



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:59 PM UTC

PDB ID : 7NVG / pdb\_00007nvg  
EMDB ID : EMD-12603  
Title : Salmonella flagellar basal body refined in C1 map  
Authors : Johnson, S.; Furlong, E.; Lea, S.M.  
Deposited on : 2021-03-15  
Resolution : 3.70 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:

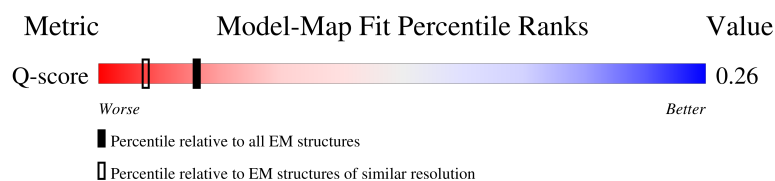
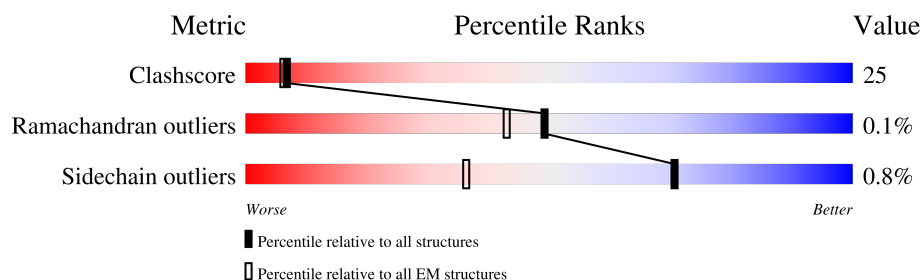
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.70 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                       | 11569 ( 3.20 - 4.20 )                                    |

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   | A1    | 560    | <div> <div>12%</div> <div>19% 8% 73%</div> </div>  |
| 1   | B1    | 560    | <div> <div>20%</div> <div>27% 18% 55%</div> </div> |
| 1   | C1    | 560    | <div> <div>16%</div> <div>27% 18% 55%</div> </div> |
| 1   | D1    | 560    | <div> <div>12%</div> <div>17% 10% 73%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E1    | 560    |                  |
| 1   | F1    | 560    |                  |
| 1   | G1    | 560    |                  |
| 1   | H1    | 560    |                  |
| 1   | I1    | 560    |                  |
| 1   | J1    | 560    |                  |
| 1   | K1    | 560    |                  |
| 1   | L1    | 560    |                  |
| 1   | M1    | 560    |                  |
| 1   | N1    | 560    |                  |
| 1   | O1    | 560    |                  |
| 1   | P1    | 560    |                  |
| 1   | Q1    | 560    |                  |
| 1   | R1    | 560    |                  |
| 1   | S1    | 560    |                  |
| 1   | T1    | 560    |                  |
| 1   | U1    | 560    |                  |
| 1   | V1    | 560    |                  |
| 1   | W1    | 560    |                  |
| 1   | X1    | 560    |                  |
| 1   | Y1    | 560    |                  |
| 1   | Z1    | 560    |                  |
| 1   | a1    | 560    |                  |
| 1   | b1    | 560    |                  |
| 1   | c1    | 560    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | d1    | 560    |                  |
| 1   | e1    | 560    |                  |
| 1   | f1    | 560    |                  |
| 1   | g1    | 560    |                  |
| 1   | h1    | 560    |                  |
| 2   | A2    | 245    |                  |
| 2   | B2    | 245    |                  |
| 2   | C2    | 245    |                  |
| 2   | D2    | 245    |                  |
| 2   | E2    | 245    |                  |
| 3   | F2    | 264    |                  |
| 4   | G2    | 89     |                  |
| 4   | H2    | 89     |                  |
| 4   | I2    | 89     |                  |
| 4   | J2    | 89     |                  |
| 5   | K2    | 104    |                  |
| 5   | L2    | 104    |                  |
| 5   | M2    | 104    |                  |
| 5   | N2    | 104    |                  |
| 5   | O2    | 104    |                  |
| 5   | P2    | 104    |                  |
| 6   | Q2    | 138    |                  |
| 6   | R2    | 138    |                  |
| 6   | S2    | 138    |                  |
| 6   | T2    | 138    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | U2    | 138    |                  |
| 7   | V2    | 134    |                  |
| 7   | W2    | 134    |                  |
| 7   | X2    | 134    |                  |
| 7   | Y2    | 134    |                  |
| 7   | Z2    | 134    |                  |
| 7   | a2    | 134    |                  |
| 8   | b2    | 251    |                  |
| 8   | c2    | 251    |                  |
| 8   | d2    | 251    |                  |
| 8   | e2    | 251    |                  |
| 8   | f2    | 251    |                  |
| 9   | 12    | 260    |                  |
| 9   | 22    | 260    |                  |
| 9   | 32    | 260    |                  |
| 9   | 42    | 260    |                  |
| 9   | g2    | 260    |                  |
| 9   | h2    | 260    |                  |
| 9   | i2    | 260    |                  |
| 9   | j2    | 260    |                  |
| 9   | k2    | 260    |                  |
| 9   | l2    | 260    |                  |
| 9   | m2    | 260    |                  |
| 9   | n2    | 260    |                  |
| 9   | o2    | 260    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9   | p2    | 260    |                  |
| 9   | q2    | 260    |                  |
| 9   | r2    | 260    |                  |
| 9   | s2    | 260    |                  |
| 9   | t2    | 260    |                  |
| 9   | u2    | 260    |                  |
| 9   | v2    | 260    |                  |
| 9   | w2    | 260    |                  |
| 9   | x2    | 260    |                  |
| 9   | y2    | 260    |                  |
| 9   | z2    | 260    |                  |
| 10  | A3    | 232    |                  |
| 10  | B3    | 232    |                  |
| 10  | C3    | 232    |                  |
| 10  | D3    | 232    |                  |
| 10  | E3    | 232    |                  |
| 10  | F3    | 232    |                  |
| 10  | G3    | 232    |                  |
| 10  | H3    | 232    |                  |
| 10  | I3    | 232    |                  |
| 10  | J3    | 232    |                  |
| 10  | K3    | 232    |                  |
| 10  | L3    | 232    |                  |
| 10  | M3    | 232    |                  |
| 10  | N3    | 232    |                  |

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| Mol | Chain | Length | Quality of chain |     |     |     |
|-----|-------|--------|------------------|-----|-----|-----|
| 10  | O3    | 232    | 86%              | 54% | 36% | 9%  |
| 10  | P3    | 232    | 87%              | 54% | 36% | 9%  |
| 10  | Q3    | 232    | 88%              | 53% | 37% | 9%  |
| 10  | R3    | 232    | 86%              | 52% | 38% | 9%  |
| 10  | S3    | 232    | 88%              | 53% | 37% | 9%  |
| 10  | T3    | 232    | 87%              | 54% | 37% | 9%  |
| 10  | U3    | 232    | 87%              | 54% | 36% | 9%  |
| 10  | V3    | 232    | 87%              | 55% | 36% | 9%  |
| 10  | W3    | 232    | 86%              | 55% | 36% | 9%  |
| 10  | X3    | 232    | 88%              | 55% | 35% | 9%  |
| 10  | Y3    | 232    | 87%              | 55% | 35% | 9%  |
| 10  | Z3    | 232    | 84%              | 53% | 37% | 9%  |
| 11  | a3    | 365    | 83%              | 40% | 42% | 16% |
| 11  | b3    | 365    | 83%              | 40% | 42% | 16% |
| 11  | c3    | 365    | 84%              | 40% | 42% | 16% |
| 11  | d3    | 365    | 83%              | 41% | 41% | 16% |
| 11  | e3    | 365    | 83%              | 41% | 42% | 16% |
| 11  | f3    | 365    | 84%              | 40% | 42% | 16% |
| 11  | g3    | 365    | 83%              | 42% | 41% | 16% |
| 11  | h3    | 365    | 84%              | 40% | 42% | 16% |
| 11  | i3    | 365    | 83%              | 40% | 42% | 16% |
| 11  | j3    | 365    | 84%              | 42% | 41% | 16% |
| 11  | k3    | 365    | 84%              | 41% | 42% | 16% |
| 11  | l3    | 365    | 84%              | 41% | 42% | 16% |
| 11  | m3    | 365    | 84%              | 41% | 42% | 16% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 11  | n3    | 365    |                  |
| 11  | o3    | 365    |                  |
| 11  | p3    | 365    |                  |
| 11  | q3    | 365    |                  |
| 11  | r3    | 365    |                  |
| 11  | s3    | 365    |                  |
| 11  | t3    | 365    |                  |
| 11  | u3    | 365    |                  |
| 11  | v3    | 365    |                  |
| 11  | w3    | 365    |                  |
| 11  | x3    | 365    |                  |
| 11  | y3    | 365    |                  |
| 11  | z3    | 365    |                  |
| 12  | A4    | 232    |                  |
| 12  | B4    | 232    |                  |
| 12  | C4    | 232    |                  |
| 12  | D4    | 232    |                  |
| 12  | E4    | 232    |                  |



## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 246311 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar M-ring protein.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | A1    | 151      | Total<br>1193 | C<br>726  | N<br>223 | O<br>241 | S<br>3 | 0       | 0     |
| 1   | B1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | C1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | D1    | 151      | Total<br>1193 | C<br>726  | N<br>223 | O<br>241 | S<br>3 | 0       | 0     |
| 1   | E1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | F1    | 151      | Total<br>1193 | C<br>726  | N<br>223 | O<br>241 | S<br>3 | 0       | 0     |
| 1   | G1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | H1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | I1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | J1    | 151      | Total<br>1193 | C<br>726  | N<br>223 | O<br>241 | S<br>3 | 0       | 0     |
| 1   | K1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | L1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | M1    | 151      | Total<br>1193 | C<br>726  | N<br>223 | O<br>241 | S<br>3 | 0       | 0     |
| 1   | N1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | O1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |
| 1   | P1    | 151      | Total<br>1193 | C<br>726  | N<br>223 | O<br>241 | S<br>3 | 0       | 0     |
| 1   | Q1    | 250      | Total<br>1931 | C<br>1187 | N<br>355 | O<br>385 | S<br>4 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | R1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | S1    | 151      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 726  | 223 | 241 | 3 |         |       |
| 1   | T1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | U1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | V1    | 151      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 726  | 223 | 241 | 3 |         |       |
| 1   | W1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | X1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | Y1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | Z1    | 151      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 726  | 223 | 241 | 3 |         |       |
| 1   | a1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | b1    | 151      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 726  | 223 | 241 | 3 |         |       |
| 1   | c1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | d1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | e1    | 151      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 726  | 223 | 241 | 3 |         |       |
| 1   | f1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | g1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |
| 1   | h1    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1187 | 355 | 385 | 4 |         |       |

- Molecule 2 is a protein called Flagellar biosynthetic protein FlIP.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | A2    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1623  | 1084 | 251 | 276 | 12 |         |       |
| 2   | B2    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1623  | 1084 | 251 | 276 | 12 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | C2    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1623  | 1084 | 251 | 276 | 12 |         |       |
| 2   | D2    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1623  | 1084 | 251 | 276 | 12 |         |       |
| 2   | E2    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1623  | 1084 | 251 | 276 | 12 |         |       |

- Molecule 3 is a protein called Flagellar biosynthetic protein FliR.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | F2    | 258      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1986  | 1329 | 314 | 327 | 16 |         |       |

- Molecule 4 is a protein called Flagellar biosynthetic protein FliQ.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | G2    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 4   | H2    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 4   | I2    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |
| 4   | J2    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 449 | 100 | 114 | 7 |         |       |

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | K2    | 39       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 296   | 183 | 51  | 56  | 6 |         |       |
| 5   | L2    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 563   | 347 | 102 | 108 | 6 |         |       |
| 5   | M2    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 563   | 347 | 102 | 108 | 6 |         |       |
| 5   | N2    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 563   | 347 | 102 | 108 | 6 |         |       |
| 5   | O2    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 563   | 347 | 102 | 108 | 6 |         |       |
| 5   | P2    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 563   | 347 | 102 | 108 | 6 |         |       |

- Molecule 6 is a protein called Flagellar basal body rod protein FlgB.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | Q2    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 630 | 188 | 200 | 5 |         |       |
| 6   | R2    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 932   | 578 | 169 | 180 | 5 |         |       |
| 6   | S2    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 583 | 173 | 181 | 5 |         |       |
| 6   | T2    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 835   | 516 | 153 | 161 | 5 |         |       |
| 6   | U2    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 925   | 573 | 168 | 179 | 5 |         |       |

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgC.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | V2    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 604 | 167 | 193 | 5 |         |       |
| 7   | W2    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 601 | 166 | 192 | 5 |         |       |
| 7   | X2    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 601 | 166 | 192 | 5 |         |       |
| 7   | Y2    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 601 | 166 | 192 | 5 |         |       |
| 7   | Z2    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 601 | 166 | 192 | 5 |         |       |
| 7   | a2    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 601 | 166 | 192 | 5 |         |       |

- Molecule 8 is a protein called Flagellar basal body protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | b2    | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1812  | 1111 | 325 | 368 | 8 |         |       |
| 8   | c2    | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1812  | 1111 | 325 | 368 | 8 |         |       |
| 8   | d2    | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1812  | 1111 | 325 | 368 | 8 |         |       |
| 8   | e2    | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1812  | 1111 | 325 | 368 | 8 |         |       |
| 8   | f2    | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1812  | 1111 | 325 | 368 | 8 |         |       |

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgG.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 9   | g2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | h2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | i2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | j2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | k2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | l2    | 249      | Total<br>1871 | C<br>1157 | N<br>328 | O<br>381 | S<br>5 | 0       | 0     |
| 9   | m2    | 249      | Total<br>1871 | C<br>1157 | N<br>328 | O<br>381 | S<br>5 | 0       | 0     |
| 9   | n2    | 249      | Total<br>1871 | C<br>1157 | N<br>328 | O<br>381 | S<br>5 | 0       | 0     |
| 9   | o2    | 249      | Total<br>1871 | C<br>1157 | N<br>328 | O<br>381 | S<br>5 | 0       | 0     |
| 9   | p2    | 249      | Total<br>1871 | C<br>1157 | N<br>328 | O<br>381 | S<br>5 | 0       | 0     |
| 9   | q2    | 251      | Total<br>1885 | C<br>1166 | N<br>330 | O<br>384 | S<br>5 | 0       | 0     |
| 9   | r2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | s2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | t2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | u2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | v2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | w2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | x2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | y2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | z2    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | 12    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |
| 9   | 22    | 260      | Total<br>1949 | C<br>1202 | N<br>341 | O<br>400 | S<br>6 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | 32    | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1948  | 1202 | 340 | 400 | 6 |         |       |
| 9   | 42    | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1949  | 1202 | 341 | 400 | 6 |         |       |

- Molecule 10 is a protein called Flagellar L-ring protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | A3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | B3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | C3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | D3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | E3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | F3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | G3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | H3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | I3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | J3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | K3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | L3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | M3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | N3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | O3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | P3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | Q3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | R3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | S3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | T3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | U3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | V3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | W3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 984 | 282 | 310 | 4 |         |       |
| 10  | X3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | Y3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |
| 10  | Z3    | 211      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 985 | 282 | 310 | 4 |         |       |

- Molecule 11 is a protein called Flagellar P-ring protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | a3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | b3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | c3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | d3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | e3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | f3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | g3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | h3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2251  | 1379 | 408 | 451 | 13 |         |       |
| 11  | i3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | j3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | k3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | l3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | m3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | n3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | o3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | p3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | q3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | r3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2251  | 1378 | 409 | 451 | 13 |         |       |
| 11  | s3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | t3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | u3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | v3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | w3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | x3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | y3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |
| 11  | z3    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2252  | 1379 | 409 | 451 | 13 |         |       |

- Molecule 12 is a protein called Basal-body rod modification protein FlgD.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | A4    | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1475  | 914 | 253 | 307 | 1 |         |       |
| 12  | B4    | 204      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1493  | 924 | 256 | 312 | 1 |         |       |
| 12  | C4    | 199      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1458  | 903 | 250 | 304 | 1 |         |       |

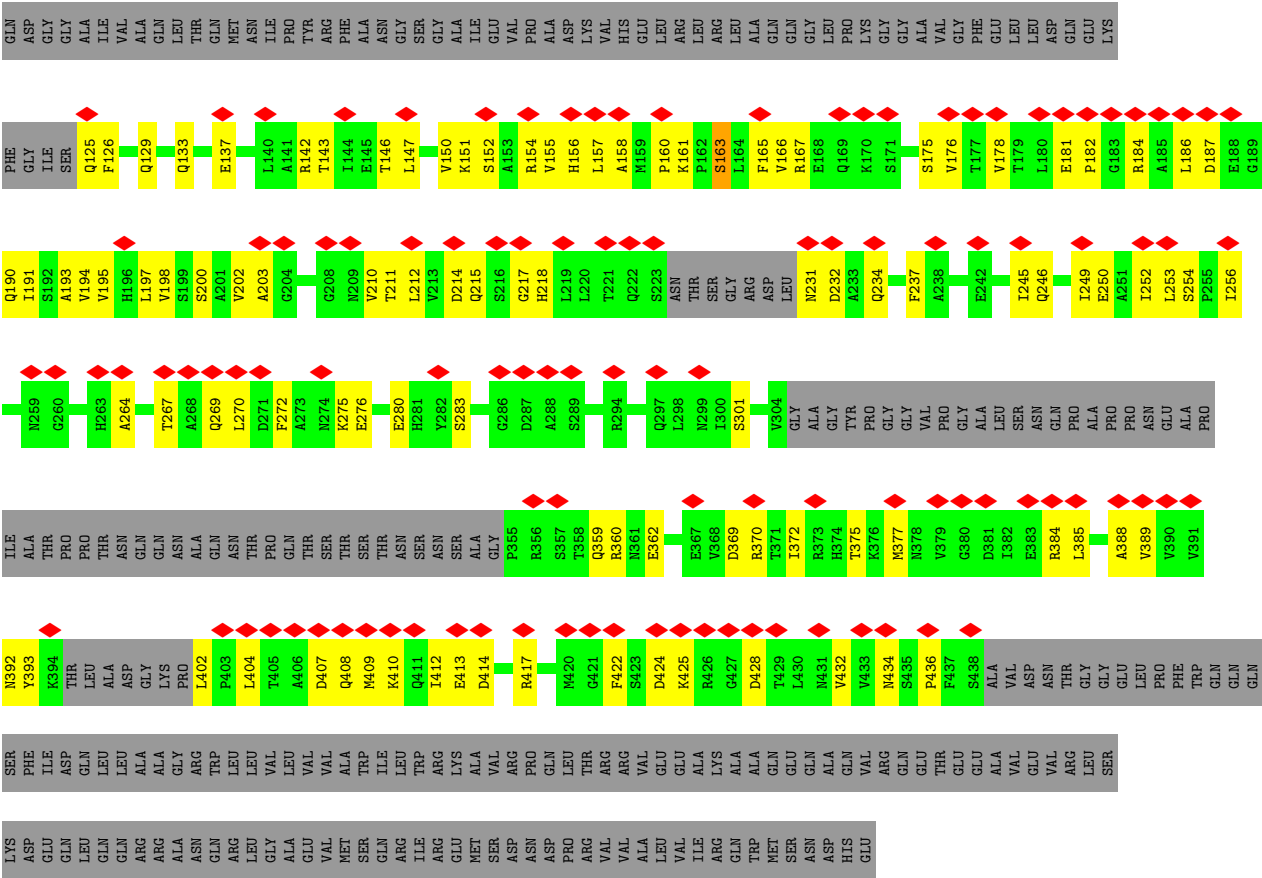
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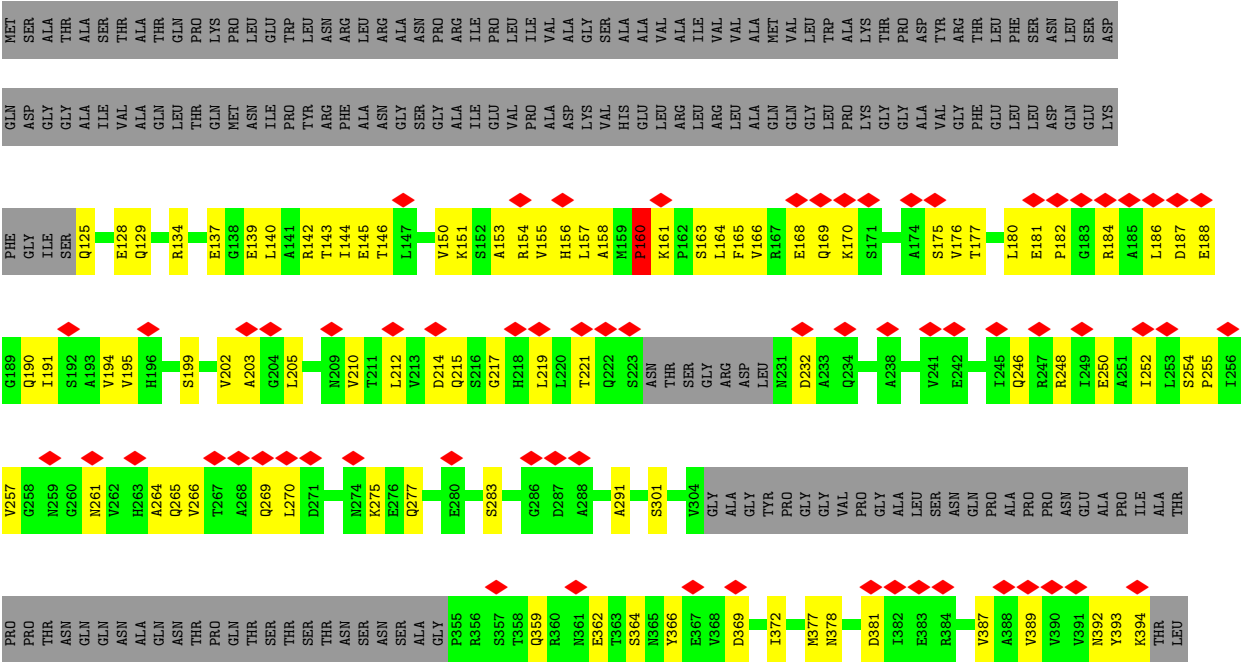
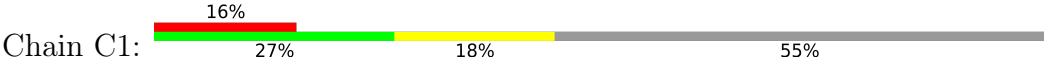
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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | D4    | 202      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1482  | 917 | 254 | 310 | 1 |         |       |
| 12  | E4    | 204      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1493  | 924 | 256 | 312 | 1 |         |       |

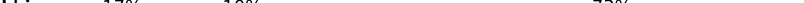


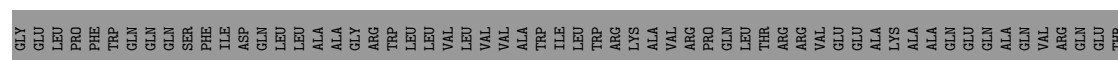
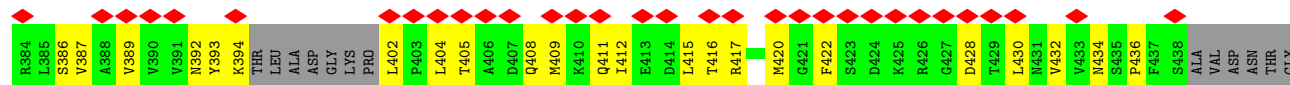
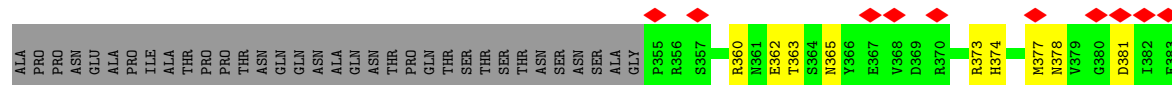
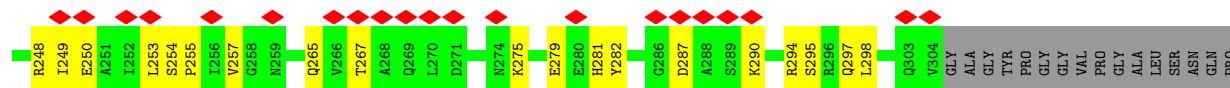
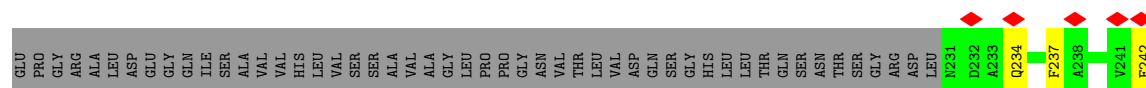


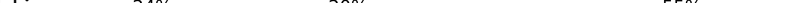
● Molecule 1: Flagellar M-ring protein

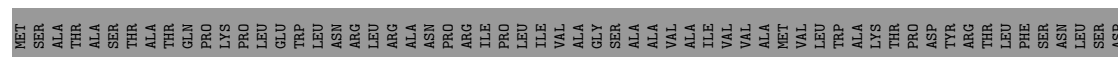




Chain D1: 



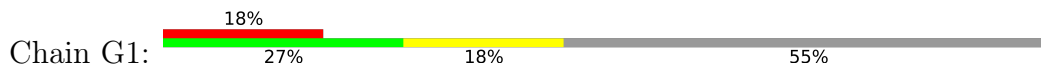
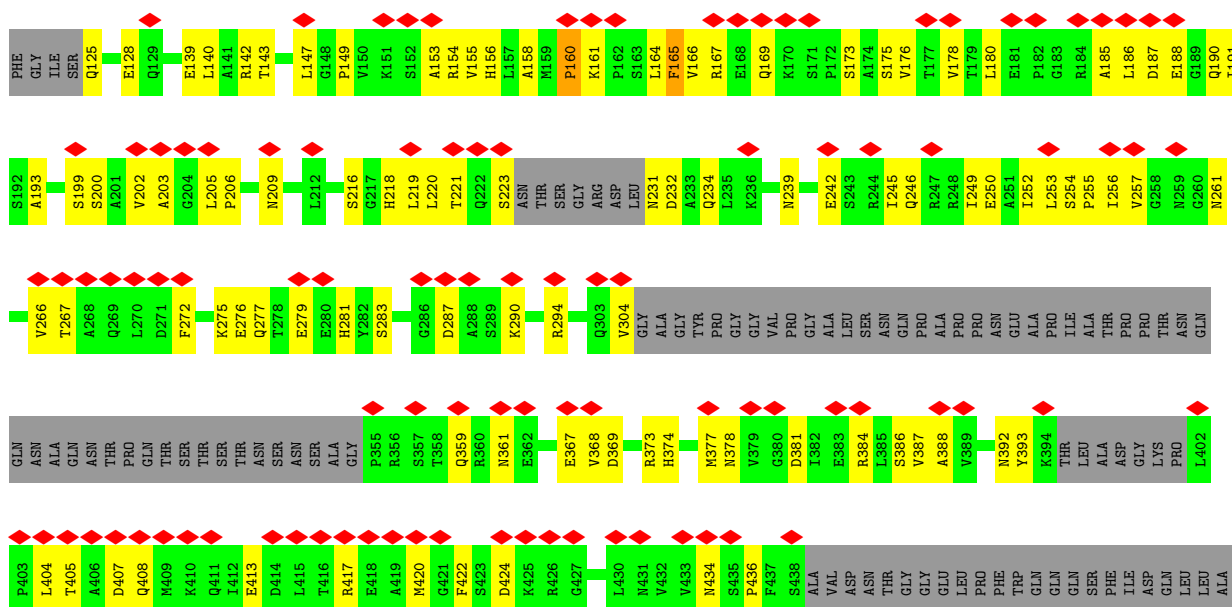
Chain E1: 



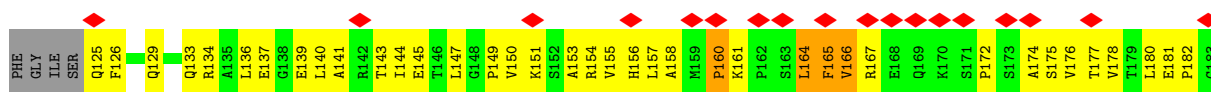


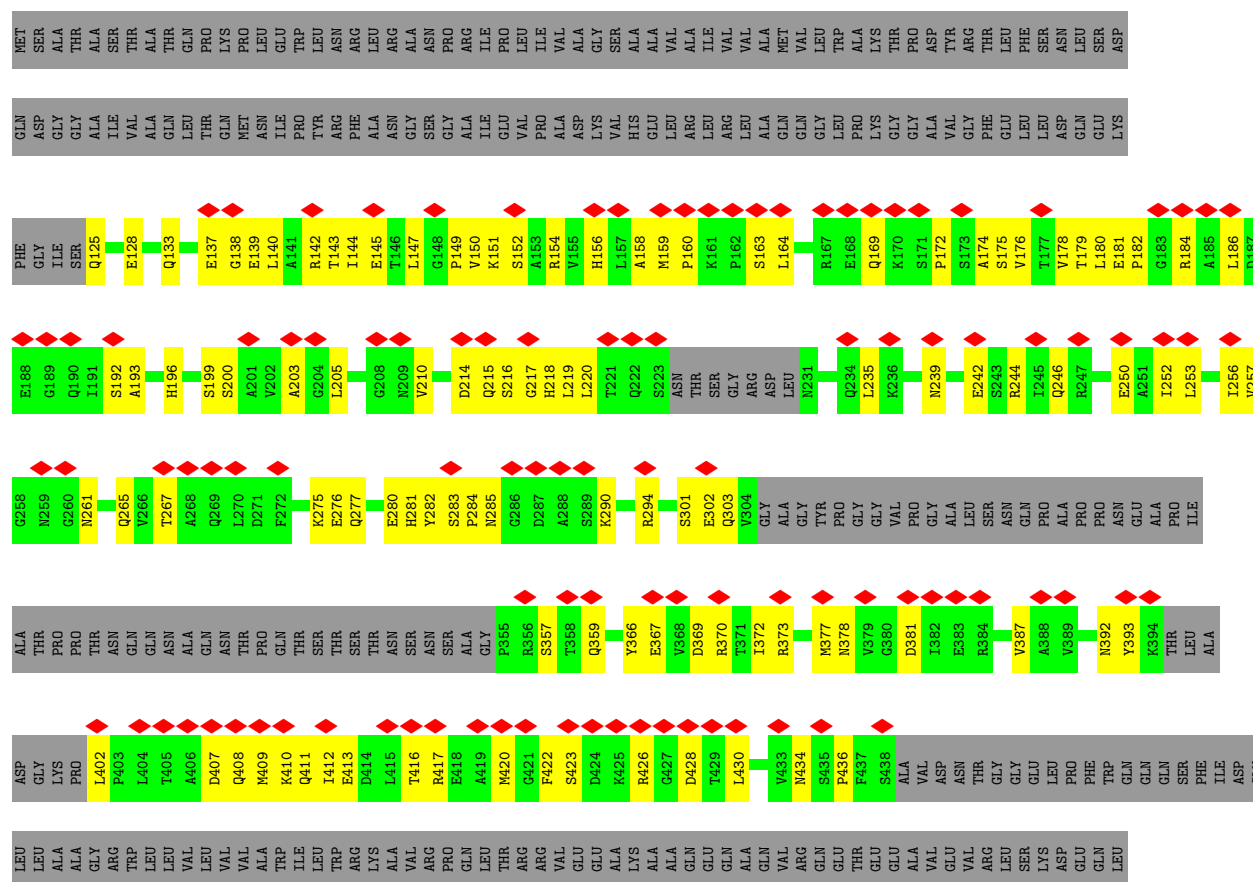
[illegible]

- Molecule 1: Flagellar M-ring protein

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- Molecule 1: Flagellar M-ring protein

[illegible]

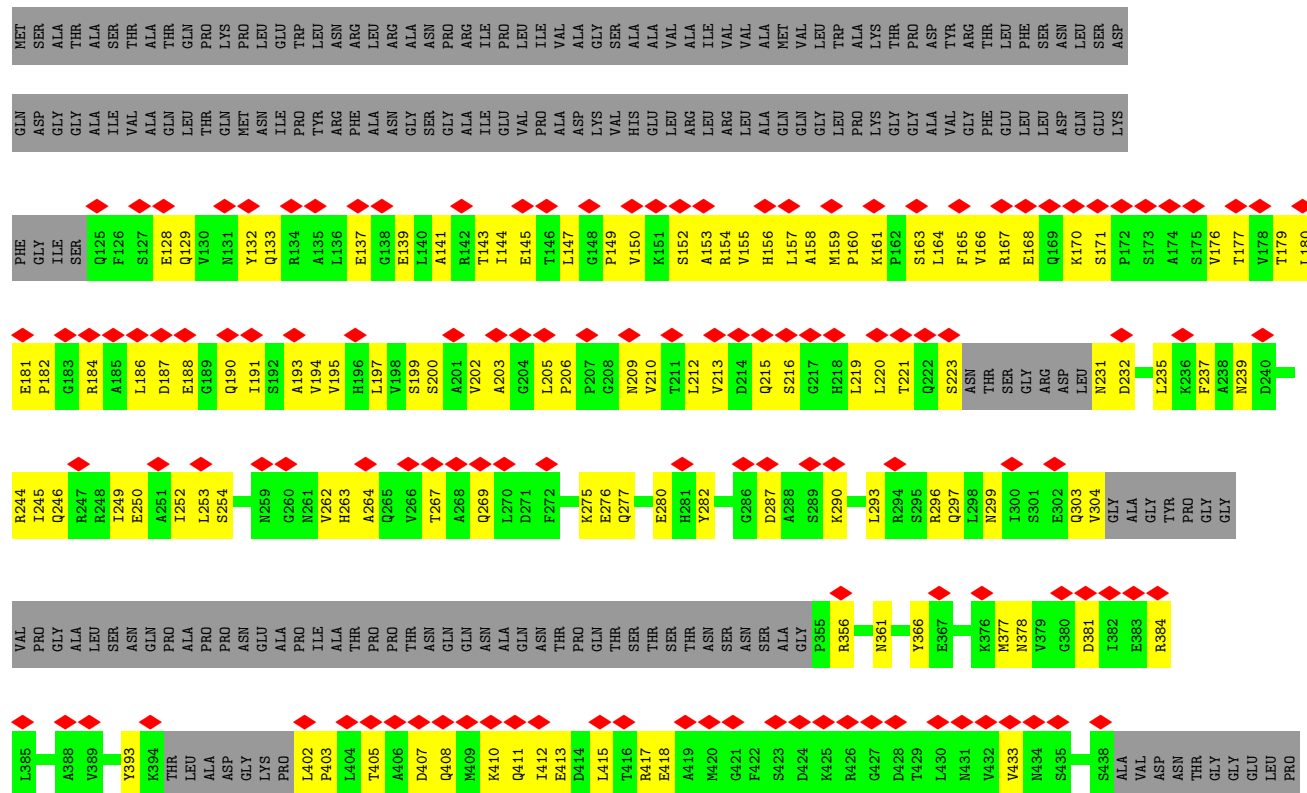








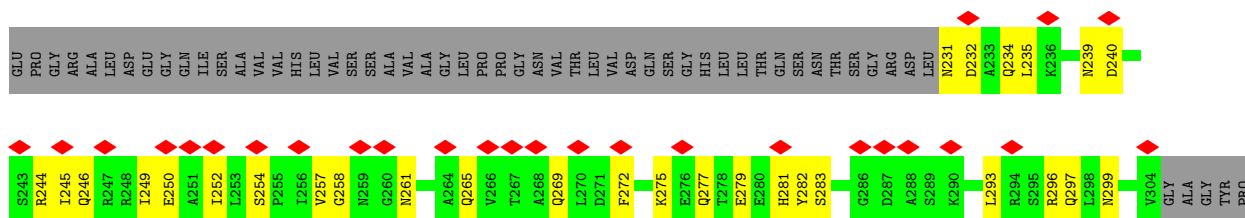




- Molecule 1: Flagellar M-ring protein



PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLY GLU GLU LEU LEU GLY VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO PRO LYS PRO SER PHE VAL ARG GLN LYS SER PRO SER ALA SER VAL THR VAL THR THR LEU



| Category | Value | Color |
|----------|-------|-------|
| GLY      | 3355  | Red   |
| GLY      | 3356  | Red   |
| VAL      | 3359  | Red   |
| PRO      | 3360  | Red   |
| GLY      | 3361  | Red   |
| ALA      | 3362  | Red   |
| LEU      | 3363  | Red   |
| SER      | 3364  | Red   |
| ASN      | 3365  | Red   |
| GLN      | 3366  | Red   |
| PRO      | 3367  | Red   |
| ALA      | 3368  | Red   |
| PRO      | 3369  | Red   |
| ASN      | 3370  | Red   |
| GLU      | 3371  | Red   |
| ALA      | 3372  | Red   |
| PRO      | 3373  | Red   |
| ILE      | 3374  | Red   |
| ALA      | 3375  | Red   |
| THR      | 3376  | Red   |
| PRO      | 3377  | Red   |
| THR      | 3378  | Red   |
| ASN      | 3379  | Red   |
| GLN      | 3380  | Red   |
| GLN      | 3381  | Red   |
| ASN      | 3382  | Red   |
| ALA      | 3383  | Red   |
| GLN      | 3384  | Red   |
| ASN      | 3385  | Red   |
| ALA      | 3386  | Red   |
| GLN      | 3387  | Red   |
| ASN      | 3388  | Red   |
| THR      | 3389  | Red   |
| PRO      | 3390  | Red   |
| GLN      | 3391  | Red   |
| THR      | 3392  | Red   |
| SER      | 3393  | Red   |
| THR      | 3394  | Red   |
| THR      | 3395  | Red   |
| ASN      | 3396  | Red   |
| SER      | 3397  | Red   |
| ASN      | 3398  | Red   |
| SER      | 3399  | Red   |
| ALA      | 3400  | Red   |
| ALA      | 3401  | Red   |
| GLY      | 3402  | Red   |
| P355     | 3403  | Red   |
| R356     | 3404  | Red   |
| Q359     | 3405  | Red   |
| R360     | 3406  | Red   |
| N361     | 3407  | Red   |
| F362     | 3408  | Red   |
| T363     | 3409  | Red   |
| D369     | 3410  | Red   |
| R370     | 3411  | Red   |
| H374     | 3412  | Red   |
| K377     | 3413  | Red   |

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| N378 | N379 | G380 | D381 | I382 | E383 | K384 | L385 | G386 | V387 | A388 | V389 | V390 | V391 | N392 | V393 | K394 | THR | LEU | ALA | ASP | GLY | LYS | PRO | L402 | P403 | L404 | T405 | A406 | D407 | Q408 | M409 | K410 | Q411 | I412 | E413 | D414 | L415 | T416 | R417 | E418 | A419 | M420 | C421 | F422 | S423 | D424 | K425 | R426 | G427 | T428 | T429 | L430 | M431 | V432 | V433 | N434 | S435 | P436 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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| ALA | GLN | VAL | ARG | GLU | THR | GLU | GLU | GLU | ALA | VAL | GLU | VAL | ARG | LEU | SER | LYS | ASP | GLU | GLN | LEU | GLN | GLN | ARG | ALA | ASN | GLN | ARG | LEU | GLY | GLU | VAL | VAL | SER | SER | GLN | ARG | ILE | GLU | ARG | ARG | GLU | GLY | NET | SER | ASP | ASN | ASP | PRO | ARG | VAL | VAL | VAL | LEU | ILE | ARG | GLN | TRP | NET | SER | GLN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

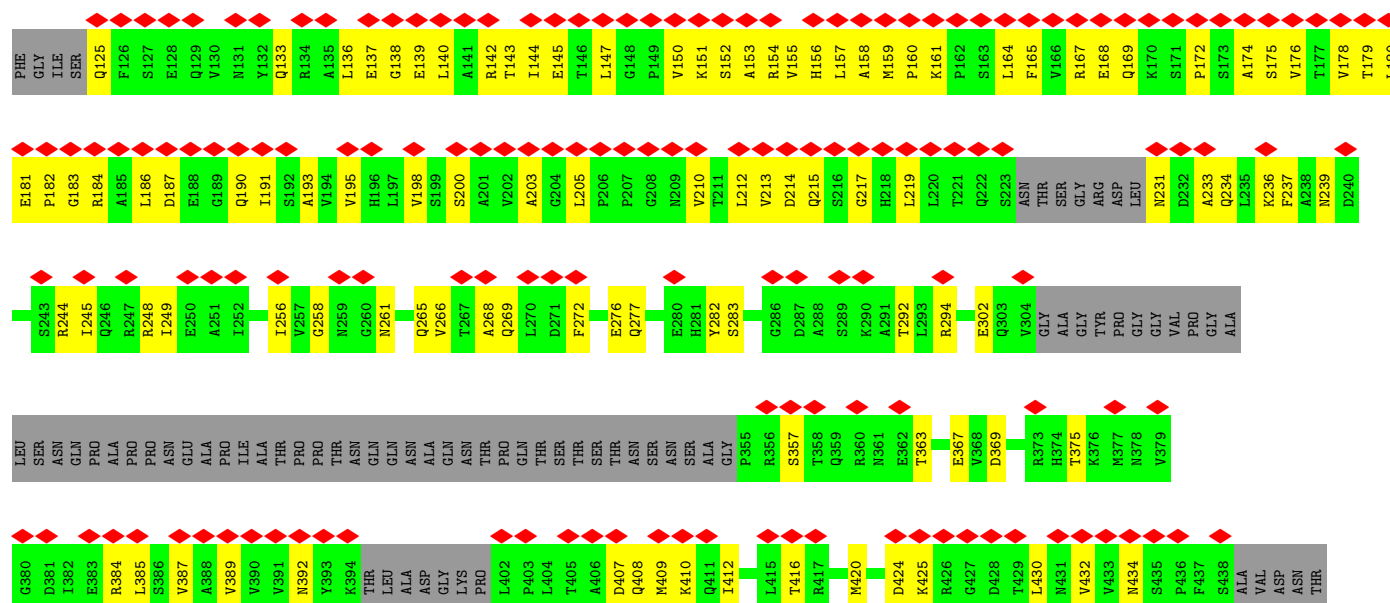
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- Molecule 1: Flagellar M-ring protein



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | ALA | THR | THR | SER | ALA | ALA | THR | PRO | LYS | PRO | GLN | LEU | GLY | TRP | LEU | ASN | ARG | ARG | ALA | ALA | ASN | PRO | ARG | ILE | PRO | LEU | ILE | VAL | GLY | SER | ALA | ALA | VAL | ALA | VAL | MET | VAL | LEU | TRP | ASP | TYR | ARG | THR | LEU | PHE | SER | ASN | LEU | SER | SER |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

GLN ASP GLY GLY GLY ALA ALA ALA VAL ILE VAL GLN LEU LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ALA ASN GLY SER GLY ALA ILE GLU VAL VAL PRO PRO ALA ASP LYS VAL VAL HIS HIS LEU LEU ARG ARG ARG LEU ALA GLN GLN GLY LEU LEU LEU LEU LYS GLY GLY ALA VAL VAL GLY PHE GLY GLU LEU LEU LEU ASP GLN GLY LYS



- Molecule 1: Flagellar M-ring protein



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PHE | GLY | ILE | SER | GLN | PHE | SER | GLU | GLN | VAL | TYR | GLN | ARG | ALA | LEU | GLY | GLU | LEU | LEU | GLY | ARG | ALA | THR | THR | ILE | GLU | THR | LEU | LEU | GLY | PRO | VAL | LYS | SER | ALA | ARG | VAL | HIS | LEU | ALA | MET | PRO | PRO | LYS | PRO | SER | LEU | VAL | VAL | GLU | ARG | GLN | LYS | SER | SER | PRO | ALA | ALA | SER | VAL | THR | VAL | THR | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| GLU | PRO | GLY | ARG | ALA | LEU | ASP | GLU | GLY | GLN | ILE | SER | VAL | ALA | VAL | HIS | LEU | VAL | SER | SER | ALA | VAL | ALA | GLY | LEU | PRO | PRO | GLY | GLY | ASN | VAL | THR | THR | LEU | VAL | ASP | GLN | SER | GLY | HIS | LEU | LEU | THR | GLN | SER | ASN | THR | SER | GLY | ARG | ASP | ASP | LEU | N231 | D232 | A233 | D234 | L235 | F242 | S243 | R244 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| Q246 | Q247 | R248 | R249 | E250 | A251 | A252 | L253 | S254 | F255 | L256 | V257 | G258 | N259 | Q260 | N261 | V262 | H263 | A264 | Q265 | V266 | T267 | A268 | Q269 | L270 | D271 | F272 | K275 | E276 | E279 | F280 | H281 | S282 | S283 | G286 | D287 | A288 | S289 | K290 | A291 | R294 | S295 | I300 | S301 | E302 | Q303 | V304 | GLY | ALA | GLY | TYR | PRO | GLY | GLY | VAL |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|

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| PRO | GLY | ALA | LEU | SER | ASN | GLN | PRO | PRO | ALA | PRO | PRO | ASN | GLU | ALA | PRO | PRO | THR | ALA | ALA | PRO | PRO | THR | ASN | GLN | GLN | GLN | ASN | ALA | ALA | GLN | ASN | THR | PRO | GLN | THR | THR | SER | THR | THR | ASN | SER | ASN | SER | ALA | ALA | GLY | P355 | P356 | P357 | P360 | P361 | P362 | P363 | P364 | P367 | P368 | P369 | P370 | P374 | P377 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

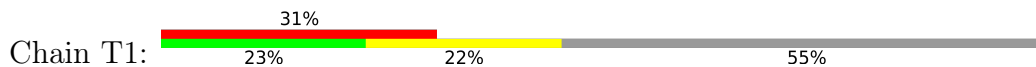
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| R378 | R379 | R380 | R381 | R382 | R383 | R384 | R385 | R386 | R387 | R388 | R389 | R390 | R391 | R392 | R393 | R394 | THR | LEU | ALA | ASP | GLY | LYS | PRO | R402 | R403 | R404 | R405 | R406 | R407 | R408 | R409 | R410 | R411 | R412 | R413 | R414 | R415 | R416 |  | R419 | R420 | R421 | R422 | R423 | R424 | R425 | R426 | R427 | R428 | R429 | R430 | R431 | R432 | R433 | R434 | R435 | R436 | R437 | R438 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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| ALA | VAL | ASP | ASN | THR | GLY | GLU | LEU | PRO | PHE | TRP | GLN | GLN | GLN | SER | PHE | TLE | ASP | GLN | LEU | LEU | LEU | ALA | ALA | GLY | ARG | TRP | LEU | LEU | VAL | LEU | VAL | VAL | ALA | ALA | TRP | TRP | TLE | LEU | TRP | ARG | LYS | ALA | LYS | VAL | ARG | PRO | ARG | GLN | GLN | LEU | LEU | THR | ARG | ARG | VAL | GLU | GLU | GLU | ALA | ALA | LYS | GLN | GLN | GLN | ALA | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLN | VAL | ARG | GLN | GLN | THR | GLU | GLU | ALA | ALA | VAL | GLU | VAL | ARG | ARG | LEU | SER | LYS | ASP | GLU | GLN | GLN | GLN | ARG | ARG | ALA | ASN | GLN | ARG | GLU | GLY | ALA | GLU | VAL | VAL | MET | MET | SER | SER | GLN | ARG | ILE | GLU | ARG | ARG | PRO | ASP | ASP | ASN | SER | ASP | GLN | VAL | VAL | LEU | LEU | ALA | VAL | VAL | ILE | GLN | ARG | GLN | TRP | GLN | GLN | MET | SER | SER | ASN | ASP |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

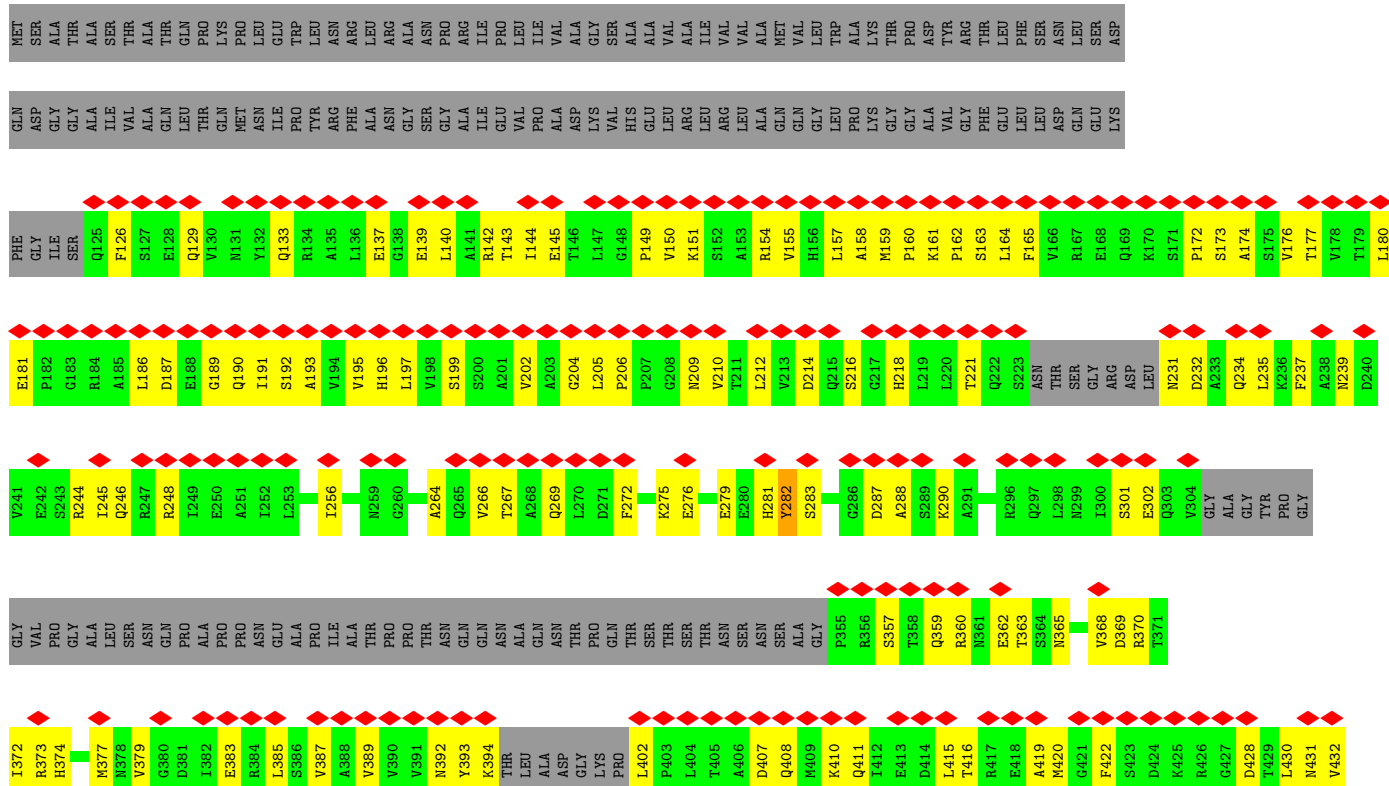
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| 5   | 0.00 | 0.00 |
| 6   | 0.00 | 0.00 |
| 7   | 0.00 | 0.00 |
| 8   | 0.00 | 0.00 |
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| 11  | 0.00 | 0.00 |
| 12  | 0.00 | 0.00 |
| 13  | 0.00 | 0.00 |
| 14  | 0.00 | 0.00 |
| 15  | 0.00 | 0.00 |
| 16  | 0.00 | 0.00 |
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| 27  | 0.00 | 0.00 |
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| 40  | 0.00 | 0.00 |
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| 45  | 0.00 | 0.00 |
| 46  | 0.00 | 0.00 |
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| 49  | 0.00 | 0.00 |
| 50  | 0.00 | 0.00 |
| 51  | 0.00 | 0.00 |
| 52  | 0.00 | 0.00 |
| 53  | 0.00 | 0.00 |
| 54  | 0.00 | 0.00 |
| 55  | 0.00 | 0.00 |
| 56  | 0.00 | 0.00 |
| 57  | 0.00 | 0.00 |
| 58  | 0.00 | 0.00 |
| 59  | 0.00 | 0.00 |
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| 61  | 0.00 | 0.00 |
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| 65  | 0.00 | 0.00 |
| 66  | 0.00 | 0.00 |
| 67  | 0.00 | 0.00 |
| 68  | 0.00 | 0.00 |
| 69  | 0.00 | 0.00 |
| 70  | 0.00 | 0.00 |
| 71  | 0.00 | 0.00 |
| 72  | 0.00 | 0.00 |
| 73  | 0.00 | 0.00 |
| 74  | 0.00 | 0.00 |
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| 79  | 0.00 | 0.00 |
| 80  | 0.00 | 0.00 |
| 81  | 0.00 | 0.00 |
| 82  | 0.00 | 0.00 |
| 83  | 0.00 | 0.00 |
| 84  | 0.00 | 0.00 |
| 85  | 0.00 | 0.00 |
| 86  | 0.00 | 0.00 |
| 87  | 0.00 | 0.00 |
| 88  | 0.00 | 0.00 |
| 89  | 0.00 | 0.00 |
| 90  | 0.00 | 0.00 |
| 91  | 0.00 | 0.00 |
| 92  | 0.00 | 0.00 |
| 93  | 0.00 | 0.00 |
| 94  | 0.00 | 0.00 |
| 95  | 0.00 | 0.00 |
| 96  | 0.00 | 0.00 |
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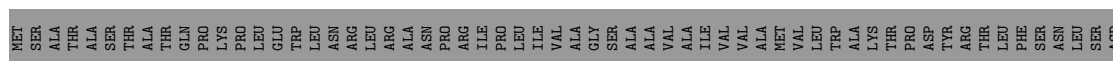
- Molecule 1: Flagellar M-ring protein



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | ALA | THR | THR | SER | SER | THR | ALA | ALA | THR | GLN | PRO | PRO | PRO | LEU | GLU | TRP | LEU | LEU | ASN | ARG | LEU | ARG | ALA | ALA | ASN | PRO | ARG | ILE | LEU | LEU | ILE | VAL | VAL | ALA | GLY | SER | ALA | ALA | VAL | VAL | VAL | VAL | VAL | VAL | MET | VAL | VAL | LEU | TRP | ALA | ALA | LYS | THR | PRO | ASP | TYR | ARG | THR | LEU | PHE | SER | ASN | LEU | LEU | SER | SER | SER |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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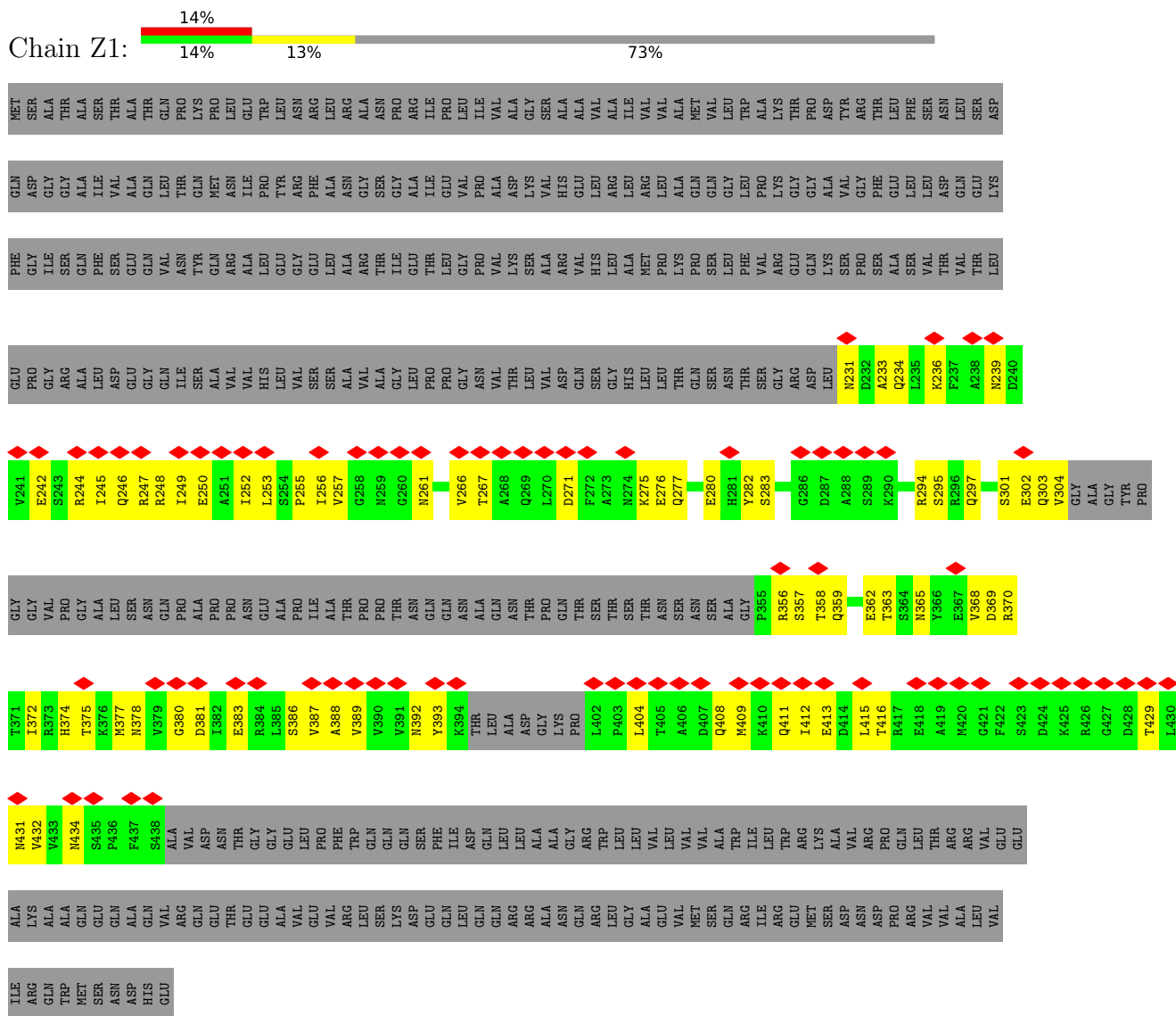




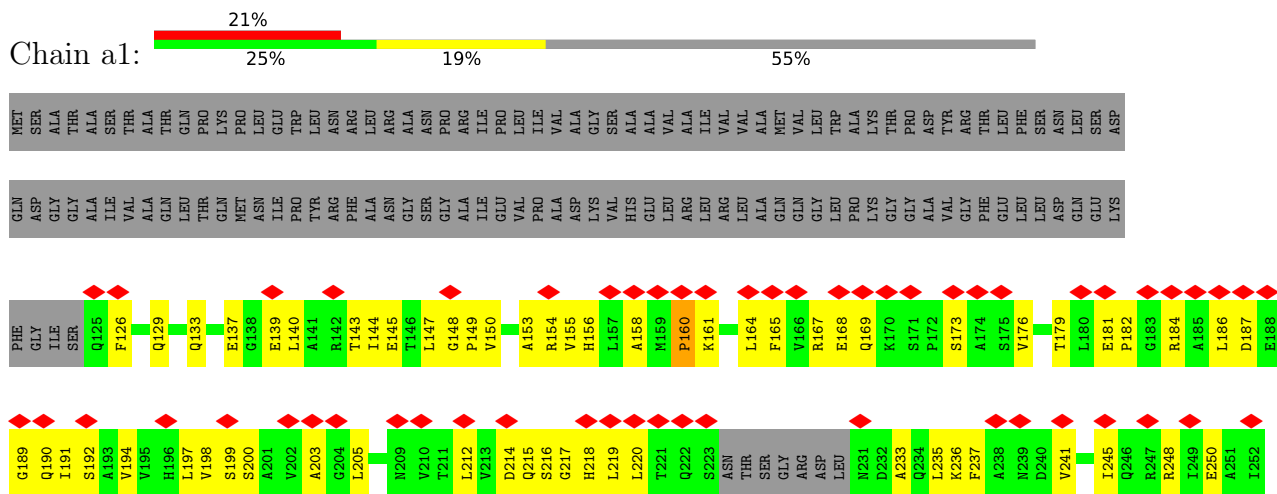




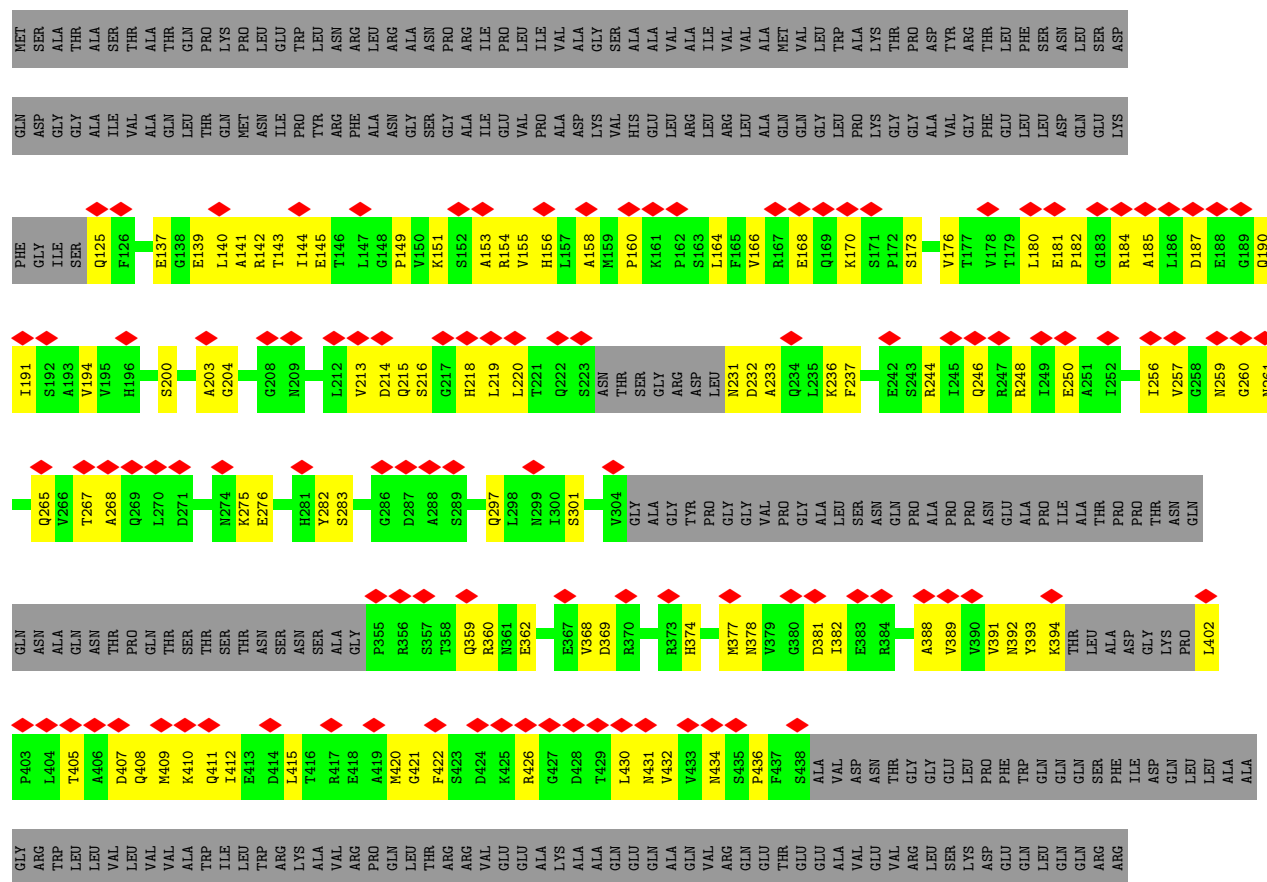




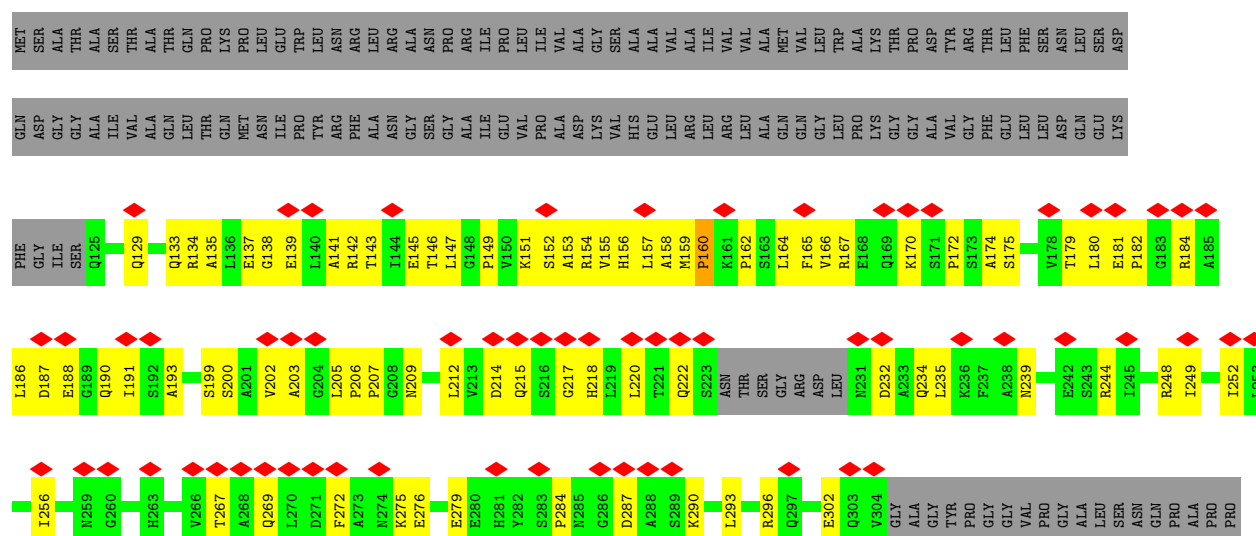
- Molecule 1: Flagellar M-ring protein

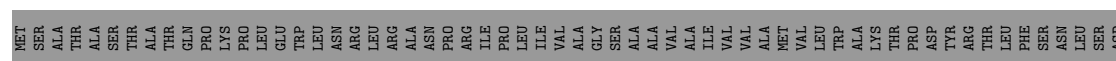




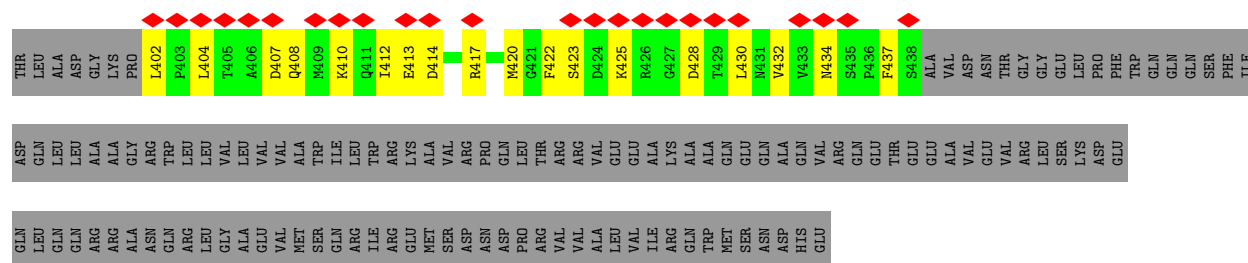


### • Molecule 1: Flagellar M-ring protein

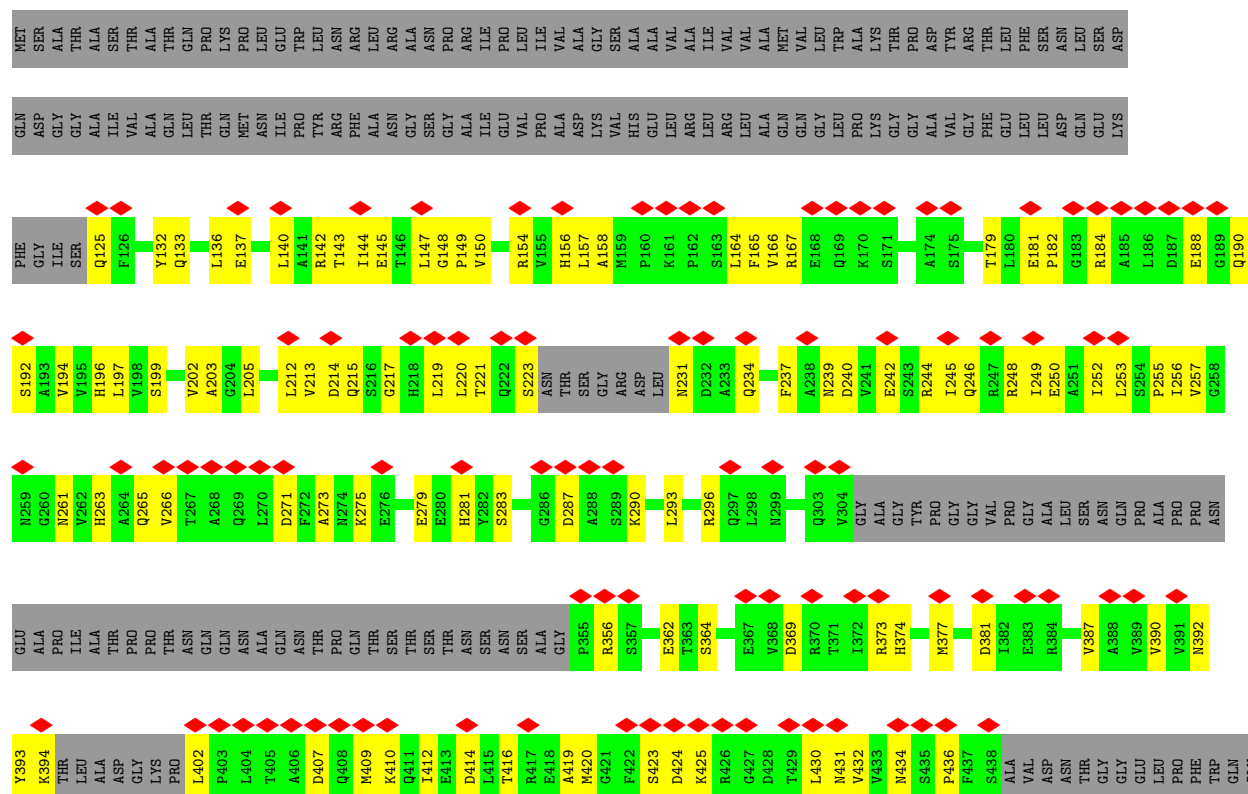
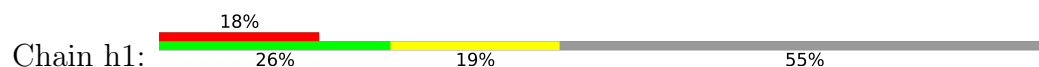




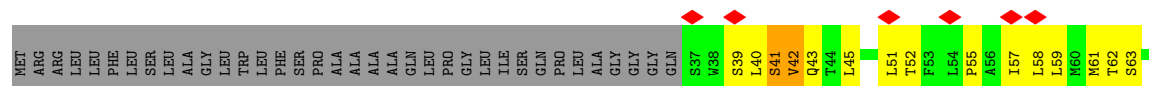
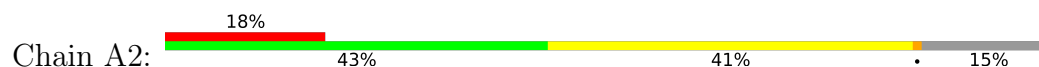




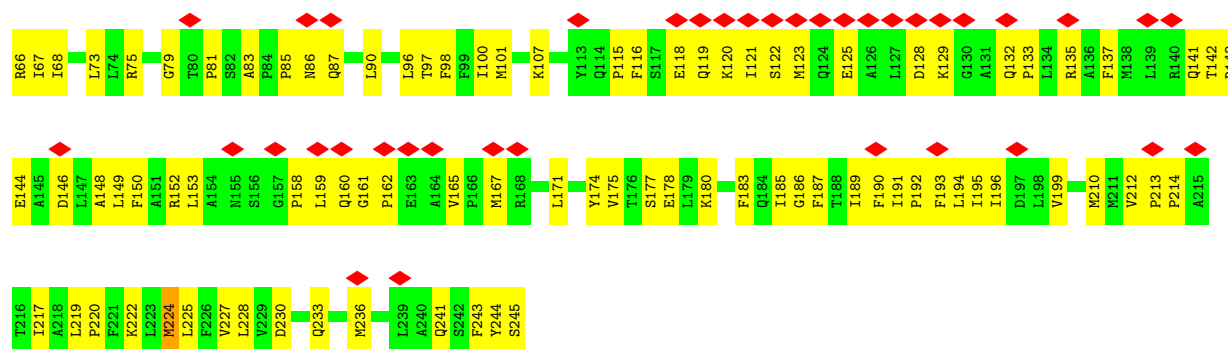
### • Molecule 1: Flagellar M-ring protein



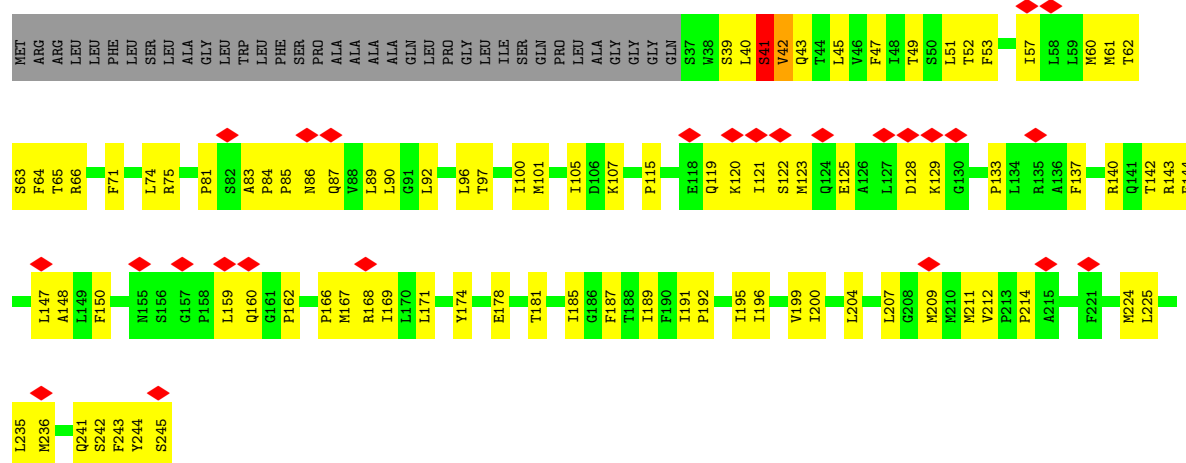
### • Molecule 2: Flagellar biosynthetic protein FlpI



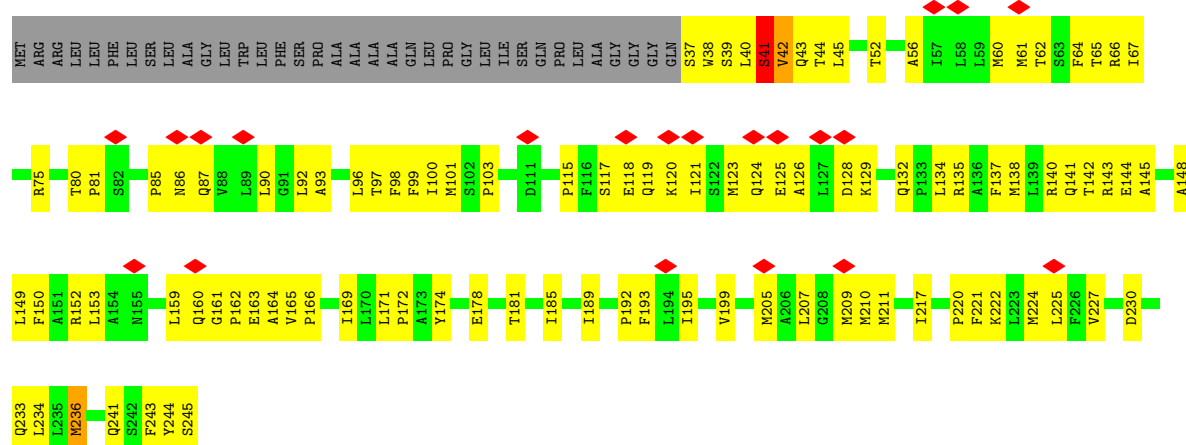




• Molecule 2: Flagellar biosynthetic protein Flp

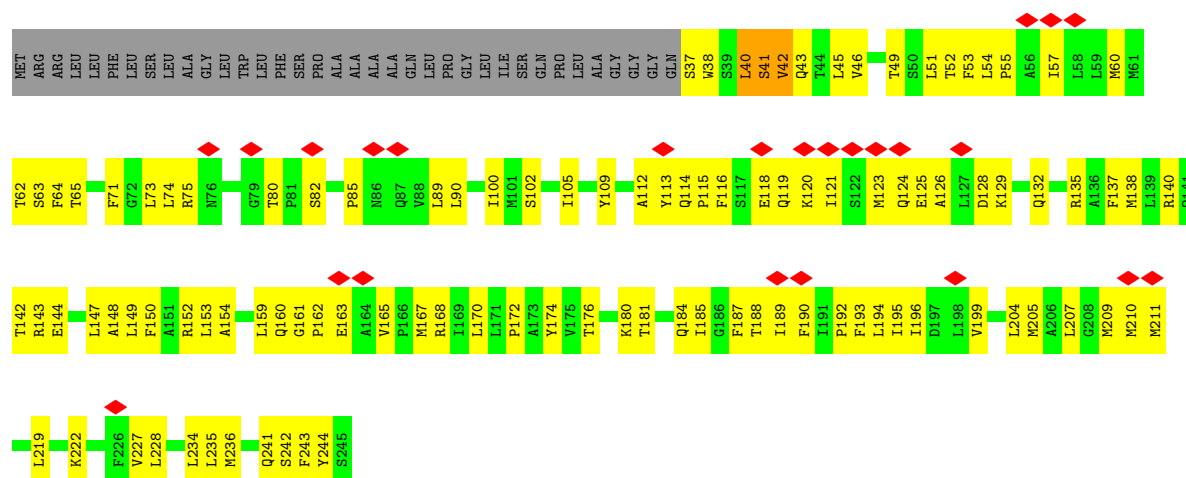


• Molecule 2: Flagellar biosynthetic protein Flp

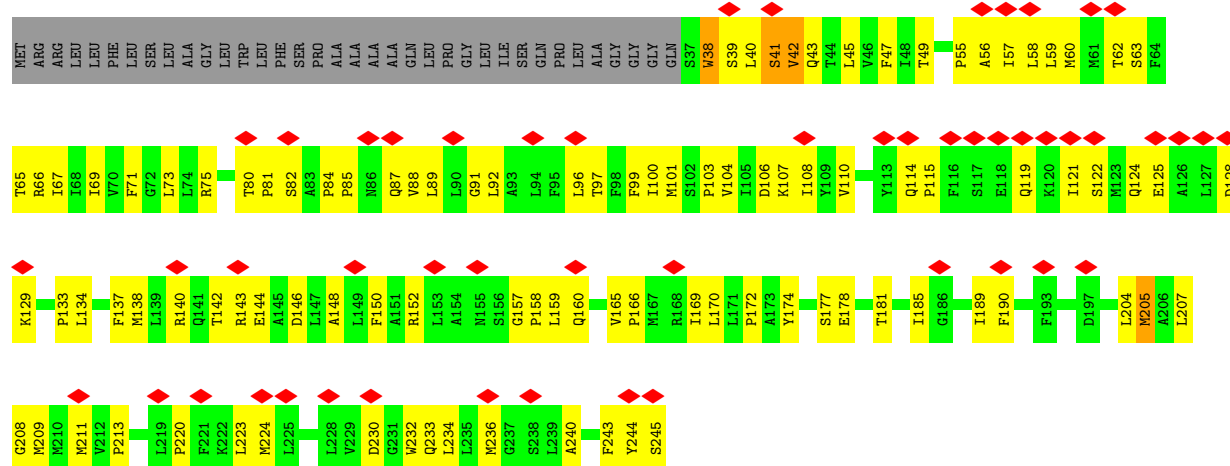
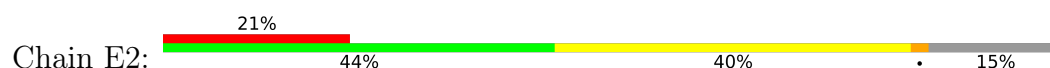


• Molecule 2: Flagellar biosynthetic protein Flp

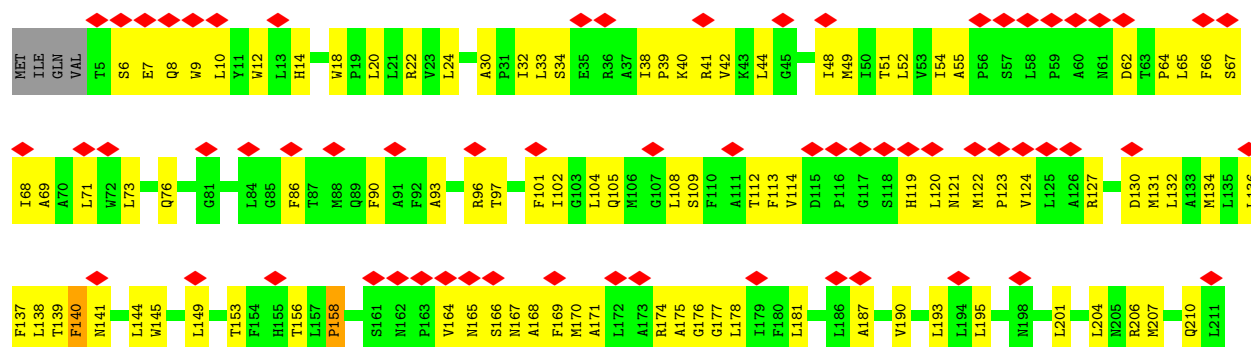


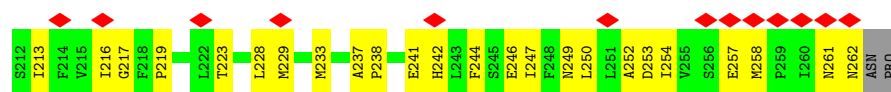


• Molecule 2: Flagellar biosynthetic protein FlpP

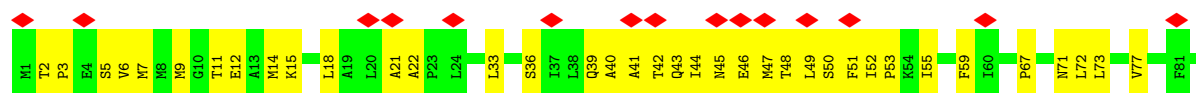


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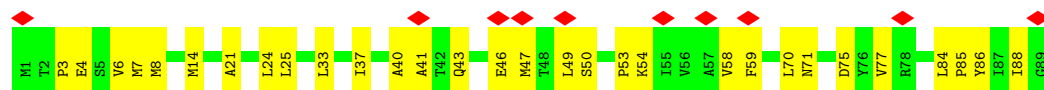




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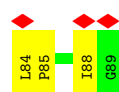
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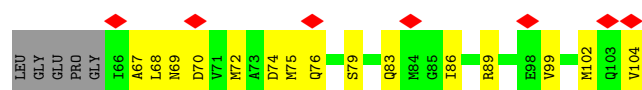
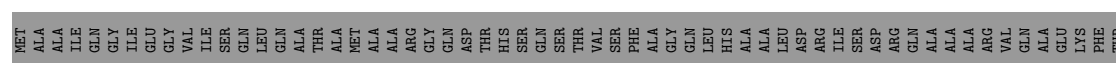
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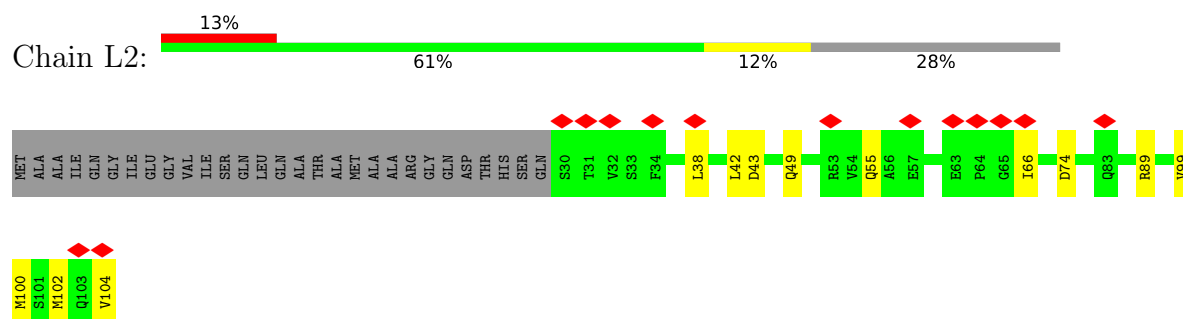
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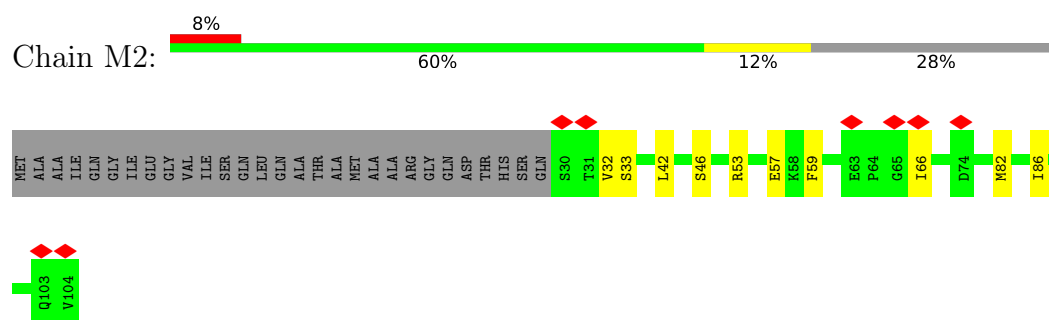
• Molecule 5: Flagellar hook-basal body complex protein FliE



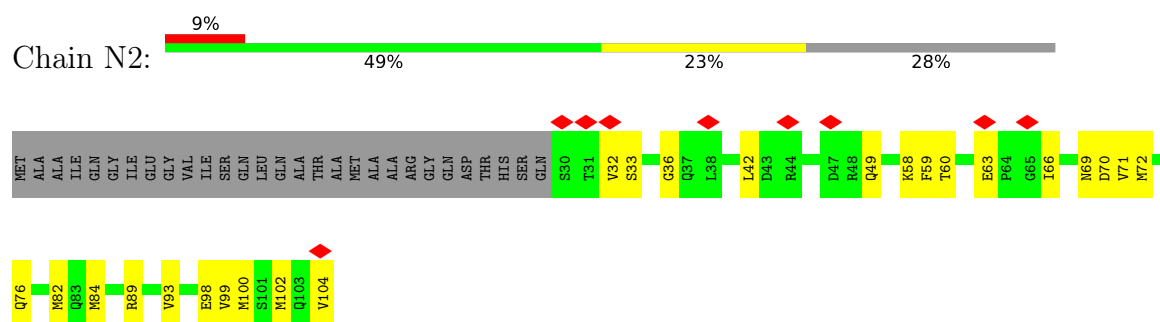
- Molecule 5: Flagellar hook-basal body complex protein FliE



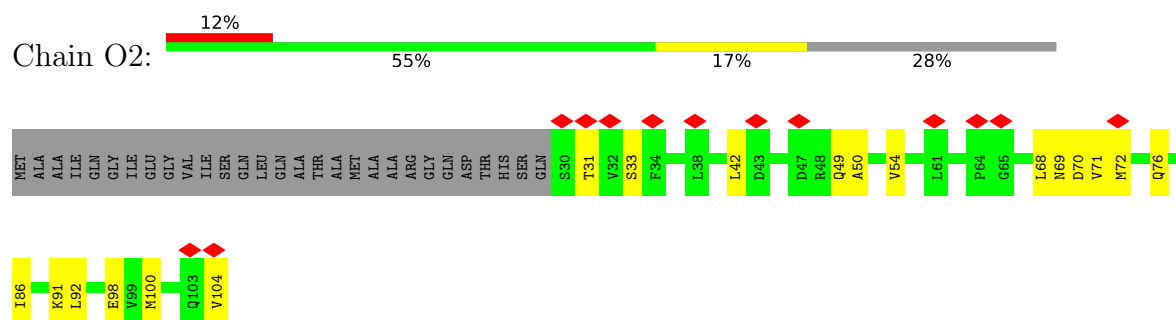
- Molecule 5: Flagellar hook-basal body complex protein FliE



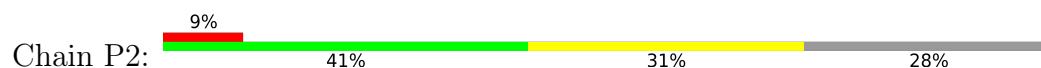
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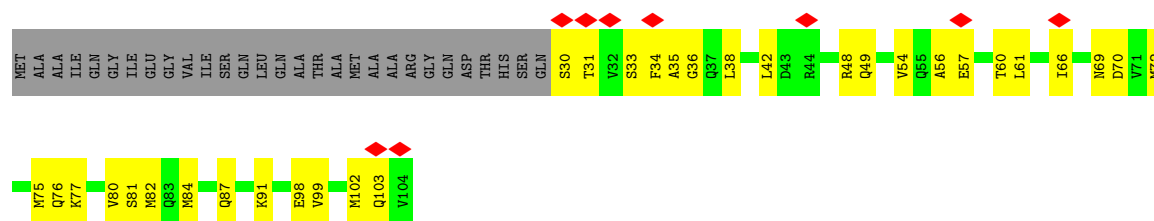


- Molecule 5: Flagellar hook-basal body complex protein FliE

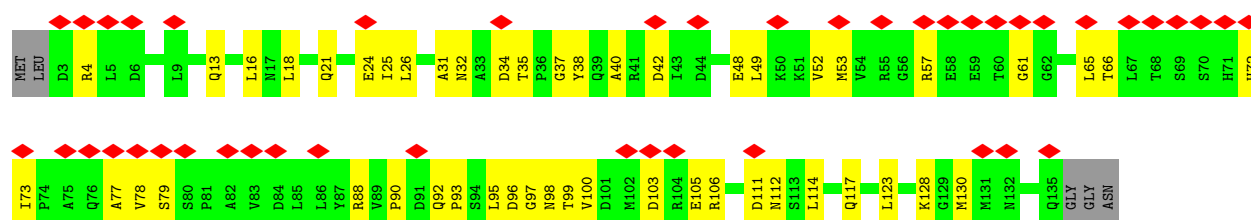


- Molecule 5: Flagellar hook-basal body complex protein FliE

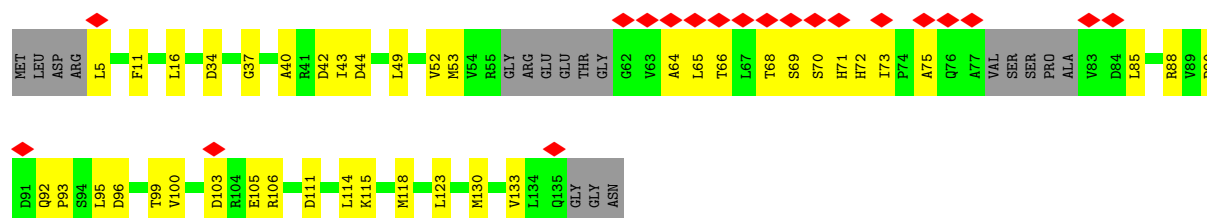




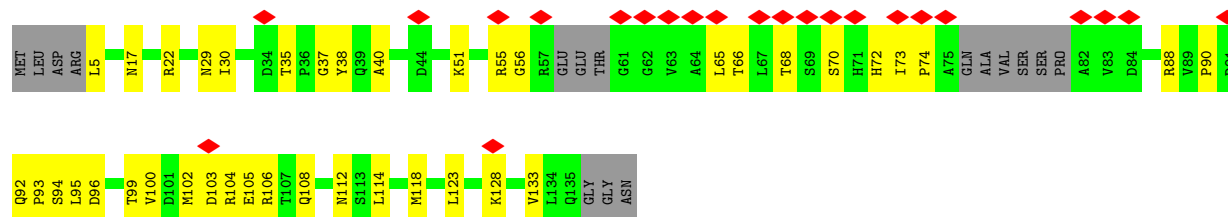
• Molecule 6: Flagellar basal body rod protein FlgB



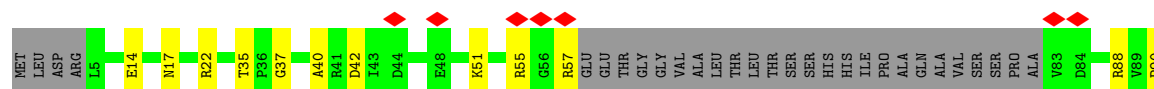
• Molecule 6: Flagellar basal body rod protein FlgB



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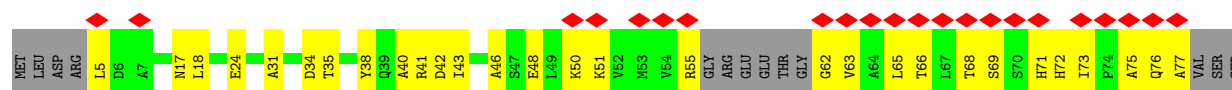


• Molecule 6: Flagellar basal body rod protein FlgB

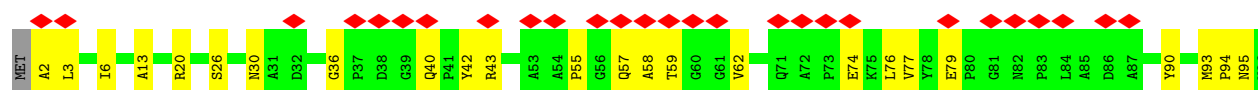
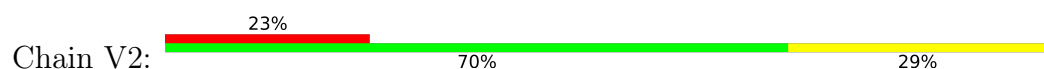




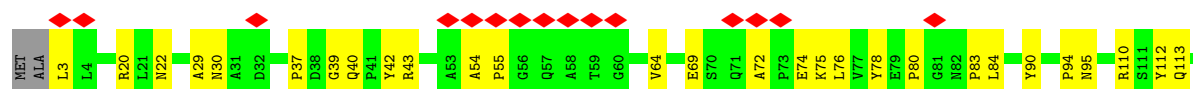
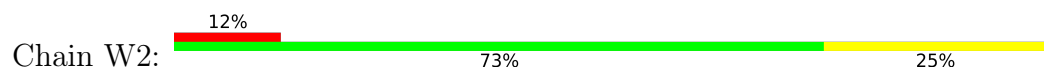
- Molecule 6: Flagellar basal body rod protein FlgB



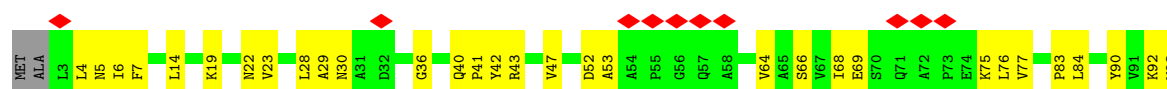
- Molecule 7: Flagellar basal-body rod protein FlgC



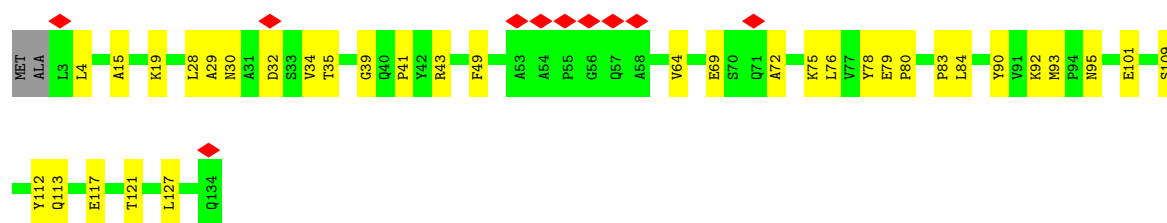
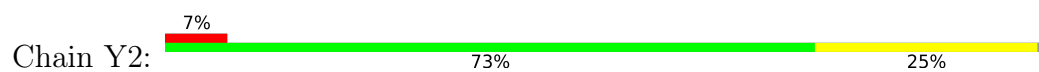
- Molecule 7: Flagellar basal-body rod protein FlgC



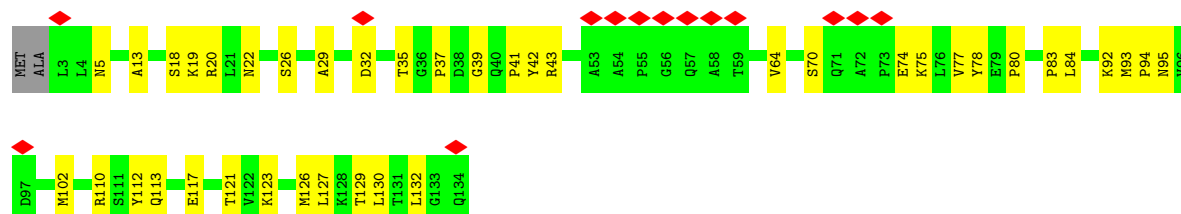
- Molecule 7: Flagellar basal-body rod protein FlgC



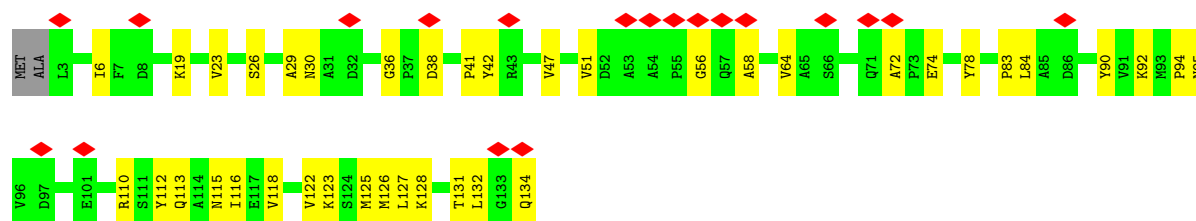
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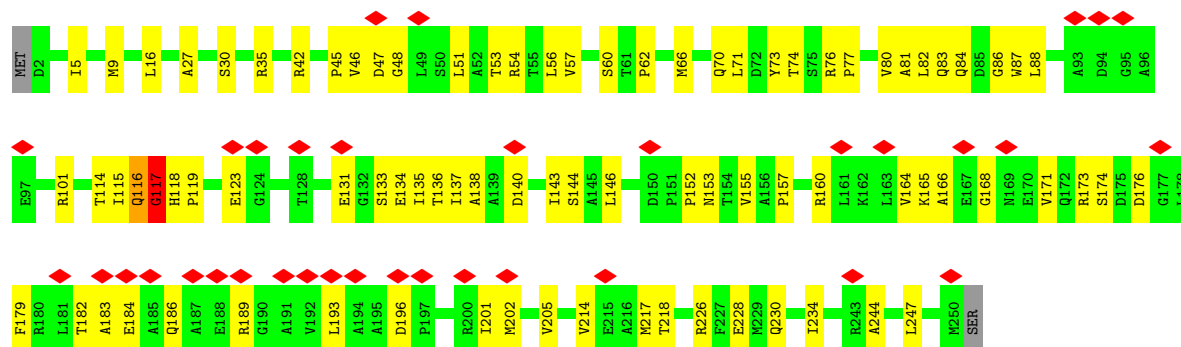
• Molecule 7: Flagellar basal-body rod protein FlgC



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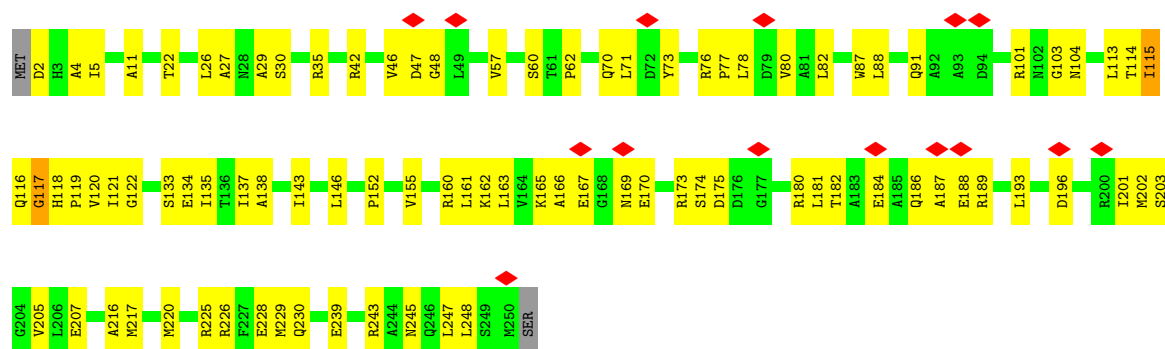


• Molecule 8: Flagellar basal body protein



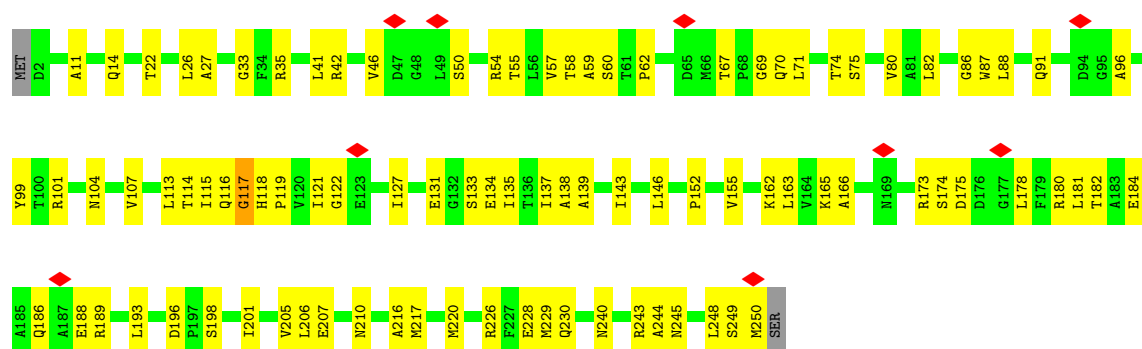
• Molecule 8: Flagellar basal body protein





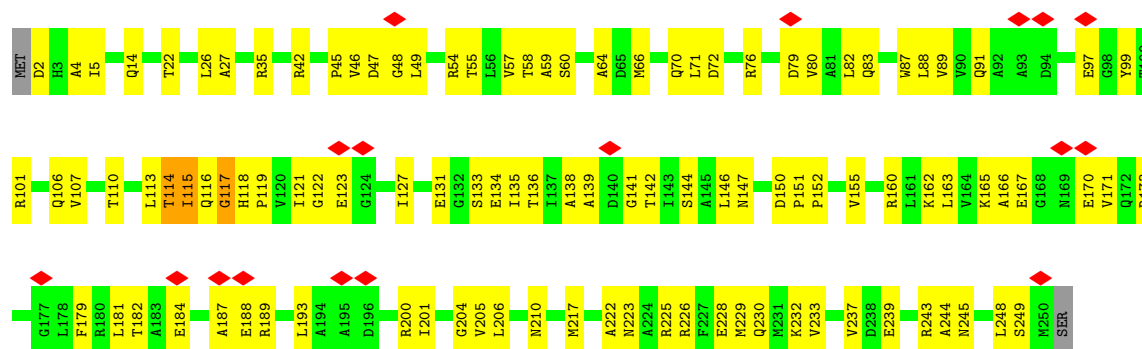
• Molecule 8: Flagellar basal body protein

Chain d2: 62% 37%



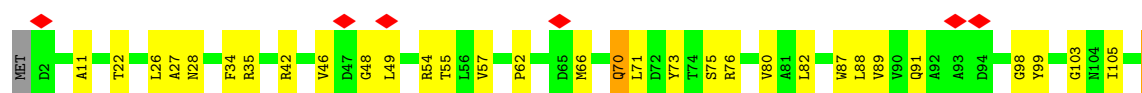
• Molecule 8: Flagellar basal body protein

Chain e2: 7% 57% 41%

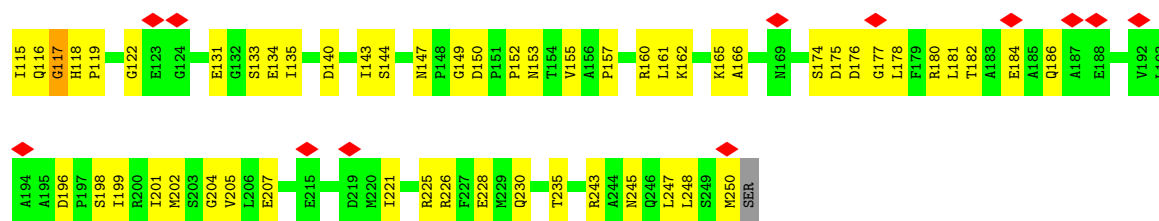


• Molecule 8: Flagellar basal body protein

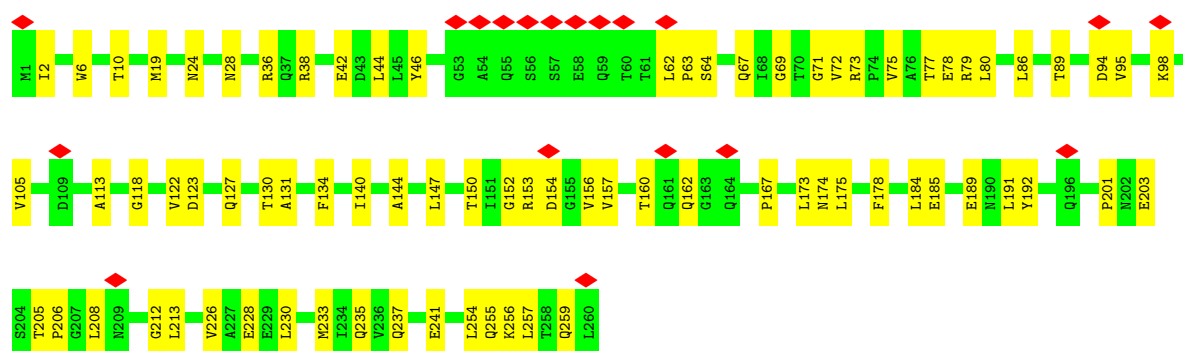
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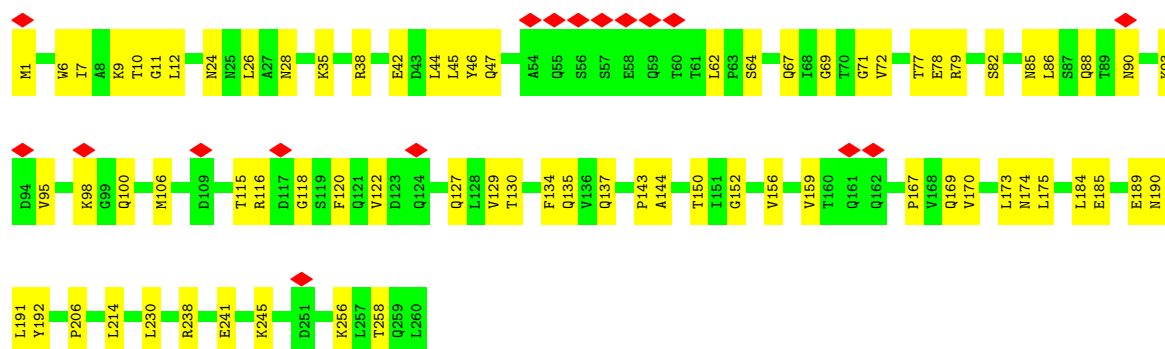
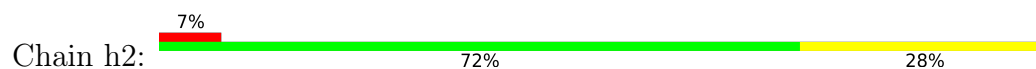




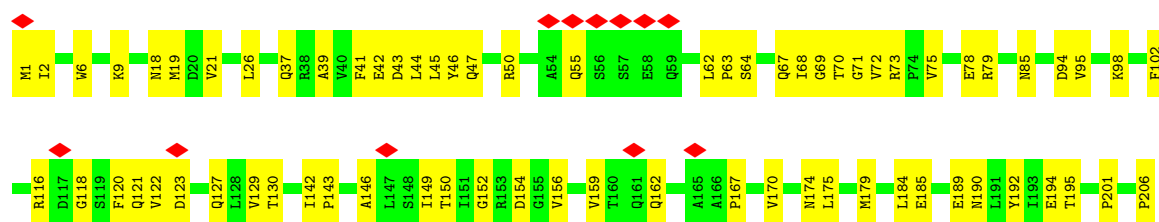
• Molecule 9: Flagellar basal-body rod protein FlgG



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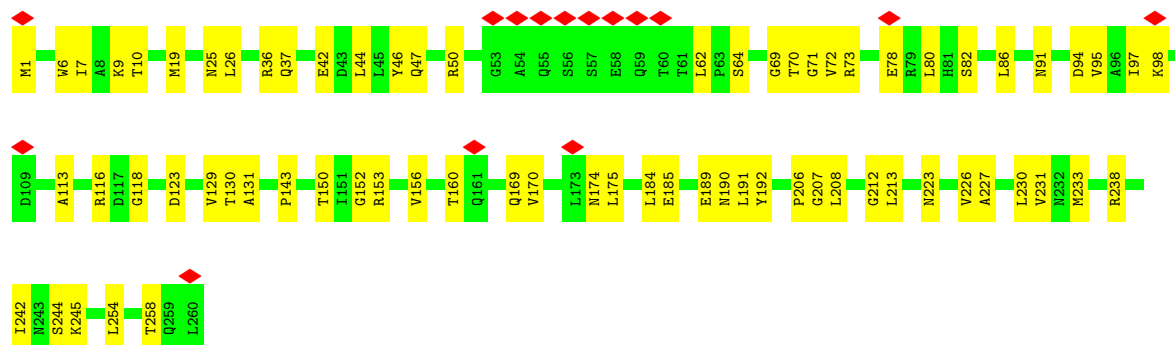
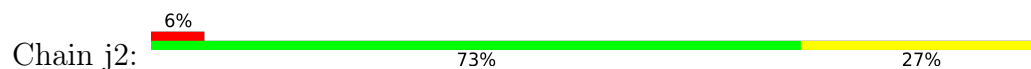


• Molecule 9: Flagellar basal-body rod protein FlgG

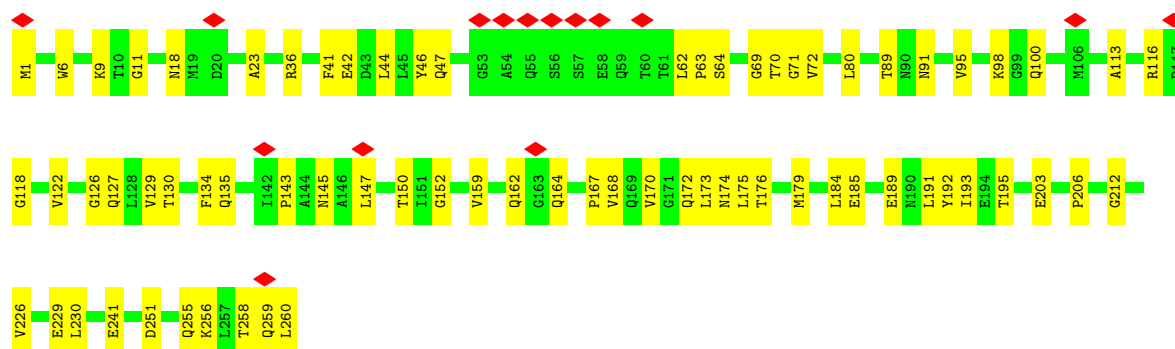
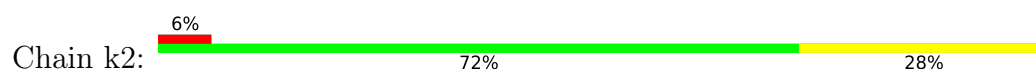




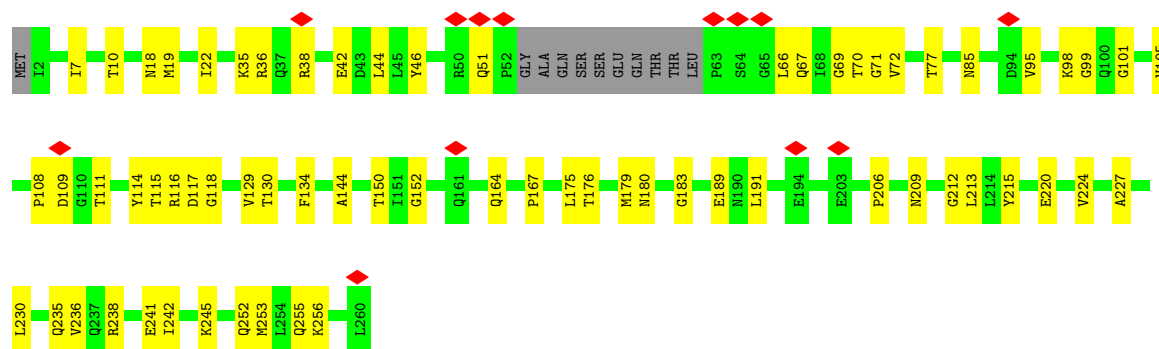
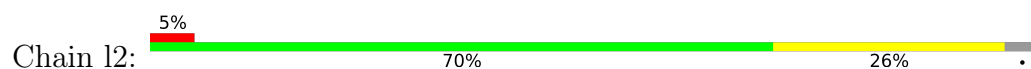
• Molecule 9: Flagellar basal-body rod protein FlgG



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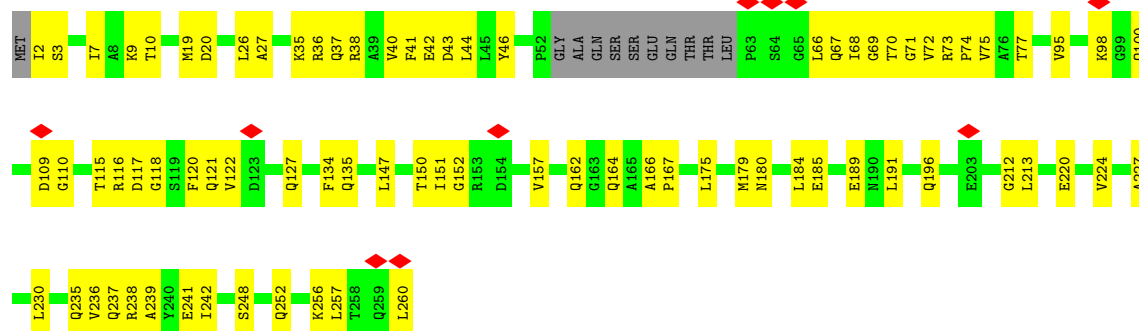


• Molecule 9: Flagellar basal-body rod protein FlgG



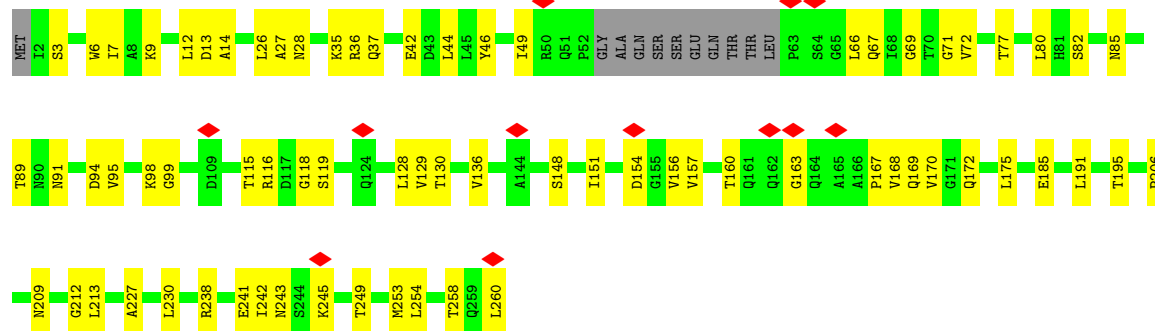
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Chain m2: 



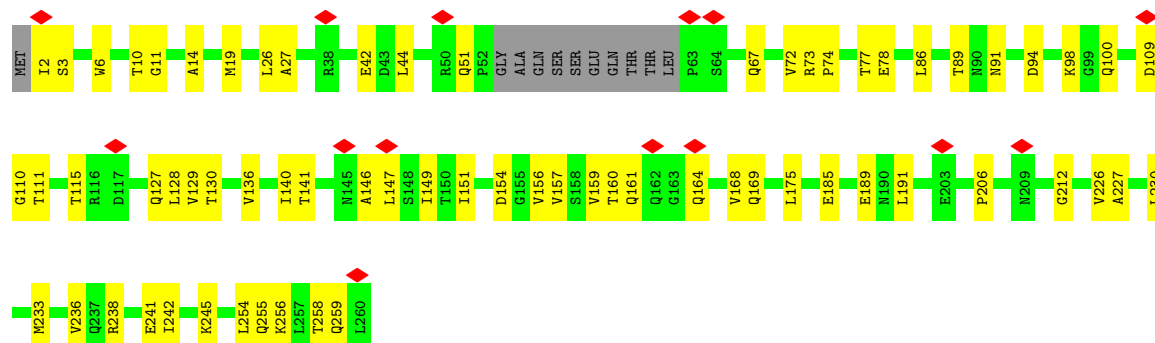
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Chain n2: 



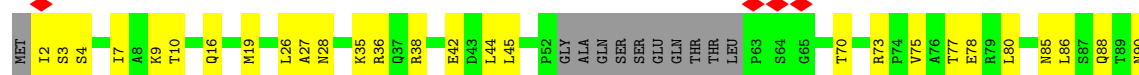
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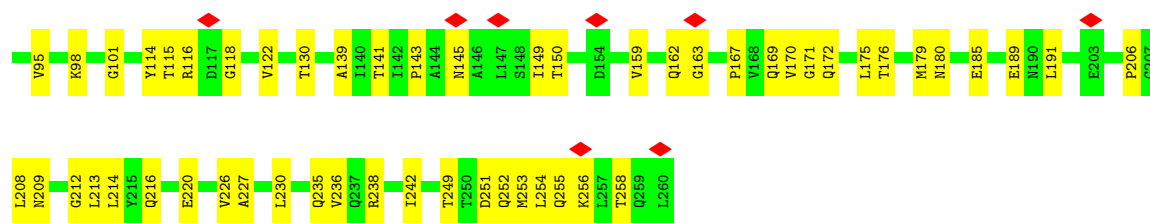
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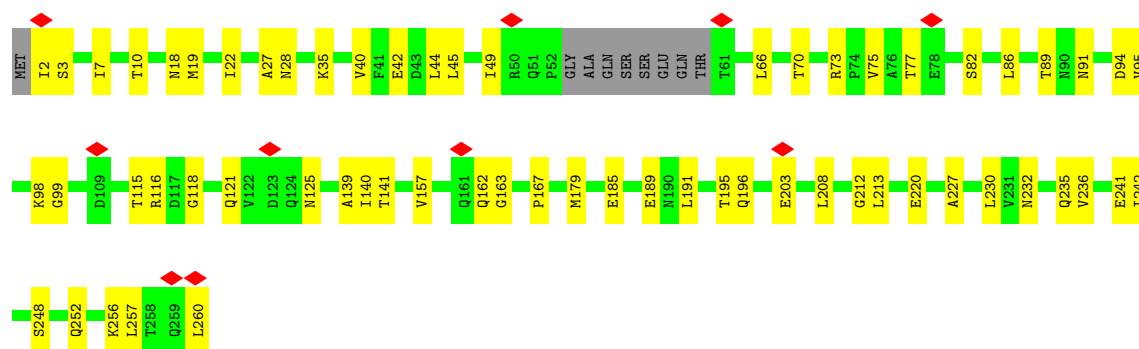
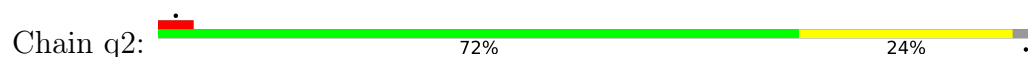
• Molecule 9: Flagellar basal-body rod protein FlgG

Chain p2: 

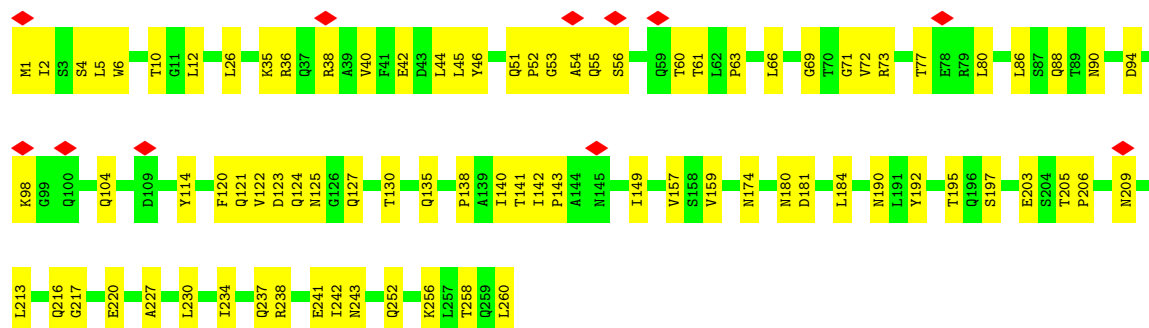




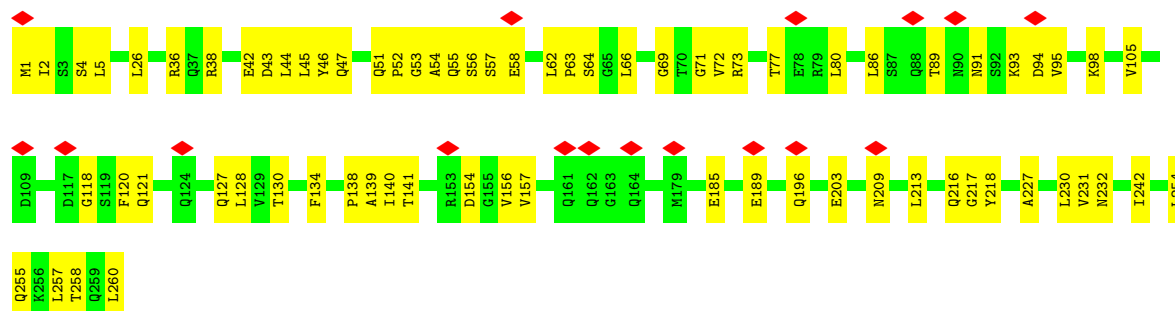
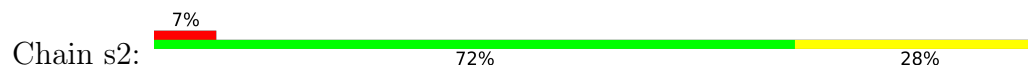
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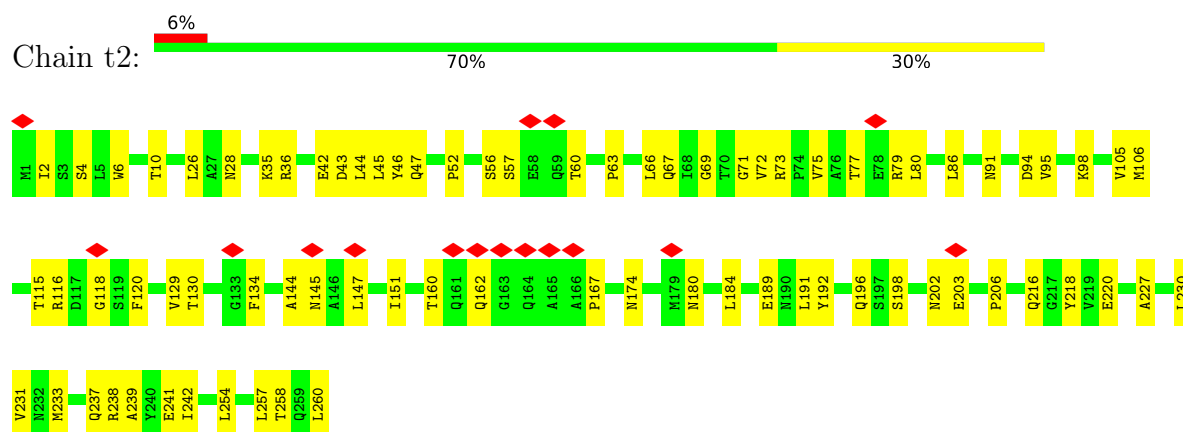
• Molecule 9: Flagellar basal-body rod protein FlgG



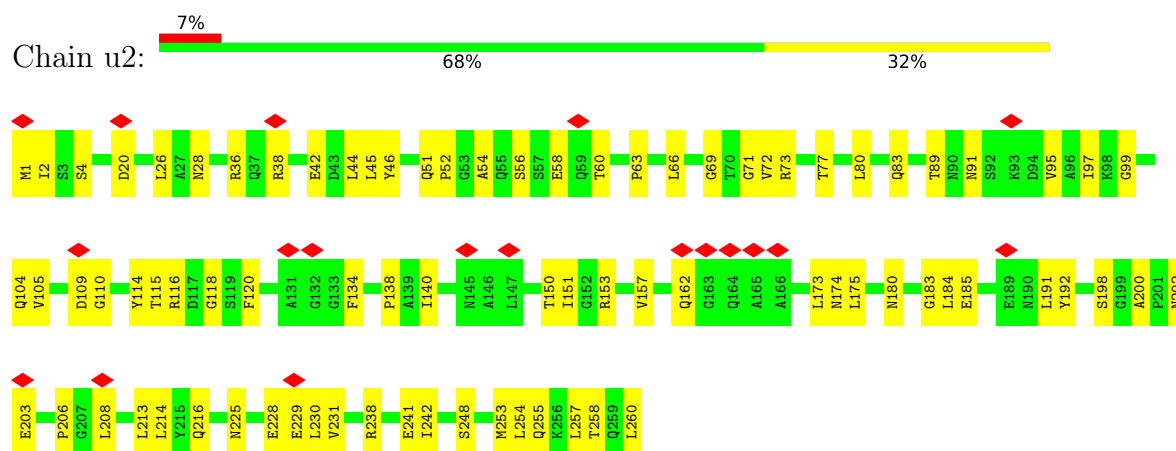
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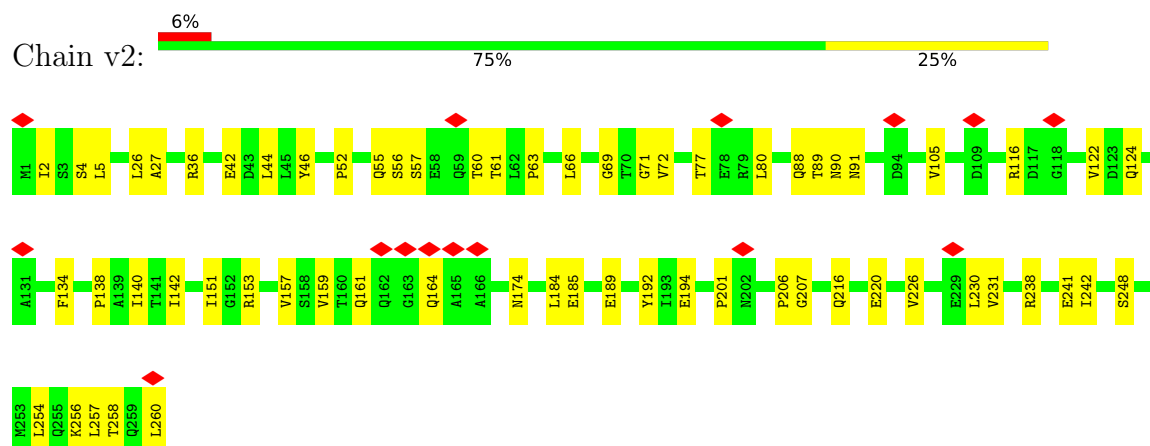
- Molecule 9: Flagellar basal-body rod protein FlgG



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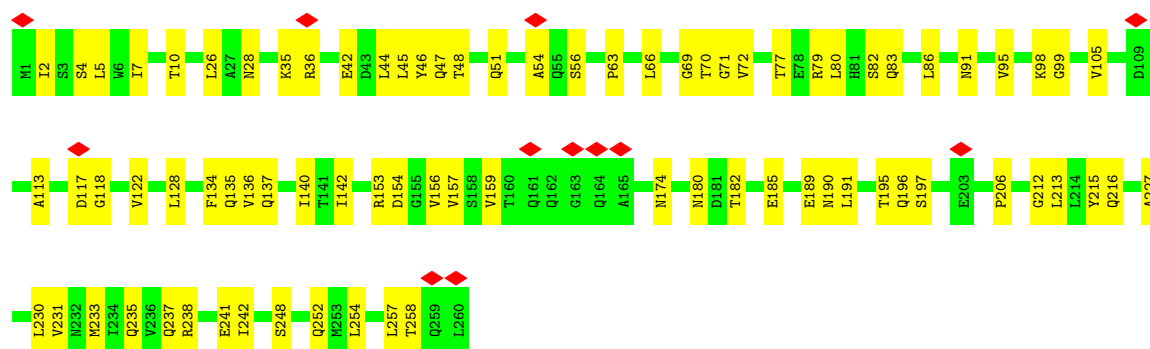


- Molecule 9: Flagellar basal-body rod protein FlgG

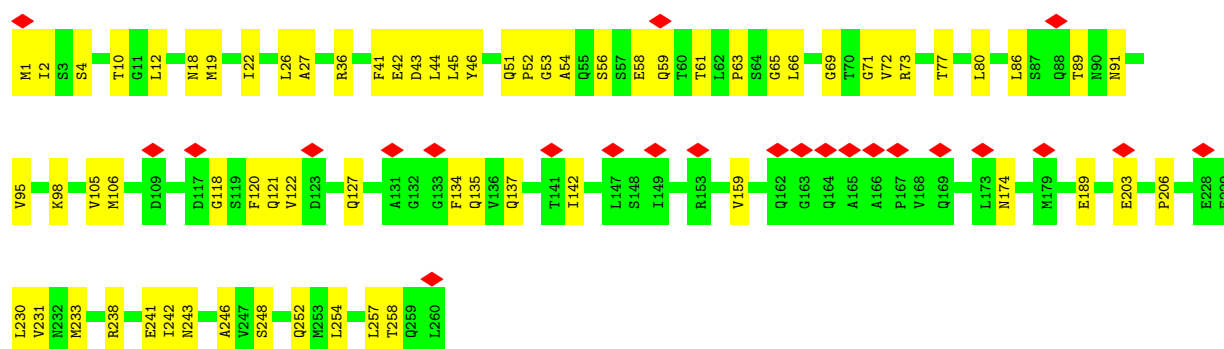


- Molecule 9: Flagellar basal-body rod protein FlgG

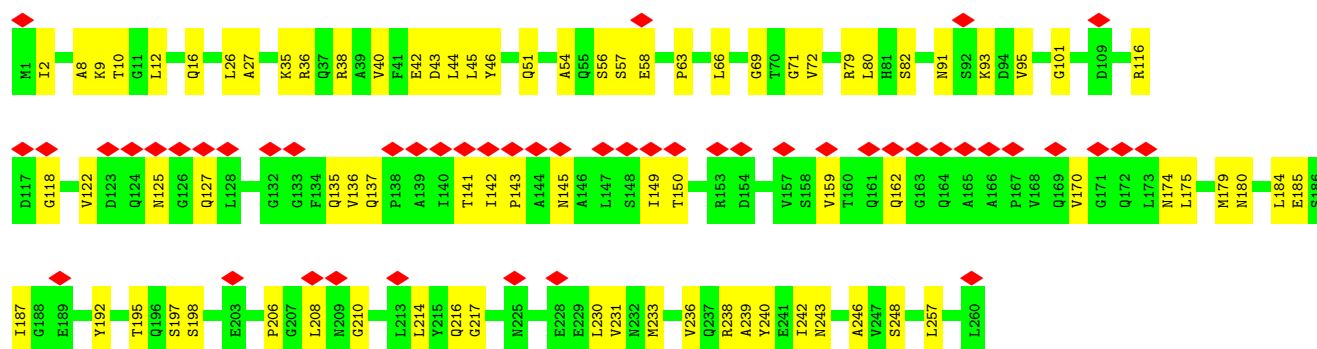




• Molecule 9: Flagellar basal-body rod protein FlgG

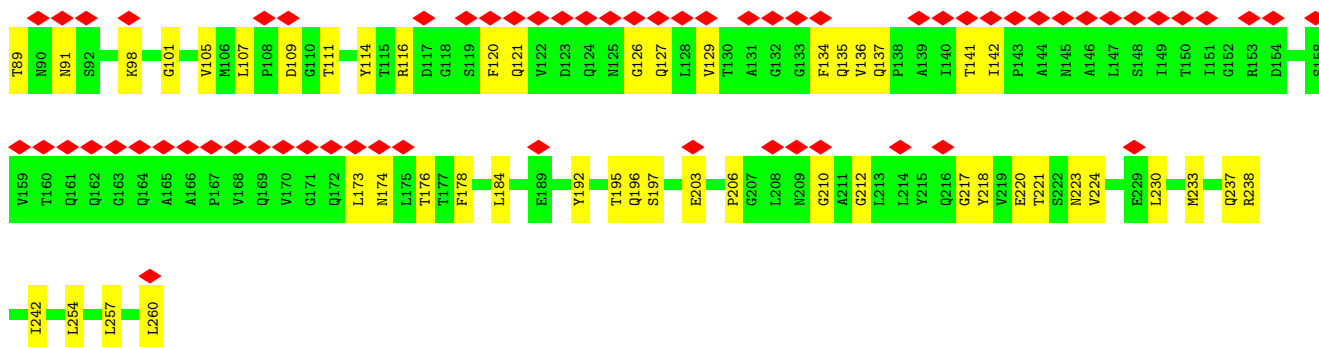


• Molecule 9: Flagellar basal-body rod protein FlgG

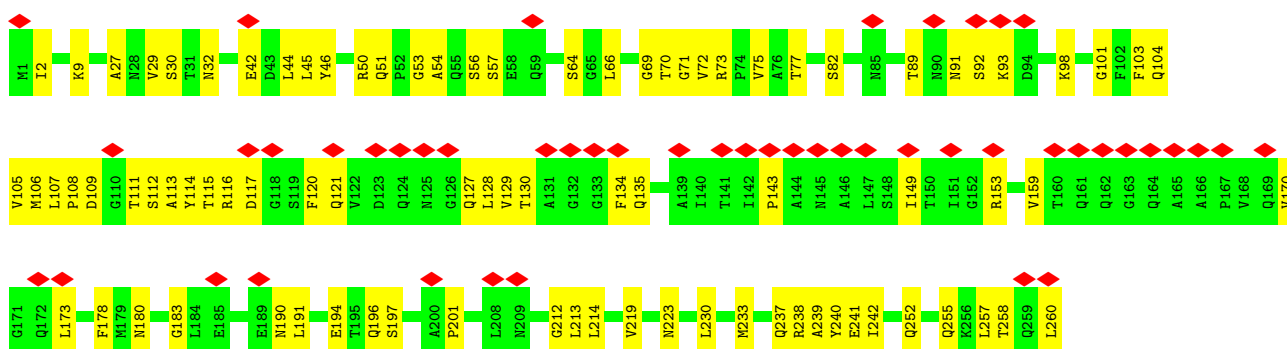


• Molecule 9: Flagellar basal-body rod protein FlgG

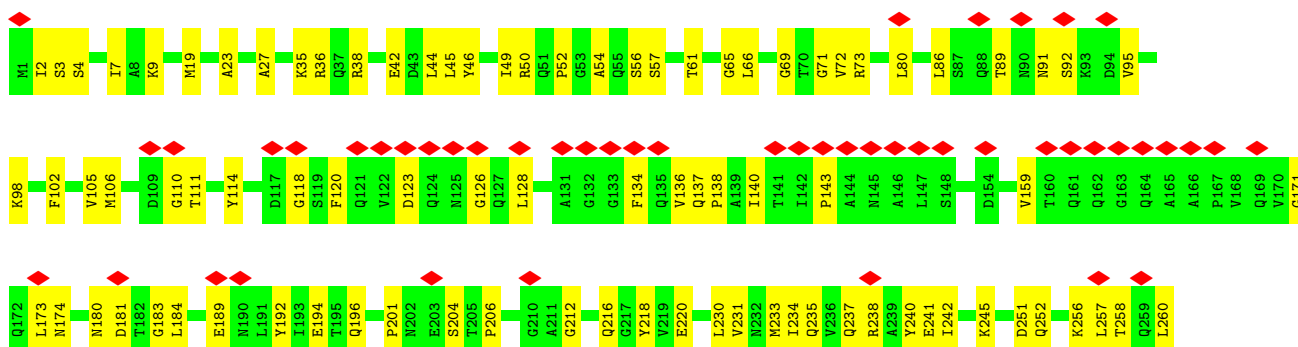




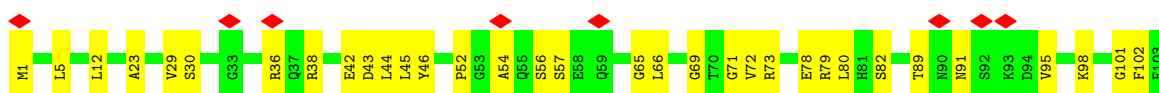
• Molecule 9: Flagellar basal-body rod protein FlgG

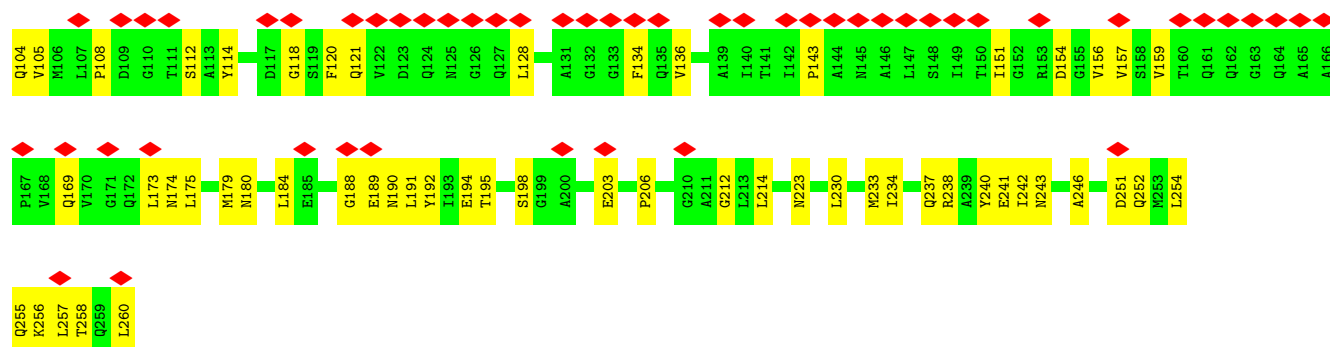


• Molecule 9: Flagellar basal-body rod protein FlgG

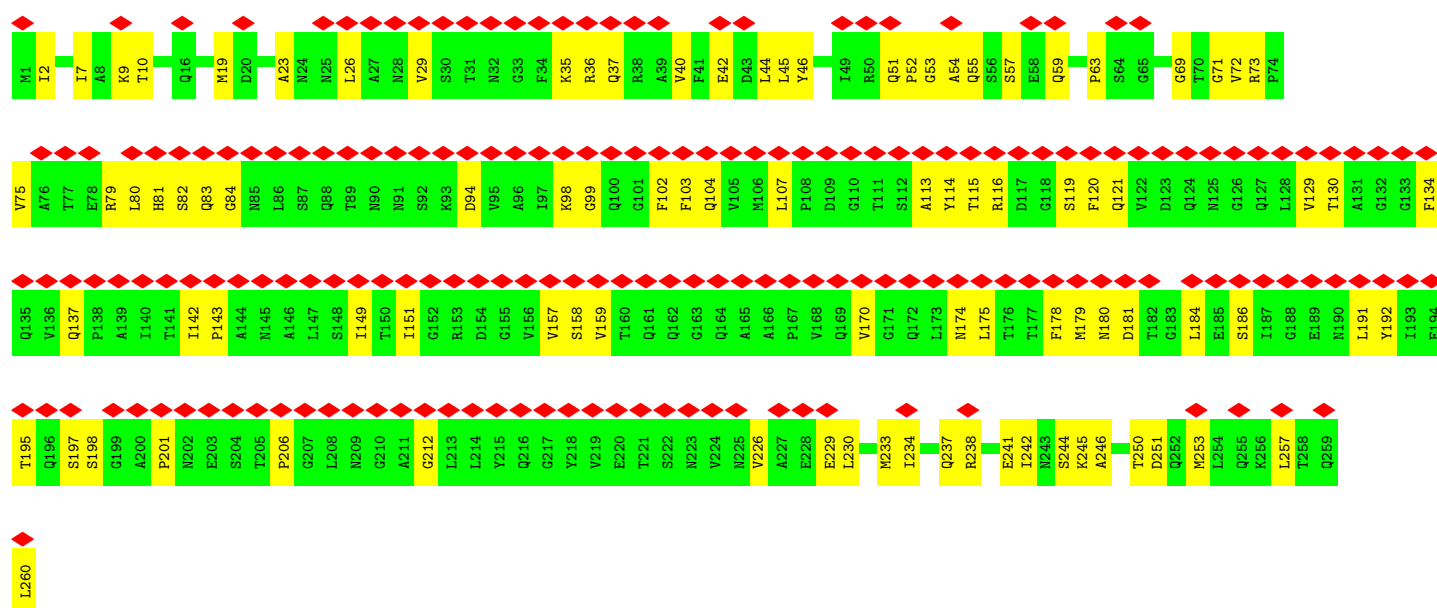
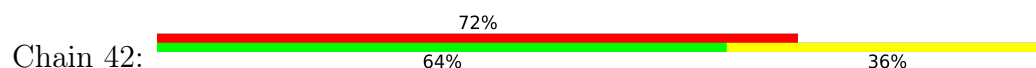


• Molecule 9: Flagellar basal-body rod protein FlgG

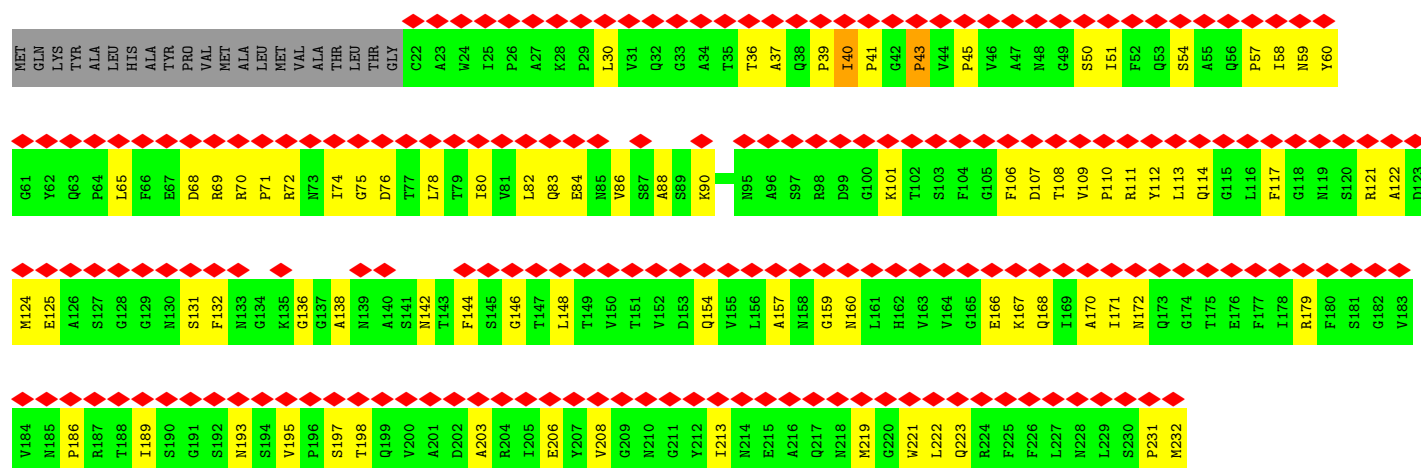
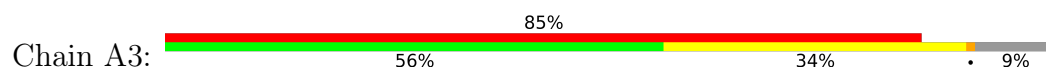




• Molecule 9: Flagellar basal-body rod protein FlgG



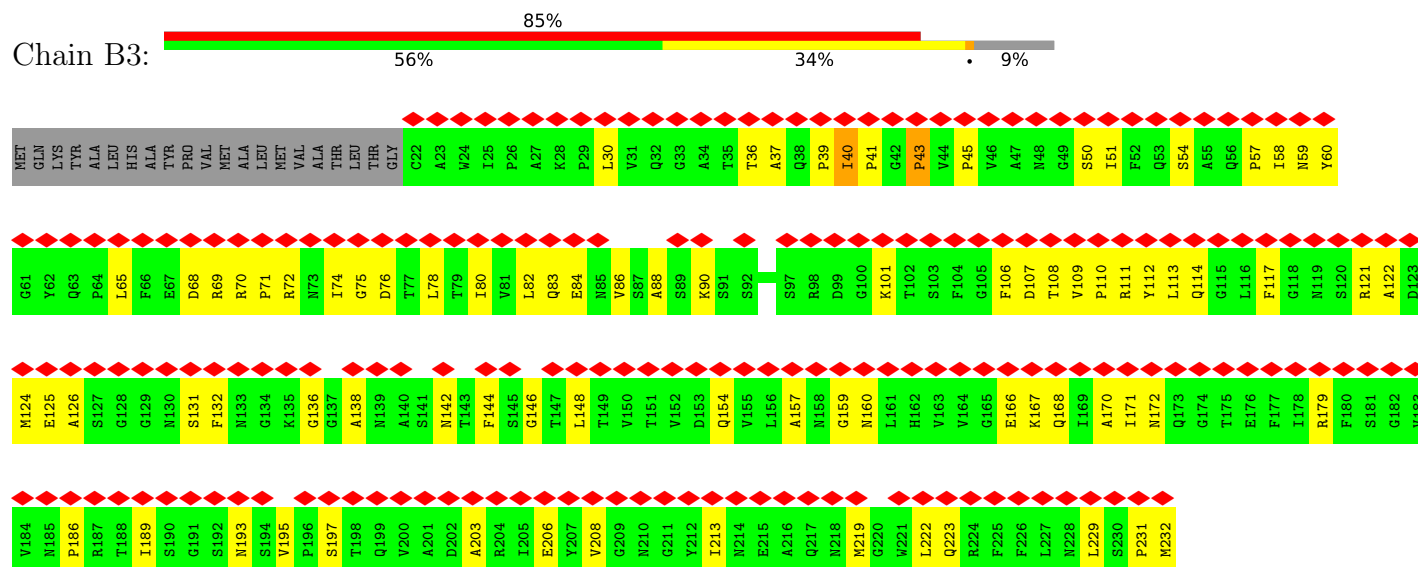
• Molecule 10: Flagellar L-ring protein





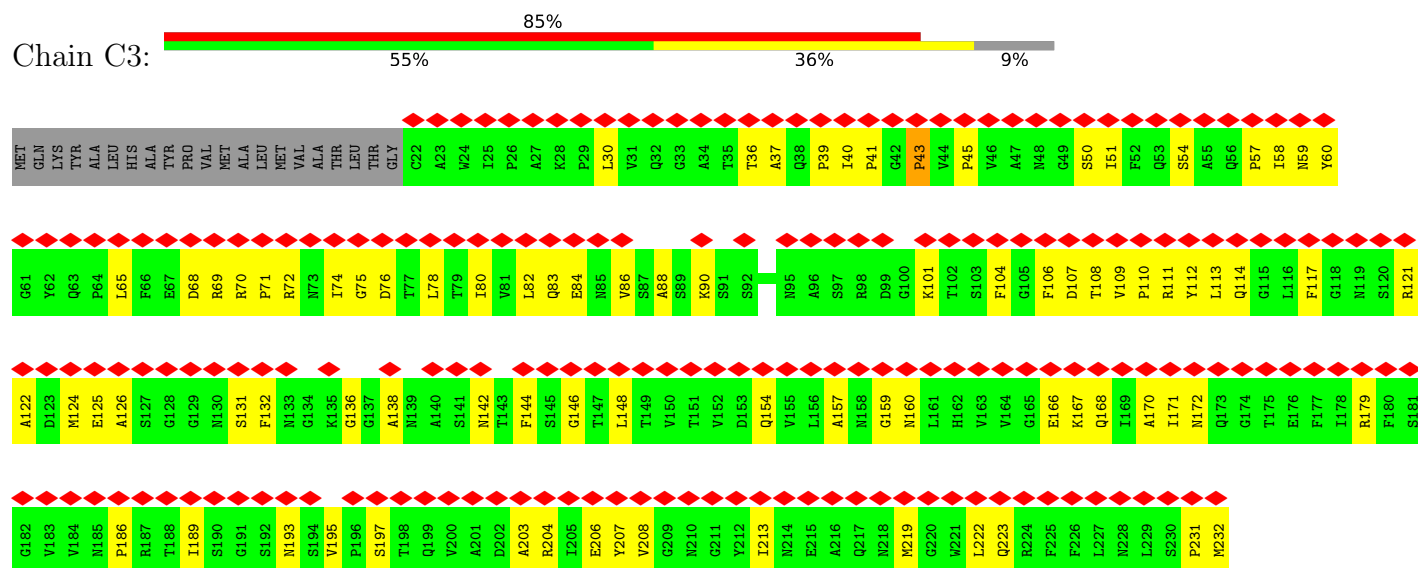
## • Molecule 10: Flagellar L-ring protein

Chain B3:



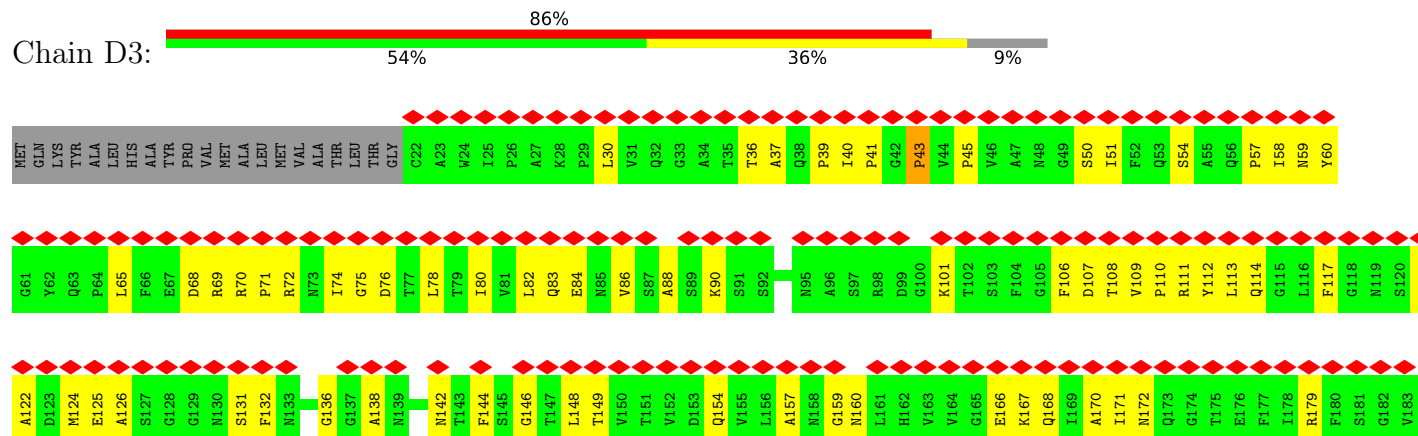
## • Molecule 10: Flagellar L-ring protein

Chain C3:



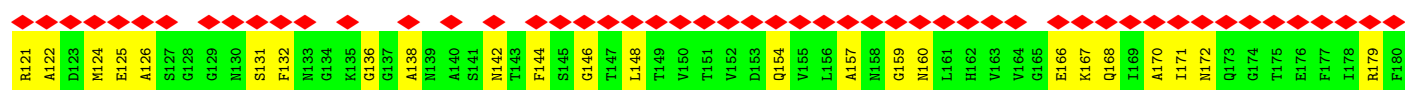
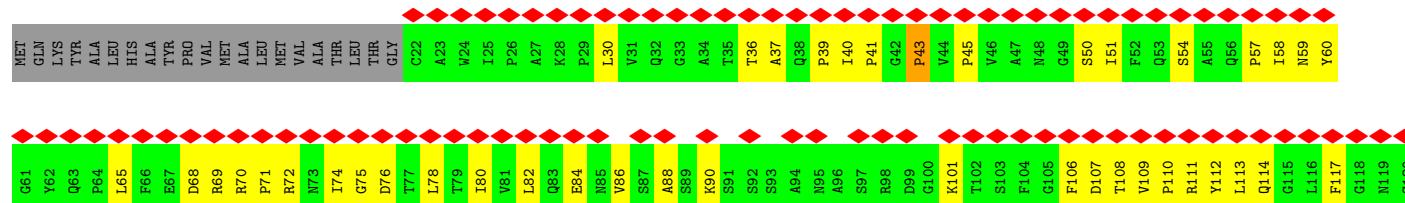
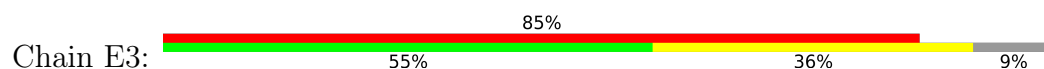
## • Molecule 10: Flagellar L-ring protein

Chain D3:

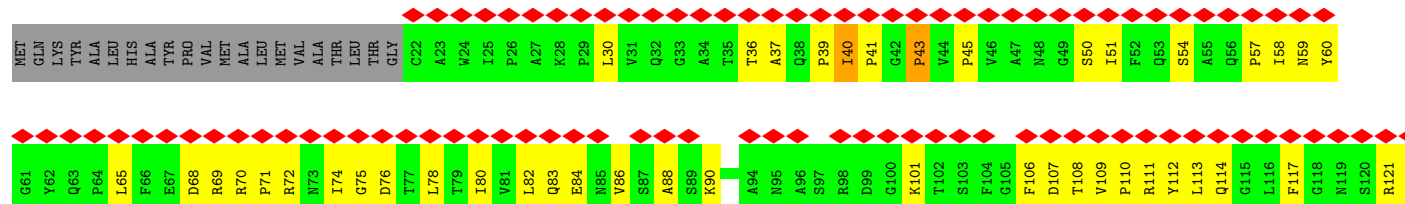
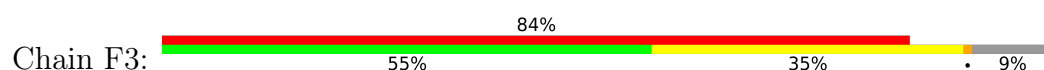




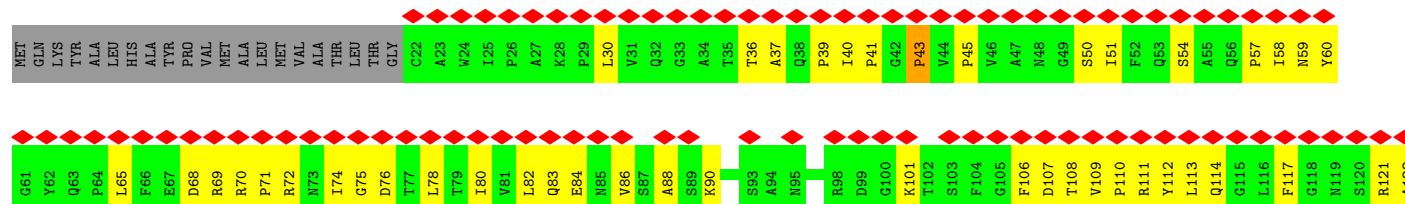
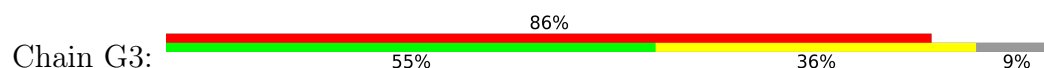
## • Molecule 10: Flagellar L-ring protein



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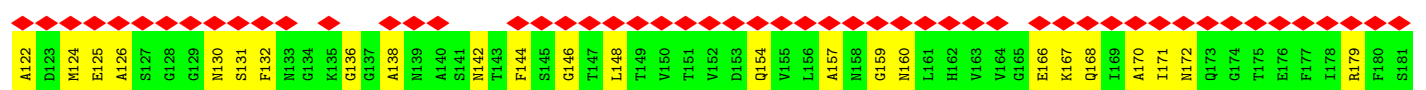
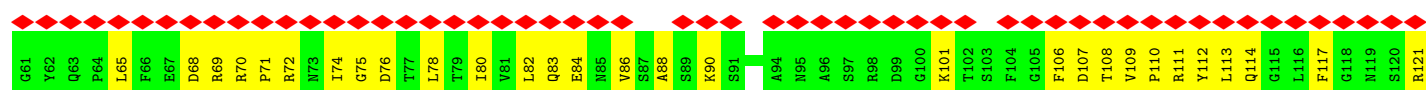


## • Molecule 10: Flagellar L-ring protein

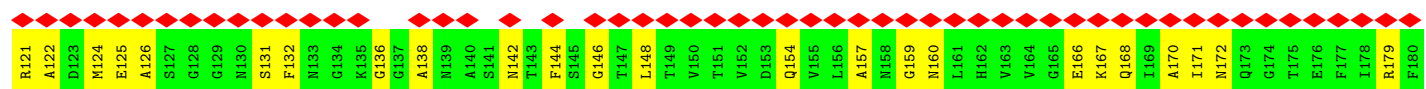




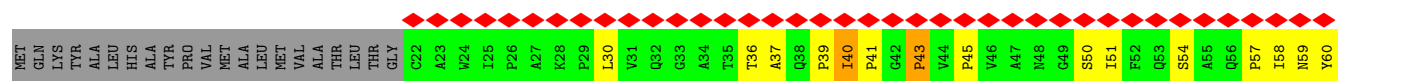
Chain H3:  86% 54% 36% 9%

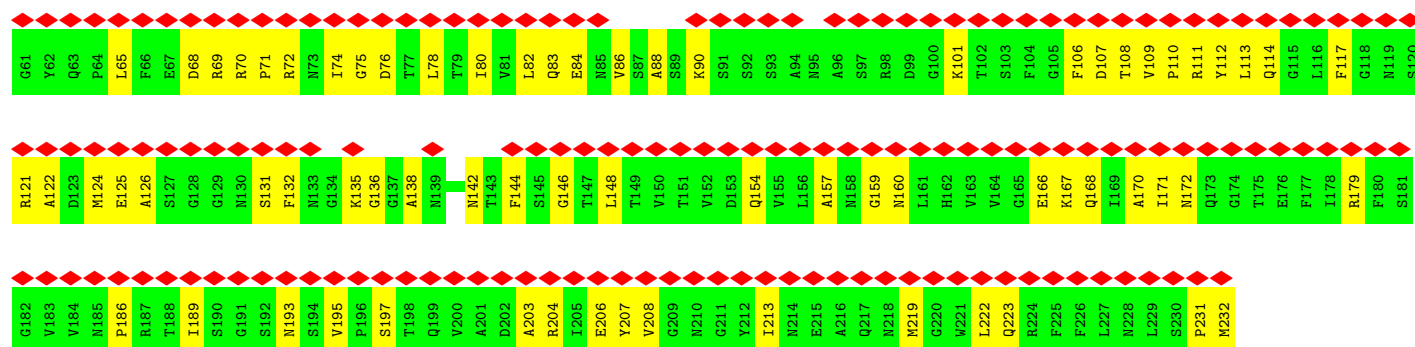


Chain I3:  87% 55% 35% 9%

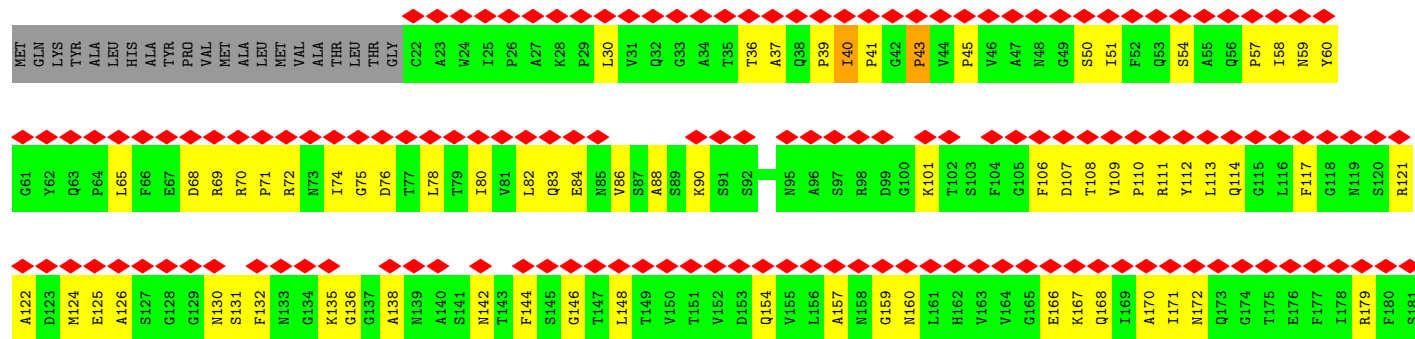
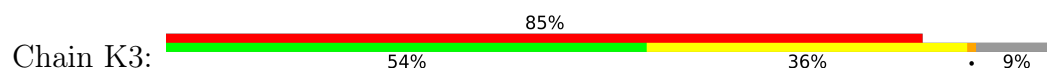


Chain J3:  85% 55% 35% 9%

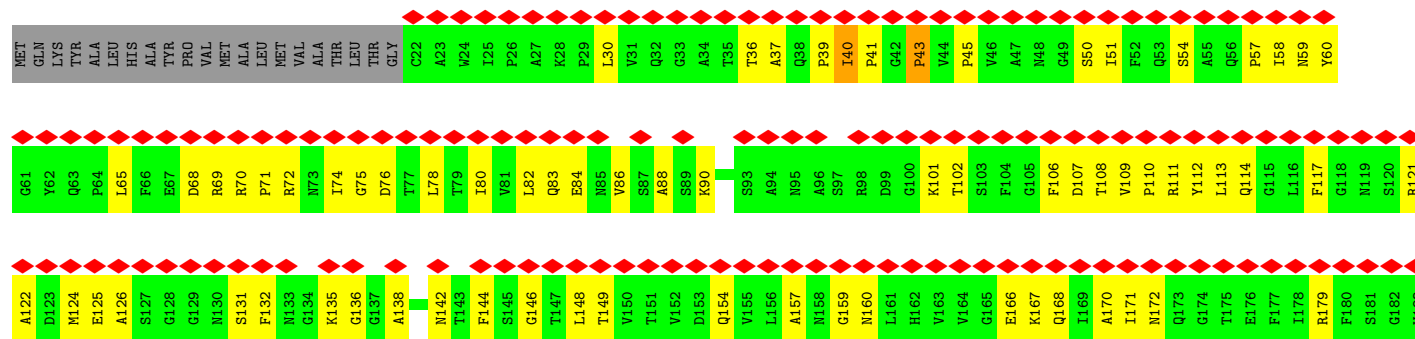
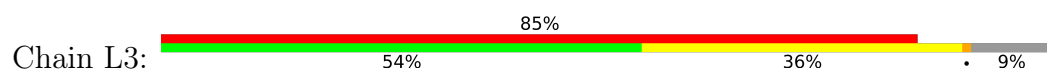




• Molecule 10: Flagellar L-ring protein

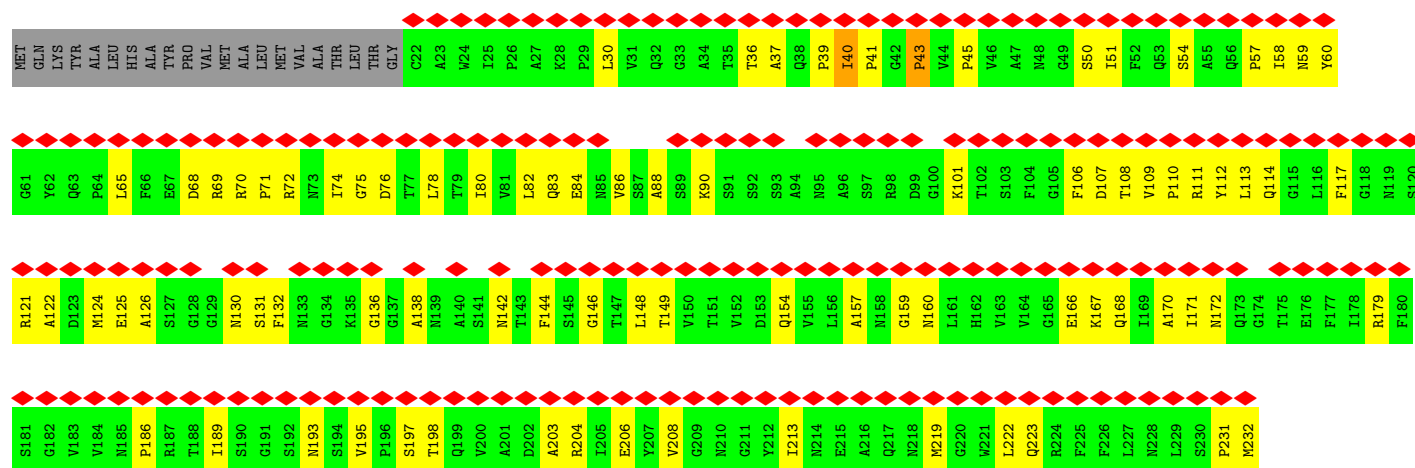


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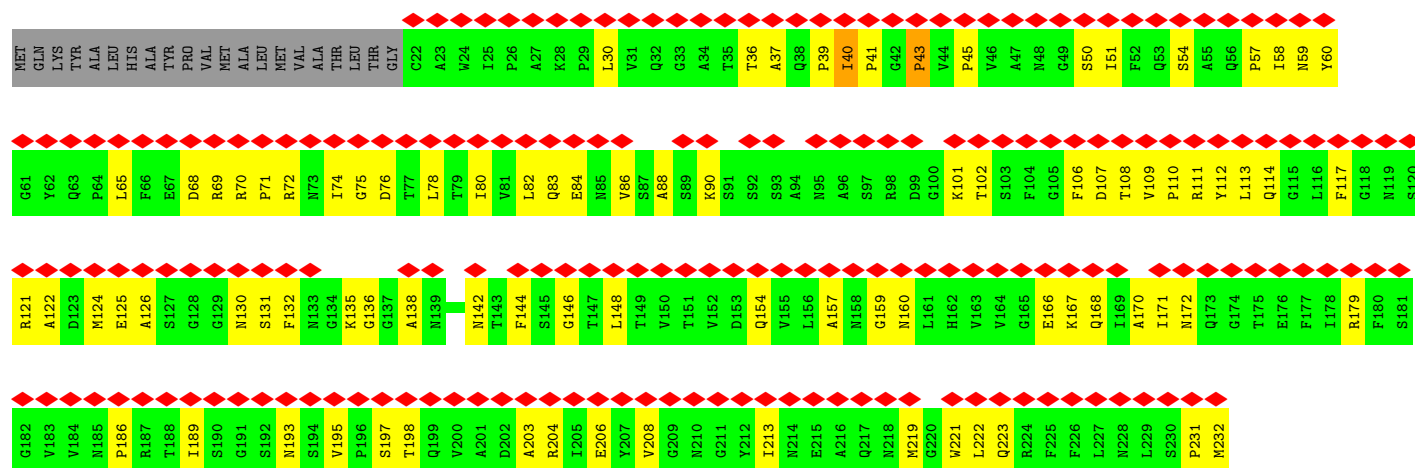
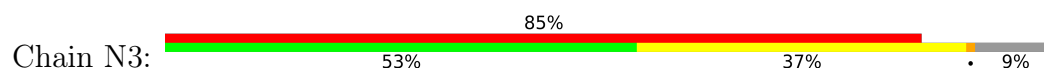


• Molecule 10: Flagellar L-ring protein

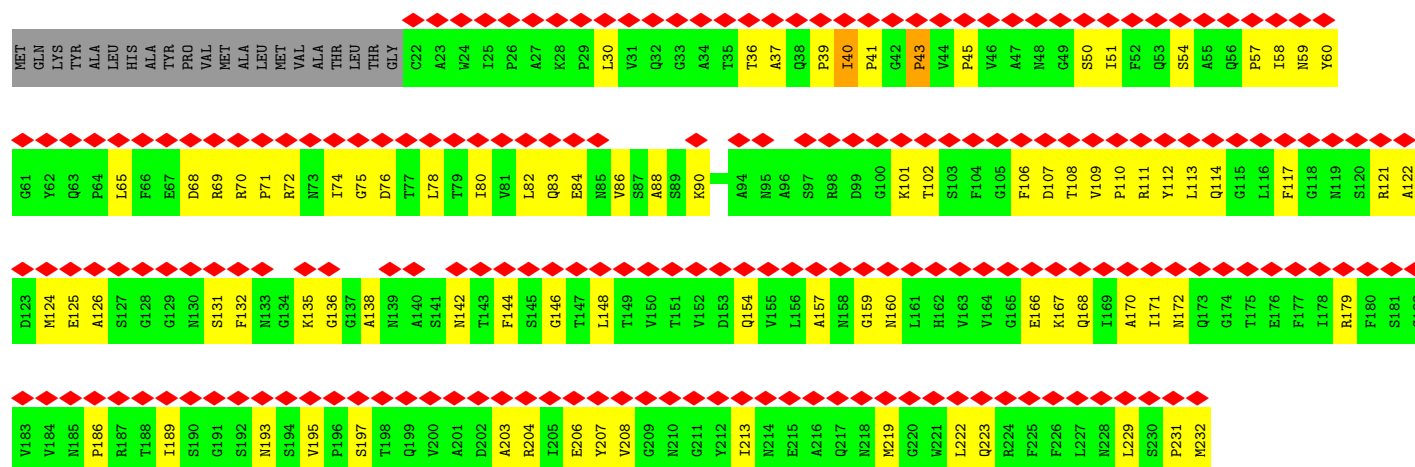
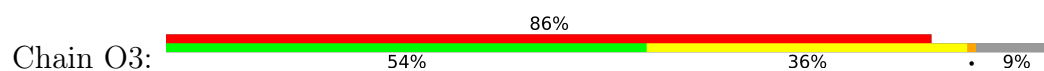




### • Molecule 10: Flagellar L-ring protein

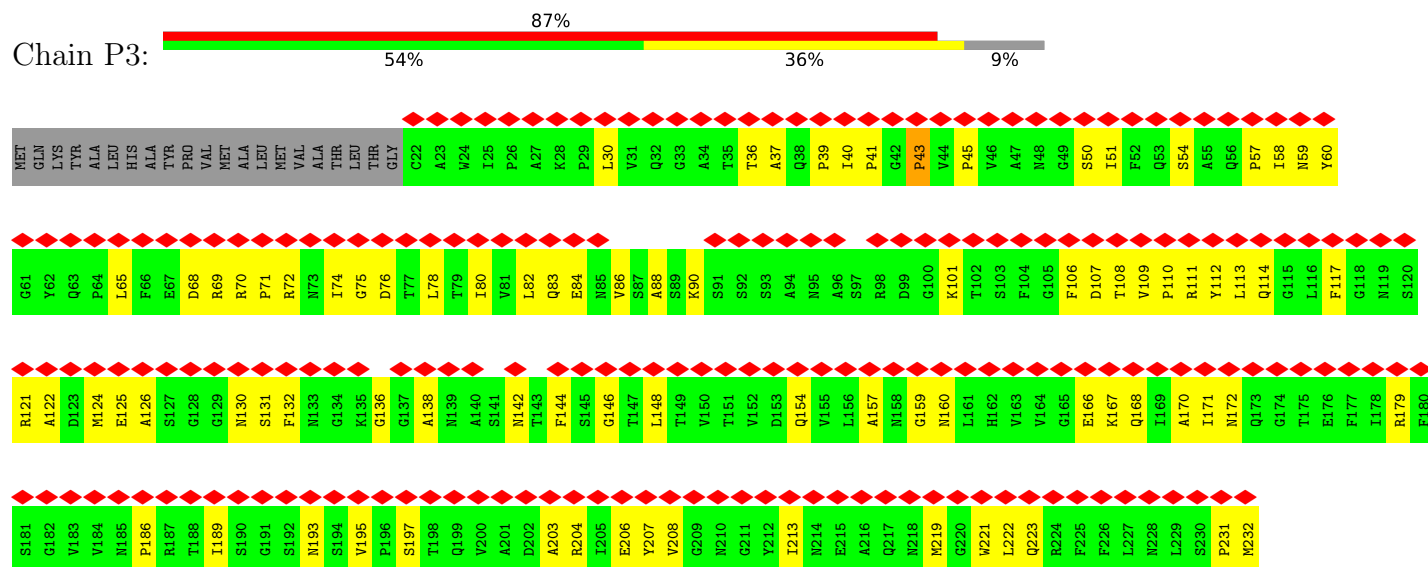


### • Molecule 10: Flagellar L-ring protein



## ● Molecule 10: Flagellar L-ring protein

Chain P3:



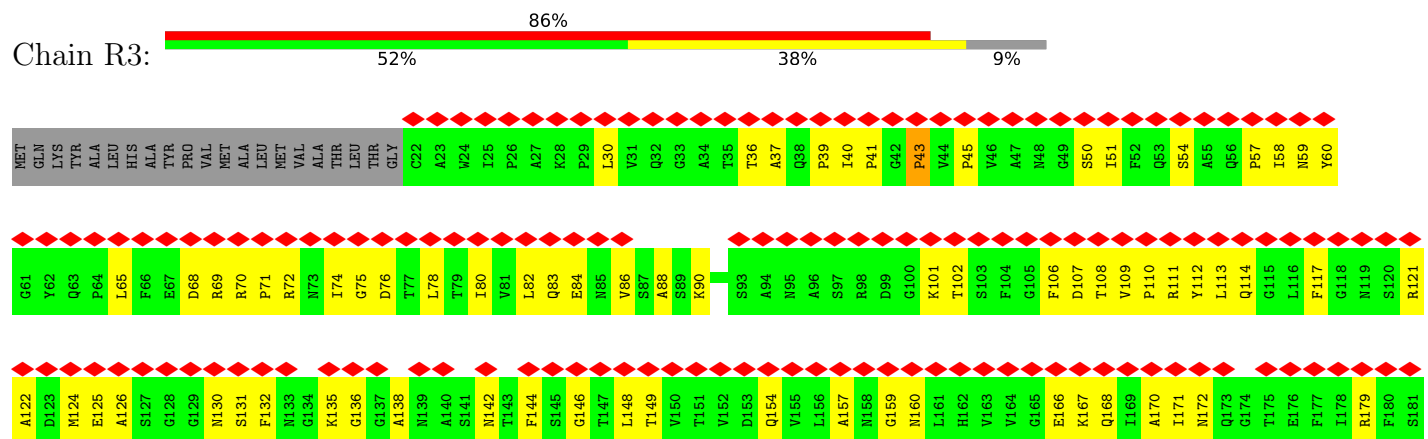
## ● Molecule 10: Flagellar L-ring protein

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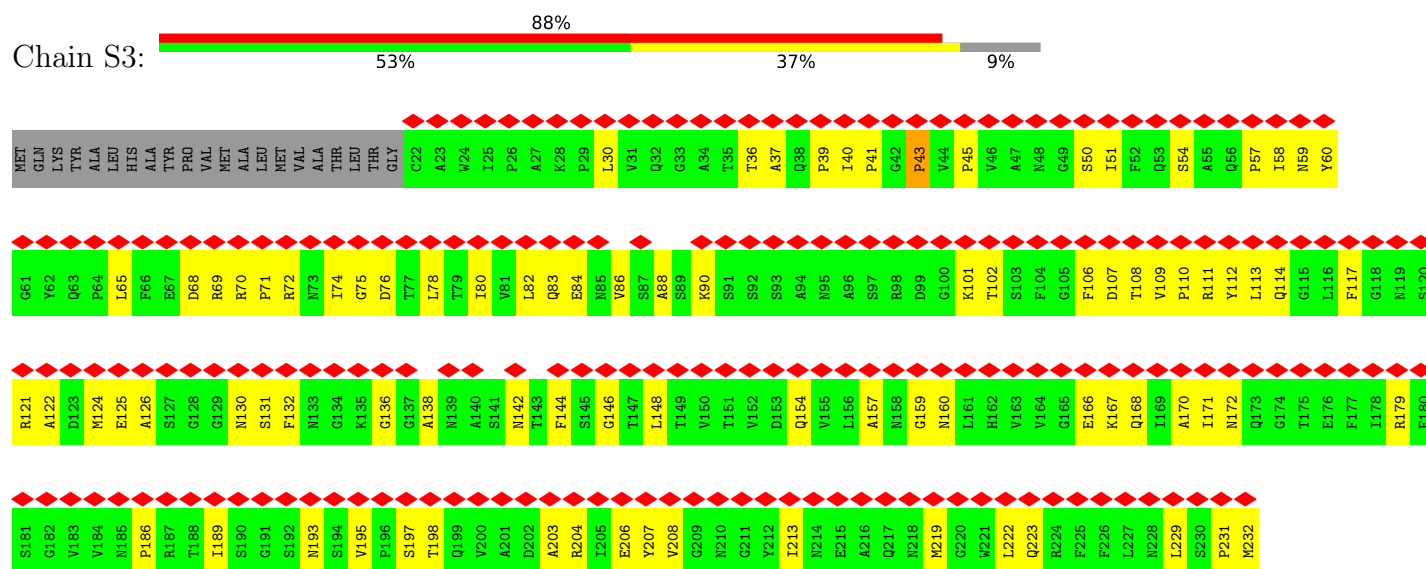
## ● Molecule 10: Flagellar L-ring protein

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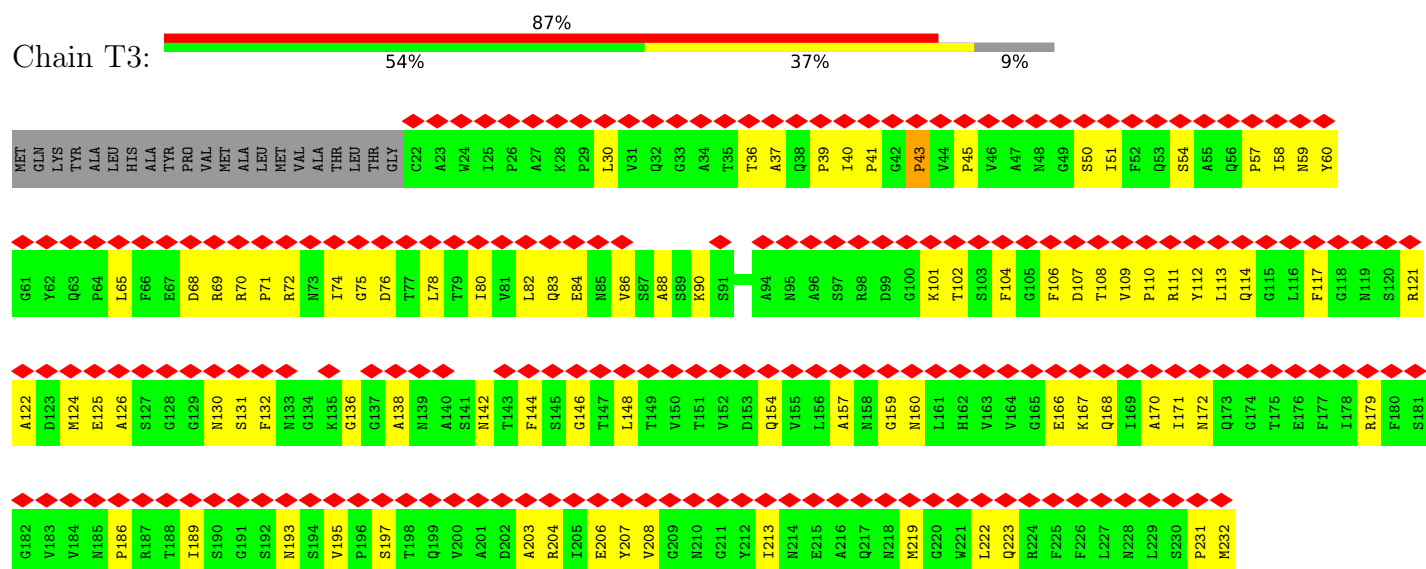




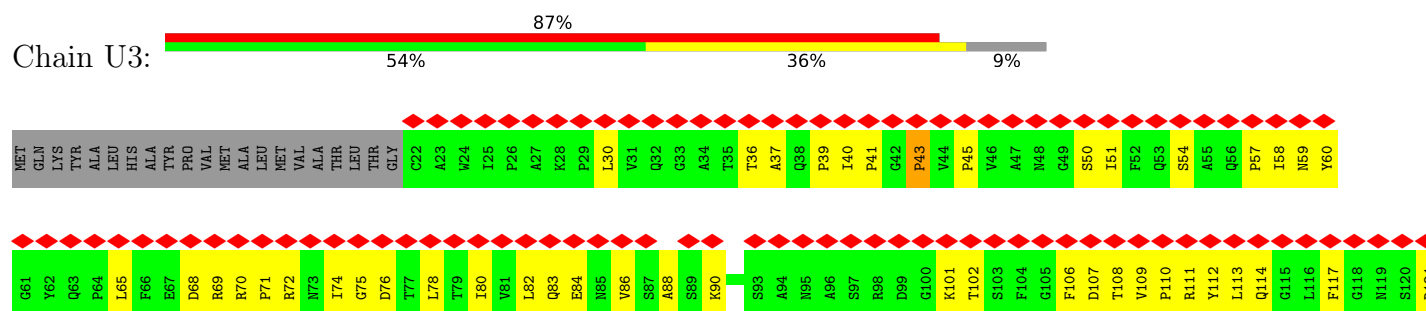
• Molecule 10: Flagellar L-ring protein



• Molecule 10: Flagellar L-ring protein

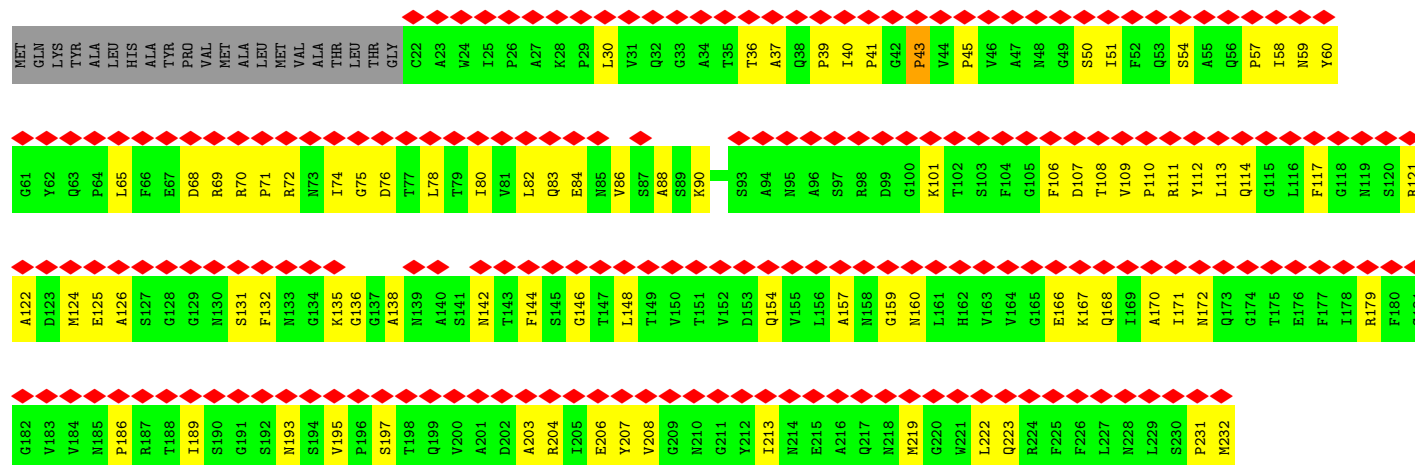
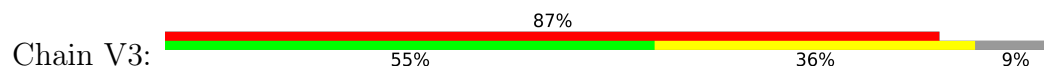


• Molecule 10: Flagellar L-ring protein

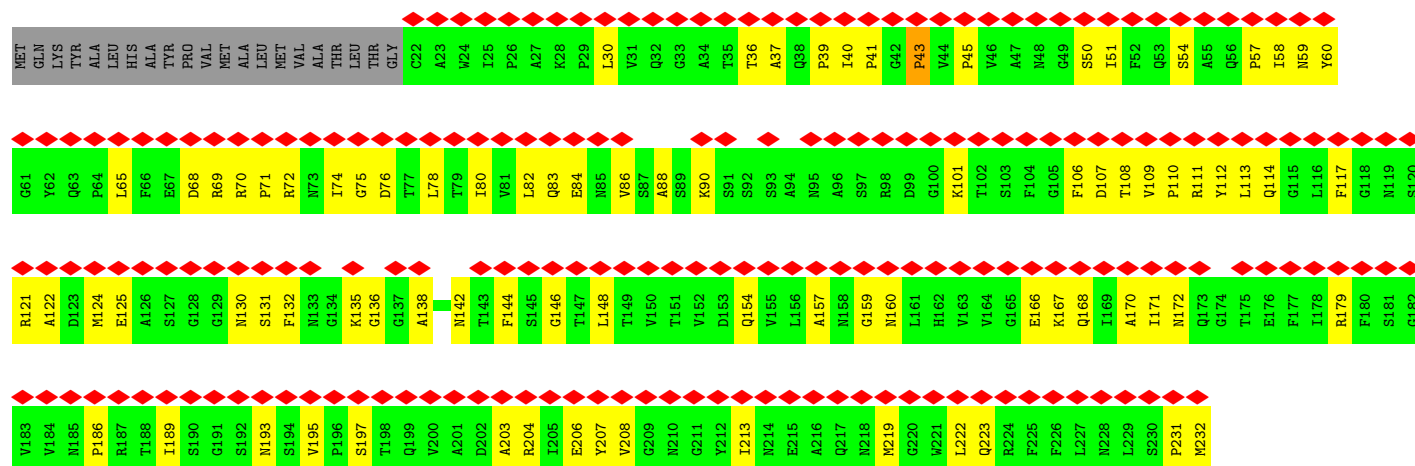




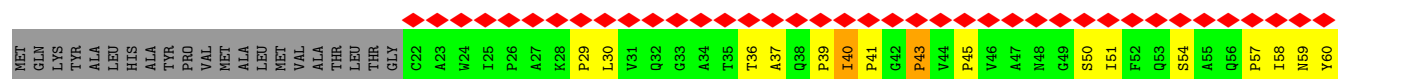
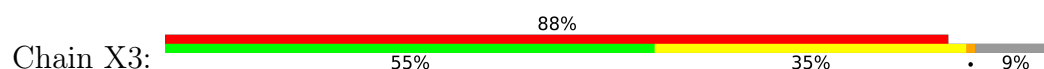
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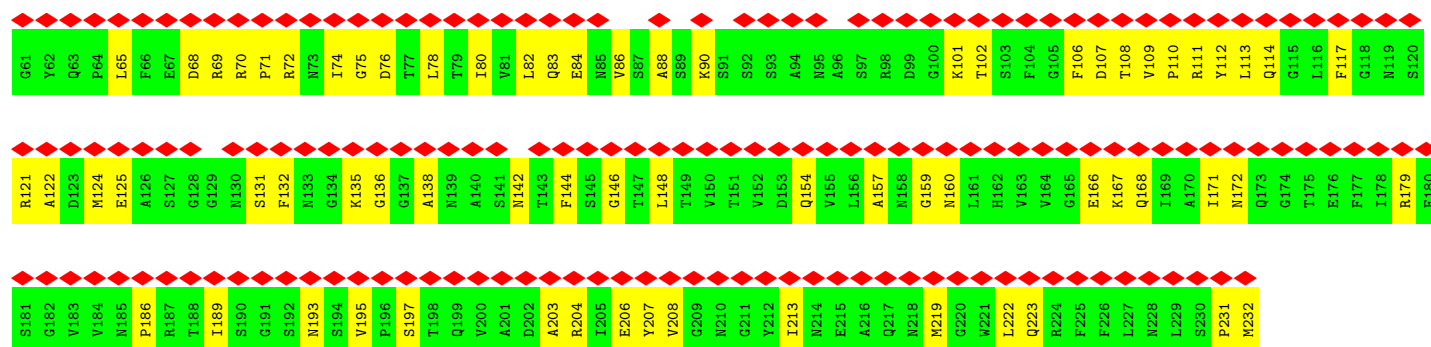
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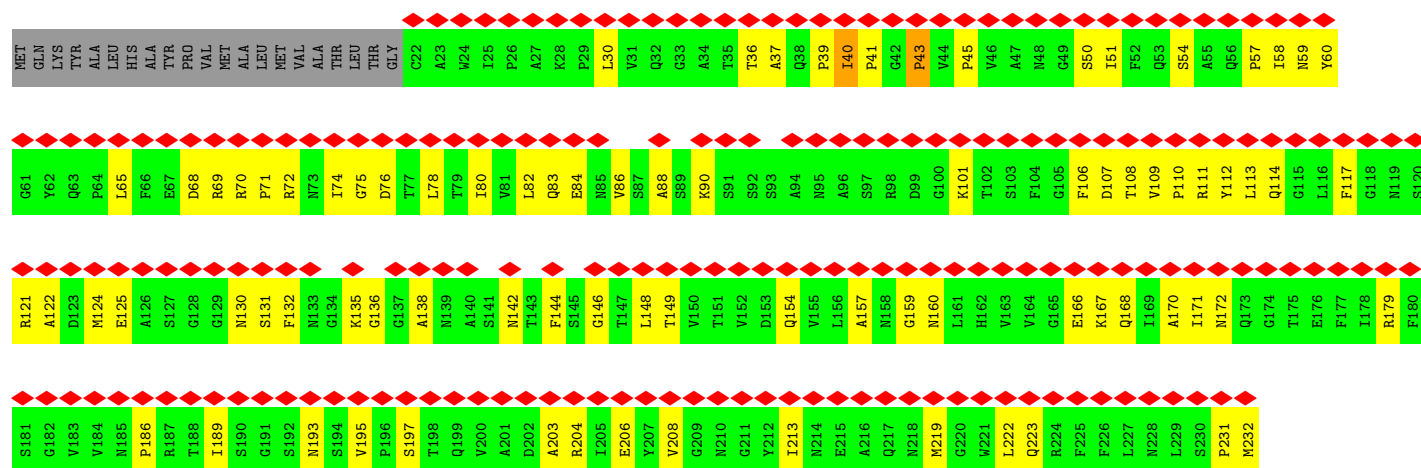
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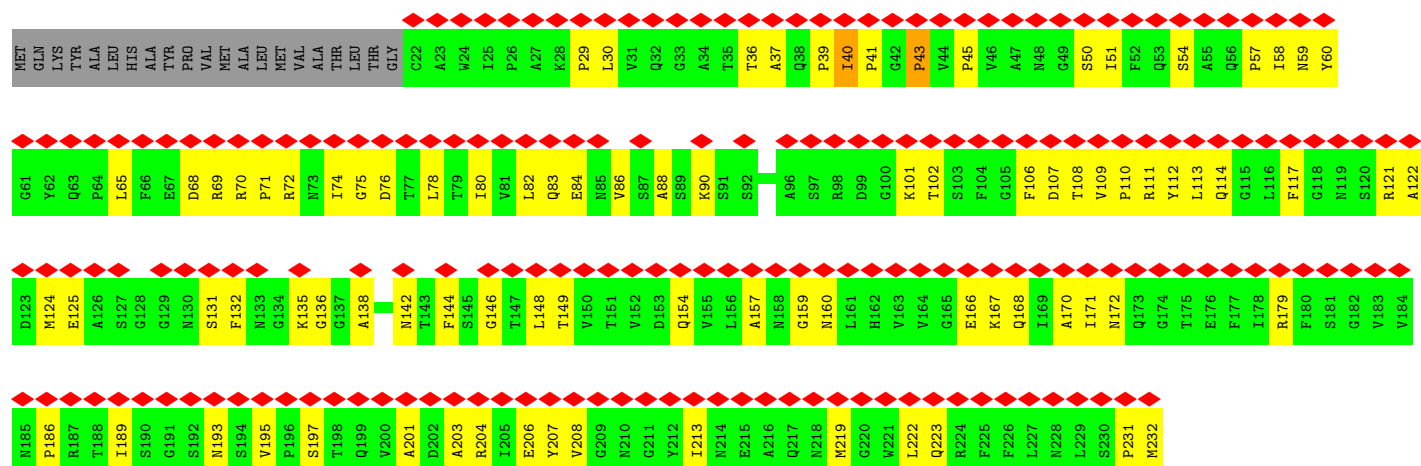
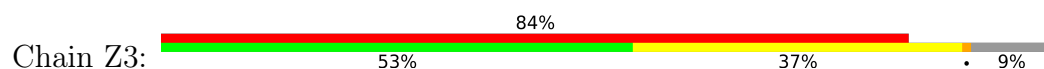




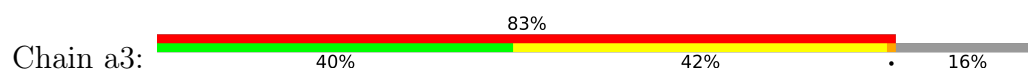
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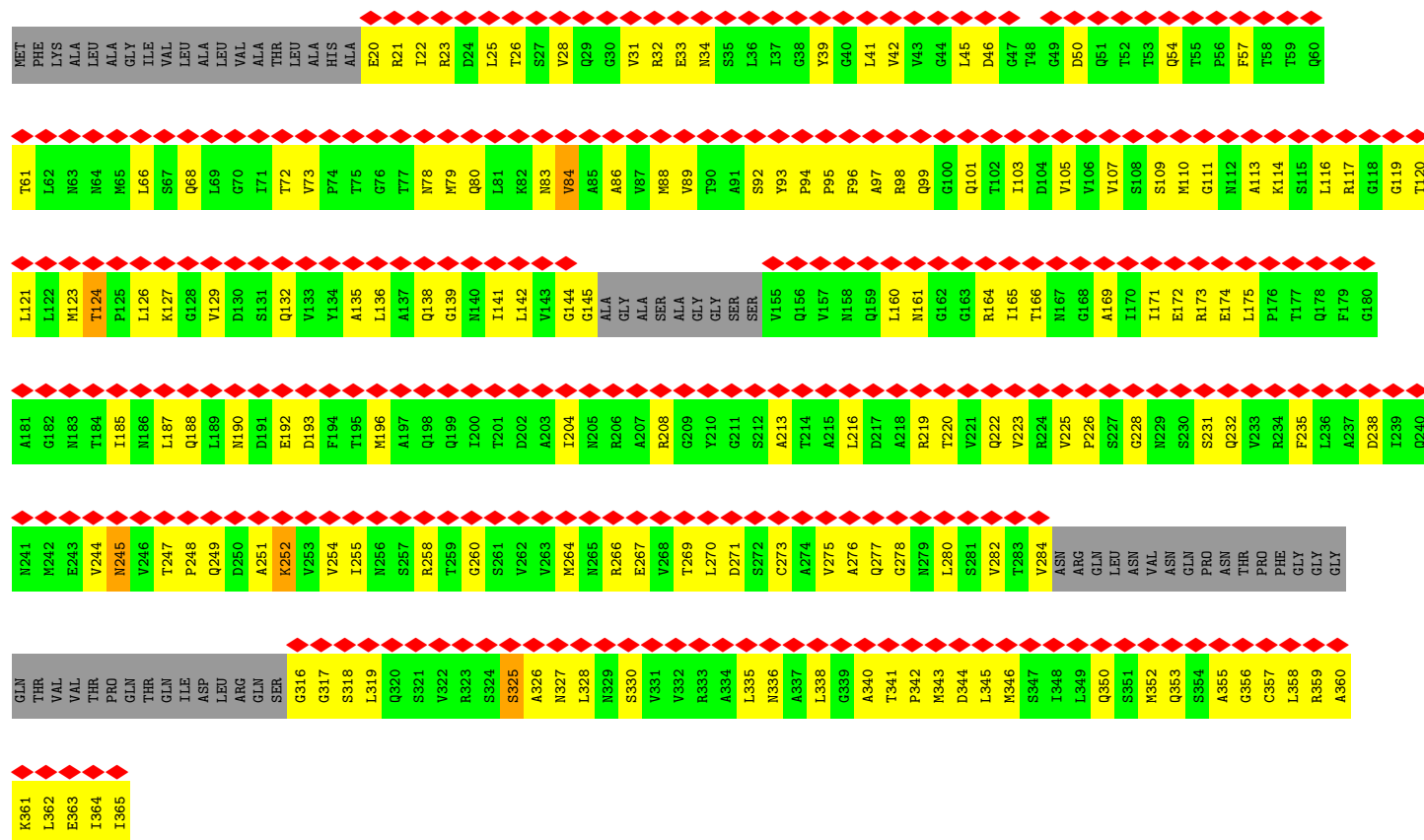


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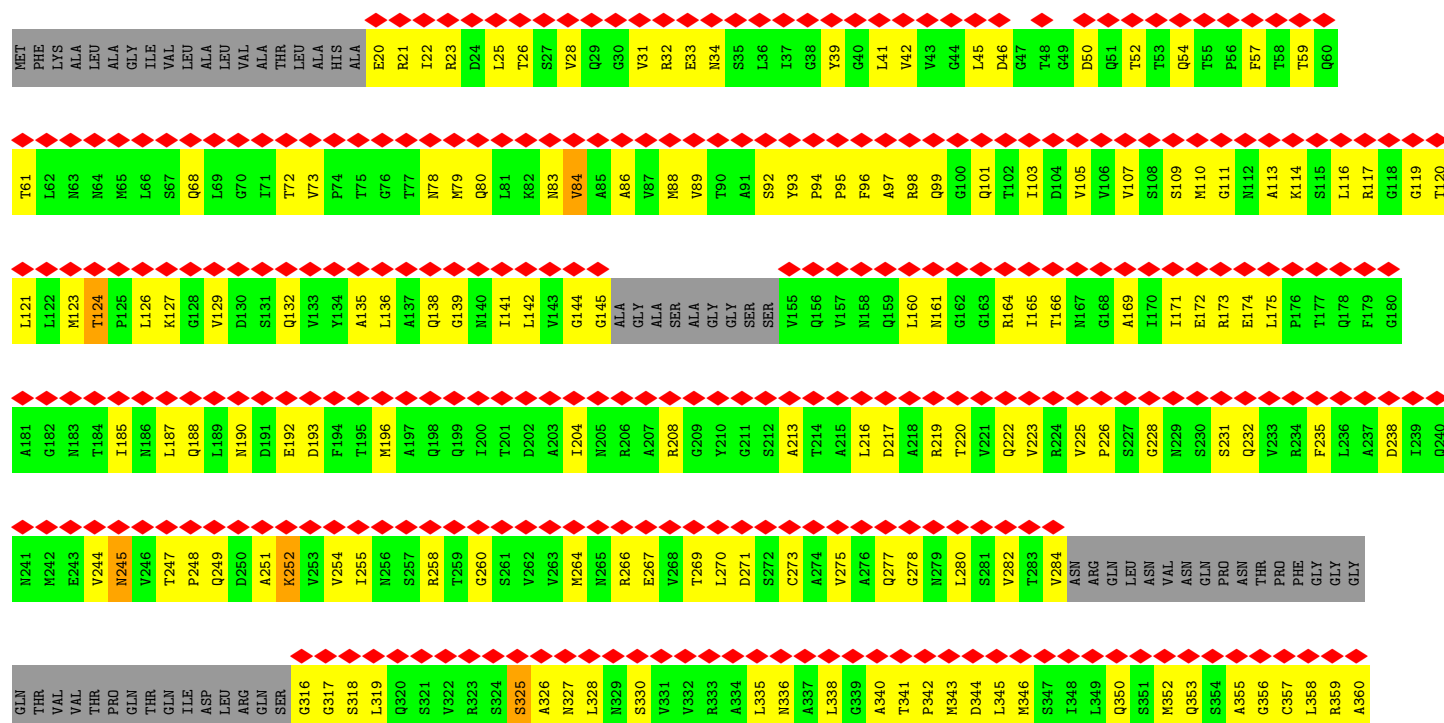
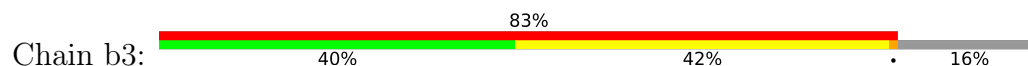


• Molecule 11: Flagellar P-ring protein



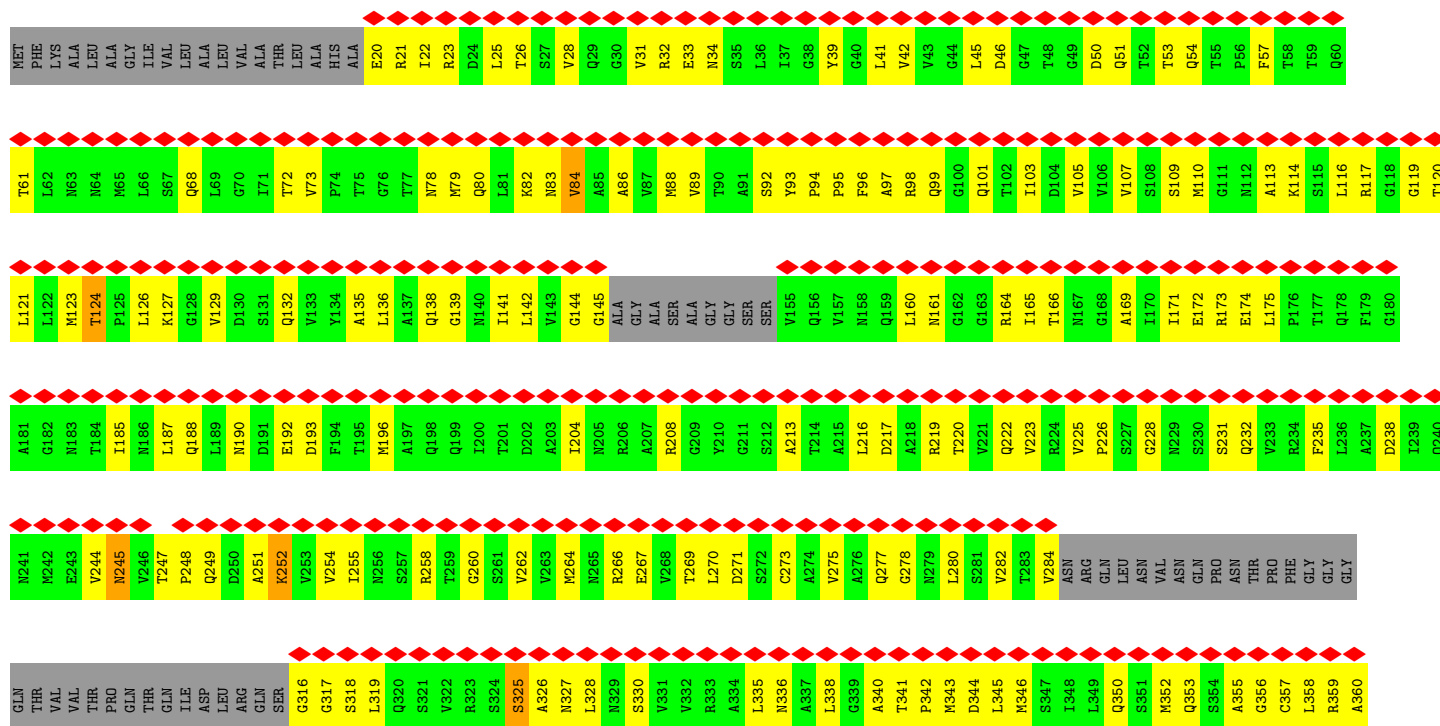
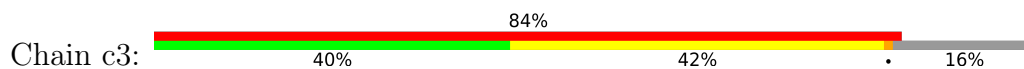


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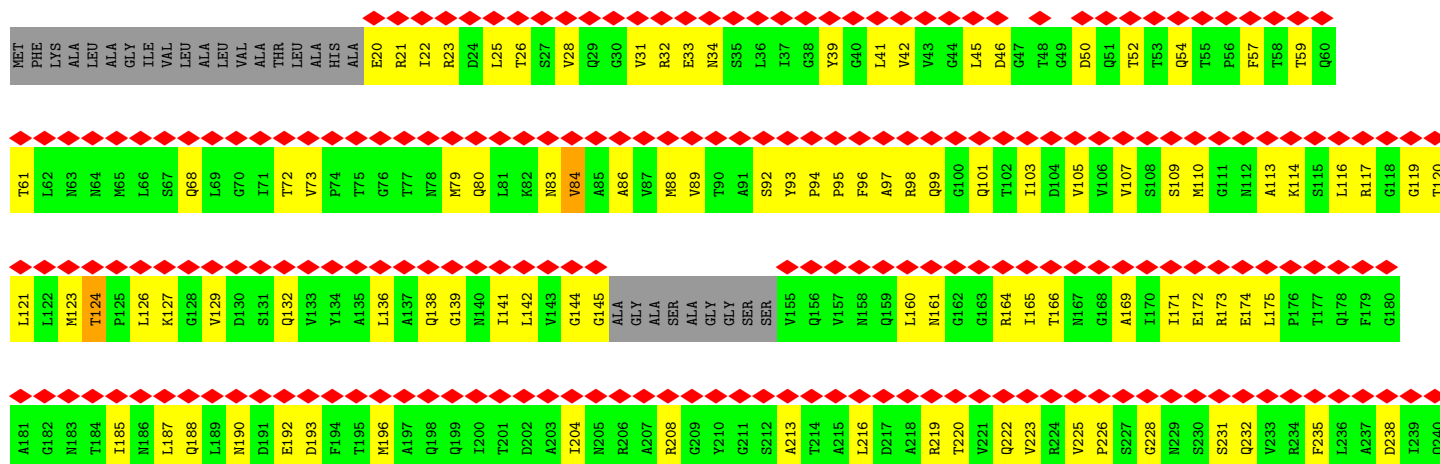
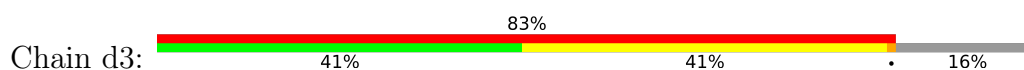




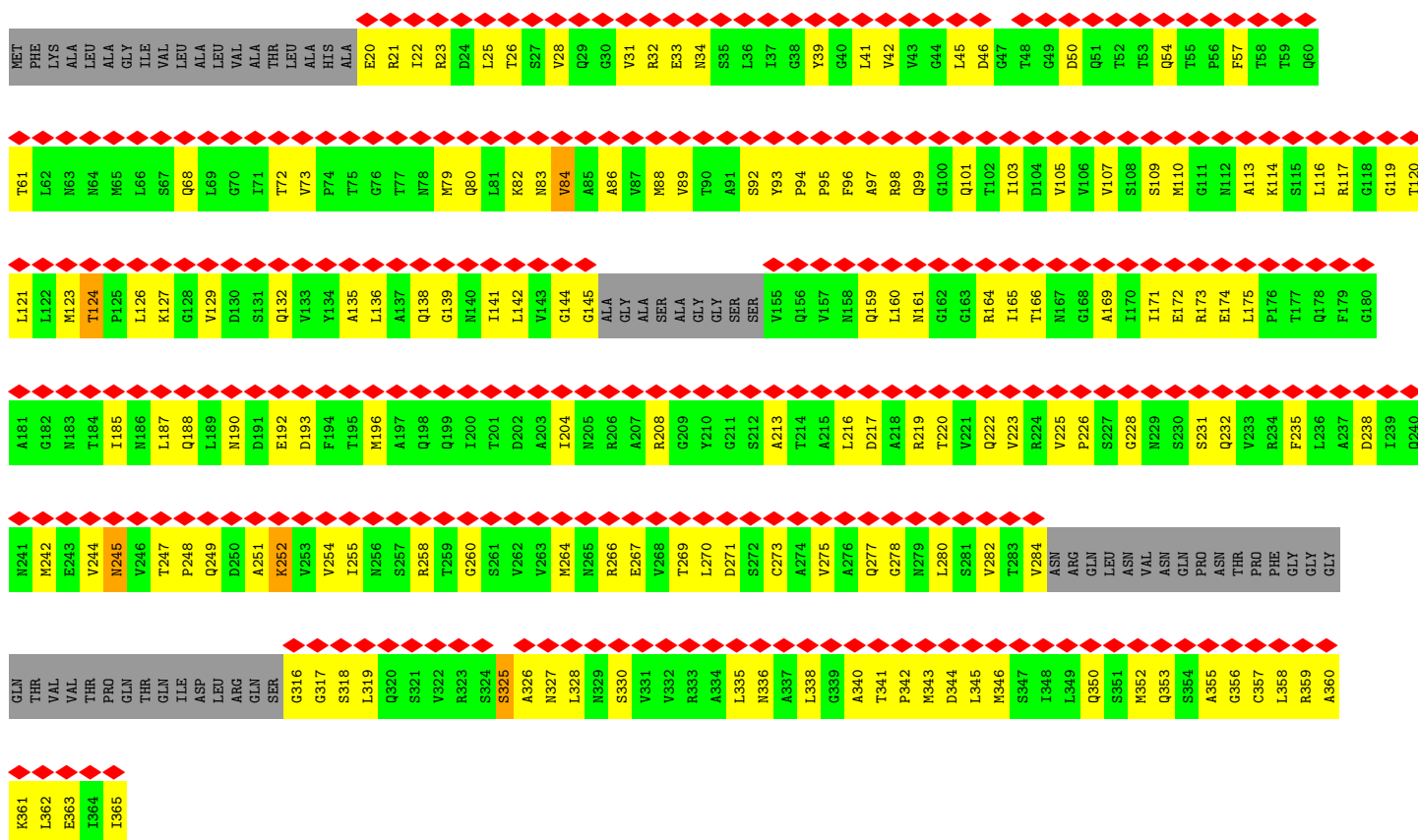
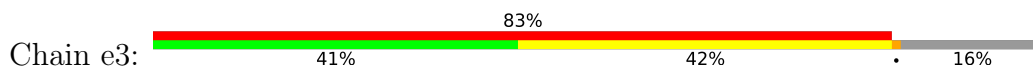
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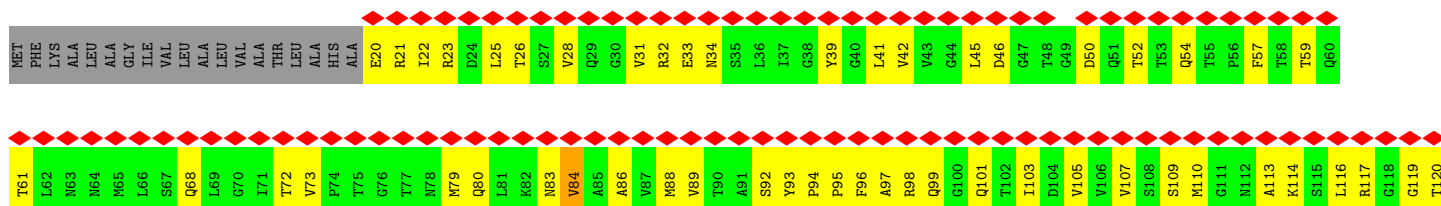
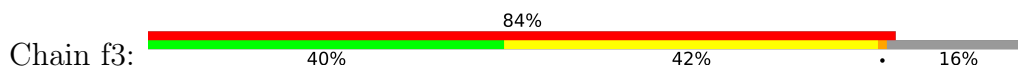
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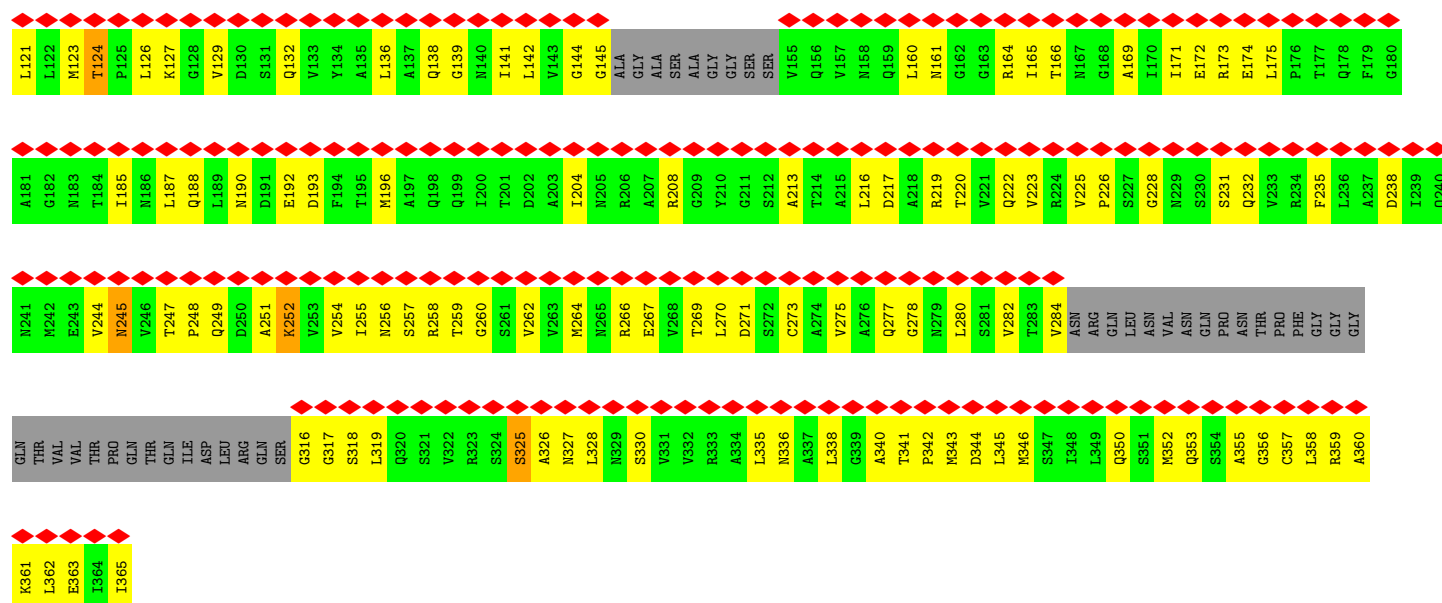


- Molecule 11: Flagellar P-ring protein

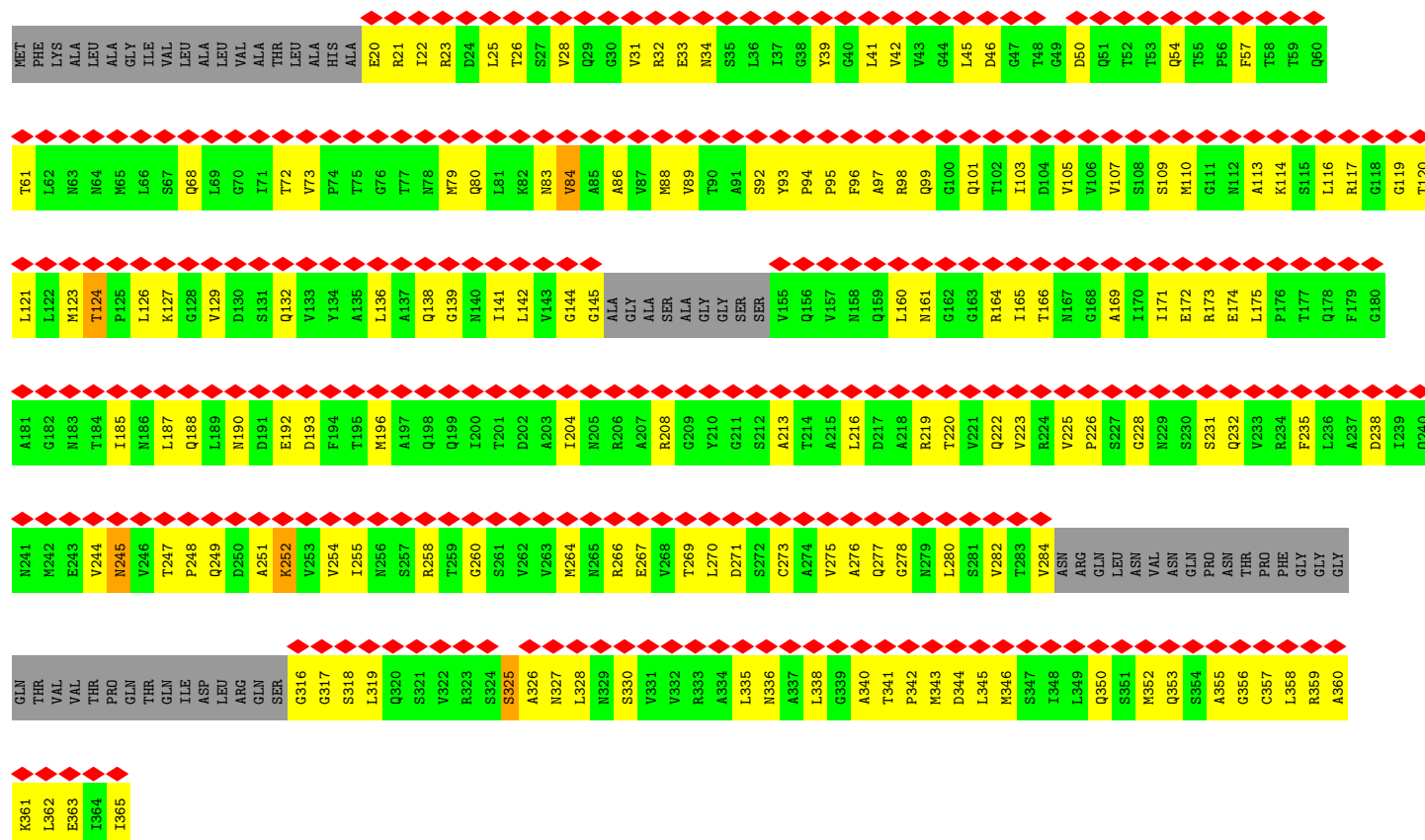
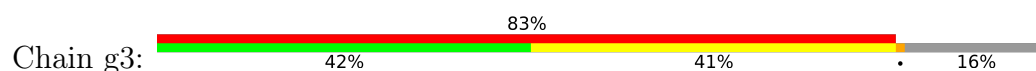


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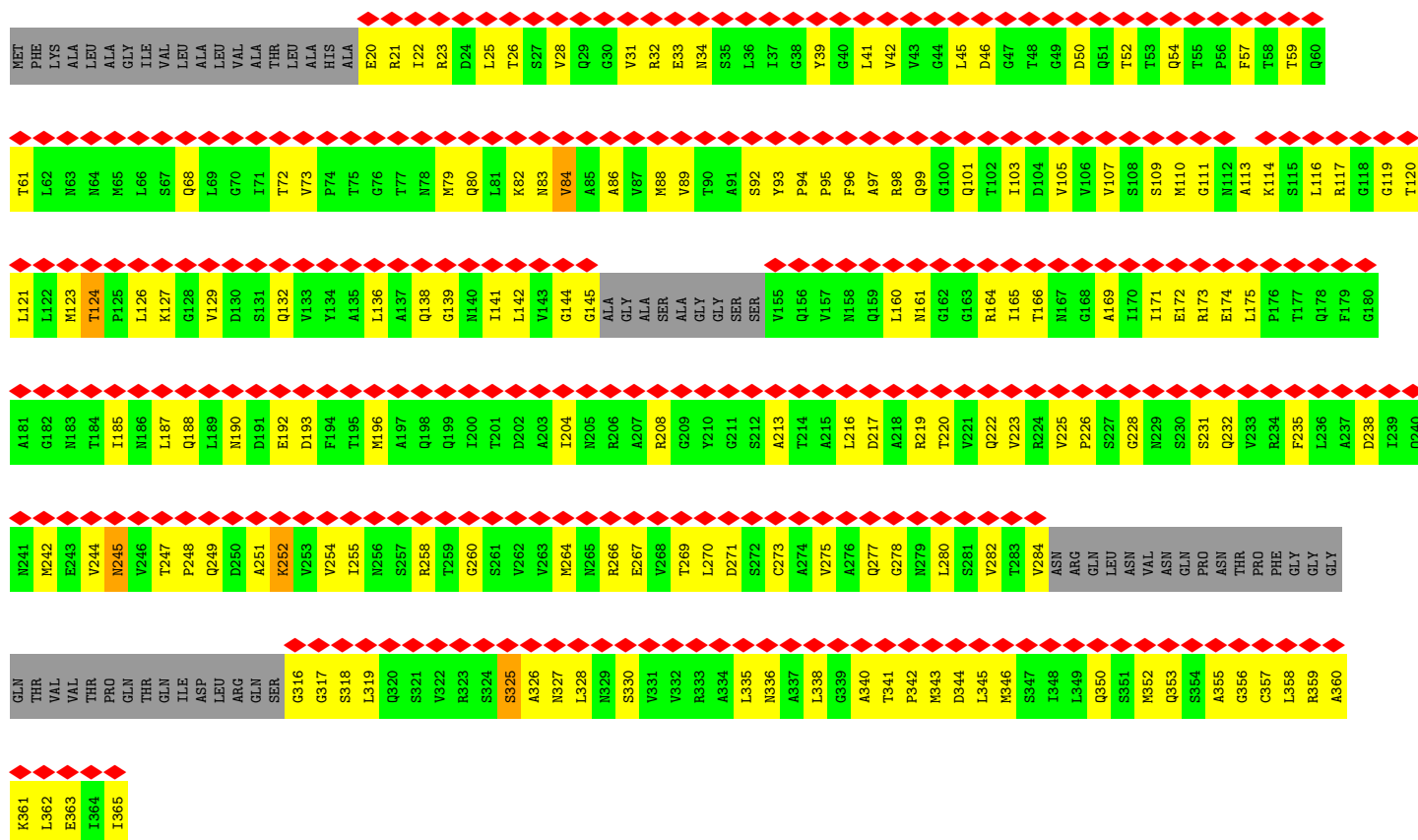
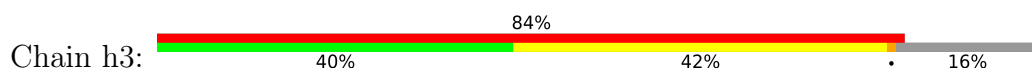




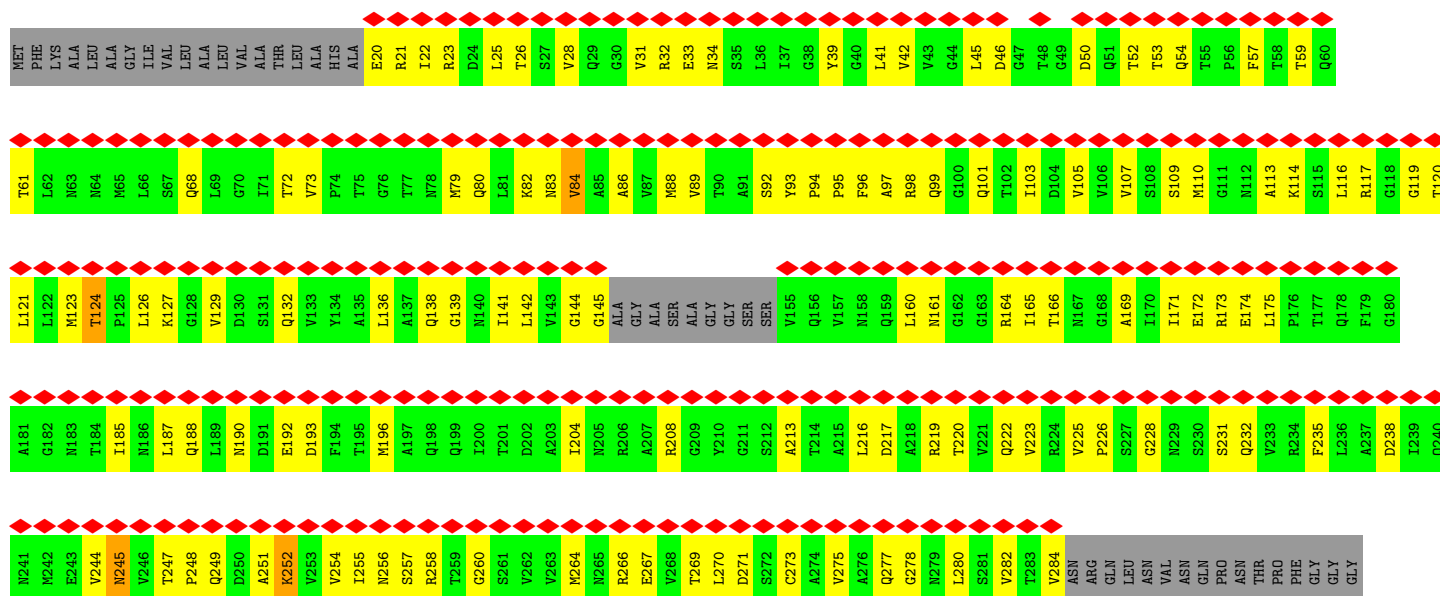
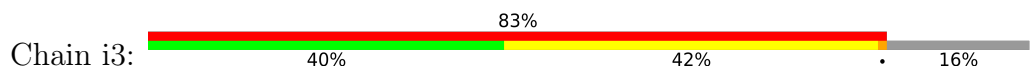
• Molecule 11: Flagellar P-ring protein

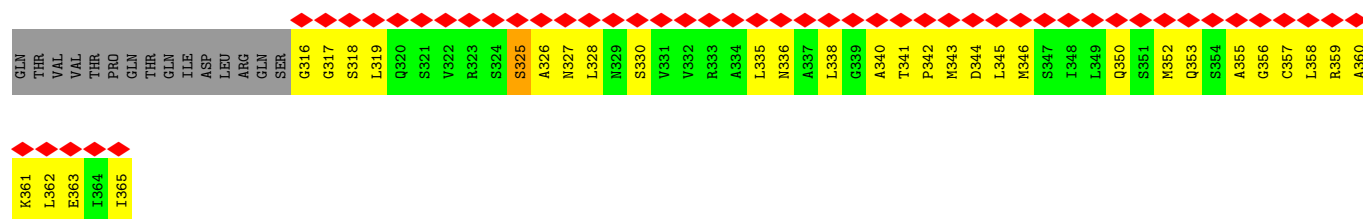


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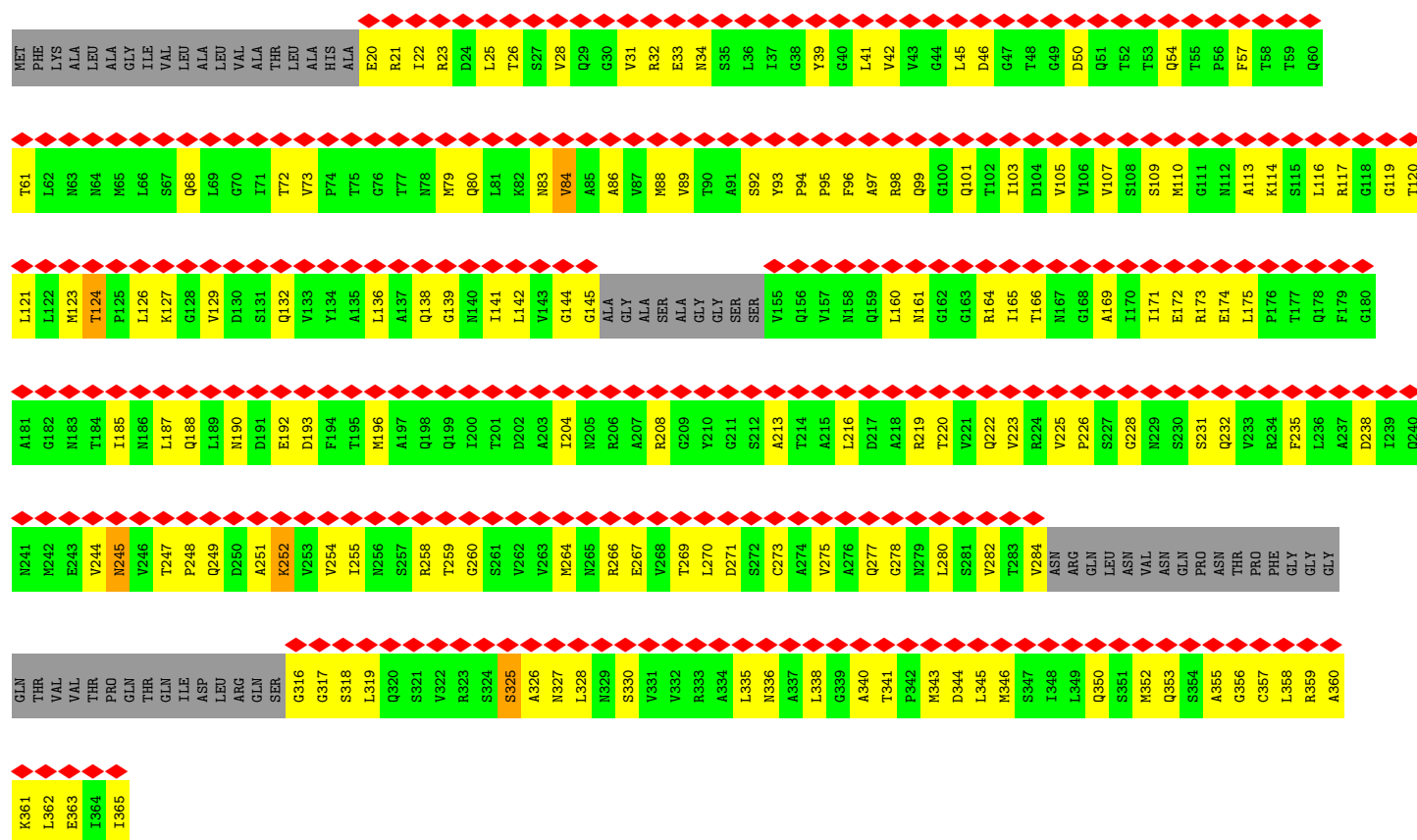
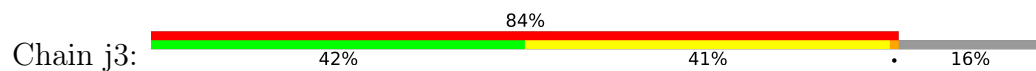


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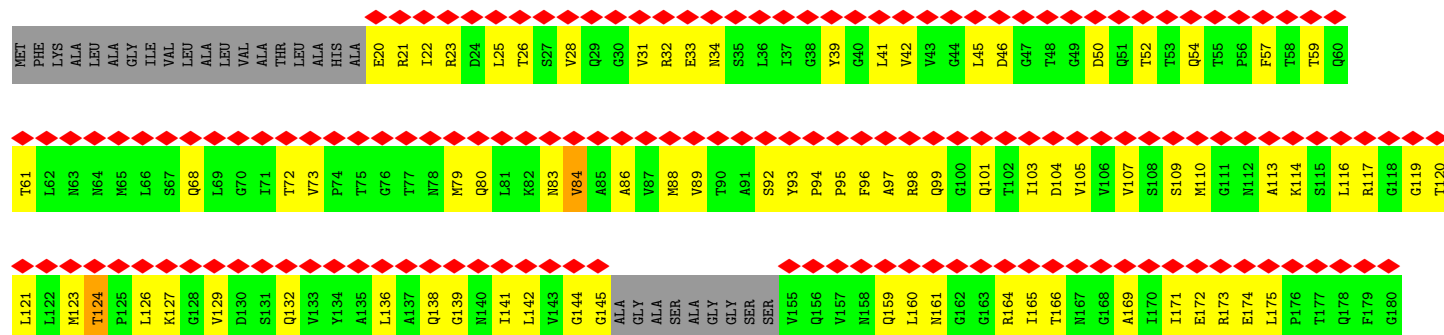
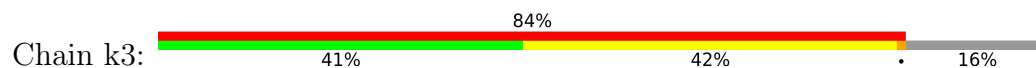




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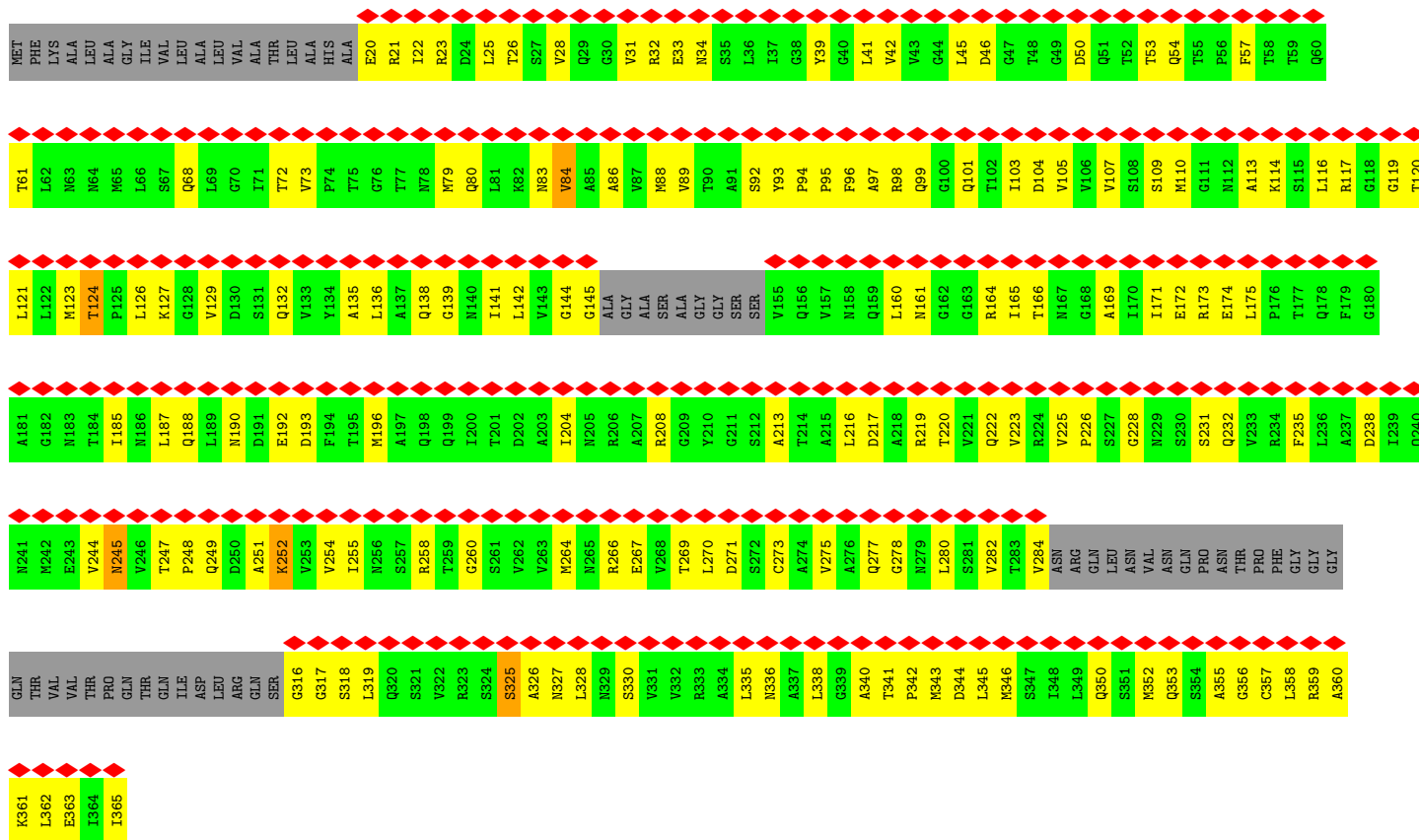
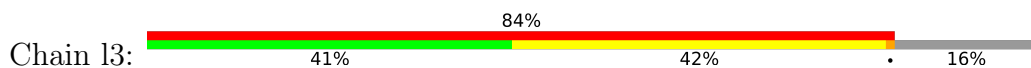


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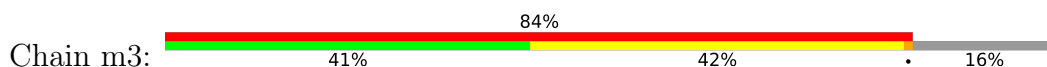




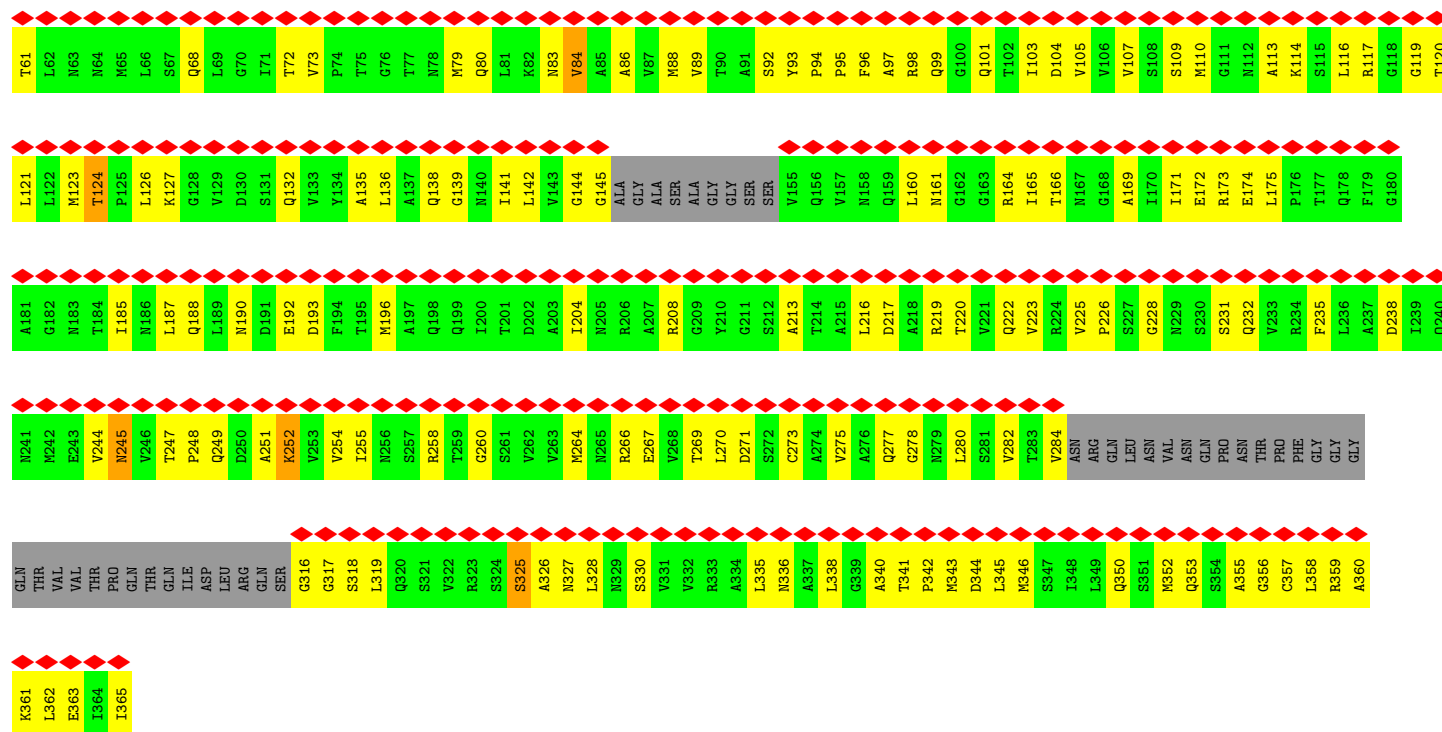
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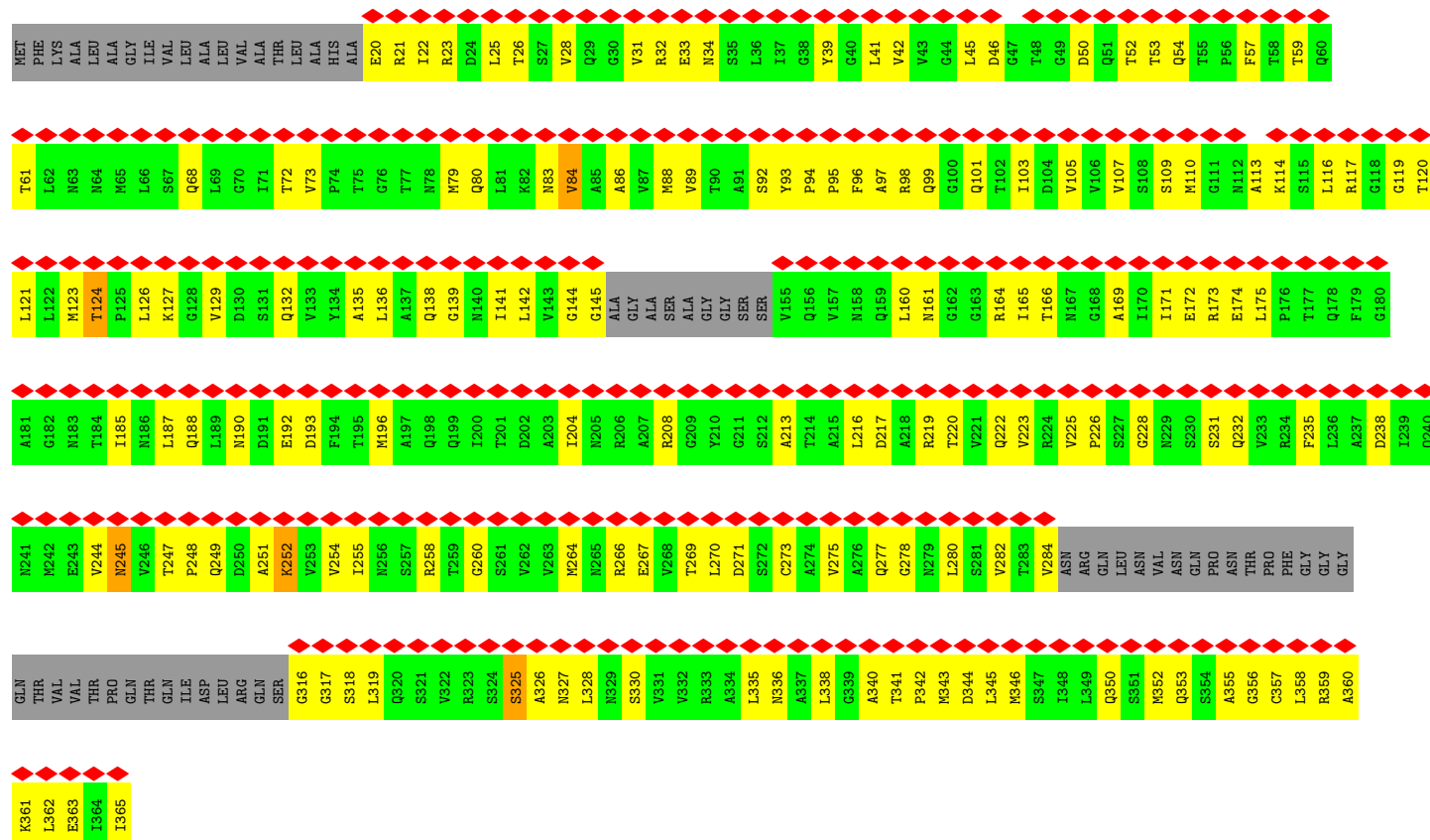
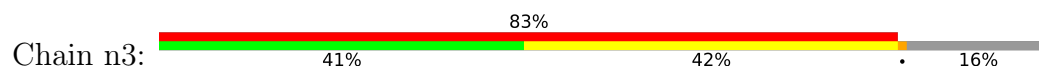
• Molecule 11: Flagellar P-ring protein



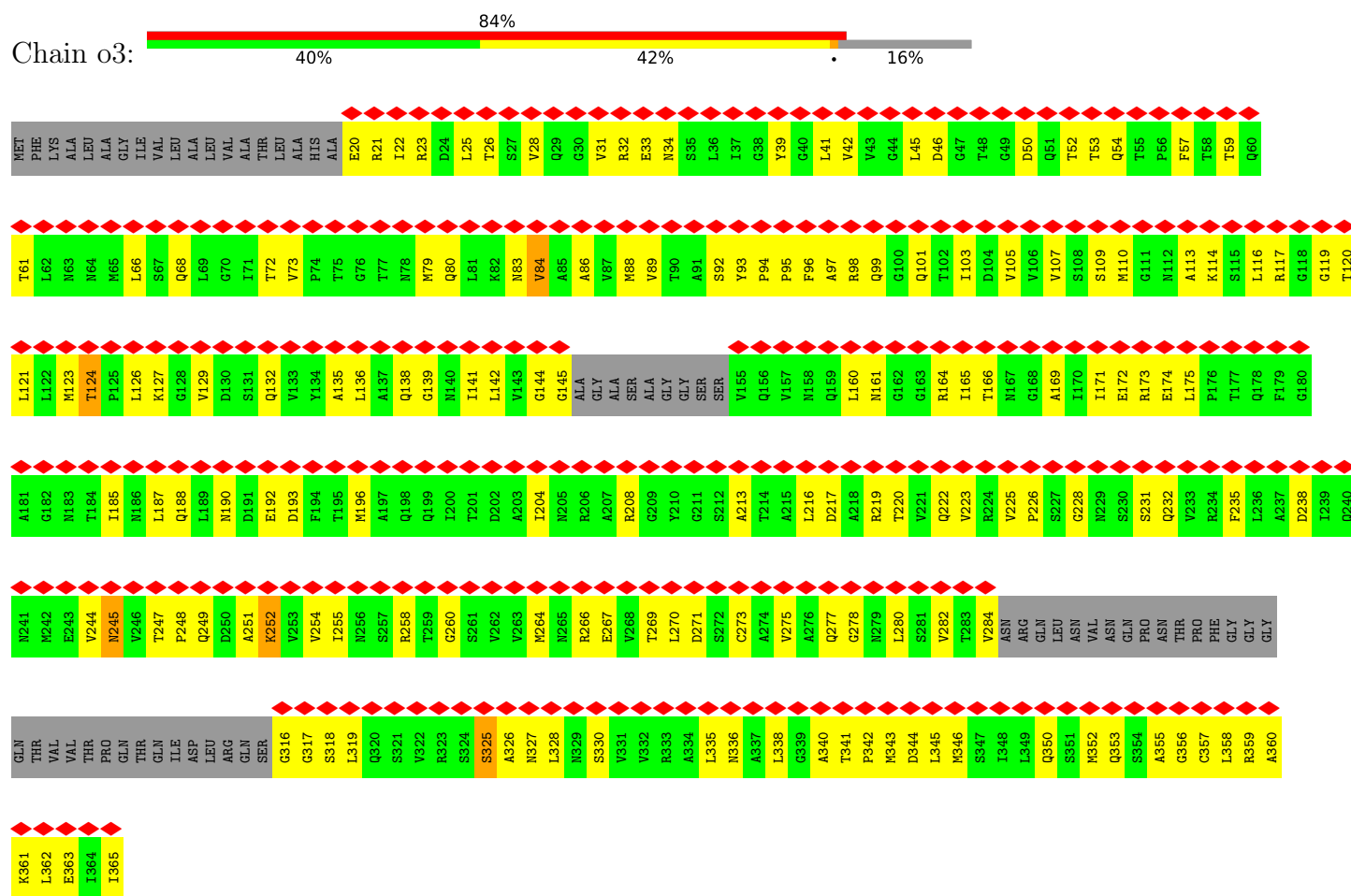




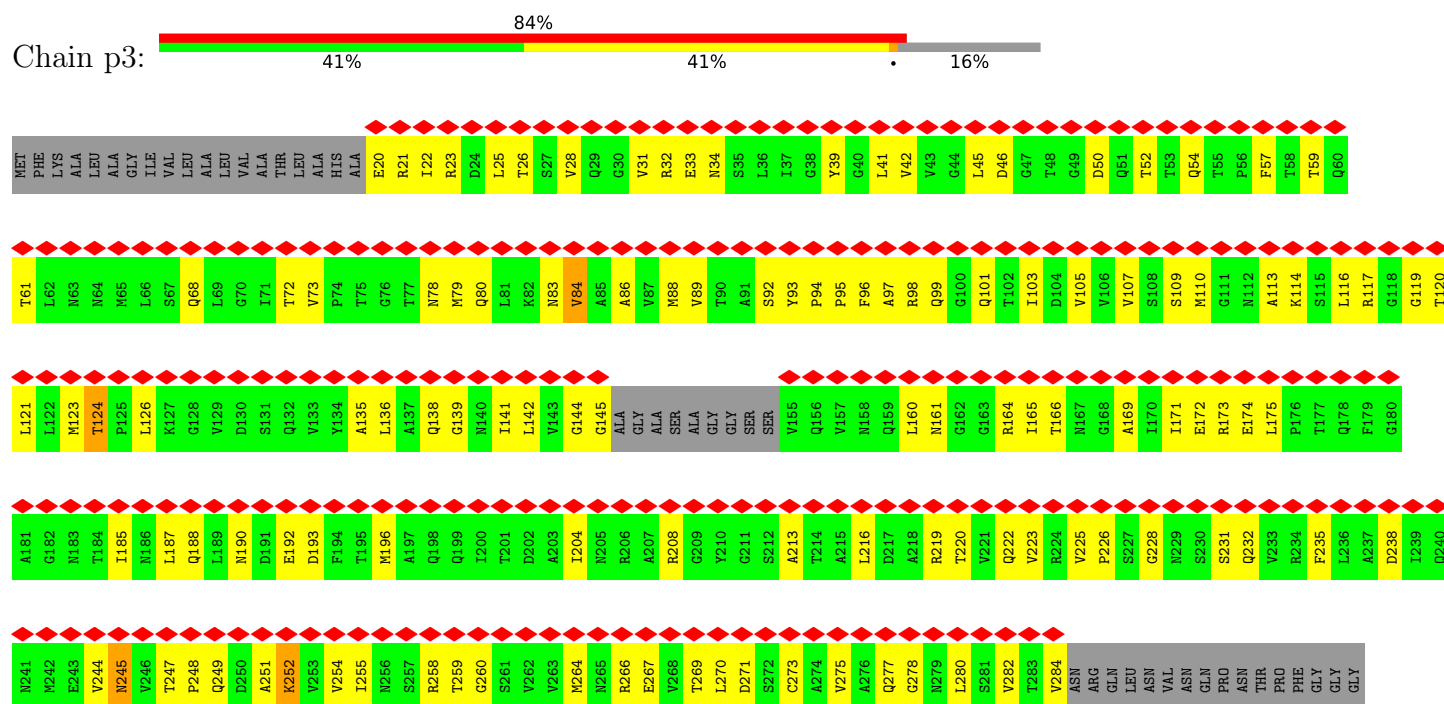
# Molecule 11: Flagellar P-ring protein

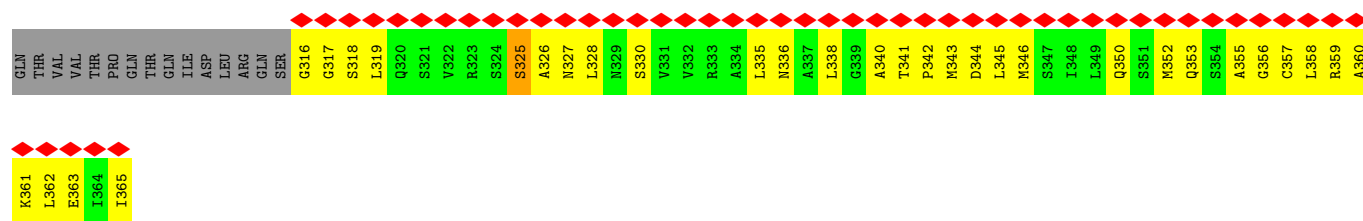


- Molecule 11: Flagellar P-ring protein

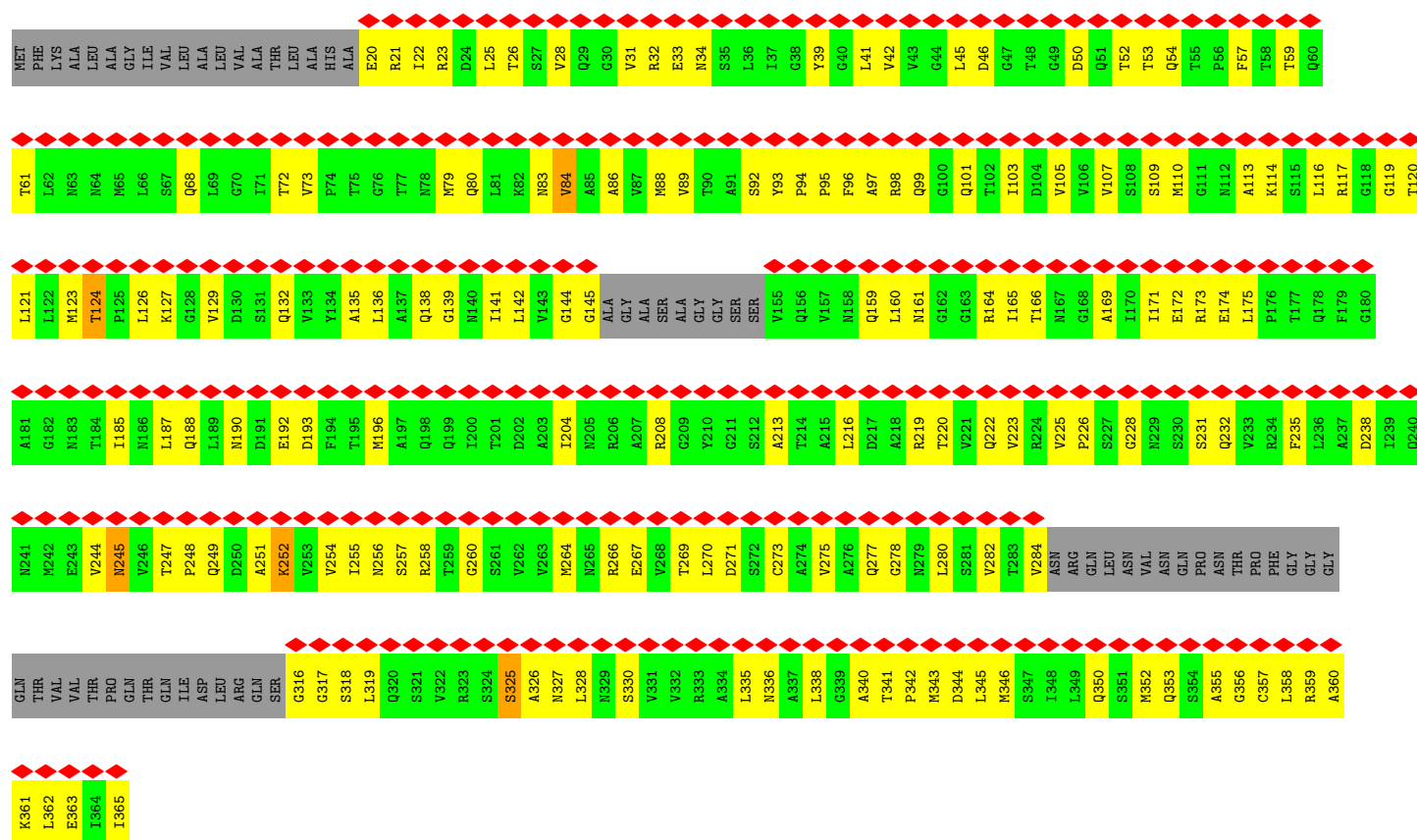
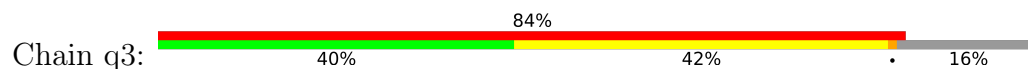


- Molecule 11: Flagellar P-ring protein

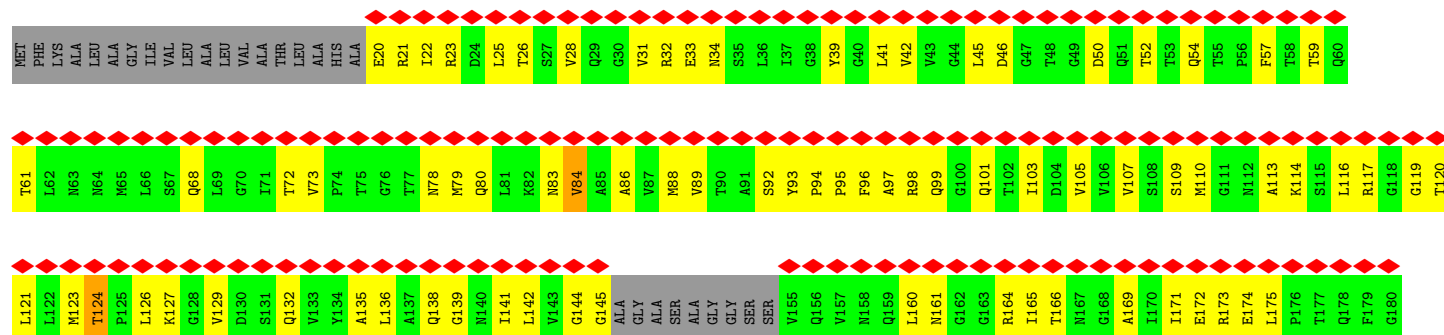
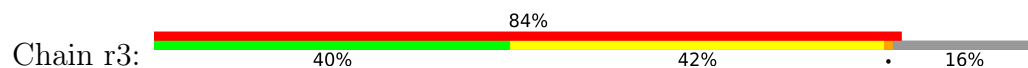




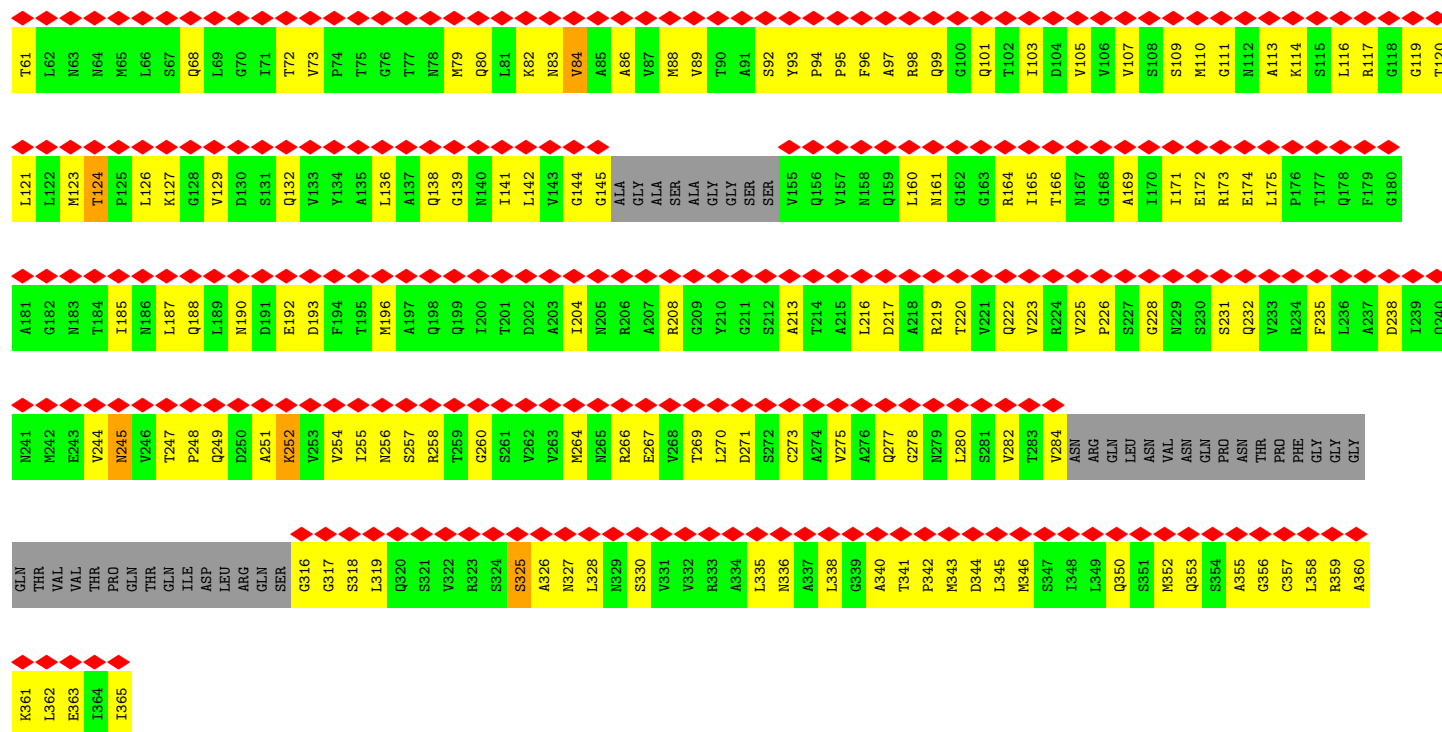
• Molecule 11: Flagellar P-ring protein



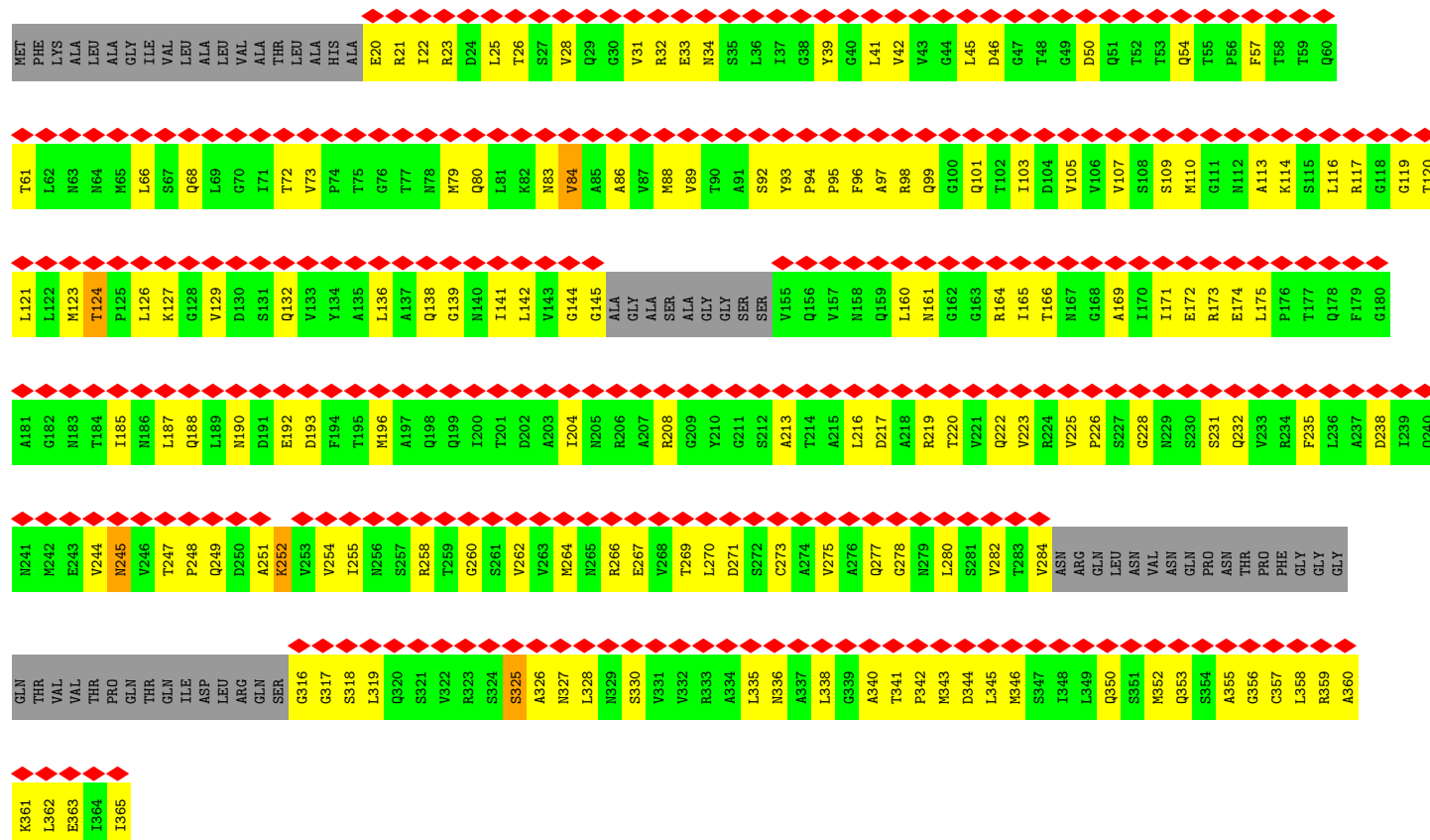
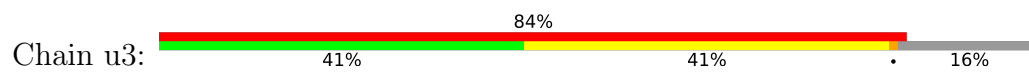
• Molecule 11: Flagellar P-ring protein



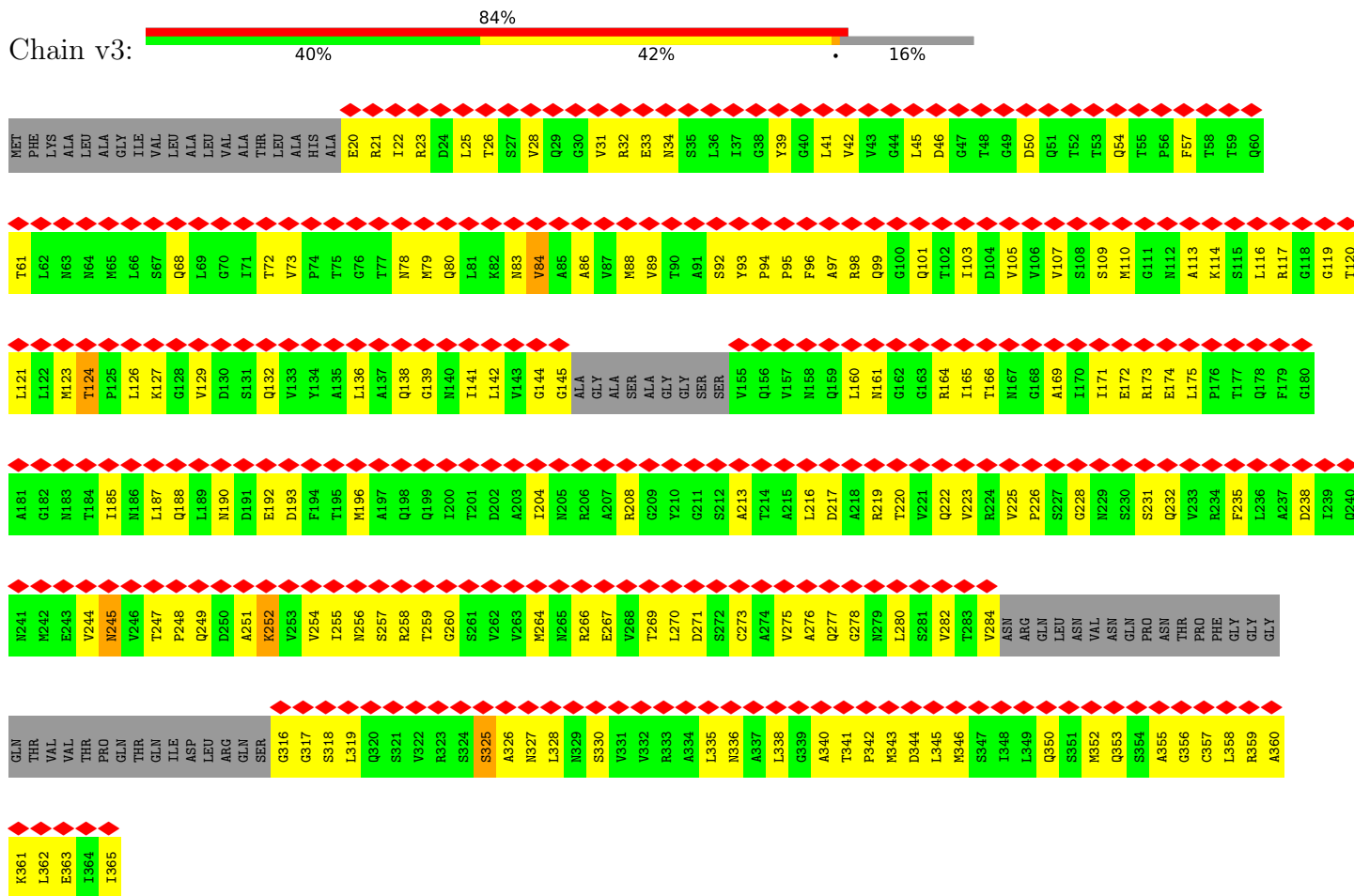




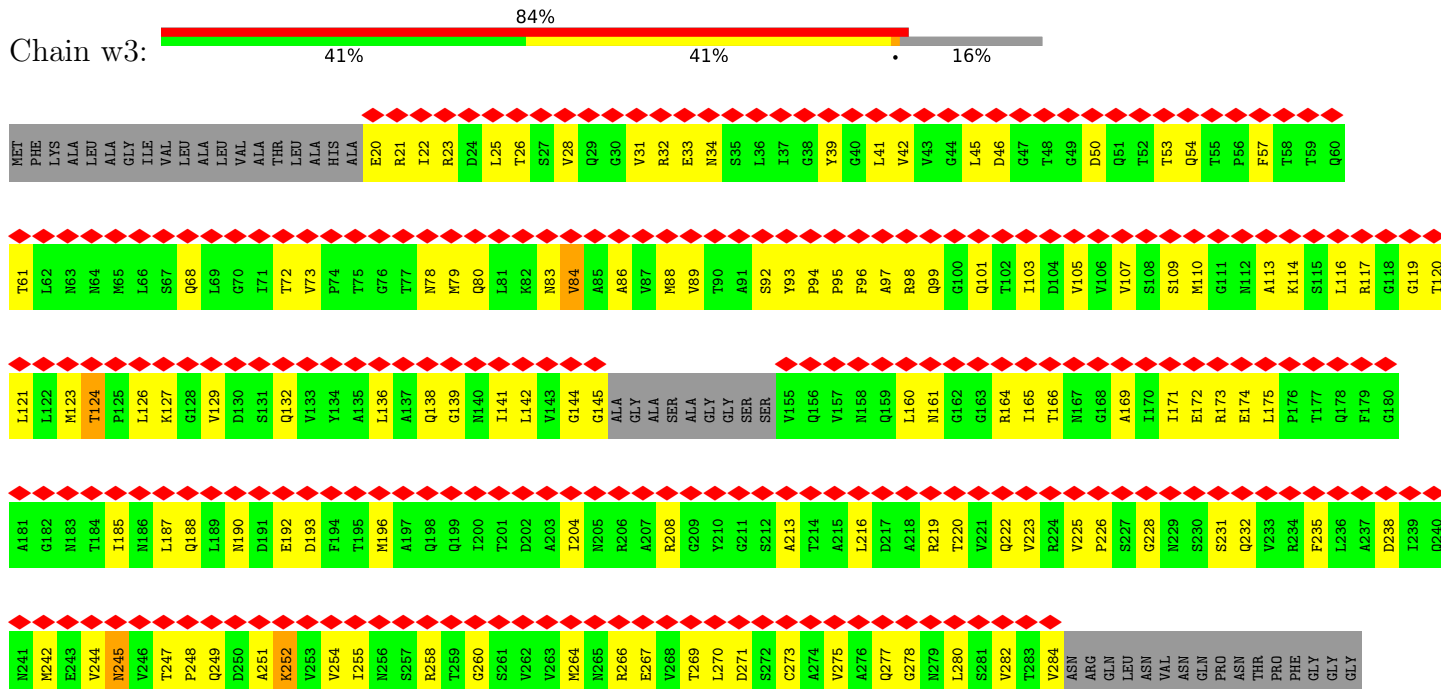
• Molecule 11: Flagellar P-ring protein

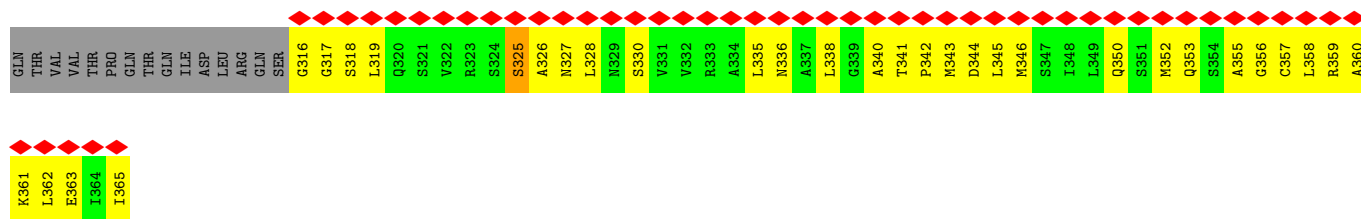


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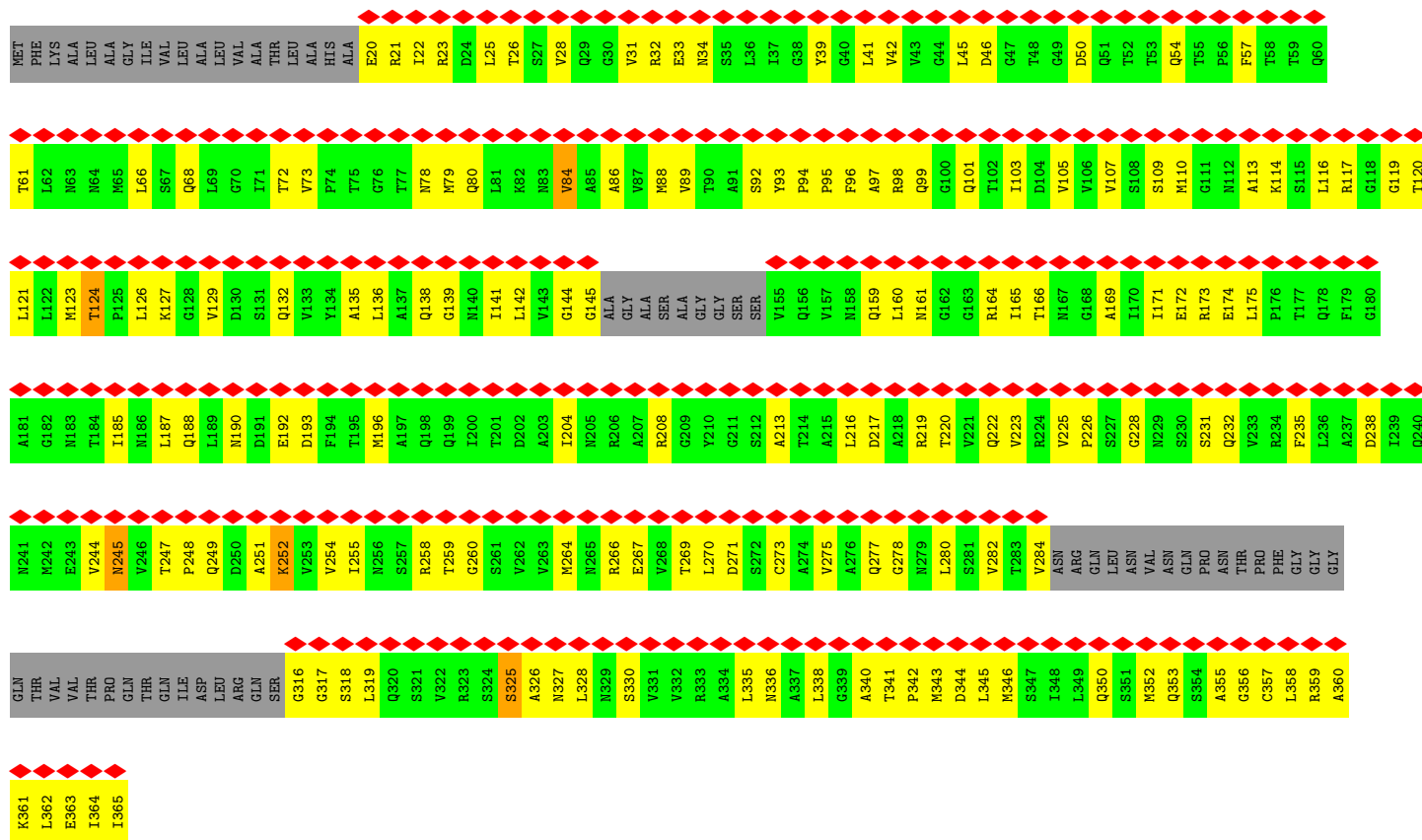
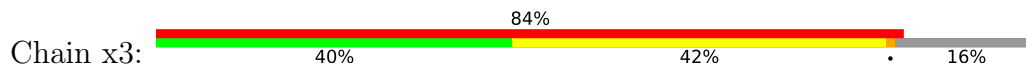


## Chain w3:

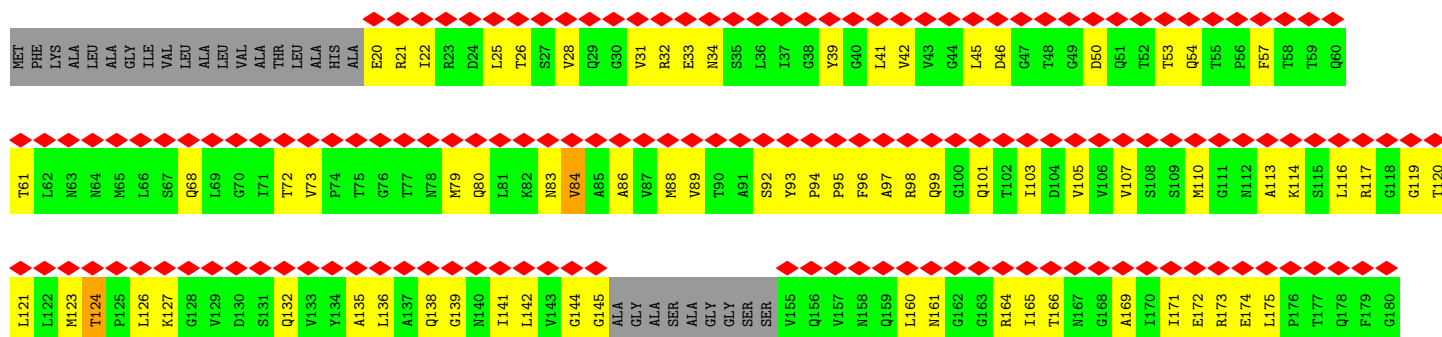
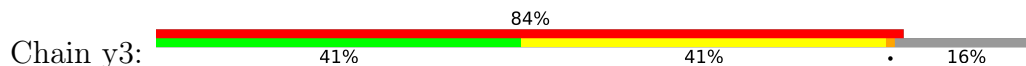




• Molecule 11: Flagellar P-ring protein

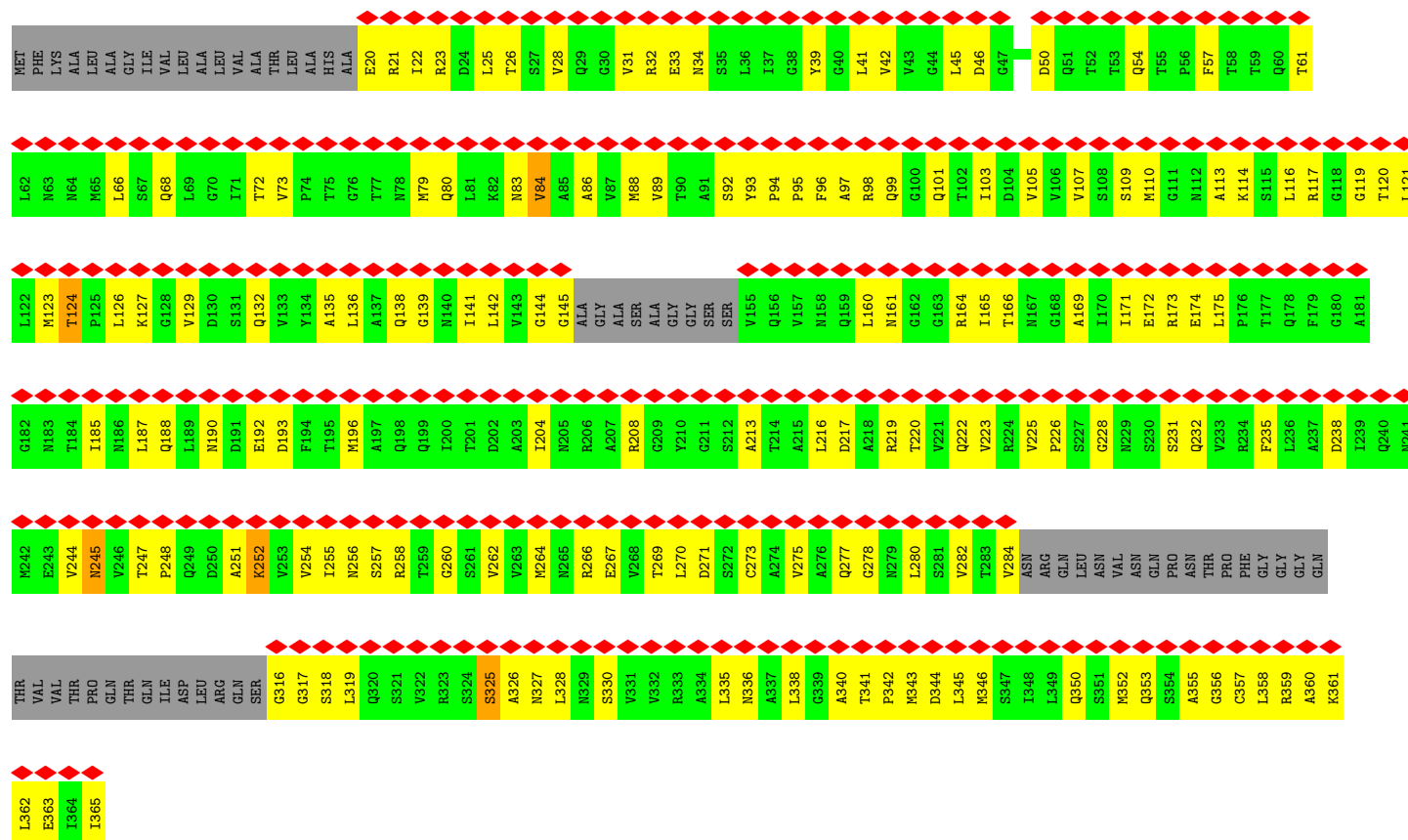
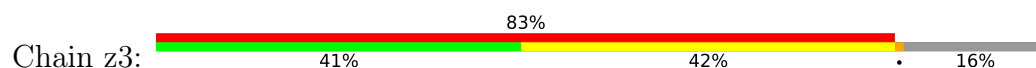


• Molecule 11: Flagellar P-ring protein

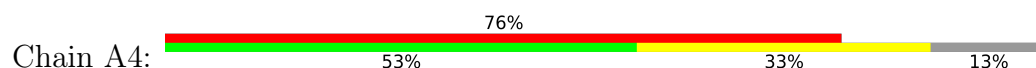




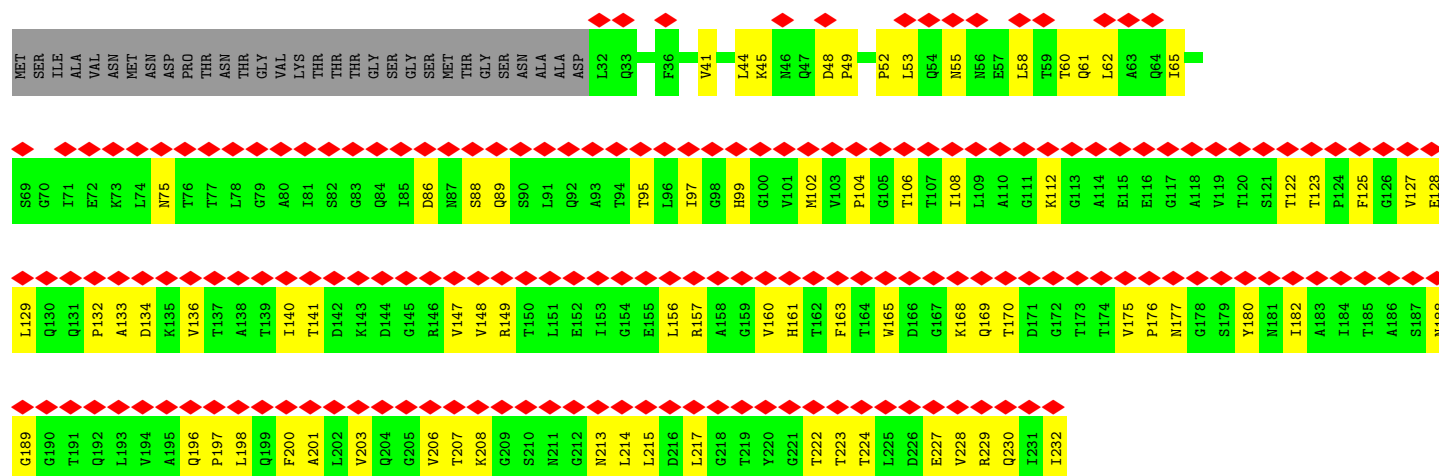
• Molecule 11: Flagellar P-ring protein



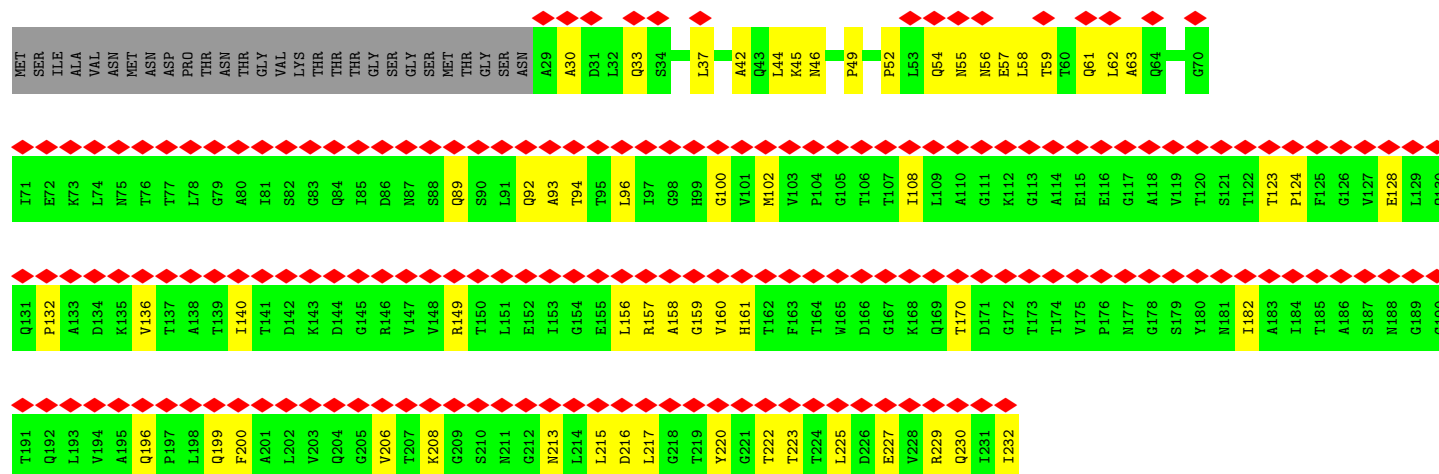
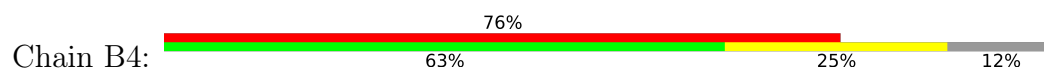
• Molecule 12: Basal-body rod modification protein FlgD



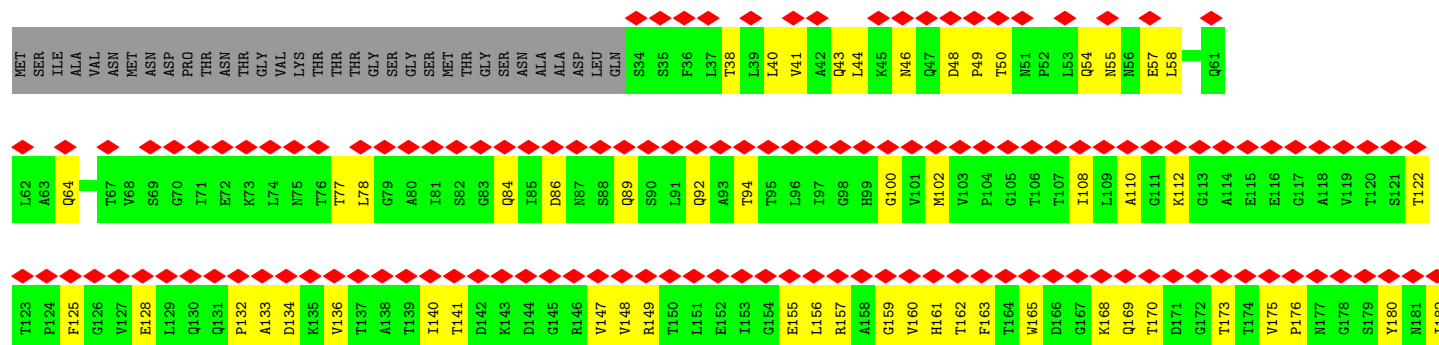
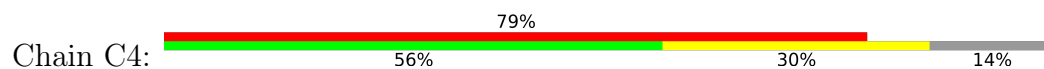




• Molecule 12: Basal-body rod modification protein FlgD

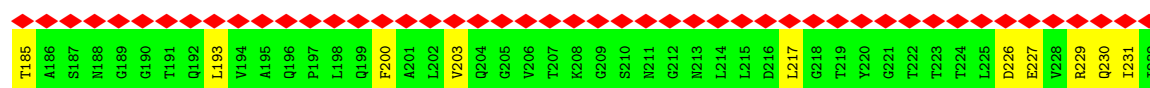
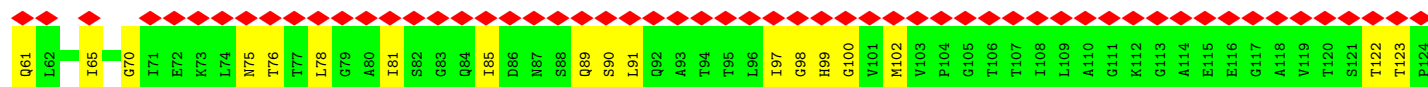
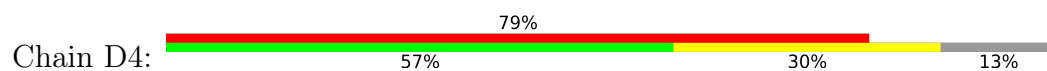


• Molecule 12: Basal-body rod modification protein FlgD

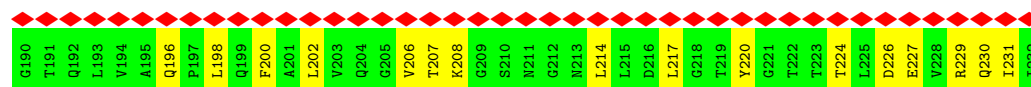
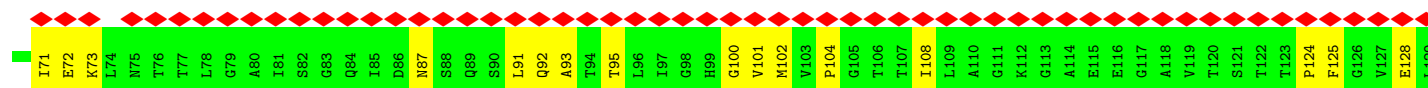
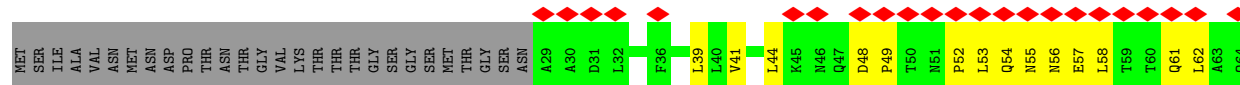
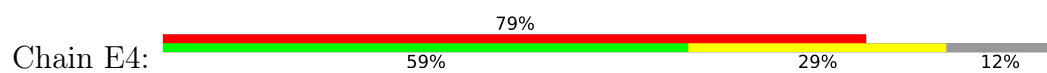




• Molecule 12: Basal-body rod modification protein FlgD



• Molecule 12: Basal-body rod modification protein FlgD



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 60497                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 59                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.023                                   | Depositor |
| Minimum map value                    | -0.010                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.0075                                  | Depositor |
| Map size (Å)                         | 638.976, 638.976, 638.976               | wwPDB     |
| Map dimensions                       | 768, 768, 768                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.832, 0.832, 0.832                     | 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   | A1    | 0.35         | 0/1205      | 0.48        | 0/1624        |
| 1   | B1    | 0.33         | 0/1955      | 0.53        | 0/2645        |
| 1   | C1    | 0.34         | 0/1955      | 0.52        | 2/2645 (0.1%) |
| 1   | D1    | 0.36         | 0/1205      | 0.50        | 0/1624        |
| 1   | E1    | 0.33         | 0/1955      | 0.53        | 0/2645        |
| 1   | F1    | 0.35         | 0/1205      | 0.51        | 0/1624        |
| 1   | G1    | 0.33         | 0/1955      | 0.50        | 0/2645        |
| 1   | H1    | 0.34         | 0/1955      | 0.56        | 2/2645 (0.1%) |
| 1   | I1    | 0.33         | 0/1955      | 0.48        | 0/2645        |
| 1   | J1    | 0.36         | 0/1205      | 0.50        | 0/1624        |
| 1   | K1    | 0.31         | 0/1955      | 0.53        | 2/2645 (0.1%) |
| 1   | L1    | 0.32         | 0/1955      | 0.51        | 1/2645 (0.0%) |
| 1   | M1    | 0.35         | 0/1205      | 0.52        | 0/1624        |
| 1   | N1    | 0.31         | 0/1955      | 0.54        | 1/2645 (0.0%) |
| 1   | O1    | 0.30         | 0/1955      | 0.49        | 0/2645        |
| 1   | P1    | 0.32         | 0/1205      | 0.49        | 0/1624        |
| 1   | Q1    | 0.30         | 0/1955      | 0.48        | 0/2645        |
| 1   | R1    | 0.29         | 0/1955      | 0.47        | 0/2645        |
| 1   | S1    | 0.33         | 0/1205      | 0.47        | 0/1624        |
| 1   | T1    | 0.29         | 0/1955      | 0.50        | 0/2645        |
| 1   | U1    | 0.30         | 0/1955      | 0.56        | 2/2645 (0.1%) |
| 1   | V1    | 0.33         | 0/1205      | 0.50        | 0/1624        |
| 1   | W1    | 0.29         | 0/1955      | 0.50        | 0/2645        |
| 1   | X1    | 0.30         | 0/1955      | 0.50        | 0/2645        |
| 1   | Y1    | 0.29         | 0/1955      | 0.49        | 0/2645        |
| 1   | Z1    | 0.35         | 0/1205      | 0.54        | 0/1624        |
| 1   | a1    | 0.30         | 0/1955      | 0.50        | 0/2645        |
| 1   | b1    | 0.35         | 0/1205      | 0.50        | 0/1624        |
| 1   | c1    | 0.31         | 0/1955      | 0.49        | 0/2645        |
| 1   | d1    | 0.32         | 0/1955      | 0.50        | 0/2645        |
| 1   | e1    | 0.35         | 0/1205      | 0.48        | 0/1624        |
| 1   | f1    | 0.32         | 0/1955      | 0.49        | 0/2645        |
| 1   | g1    | 0.32         | 0/1955      | 0.50        | 0/2645        |
| 1   | h1    | 0.32         | 0/1955      | 0.46        | 0/2645        |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 2   | A2    | 0.34         | 0/1662        | 0.63        | 2/2263 (0.1%) |
| 2   | B2    | 0.35         | 0/1662        | 0.62        | 0/2263        |
| 2   | C2    | 0.36         | 0/1662        | 0.64        | 1/2263 (0.0%) |
| 2   | D2    | 0.36         | 0/1662        | 0.62        | 2/2263 (0.1%) |
| 2   | E2    | 1.11         | 1/1662 (0.1%) | 0.64        | 2/2263 (0.1%) |
| 3   | F2    | 0.31         | 0/2035        | 0.60        | 2/2777 (0.1%) |
| 4   | G2    | 0.28         | 0/681         | 0.60        | 0/930         |
| 4   | H2    | 0.29         | 0/681         | 0.56        | 0/930         |
| 4   | I2    | 0.31         | 0/681         | 0.51        | 0/930         |
| 4   | J2    | 1.86         | 6/681 (0.9%)  | 0.56        | 0/930         |
| 5   | K2    | 0.31         | 0/296         | 0.53        | 0/395         |
| 5   | L2    | 0.28         | 0/567         | 0.39        | 0/761         |
| 5   | M2    | 0.31         | 0/567         | 0.45        | 0/761         |
| 5   | N2    | 0.30         | 0/567         | 0.42        | 0/761         |
| 5   | O2    | 0.29         | 0/567         | 0.44        | 0/761         |
| 5   | P2    | 0.30         | 0/567         | 0.43        | 0/761         |
| 6   | Q2    | 0.34         | 0/1035        | 0.52        | 0/1399        |
| 6   | R2    | 0.34         | 0/941         | 0.49        | 0/1269        |
| 6   | S2    | 0.38         | 0/951         | 0.52        | 0/1281        |
| 6   | T2    | 0.37         | 0/842         | 0.48        | 0/1132        |
| 6   | U2    | 0.33         | 0/934         | 0.46        | 0/1259        |
| 7   | V2    | 0.40         | 0/981         | 0.66        | 0/1334        |
| 7   | W2    | 0.37         | 0/976         | 0.56        | 0/1327        |
| 7   | X2    | 0.40         | 0/976         | 0.56        | 0/1327        |
| 7   | Y2    | 0.38         | 0/976         | 0.54        | 0/1327        |
| 7   | Z2    | 0.37         | 0/976         | 0.54        | 0/1327        |
| 7   | a2    | 0.36         | 0/976         | 0.56        | 0/1327        |
| 8   | b2    | 0.35         | 0/1836        | 0.57        | 0/2502        |
| 8   | c2    | 0.39         | 0/1836        | 0.58        | 0/2502        |
| 8   | d2    | 0.40         | 0/1836        | 0.58        | 0/2502        |
| 8   | e2    | 0.38         | 0/1836        | 0.55        | 0/2502        |
| 8   | f2    | 0.36         | 0/1836        | 0.54        | 0/2502        |
| 9   | l2    | 0.31         | 0/1973        | 0.48        | 0/2682        |
| 9   | 22    | 0.30         | 0/1973        | 0.47        | 0/2682        |
| 9   | 32    | 0.29         | 0/1971        | 0.47        | 0/2677        |
| 9   | 42    | 0.23         | 0/1973        | 0.47        | 0/2682        |
| 9   | g2    | 0.34         | 0/1973        | 0.46        | 0/2682        |
| 9   | h2    | 0.37         | 0/1973        | 0.46        | 0/2682        |
| 9   | i2    | 0.37         | 0/1973        | 0.47        | 0/2682        |
| 9   | j2    | 0.38         | 0/1973        | 0.47        | 0/2682        |
| 9   | k2    | 0.37         | 0/1973        | 0.47        | 0/2682        |
| 9   | l2    | 0.37         | 0/1894        | 0.45        | 0/2573        |
| 9   | m2    | 0.39         | 0/1894        | 0.47        | 0/2573        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 9   | n2    | 0.37         | 0/1894  | 0.45        | 0/2573        |
| 9   | o2    | 0.38         | 0/1894  | 0.46        | 0/2573        |
| 9   | p2    | 0.38         | 0/1894  | 0.47        | 0/2573        |
| 9   | q2    | 0.37         | 0/1907  | 0.45        | 0/2590        |
| 9   | r2    | 0.37         | 0/1973  | 0.50        | 0/2682        |
| 9   | s2    | 0.37         | 0/1973  | 0.53        | 0/2682        |
| 9   | t2    | 0.37         | 0/1973  | 0.52        | 1/2682 (0.0%) |
| 9   | u2    | 0.36         | 0/1973  | 0.50        | 0/2682        |
| 9   | v2    | 0.38         | 0/1973  | 0.49        | 0/2682        |
| 9   | w2    | 0.37         | 0/1973  | 0.50        | 0/2682        |
| 9   | x2    | 0.33         | 0/1973  | 0.47        | 0/2682        |
| 9   | y2    | 0.30         | 0/1973  | 0.45        | 0/2682        |
| 9   | z2    | 0.29         | 0/1973  | 0.44        | 0/2682        |
| 10  | A3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | B3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | C3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | D3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | E3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | F3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | G3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | H3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | I3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | J3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | K3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | L3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | M3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | N3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | O3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | P3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | Q3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | R3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | S3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | T3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | U3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | V3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | W3    | 0.12         | 0/1611  | 0.29        | 1/2188 (0.0%) |
| 10  | X3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | Y3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 10  | Z3    | 0.12         | 0/1614  | 0.29        | 1/2194 (0.0%) |
| 11  | a3    | 0.07         | 0/2267  | 0.21        | 0/3073        |
| 11  | b3    | 0.08         | 0/2267  | 0.21        | 0/3073        |
| 11  | c3    | 0.08         | 0/2267  | 0.22        | 0/3073        |
| 11  | d3    | 0.08         | 0/2267  | 0.21        | 0/3073        |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 11  | e3    | 0.08         | 0/2267          | 0.21        | 0/3073           |
| 11  | f3    | 0.07         | 0/2267          | 0.21        | 0/3073           |
| 11  | g3    | 0.07         | 0/2267          | 0.22        | 0/3073           |
| 11  | h3    | 0.08         | 0/2266          | 0.21        | 0/3071           |
| 11  | i3    | 0.07         | 0/2267          | 0.21        | 0/3073           |
| 11  | j3    | 0.08         | 0/2267          | 0.22        | 0/3073           |
| 11  | k3    | 0.07         | 0/2267          | 0.21        | 0/3073           |
| 11  | l3    | 0.08         | 0/2267          | 0.22        | 0/3073           |
| 11  | m3    | 0.07         | 0/2267          | 0.21        | 0/3073           |
| 11  | n3    | 0.08         | 0/2267          | 0.22        | 0/3073           |
| 11  | o3    | 0.07         | 0/2267          | 0.22        | 0/3073           |
| 11  | p3    | 0.08         | 0/2267          | 0.21        | 0/3073           |
| 11  | q3    | 0.07         | 0/2267          | 0.22        | 0/3073           |
| 11  | r3    | 0.08         | 0/2264          | 0.22        | 0/3066           |
| 11  | s3    | 0.07         | 0/2267          | 0.21        | 0/3073           |
| 11  | t3    | 0.07         | 0/2267          | 0.21        | 0/3073           |
| 11  | u3    | 0.08         | 0/2267          | 0.21        | 0/3073           |
| 11  | v3    | 0.07         | 0/2267          | 0.22        | 0/3073           |
| 11  | w3    | 0.08         | 0/2267          | 0.21        | 0/3073           |
| 11  | x3    | 0.08         | 0/2267          | 0.21        | 0/3073           |
| 11  | y3    | 0.08         | 0/2267          | 0.22        | 0/3073           |
| 11  | z3    | 0.08         | 0/2267          | 0.22        | 0/3073           |
| 12  | A4    | 0.13         | 0/1491          | 0.25        | 0/2033           |
| 12  | B4    | 0.14         | 0/1509          | 0.27        | 0/2058           |
| 12  | C4    | 0.13         | 0/1474          | 0.27        | 0/2010           |
| 12  | D4    | 0.14         | 0/1496          | 0.35        | 0/2040           |
| 12  | E4    | 0.14         | 0/1509          | 0.28        | 0/2058           |
| All | All   | 0.29         | 7/249431 (0.0%) | 0.42        | 46/338382 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B1    | 0                   | 1                   |
| 1   | E1    | 0                   | 1                   |
| 1   | G1    | 0                   | 1                   |
| 1   | H1    | 0                   | 1                   |
| 1   | L1    | 0                   | 1                   |
| 1   | N1    | 0                   | 1                   |
| 2   | B2    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | C2    | 0                   | 2                   |
| 2   | D2    | 0                   | 2                   |
| 2   | E2    | 0                   | 1                   |
| 3   | F2    | 0                   | 2                   |
| 4   | G2    | 0                   | 1                   |
| 4   | H2    | 0                   | 1                   |
| 4   | I2    | 0                   | 1                   |
| 4   | J2    | 0                   | 1                   |
| 6   | U2    | 0                   | 1                   |
| 8   | b2    | 0                   | 2                   |
| 8   | c2    | 0                   | 2                   |
| 8   | d2    | 0                   | 1                   |
| 8   | e2    | 0                   | 3                   |
| 8   | f2    | 0                   | 3                   |
| All | All   | 0                   | 31                  |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E2    | 205 | MET  | SD-CE   | 43.51 | 2.88        | 1.79     |
| 4   | J2    | 51  | PHE  | CD1-CE1 | 21.93 | 2.04        | 1.38     |
| 4   | J2    | 51  | PHE  | CE2-CZ  | 21.65 | 2.03        | 1.38     |
| 4   | J2    | 51  | PHE  | CD2-CE2 | 21.09 | 2.02        | 1.38     |
| 4   | J2    | 51  | PHE  | CE1-CZ  | 20.92 | 2.01        | 1.38     |
| 4   | J2    | 51  | PHE  | CG-CD1  | 15.55 | 1.71        | 1.38     |
| 4   | J2    | 51  | PHE  | CG-CD2  | 15.18 | 1.70        | 1.38     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | E2    | 205 | MET  | CG-SD-CE | 14.35 | 132.46      | 100.90   |
| 9   | t2    | 167 | PRO  | CA-N-CD  | -8.81 | 99.66       | 112.00   |
| 1   | K1    | 282 | TYR  | CA-C-N   | -7.46 | 111.24      | 121.61   |
| 1   | K1    | 282 | TYR  | C-N-CA   | -7.46 | 111.24      | 121.61   |
| 10  | Z3    | 43  | PRO  | CA-N-CD  | -6.72 | 102.59      | 112.00   |
| 10  | N3    | 43  | PRO  | CA-N-CD  | -6.72 | 102.59      | 112.00   |
| 10  | M3    | 43  | PRO  | CA-N-CD  | -6.71 | 102.60      | 112.00   |
| 10  | A3    | 43  | PRO  | CA-N-CD  | -6.71 | 102.61      | 112.00   |
| 10  | J3    | 43  | PRO  | CA-N-CD  | -6.70 | 102.62      | 112.00   |
| 10  | Y3    | 43  | PRO  | CA-N-CD  | -6.70 | 102.62      | 112.00   |
| 10  | W3    | 43  | PRO  | CA-N-CD  | -6.70 | 102.63      | 112.00   |
| 10  | V3    | 43  | PRO  | CA-N-CD  | -6.69 | 102.63      | 112.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 10  | B3    | 43  | PRO  | CA-N-CD  | -6.69 | 102.63      | 112.00   |
| 10  | Q3    | 43  | PRO  | CA-N-CD  | -6.69 | 102.63      | 112.00   |
| 10  | D3    | 43  | PRO  | CA-N-CD  | -6.68 | 102.64      | 112.00   |
| 10  | H3    | 43  | PRO  | CA-N-CD  | -6.68 | 102.64      | 112.00   |
| 10  | R3    | 43  | PRO  | CA-N-CD  | -6.68 | 102.65      | 112.00   |
| 10  | I3    | 43  | PRO  | CA-N-CD  | -6.68 | 102.65      | 112.00   |
| 10  | F3    | 43  | PRO  | CA-N-CD  | -6.68 | 102.65      | 112.00   |
| 10  | S3    | 43  | PRO  | CA-N-CD  | -6.67 | 102.66      | 112.00   |
| 10  | G3    | 43  | PRO  | CA-N-CD  | -6.67 | 102.67      | 112.00   |
| 10  | T3    | 43  | PRO  | CA-N-CD  | -6.66 | 102.67      | 112.00   |
| 10  | C3    | 43  | PRO  | CA-N-CD  | -6.66 | 102.67      | 112.00   |
| 10  | K3    | 43  | PRO  | CA-N-CD  | -6.65 | 102.69      | 112.00   |
| 10  | L3    | 43  | PRO  | CA-N-CD  | -6.65 | 102.69      | 112.00   |
| 10  | O3    | 43  | PRO  | CA-N-CD  | -6.65 | 102.69      | 112.00   |
| 10  | U3    | 43  | PRO  | CA-N-CD  | -6.65 | 102.69      | 112.00   |
| 10  | P3    | 43  | PRO  | CA-N-CD  | -6.65 | 102.70      | 112.00   |
| 10  | X3    | 43  | PRO  | CA-N-CD  | -6.64 | 102.70      | 112.00   |
| 10  | E3    | 43  | PRO  | CA-N-CD  | -6.64 | 102.70      | 112.00   |
| 1   | L1    | 166 | VAL  | N-CA-C   | -6.58 | 106.05      | 111.91   |
| 2   | C2    | 41  | SER  | N-CA-C   | -6.43 | 100.19      | 109.31   |
| 2   | A2    | 224 | MET  | CB-CG-SD | -6.32 | 93.75       | 112.70   |
| 1   | U1    | 282 | TYR  | CA-C-N   | -5.97 | 109.30      | 121.48   |
| 1   | U1    | 282 | TYR  | C-N-CA   | -5.97 | 109.30      | 121.48   |
| 2   | D2    | 113 | TYR  | CA-C-N   | -5.64 | 113.57      | 119.83   |
| 2   | D2    | 113 | TYR  | C-N-CA   | -5.64 | 113.57      | 119.83   |
| 1   | H1    | 164 | LEU  | CA-C-N   | 5.58  | 132.19      | 121.54   |
| 1   | H1    | 164 | LEU  | C-N-CA   | 5.58  | 132.19      | 121.54   |
| 1   | N1    | 166 | VAL  | N-CA-C   | -5.58 | 97.74       | 109.34   |
| 2   | A2    | 40  | LEU  | N-CA-C   | -5.50 | 106.94      | 113.38   |
| 3   | F2    | 139 | THR  | CA-C-N   | -5.29 | 114.35      | 121.71   |
| 3   | F2    | 139 | THR  | C-N-CA   | -5.29 | 114.35      | 121.71   |
| 2   | E2    | 119 | GLN  | N-CA-C   | 5.28  | 116.98      | 108.32   |
| 1   | C1    | 160 | PRO  | CA-C-N   | 5.12  | 134.28      | 121.80   |
| 1   | C1    | 160 | PRO  | C-N-CA   | 5.12  | 134.28      | 121.80   |

There are no chirality outliers.

All (31) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B1    | 163 | SER  | Peptide |
| 2   | B2    | 40  | LEU  | Peptide |
| 2   | B2    | 41  | SER  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | C2    | 40  | LEU  | Peptide |
| 2   | C2    | 41  | SER  | Peptide |
| 2   | D2    | 40  | LEU  | Peptide |
| 2   | D2    | 41  | SER  | Peptide |
| 1   | E1    | 162 | PRO  | Peptide |
| 2   | E2    | 38  | TRP  | Peptide |
| 3   | F2    | 113 | PHE  | Peptide |
| 3   | F2    | 140 | PHE  | Peptide |
| 1   | G1    | 165 | PHE  | Peptide |
| 4   | G2    | 41  | ALA  | Peptide |
| 1   | H1    | 165 | PHE  | Peptide |
| 4   | H2    | 41  | ALA  | Peptide |
| 4   | I2    | 41  | ALA  | Peptide |
| 4   | J2    | 41  | ALA  | Peptide |
| 1   | L1    | 125 | GLN  | Peptide |
| 1   | N1    | 165 | PHE  | Peptide |
| 6   | U2    | 95  | LEU  | Peptide |
| 8   | b2    | 116 | GLN  | Peptide |
| 8   | b2    | 117 | GLY  | Peptide |
| 8   | c2    | 115 | ILE  | Peptide |
| 8   | c2    | 117 | GLY  | Peptide |
| 8   | d2    | 117 | GLY  | Peptide |
| 8   | e2    | 114 | THR  | Peptide |
| 8   | e2    | 115 | ILE  | Peptide |
| 8   | e2    | 117 | GLY  | Peptide |
| 8   | f2    | 114 | THR  | Peptide |
| 8   | f2    | 117 | GLY  | Peptide |
| 8   | f2    | 70  | GLN  | 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   | A1    | 1193  | 0        | 1173     | 46      | 0            |
| 1   | B1    | 1931  | 0        | 1922     | 130     | 0            |
| 1   | C1    | 1931  | 0        | 1921     | 112     | 0            |
| 1   | D1    | 1193  | 0        | 1173     | 62      | 0            |
| 1   | E1    | 1931  | 0        | 1922     | 159     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | F1    | 1193  | 0        | 1173     | 64      | 0            |
| 1   | G1    | 1931  | 0        | 1919     | 121     | 0            |
| 1   | H1    | 1931  | 0        | 1925     | 124     | 0            |
| 1   | I1    | 1931  | 0        | 1919     | 100     | 0            |
| 1   | J1    | 1193  | 0        | 1173     | 56      | 0            |
| 1   | K1    | 1931  | 0        | 1921     | 107     | 0            |
| 1   | L1    | 1931  | 0        | 1924     | 121     | 0            |
| 1   | M1    | 1193  | 0        | 1173     | 89      | 0            |
| 1   | N1    | 1931  | 0        | 1924     | 149     | 0            |
| 1   | O1    | 1931  | 0        | 1921     | 110     | 0            |
| 1   | P1    | 1193  | 0        | 1173     | 50      | 0            |
| 1   | Q1    | 1931  | 0        | 1921     | 135     | 0            |
| 1   | R1    | 1931  | 0        | 1921     | 134     | 0            |
| 1   | S1    | 1193  | 0        | 1173     | 55      | 0            |
| 1   | T1    | 1931  | 0        | 1922     | 199     | 0            |
| 1   | U1    | 1931  | 0        | 1925     | 135     | 0            |
| 1   | V1    | 1193  | 0        | 1173     | 59      | 0            |
| 1   | W1    | 1931  | 0        | 1922     | 134     | 0            |
| 1   | X1    | 1931  | 0        | 1922     | 116     | 0            |
| 1   | Y1    | 1931  | 0        | 1918     | 134     | 0            |
| 1   | Z1    | 1193  | 0        | 1171     | 85      | 0            |
| 1   | a1    | 1931  | 0        | 1924     | 121     | 0            |
| 1   | b1    | 1193  | 0        | 1173     | 52      | 0            |
| 1   | c1    | 1931  | 0        | 1923     | 96      | 0            |
| 1   | d1    | 1931  | 0        | 1923     | 135     | 0            |
| 1   | e1    | 1193  | 0        | 1173     | 41      | 0            |
| 1   | f1    | 1931  | 0        | 1918     | 102     | 0            |
| 1   | g1    | 1931  | 0        | 1921     | 114     | 0            |
| 1   | h1    | 1931  | 0        | 1923     | 132     | 0            |
| 2   | A2    | 1623  | 0        | 1706     | 141     | 0            |
| 2   | B2    | 1623  | 0        | 1707     | 161     | 0            |
| 2   | C2    | 1623  | 0        | 1707     | 197     | 0            |
| 2   | D2    | 1623  | 0        | 1708     | 172     | 0            |
| 2   | E2    | 1623  | 0        | 1709     | 246     | 0            |
| 3   | F2    | 1986  | 0        | 2098     | 230     | 0            |
| 4   | G2    | 670   | 0        | 739      | 40      | 0            |
| 4   | H2    | 670   | 0        | 739      | 47      | 0            |
| 4   | I2    | 670   | 0        | 737      | 48      | 0            |
| 4   | J2    | 670   | 0        | 738      | 67      | 0            |
| 5   | K2    | 296   | 0        | 308      | 18      | 0            |
| 5   | L2    | 563   | 0        | 571      | 11      | 0            |
| 5   | M2    | 563   | 0        | 571      | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | N2    | 563   | 0        | 571      | 24      | 0            |
| 5   | O2    | 563   | 0        | 571      | 20      | 0            |
| 5   | P2    | 563   | 0        | 571      | 39      | 0            |
| 6   | Q2    | 1023  | 0        | 1020     | 71      | 0            |
| 6   | R2    | 932   | 0        | 931      | 67      | 0            |
| 6   | S2    | 942   | 0        | 943      | 73      | 0            |
| 6   | T2    | 835   | 0        | 838      | 34      | 0            |
| 6   | U2    | 925   | 0        | 923      | 101     | 0            |
| 7   | V2    | 969   | 0        | 979      | 45      | 0            |
| 7   | W2    | 964   | 0        | 976      | 32      | 0            |
| 7   | X2    | 964   | 0        | 976      | 47      | 0            |
| 7   | Y2    | 964   | 0        | 976      | 35      | 0            |
| 7   | Z2    | 964   | 0        | 976      | 44      | 0            |
| 7   | a2    | 964   | 0        | 976      | 41      | 0            |
| 8   | b2    | 1812  | 0        | 1800     | 80      | 0            |
| 8   | c2    | 1812  | 0        | 1800     | 89      | 0            |
| 8   | d2    | 1812  | 0        | 1800     | 98      | 0            |
| 8   | e2    | 1812  | 0        | 1800     | 91      | 0            |
| 8   | f2    | 1812  | 0        | 1800     | 82      | 0            |
| 9   | l2    | 1949  | 0        | 1925     | 94      | 0            |
| 9   | 22    | 1949  | 0        | 1924     | 108     | 0            |
| 9   | 32    | 1948  | 0        | 1922     | 121     | 0            |
| 9   | 42    | 1949  | 0        | 1925     | 107     | 0            |
| 9   | g2    | 1949  | 0        | 1926     | 71      | 0            |
| 9   | h2    | 1949  | 0        | 1926     | 83      | 0            |
| 9   | i2    | 1949  | 0        | 1926     | 86      | 0            |
| 9   | j2    | 1949  | 0        | 1925     | 76      | 0            |
| 9   | k2    | 1949  | 0        | 1926     | 76      | 0            |
| 9   | l2    | 1871  | 0        | 1849     | 65      | 0            |
| 9   | m2    | 1871  | 0        | 1849     | 91      | 0            |
| 9   | n2    | 1871  | 0        | 1849     | 94      | 0            |
| 9   | o2    | 1871  | 0        | 1849     | 92      | 0            |
| 9   | p2    | 1871  | 0        | 1849     | 101     | 0            |
| 9   | q2    | 1885  | 0        | 1862     | 66      | 0            |
| 9   | r2    | 1949  | 0        | 1926     | 101     | 0            |
| 9   | s2    | 1949  | 0        | 1924     | 95      | 0            |
| 9   | t2    | 1949  | 0        | 1926     | 89      | 0            |
| 9   | u2    | 1949  | 0        | 1926     | 107     | 0            |
| 9   | v2    | 1949  | 0        | 1926     | 55      | 0            |
| 9   | w2    | 1949  | 0        | 1926     | 95      | 0            |
| 9   | x2    | 1949  | 0        | 1926     | 65      | 0            |
| 9   | y2    | 1949  | 0        | 1926     | 88      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | z2    | 1949  | 0        | 1926     | 91      | 0            |
| 10  | A3    | 1581  | 0        | 1534     | 92      | 0            |
| 10  | B3    | 1581  | 0        | 1534     | 92      | 0            |
| 10  | C3    | 1581  | 0        | 1534     | 95      | 0            |
| 10  | D3    | 1581  | 0        | 1534     | 94      | 0            |
| 10  | E3    | 1581  | 0        | 1534     | 95      | 0            |
| 10  | F3    | 1581  | 0        | 1534     | 93      | 0            |
| 10  | G3    | 1581  | 0        | 1534     | 94      | 0            |
| 10  | H3    | 1581  | 0        | 1534     | 94      | 0            |
| 10  | I3    | 1581  | 0        | 1534     | 96      | 0            |
| 10  | J3    | 1581  | 0        | 1534     | 95      | 0            |
| 10  | K3    | 1581  | 0        | 1534     | 96      | 0            |
| 10  | L3    | 1581  | 0        | 1534     | 95      | 0            |
| 10  | M3    | 1581  | 0        | 1534     | 95      | 0            |
| 10  | N3    | 1581  | 0        | 1534     | 99      | 0            |
| 10  | O3    | 1581  | 0        | 1534     | 98      | 0            |
| 10  | P3    | 1581  | 0        | 1534     | 93      | 0            |
| 10  | Q3    | 1581  | 0        | 1534     | 100     | 0            |
| 10  | R3    | 1581  | 0        | 1534     | 100     | 0            |
| 10  | S3    | 1581  | 0        | 1534     | 98      | 0            |
| 10  | T3    | 1581  | 0        | 1534     | 95      | 0            |
| 10  | U3    | 1581  | 0        | 1534     | 93      | 0            |
| 10  | V3    | 1581  | 0        | 1534     | 91      | 0            |
| 10  | W3    | 1580  | 0        | 1529     | 94      | 0            |
| 10  | X3    | 1581  | 0        | 1534     | 95      | 0            |
| 10  | Y3    | 1581  | 0        | 1534     | 96      | 0            |
| 10  | Z3    | 1581  | 0        | 1534     | 101     | 0            |
| 11  | a3    | 2252  | 0        | 2292     | 193     | 0            |
| 11  | b3    | 2252  | 0        | 2293     | 194     | 0            |
| 11  | c3    | 2252  | 0        | 2292     | 205     | 0            |
| 11  | d3    | 2252  | 0        | 2293     | 188     | 0            |
| 11  | e3    | 2252  | 0        | 2293     | 189     | 0            |
| 11  | f3    | 2252  | 0        | 2293     | 197     | 0            |
| 11  | g3    | 2252  | 0        | 2293     | 192     | 0            |
| 11  | h3    | 2251  | 0        | 2291     | 190     | 0            |
| 11  | i3    | 2252  | 0        | 2291     | 189     | 0            |
| 11  | j3    | 2252  | 0        | 2293     | 187     | 0            |
| 11  | k3    | 2252  | 0        | 2293     | 185     | 0            |
| 11  | l3    | 2252  | 0        | 2291     | 197     | 0            |
| 11  | m3    | 2252  | 0        | 2293     | 193     | 0            |
| 11  | n3    | 2252  | 0        | 2293     | 185     | 0            |
| 11  | o3    | 2252  | 0        | 2291     | 193     | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 11  | p3    | 2252   | 0        | 2293     | 188     | 0            |
| 11  | q3    | 2252   | 0        | 2293     | 195     | 0            |
| 11  | r3    | 2251   | 0        | 2287     | 192     | 0            |
| 11  | s3    | 2252   | 0        | 2293     | 198     | 0            |
| 11  | t3    | 2252   | 0        | 2293     | 198     | 0            |
| 11  | u3    | 2252   | 0        | 2293     | 187     | 0            |
| 11  | v3    | 2252   | 0        | 2293     | 199     | 0            |
| 11  | w3    | 2252   | 0        | 2293     | 190     | 0            |
| 11  | x3    | 2252   | 0        | 2293     | 198     | 0            |
| 11  | y3    | 2252   | 0        | 2291     | 198     | 0            |
| 11  | z3    | 2252   | 0        | 2293     | 205     | 0            |
| 12  | A4    | 1475   | 0        | 1488     | 85      | 0            |
| 12  | B4    | 1493   | 0        | 1501     | 86      | 0            |
| 12  | C4    | 1458   | 0        | 1468     | 73      | 0            |
| 12  | D4    | 1482   | 0        | 1487     | 89      | 0            |
| 12  | E4    | 1493   | 0        | 1502     | 63      | 0            |
| All | All   | 246311 | 0        | 246056   | 12078   | 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 25.

All (12078) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B2:96:LEU:HD22  | 2:B2:236:MET:CE   | 1.21                     | 1.65              |
| 1:T1:167:ARG:CZ   | 2:E2:107:LYS:CD   | 1.74                     | 1.64              |
| 1:R1:125:GLN:CG   | 2:E2:230:ASP:HB3  | 1.32                     | 1.58              |
| 1:a1:167:ARG:HD3  | 2:D2:244:TYR:CD2  | 1.36                     | 1.58              |
| 1:W1:164:LEU:HD11 | 2:E2:143:ARG:CA   | 1.11                     | 1.57              |
| 2:E2:96:LEU:HD22  | 2:E2:236:MET:CE   | 1.29                     | 1.53              |
| 1:N1:125:GLN:CG   | 3:F2:238:PRO:HG3  | 1.36                     | 1.51              |
| 1:E1:167:ARG:CB   | 2:B2:140:ARG:NH2  | 1.72                     | 1.51              |
| 1:M1:363:THR:HG23 | 6:Q2:73:ILE:CD1   | 1.37                     | 1.49              |
| 1:Q1:167:ARG:CD   | 3:F2:156:THR:HG22 | 1.22                     | 1.48              |
| 4:J2:51:PHE:CE1   | 4:J2:51:PHE:CZ    | 2.01                     | 1.48              |
| 1:R1:167:ARG:CG   | 3:F2:167:ASN:HB3  | 1.40                     | 1.48              |
| 4:J2:51:PHE:CZ    | 4:J2:51:PHE:CE2   | 2.03                     | 1.47              |
| 1:R1:125:GLN:HG3  | 2:E2:230:ASP:CB   | 1.43                     | 1.46              |
| 1:W1:165:PHE:CE1  | 2:E2:244:TYR:O    | 1.66                     | 1.46              |
| 4:J2:51:PHE:CE1   | 4:J2:51:PHE:CD1   | 2.04                     | 1.45              |
| 4:J2:51:PHE:CE2   | 4:J2:51:PHE:CD2   | 2.01                     | 1.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:g1:167:ARG:HD3  | 2:C2:245:SER:C    | 1.37                     | 1.45              |
| 1:g1:167:ARG:CD   | 2:C2:245:SER:C    | 1.87                     | 1.44              |
| 9:42:238:ARG:NH1  | 12:C4:55:ASN:HB2  | 1.32                     | 1.44              |
| 1:M1:363:THR:CG2  | 6:Q2:73:ILE:HD12  | 1.47                     | 1.44              |
| 1:h1:125:GLN:CG   | 4:I2:4:GLU:OE1    | 1.64                     | 1.44              |
| 9:u2:110:GLY:HA3  | 11:z3:80:GLN:NE2  | 1.14                     | 1.44              |
| 1:B1:165:PHE:CE2  | 2:C2:161:GLY:O    | 1.69                     | 1.43              |
| 1:T1:167:ARG:HH22 | 2:E2:107:LYS:N    | 1.09                     | 1.42              |
| 9:u2:110:GLY:CA   | 11:z3:80:GLN:HE22 | 1.28                     | 1.42              |
| 1:T1:165:PHE:CD1  | 3:F2:167:ASN:N    | 1.77                     | 1.41              |
| 9:z2:27:ALA:CA    | 12:D4:45:LYS:CD   | 1.76                     | 1.41              |
| 1:Q1:162:PRO:CB   | 3:F2:253:ASP:OD1  | 1.66                     | 1.41              |
| 9:o2:168:VAL:HB   | 11:t3:54:GLN:NE2  | 1.24                     | 1.41              |
| 1:L1:165:PHE:O    | 2:A2:144:GLU:CG   | 1.70                     | 1.40              |
| 2:B2:71:PHE:HZ    | 2:B2:236:MET:SD   | 1.44                     | 1.40              |
| 1:U1:365:ASN:OD1  | 6:R2:65:LEU:C     | 1.65                     | 1.39              |
| 9:32:238:ARG:NH2  | 12:B4:55:ASN:C    | 1.81                     | 1.38              |
| 9:r2:141:THR:HG21 | 11:l3:53:THR:CG2  | 1.54                     | 1.38              |
| 2:E2:96:LEU:CD2   | 2:E2:236:MET:HE1  | 1.49                     | 1.38              |
| 9:42:238:ARG:CZ   | 12:C4:55:ASN:HB2  | 1.36                     | 1.38              |
| 9:k2:168:VAL:HG23 | 11:f3:114:LYS:NZ  | 1.28                     | 1.37              |
| 9:z2:233:MET:HE1  | 12:D4:58:LEU:CD2  | 1.53                     | 1.36              |
| 1:R1:167:ARG:CD   | 3:F2:166:SER:O    | 1.71                     | 1.36              |
| 1:c1:297:GLN:OE1  | 6:S2:55:ARG:NH2   | 1.58                     | 1.36              |
| 1:K1:167:ARG:HD3  | 2:A2:245:SER:O    | 1.21                     | 1.35              |
| 1:W1:164:LEU:CD1  | 2:E2:143:ARG:HA   | 0.88                     | 1.35              |
| 2:E2:96:LEU:CD2   | 2:E2:236:MET:CE   | 2.01                     | 1.35              |
| 1:T1:167:ARG:NH1  | 2:E2:107:LYS:HD3  | 1.43                     | 1.34              |
| 9:32:238:ARG:HH22 | 12:B4:55:ASN:C    | 1.36                     | 1.33              |
| 1:H1:165:PHE:CZ   | 2:B2:147:LEU:HD13 | 1.64                     | 1.33              |
| 1:d1:165:PHE:CE2  | 2:D2:144:GLU:HB3  | 1.62                     | 1.33              |
| 1:h1:125:GLN:HG3  | 4:I2:4:GLU:CD     | 1.51                     | 1.33              |
| 1:Q1:167:ARG:HD2  | 3:F2:156:THR:CG2  | 1.10                     | 1.32              |
| 1:Y1:164:LEU:CD1  | 2:E2:152:ARG:HD2  | 1.60                     | 1.31              |
| 1:E1:167:ARG:HG3  | 2:B2:140:ARG:NH1  | 1.45                     | 1.31              |
| 1:W1:165:PHE:CZ   | 2:E2:244:TYR:O    | 1.83                     | 1.31              |
| 1:H1:165:PHE:HZ   | 2:B2:147:LEU:CD1  | 1.43                     | 1.31              |
| 1:R1:167:ARG:HG3  | 3:F2:167:ASN:CB   | 1.61                     | 1.30              |
| 1:S1:295:SER:HB3  | 6:R2:73:ILE:CD1   | 1.60                     | 1.30              |
| 1:g1:167:ARG:HG2  | 2:C2:244:TYR:CD2  | 1.67                     | 1.30              |
| 9:r2:138:PRO:HB2  | 11:m3:54:GLN:NE2  | 1.46                     | 1.29              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B1:165:PHE:CE2  | 2:C2:162:PRO:HA   | 1.67                     | 1.29              |
| 2:B2:96:LEU:CD2   | 2:B2:236:MET:CE   | 2.11                     | 1.29              |
| 9:42:238:ARG:NH1  | 12:C4:55:ASN:CB   | 1.93                     | 1.29              |
| 1:T1:167:ARG:CZ   | 2:E2:107:LYS:HD3  | 0.81                     | 1.29              |
| 9:t2:203:GLU:CB   | 11:v3:78:ASN:HD21 | 1.46                     | 1.29              |
| 1:U1:365:ASN:ND2  | 6:R2:64:ALA:O     | 1.65                     | 1.28              |
| 1:N1:125:GLN:HG3  | 3:F2:238:PRO:CG   | 1.60                     | 1.28              |
| 9:o2:164:GLN:NE2  | 11:s3:80:GLN:OE1  | 1.65                     | 1.28              |
| 9:s2:139:ALA:HB3  | 11:q3:53:THR:CG2  | 1.63                     | 1.28              |
| 1:G1:166:VAL:H    | 2:B2:144:GLU:CG   | 1.47                     | 1.28              |
| 1:T1:167:ARG:NH2  | 2:E2:107:LYS:N    | 1.82                     | 1.27              |
| 9:12:238:ARG:NH1  | 12:E4:54:GLN:HE22 | 1.31                     | 1.27              |
| 9:22:233:MET:SD   | 12:A4:44:LEU:HD11 | 1.67                     | 1.27              |
| 9:22:237:GLN:HE22 | 12:A4:53:LEU:CD1  | 1.47                     | 1.27              |
| 9:z2:27:ALA:HA    | 12:D4:45:LYS:CD   | 1.34                     | 1.27              |
| 2:B2:96:LEU:CD2   | 2:B2:236:MET:HE3  | 1.64                     | 1.26              |
| 9:m2:164:GLN:HE21 | 11:o3:54:GLN:CD   | 1.17                     | 1.26              |
| 1:E1:167:ARG:HB3  | 2:B2:140:ARG:CZ   | 1.65                     | 1.26              |
| 1:T1:165:PHE:CG   | 3:F2:167:ASN:N    | 2.04                     | 1.26              |
| 9:z2:237:GLN:CG   | 12:D4:53:LEU:HD13 | 1.65                     | 1.26              |
| 9:u2:202:ASN:ND2  | 11:a3:78:ASN:HD22 | 1.33                     | 1.25              |
| 1:Q1:162:PRO:HB2  | 3:F2:253:ASP:OD1  | 1.14                     | 1.25              |
| 1:D1:295:SER:OG   | 6:U2:72:HIS:HA    | 1.09                     | 1.25              |
| 1:T1:167:ARG:NH2  | 2:E2:107:LYS:HD3  | 1.48                     | 1.25              |
| 1:E1:167:ARG:CG   | 2:B2:140:ARG:HH12 | 1.51                     | 1.24              |
| 9:m2:164:GLN:NE2  | 11:o3:54:GLN:CG   | 2.01                     | 1.24              |
| 9:12:241:GLU:OE2  | 12:E4:52:PRO:CB   | 1.71                     | 1.24              |
| 1:d1:165:PHE:CE2  | 2:D2:144:GLU:CB   | 2.20                     | 1.24              |
| 2:B2:71:PHE:CZ    | 2:B2:236:MET:SD   | 2.31                     | 1.22              |
| 9:32:238:ARG:HH22 | 12:B4:55:ASN:CA   | 1.33                     | 1.22              |
| 9:r2:138:PRO:CB   | 11:m3:54:GLN:NE2  | 1.99                     | 1.22              |
| 2:D2:71:PHE:HZ    | 2:D2:236:MET:SD   | 1.63                     | 1.22              |
| 9:o2:168:VAL:CB   | 11:t3:54:GLN:HE21 | 1.52                     | 1.21              |
| 1:K1:167:ARG:CD   | 2:A2:245:SER:O    | 1.86                     | 1.21              |
| 1:g1:167:ARG:HG3  | 2:C2:140:ARG:NH2  | 1.55                     | 1.21              |
| 9:m2:164:GLN:HE21 | 11:o3:54:GLN:CG   | 1.52                     | 1.21              |
| 9:t2:106:MET:HG3  | 11:v3:54:GLN:NE2  | 1.55                     | 1.21              |
| 1:R1:125:GLN:CD   | 2:E2:230:ASP:OD2  | 1.84                     | 1.21              |
| 9:t2:203:GLU:HB3  | 11:v3:78:ASN:ND2  | 1.55                     | 1.21              |
| 9:o2:164:GLN:CB   | 11:s3:78:ASN:HD21 | 1.55                     | 1.20              |
| 9:o2:164:GLN:HB3  | 11:s3:78:ASN:ND2  | 1.56                     | 1.20              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:u2:202:ASN:ND2  | 11:a3:78:ASN:ND2  | 1.90                     | 1.20              |
| 1:W1:164:LEU:CD1  | 2:E2:143:ARG:CA   | 1.83                     | 1.20              |
| 2:E2:96:LEU:CD1   | 2:E2:236:MET:HE3  | 1.70                     | 1.19              |
| 9:r2:141:THR:CG2  | 11:l3:53:THR:HG21 | 1.72                     | 1.19              |
| 9:u2:110:GLY:HA3  | 11:z3:80:GLN:CD   | 1.65                     | 1.19              |
| 1:R1:125:GLN:OE1  | 2:E2:233:GLN:CB   | 1.89                     | 1.19              |
| 1:h1:164:LEU:CD1  | 2:C2:143:ARG:HD2  | 1.72                     | 1.19              |
| 1:h1:164:LEU:CD1  | 2:C2:143:ARG:CD   | 2.21                     | 1.19              |
| 9:o2:168:VAL:CB   | 11:t3:54:GLN:NE2  | 2.07                     | 1.18              |
| 9:p2:171:GLY:HA2  | 11:c3:80:GLN:NE2  | 1.58                     | 1.18              |
| 9:q2:125:ASN:OD1  | 11:g3:54:GLN:NE2  | 1.74                     | 1.18              |
| 1:T1:165:PHE:CG   | 3:F2:167:ASN:CA   | 2.27                     | 1.18              |
| 1:T1:167:ARG:NH2  | 2:E2:107:LYS:H    | 1.38                     | 1.18              |
| 2:E2:205:MET:SD   | 4:J2:51:PHE:CD1   | 2.36                     | 1.18              |
| 1:B1:165:PHE:CE1  | 2:C2:159:LEU:HD13 | 1.79                     | 1.17              |
| 1:K1:125:GLN:OE1  | 4:G2:15:LYS:NZ    | 1.77                     | 1.17              |
| 9:s2:139:ALA:CB   | 11:q3:53:THR:HG21 | 1.74                     | 1.17              |
| 9:22:237:GLN:NE2  | 12:A4:53:LEU:HD12 | 1.56                     | 1.17              |
| 1:E1:162:PRO:HB2  | 4:H2:86:TYR:OH    | 1.37                     | 1.17              |
| 2:E2:205:MET:SD   | 4:J2:51:PHE:CE1   | 2.37                     | 1.17              |
| 9:32:238:ARG:NH2  | 12:B4:56:ASN:N    | 1.89                     | 1.17              |
| 9:32:233:MET:HE3  | 12:B4:58:LEU:HD13 | 1.20                     | 1.16              |
| 2:E2:96:LEU:HD13  | 2:E2:236:MET:CE   | 1.75                     | 1.16              |
| 9:z2:233:MET:CE   | 12:D4:58:LEU:HD21 | 1.73                     | 1.16              |
| 9:22:234:ILE:HG23 | 12:A4:55:ASN:ND2  | 1.59                     | 1.16              |
| 1:T1:167:ARG:NH2  | 2:E2:103:PRO:O    | 1.76                     | 1.15              |
| 1:D1:295:SER:HB3  | 6:U2:73:ILE:HD13  | 1.20                     | 1.15              |
| 1:B1:165:PHE:CE2  | 2:C2:162:PRO:CA   | 2.29                     | 1.15              |
| 1:H1:166:VAL:HG12 | 2:B2:160:GLN:O    | 1.45                     | 1.15              |
| 1:K1:164:LEU:HD11 | 2:A2:241:GLN:C    | 1.43                     | 1.15              |
| 1:T1:167:ARG:NH2  | 2:E2:107:LYS:CG   | 2.09                     | 1.15              |
| 1:Q1:161:LYS:CE   | 3:F2:249:ASN:ND2  | 2.10                     | 1.14              |
| 9:m2:164:GLN:NE2  | 11:o3:54:GLN:HG3  | 1.56                     | 1.14              |
| 9:n2:168:VAL:HA   | 11:x3:78:ASN:ND2  | 1.59                     | 1.14              |
| 1:S1:295:SER:OG   | 6:R2:71:HIS:O     | 1.62                     | 1.14              |
| 9:p2:139:ALA:HB3  | 11:c3:51:GLN:HE21 | 1.06                     | 1.14              |
| 2:E2:205:MET:SD   | 4:J2:51:PHE:CD2   | 2.41                     | 1.14              |
| 1:N1:165:PHE:CE2  | 2:A2:148:ALA:HB2  | 1.82                     | 1.14              |
| 9:s2:139:ALA:CB   | 11:q3:53:THR:CG2  | 2.24                     | 1.14              |
| 9:12:241:GLU:OE2  | 12:E4:52:PRO:HB3  | 1.38                     | 1.14              |
| 1:B1:165:PHE:CD1  | 2:C2:159:LEU:HD13 | 1.81                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R1:125:GLN:OE1  | 2:E2:233:GLN:HB2  | 0.96                     | 1.14              |
| 1:W1:164:LEU:HA   | 2:E2:144:GLU:CD   | 1.72                     | 1.13              |
| 1:h1:125:GLN:HG3  | 4:I2:4:GLU:OE1    | 1.18                     | 1.13              |
| 2:B2:96:LEU:HD22  | 2:B2:236:MET:HE3  | 1.14                     | 1.13              |
| 2:D2:71:PHE:CZ    | 2:D2:236:MET:SD   | 2.41                     | 1.13              |
| 9:z2:27:ALA:CB    | 12:D4:45:LYS:HD3  | 1.78                     | 1.13              |
| 9:22:23:ALA:HB1   | 12:A4:45:LYS:HD2  | 1.27                     | 1.13              |
| 1:Q1:161:LYS:CE   | 3:F2:249:ASN:HD21 | 1.62                     | 1.12              |
| 1:E1:294:ARG:HG3  | 6:U2:66:THR:HB    | 1.14                     | 1.12              |
| 1:M1:363:THR:CG2  | 6:Q2:73:ILE:CD1   | 2.12                     | 1.12              |
| 1:a1:167:ARG:CD   | 2:D2:244:TYR:CD2  | 2.31                     | 1.12              |
| 2:E2:205:MET:SD   | 4:J2:51:PHE:CE2   | 2.42                     | 1.12              |
| 2:E2:205:MET:CE   | 4:J2:51:PHE:CZ    | 2.33                     | 1.12              |
| 1:D1:295:SER:CB   | 6:U2:73:ILE:HD13  | 1.79                     | 1.12              |
| 1:W1:164:LEU:HA   | 2:E2:144:GLU:OE2  | 1.50                     | 1.12              |
| 9:u2:200:ALA:HB3  | 11:b3:54:GLN:CD   | 1.75                     | 1.12              |
| 1:B1:165:PHE:HE2  | 2:C2:162:PRO:CA   | 1.59                     | 1.11              |
| 1:E1:363:THR:HG21 | 6:U2:75:ALA:HB3   | 1.22                     | 1.11              |
| 1:Q1:161:LYS:NZ   | 3:F2:249:ASN:ND2  | 1.98                     | 1.11              |
| 2:E2:205:MET:SD   | 4:J2:51:PHE:CG    | 2.42                     | 1.11              |
| 1:E1:297:GLN:HE22 | 6:U2:76:GLN:HA    | 0.98                     | 1.11              |
| 1:Q1:165:PHE:CE2  | 3:F2:145:TRP:CZ3  | 2.39                     | 1.11              |
| 1:R1:165:PHE:CE2  | 3:F2:250:LEU:HA   | 1.80                     | 1.11              |
| 1:T1:165:PHE:CE2  | 3:F2:167:ASN:HA   | 1.83                     | 1.11              |
| 1:Y1:164:LEU:HD12 | 2:E2:152:ARG:HD2  | 1.16                     | 1.11              |
| 9:32:233:MET:SD   | 12:B4:44:LEU:HD11 | 1.90                     | 1.11              |
| 9:r2:138:PRO:CG   | 11:m3:54:GLN:NE2  | 2.13                     | 1.11              |
| 9:z2:237:GLN:HG3  | 12:D4:53:LEU:HD13 | 1.22                     | 1.11              |
| 1:D1:295:SER:OG   | 6:U2:72:HIS:CA    | 1.99                     | 1.10              |
| 1:E1:167:ARG:HB3  | 2:B2:140:ARG:NH2  | 0.79                     | 1.10              |
| 1:E1:294:ARG:CG   | 6:U2:66:THR:HB    | 1.81                     | 1.10              |
| 1:T1:165:PHE:CD2  | 3:F2:167:ASN:CB   | 2.34                     | 1.10              |
| 1:g1:167:ARG:CG   | 2:C2:244:TYR:HD2  | 1.62                     | 1.10              |
| 9:n2:169:GLN:HE21 | 11:y3:54:GLN:CG   | 1.64                     | 1.10              |
| 9:r2:138:PRO:CG   | 11:m3:54:GLN:HE21 | 1.63                     | 1.10              |
| 9:y2:231:VAL:HG22 | 12:D4:46:ASN:HD22 | 1.04                     | 1.10              |
| 9:32:238:ARG:NH2  | 12:B4:55:ASN:CA   | 1.77                     | 1.10              |
| 1:N1:125:GLN:CG   | 3:F2:238:PRO:CG   | 2.25                     | 1.10              |
| 9:u2:200:ALA:HB3  | 11:b3:54:GLN:NE2  | 1.64                     | 1.10              |
| 1:T1:165:PHE:CD2  | 3:F2:167:ASN:CG   | 2.30                     | 1.10              |
| 2:E2:205:MET:SD   | 4:J2:51:PHE:CZ    | 2.44                     | 1.10              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:l2:98:LYS:O     | 9:l2:212:GLY:HA3  | 1.52                     | 1.10              |
| 9:n2:169:GLN:HE21 | 11:y3:54:GLN:HG2  | 0.95                     | 1.10              |
| 9:n2:169:GLN:NE2  | 11:y3:54:GLN:HG2  | 1.66                     | 1.10              |
| 1:D1:295:SER:CB   | 6:U2:73:ILE:CD1   | 2.28                     | 1.09              |
| 9:n2:168:VAL:HA   | 11:x3:78:ASN:HD21 | 1.08                     | 1.09              |
| 1:W1:164:LEU:HD12 | 2:E2:143:ARG:HA   | 1.30                     | 1.09              |
| 2:E2:205:MET:CE   | 4:J2:51:PHE:CE2   | 2.35                     | 1.09              |
| 9:22:234:ILE:HG23 | 12:A4:55:ASN:HD21 | 1.04                     | 1.09              |
| 1:B1:166:VAL:HG22 | 2:C2:162:PRO:HD3  | 1.25                     | 1.09              |
| 9:n2:169:GLN:NE2  | 11:y3:53:THR:OG1  | 1.85                     | 1.09              |
| 1:G1:166:VAL:N    | 2:B2:144:GLU:CG   | 2.14                     | 1.09              |
| 1:U1:363:THR:HG23 | 6:R2:65:LEU:HD21  | 1.32                     | 1.08              |
| 1:D1:295:SER:HB3  | 6:U2:73:ILE:CD1   | 1.83                     | 1.08              |
| 1:H1:125:GLN:HG2  | 4:G2:67:PRO:HB3   | 1.32                     | 1.08              |
| 9:y2:231:VAL:HG22 | 12:D4:46:ASN:ND2  | 1.66                     | 1.08              |
| 1:G1:166:VAL:N    | 2:B2:144:GLU:HG3  | 1.67                     | 1.08              |
| 9:r2:138:PRO:CB   | 11:m3:54:GLN:HE21 | 1.63                     | 1.08              |
| 9:42:238:ARG:CZ   | 12:C4:55:ASN:CB   | 2.02                     | 1.08              |
| 1:S1:295:SER:HB3  | 6:R2:73:ILE:HD13  | 1.35                     | 1.08              |
| 1:a1:167:ARG:NH1  | 2:D2:244:TYR:CG   | 2.04                     | 1.08              |
| 1:U1:365:ASN:OD1  | 6:R2:65:LEU:CA    | 2.01                     | 1.08              |
| 9:l2:164:GLN:HG3  | 11:j3:80:GLN:NE2  | 1.67                     | 1.08              |
| 1:R1:164:LEU:HD11 | 3:F2:174:ARG:HG3  | 1.31                     | 1.07              |
| 1:a1:167:ARG:HG3  | 2:D2:140:ARG:HH22 | 1.14                     | 1.07              |
| 9:q2:203:GLU:OE1  | 11:h3:82:LYS:NZ   | 1.88                     | 1.07              |
| 1:T1:165:PHE:CZ   | 3:F2:167:ASN:HA   | 1.88                     | 1.07              |
| 9:z2:27:ALA:HA    | 12:D4:45:LYS:HD2  | 1.11                     | 1.07              |
| 1:g1:167:ARG:CG   | 2:C2:244:TYR:CD2  | 2.37                     | 1.07              |
| 2:E2:205:MET:CE   | 4:J2:51:PHE:CE1   | 2.37                     | 1.07              |
| 9:t2:203:GLU:CG   | 11:v3:78:ASN:HD21 | 1.48                     | 1.07              |
| 2:E2:96:LEU:CD1   | 2:E2:236:MET:CE   | 2.32                     | 1.07              |
| 1:Q1:161:LYS:HE2  | 3:F2:249:ASN:ND2  | 1.68                     | 1.06              |
| 1:Q1:161:LYS:HZ1  | 3:F2:249:ASN:CG   | 1.62                     | 1.06              |
| 1:Y1:167:ARG:NH1  | 2:E2:157:GLY:O    | 1.85                     | 1.06              |
| 9:o2:161:GLN:NE2  | 11:s3:80:GLN:NE2  | 2.01                     | 1.06              |
| 1:E1:167:ARG:CG   | 2:B2:140:ARG:NH1  | 2.10                     | 1.06              |
| 1:T1:167:ARG:NE   | 2:E2:107:LYS:CE   | 2.17                     | 1.06              |
| 1:N1:297:GLN:NE2  | 6:Q2:77:ALA:CB    | 2.18                     | 1.06              |
| 9:u2:110:GLY:CA   | 11:z3:80:GLN:NE2  | 2.00                     | 1.06              |
| 1:E1:297:GLN:NE2  | 6:U2:76:GLN:HA    | 1.68                     | 1.06              |
| 1:N1:297:GLN:HE22 | 6:Q2:77:ALA:CB    | 1.68                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:h1:164:LEU:HD13 | 2:C2:143:ARG:HD2  | 1.06                     | 1.06              |
| 9:22:23:ALA:HB1   | 12:A4:45:LYS:CD   | 1.86                     | 1.06              |
| 1:Y1:167:ARG:NH1  | 2:E2:157:GLY:C    | 2.11                     | 1.05              |
| 9:s2:139:ALA:HB3  | 11:q3:53:THR:HG22 | 1.35                     | 1.05              |
| 9:t2:203:GLU:CG   | 11:v3:78:ASN:ND2  | 2.11                     | 1.05              |
| 9:42:59:GLN:HE22  | 11:u3:80:GLN:NE2  | 1.52                     | 1.05              |
| 1:N1:125:GLN:HG2  | 3:F2:238:PRO:HG3  | 1.34                     | 1.05              |
| 1:K1:164:LEU:HD11 | 2:A2:241:GLN:O    | 1.55                     | 1.04              |
| 9:n2:209:ASN:HD21 | 11:z3:114:LYS:NZ  | 1.55                     | 1.04              |
| 1:d1:164:LEU:HD12 | 2:D2:148:ALA:HB2  | 1.39                     | 1.04              |
| 1:d1:167:ARG:HH21 | 2:D2:159:LEU:HG   | 1.22                     | 1.04              |
| 1:H1:165:PHE:HZ   | 2:B2:147:LEU:HD13 | 0.88                     | 1.04              |
| 9:r2:141:THR:CG2  | 11:l3:53:THR:CG2  | 2.33                     | 1.04              |
| 9:22:234:ILE:CG2  | 12:A4:55:ASN:HD21 | 1.70                     | 1.04              |
| 1:R1:165:PHE:O    | 3:F2:257:GLU:CD   | 2.00                     | 1.03              |
| 1:T1:165:PHE:CD1  | 3:F2:167:ASN:CA   | 2.41                     | 1.03              |
| 9:p2:171:GLY:HA2  | 11:c3:80:GLN:HE22 | 0.87                     | 1.03              |
| 9:t2:203:GLU:HB3  | 11:v3:78:ASN:HD21 | 1.13                     | 1.03              |
| 1:S1:295:SER:CB   | 6:R2:73:ILE:CD1   | 2.34                     | 1.03              |
| 1:E1:167:ARG:HG2  | 2:B2:244:TYR:CD2  | 1.93                     | 1.03              |
| 1:L1:167:ARG:NH2  | 2:A2:245:SER:HB2  | 1.73                     | 1.03              |
| 9:k2:168:VAL:CG2  | 11:f3:114:LYS:NZ  | 2.19                     | 1.03              |
| 9:o2:164:GLN:HB3  | 11:s3:78:ASN:HD21 | 0.95                     | 1.03              |
| 1:F1:297:GLN:OE1  | 6:U2:62:GLY:N     | 1.92                     | 1.03              |
| 1:Q1:161:LYS:NZ   | 3:F2:249:ASN:CG   | 2.17                     | 1.03              |
| 1:T1:165:PHE:CA   | 3:F2:166:SER:OG   | 2.06                     | 1.03              |
| 1:X1:165:PHE:CZ   | 2:E2:144:GLU:HB3  | 1.94                     | 1.03              |
| 1:E1:294:ARG:HG3  | 6:U2:66:THR:CB    | 1.89                     | 1.02              |
| 9:z2:27:ALA:CA    | 12:D4:45:LYS:HD3  | 1.46                     | 1.02              |
| 1:G1:166:VAL:H    | 2:B2:144:GLU:HG3  | 0.89                     | 1.02              |
| 2:E2:205:MET:CE   | 4:J2:51:PHE:CD2   | 2.43                     | 1.02              |
| 1:R1:167:ARG:CD   | 3:F2:167:ASN:HB3  | 1.88                     | 1.02              |
| 1:Z1:297:GLN:HE21 | 6:S2:65:LEU:HD21  | 1.25                     | 1.02              |
| 9:o2:164:GLN:OE1  | 11:s3:78:ASN:ND2  | 1.65                     | 1.02              |
| 1:N1:365:ASN:OD1  | 6:Q2:66:THR:HG23  | 1.58                     | 1.02              |
| 1:C1:165:PHE:HZ   | 2:C2:145:ALA:HB2  | 1.23                     | 1.02              |
| 1:E1:167:ARG:CB   | 2:B2:140:ARG:NH1  | 2.22                     | 1.02              |
| 1:G1:166:VAL:HB   | 2:B2:144:GLU:HG2  | 1.39                     | 1.02              |
| 1:R1:167:ARG:HD3  | 3:F2:166:SER:C    | 1.84                     | 1.02              |
| 1:d1:165:PHE:HE2  | 2:D2:144:GLU:HB3  | 0.88                     | 1.02              |
| 1:d1:166:VAL:HG23 | 2:D2:161:GLY:HA2  | 1.38                     | 1.02              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:12:241:GLU:OE2  | 12:E4:52:PRO:HB2  | 1.57                     | 1.02              |
| 1:E1:167:ARG:CB   | 2:B2:140:ARG:HH12 | 1.73                     | 1.01              |
| 2:E2:205:MET:CE   | 4:J2:51:PHE:CD1   | 2.43                     | 1.01              |
| 1:F1:363:THR:HG21 | 6:U2:63:VAL:HG23  | 1.38                     | 1.01              |
| 1:T1:165:PHE:CD2  | 3:F2:167:ASN:CA   | 2.43                     | 1.01              |
| 1:W1:164:LEU:HD13 | 2:E2:143:ARG:HA   | 1.39                     | 1.01              |
| 1:d1:167:ARG:NH2  | 2:D2:159:LEU:HG   | 1.73                     | 1.01              |
| 9:u2:202:ASN:HD22 | 11:a3:78:ASN:HD22 | 1.02                     | 1.01              |
| 1:N1:297:GLN:HE22 | 6:Q2:77:ALA:HB1   | 1.20                     | 1.01              |
| 1:Y1:125:GLN:HB2  | 4:J2:75:ASP:OD2   | 1.60                     | 1.01              |
| 9:m2:164:GLN:NE2  | 11:o3:54:GLN:CD   | 1.94                     | 1.01              |
| 1:N1:297:GLN:NE2  | 6:Q2:77:ALA:HB1   | 1.73                     | 1.01              |
| 9:t2:203:GLU:CB   | 11:v3:78:ASN:ND2  | 2.14                     | 1.01              |
| 9:22:237:GLN:HE22 | 12:A4:53:LEU:HD12 | 0.89                     | 1.01              |
| 1:T1:165:PHE:CD2  | 3:F2:167:ASN:HA   | 1.95                     | 1.00              |
| 1:T1:167:ARG:NH2  | 2:E2:107:LYS:CD   | 2.06                     | 1.00              |
| 1:h1:164:LEU:HD13 | 2:C2:143:ARG:CD   | 1.90                     | 1.00              |
| 9:32:238:ARG:HH22 | 12:B4:56:ASN:N    | 1.47                     | 1.00              |
| 1:Q1:162:PRO:HB3  | 3:F2:253:ASP:OD1  | 1.52                     | 1.00              |
| 1:T1:165:PHE:O    | 3:F2:166:SER:OG   | 1.78                     | 1.00              |
| 1:T1:167:ARG:NE   | 2:E2:107:LYS:HD3  | 1.76                     | 1.00              |
| 9:32:233:MET:CE   | 12:B4:58:LEU:HD13 | 1.91                     | 1.00              |
| 1:h1:125:GLN:CG   | 4:I2:4:GLU:CD     | 2.19                     | 1.00              |
| 2:E2:96:LEU:CD2   | 2:E2:236:MET:HE3  | 1.90                     | 1.00              |
| 9:12:238:ARG:NH1  | 12:E4:54:GLN:NE2  | 2.10                     | 1.00              |
| 1:E1:167:ARG:HG3  | 2:B2:140:ARG:HH12 | 1.01                     | 1.00              |
| 2:B2:96:LEU:CD2   | 2:B2:236:MET:HE1  | 1.84                     | 1.00              |
| 1:E1:167:ARG:CB   | 2:B2:140:ARG:CZ   | 2.27                     | 0.99              |
| 9:22:231:VAL:HG23 | 12:B4:42:ALA:CB   | 1.91                     | 0.99              |
| 1:K1:164:LEU:CD1  | 2:A2:241:GLN:C    | 2.36                     | 0.99              |
| 1:T1:167:ARG:CD   | 2:E2:107:LYS:HE2  | 1.91                     | 0.99              |
| 9:p2:141:THR:HB   | 11:c3:54:GLN:HE21 | 1.25                     | 0.98              |
| 1:D1:365:ASN:HD22 | 6:U2:73:ILE:HD11  | 1.28                     | 0.98              |
| 1:Z1:294:ARG:HG2  | 6:S2:68:THR:CG2   | 1.93                     | 0.98              |
| 9:p2:171:GLY:CA   | 11:c3:80:GLN:HE22 | 1.75                     | 0.98              |
| 1:a1:164:LEU:O    | 2:D2:241:GLN:OE1  | 1.81                     | 0.98              |
| 9:z2:27:ALA:CB    | 12:D4:45:LYS:CD   | 2.35                     | 0.98              |
| 1:N1:365:ASN:OD1  | 6:Q2:66:THR:CG2   | 2.10                     | 0.98              |
| 9:r2:141:THR:HG21 | 11:l3:53:THR:HG21 | 1.23                     | 0.98              |
| 1:H1:125:GLN:CG   | 4:G2:67:PRO:HB3   | 1.94                     | 0.98              |
| 1:B1:165:PHE:CE2  | 2:C2:161:GLY:C    | 2.41                     | 0.98              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:k2:168:VAL:CG2   | 11:f3:114:LYS:HZ3 | 1.73                     | 0.98              |
| 9:i2:98:LYS:O      | 9:i2:212:GLY:HA3  | 1.64                     | 0.98              |
| 11:s3:271:ASP:HB3  | 11:s3:357:CYS:HA  | 1.46                     | 0.98              |
| 11:u3:271:ASP:HB3  | 11:u3:357:CYS:HA  | 1.46                     | 0.98              |
| 1:E1:167:ARG:CD    | 2:B2:244:TYR:CD2  | 2.45                     | 0.98              |
| 9:l2:164:GLN:HG3   | 11:j3:80:GLN:HE21 | 1.29                     | 0.98              |
| 9:n2:168:VAL:CA    | 11:x3:78:ASN:HD21 | 1.76                     | 0.98              |
| 11:e3:271:ASP:HB3  | 11:e3:357:CYS:HA  | 1.46                     | 0.97              |
| 11:g3:271:ASP:HB3  | 11:g3:357:CYS:HA  | 1.46                     | 0.97              |
| 11:z3:271:ASP:HB3  | 11:z3:357:CYS:HA  | 1.46                     | 0.97              |
| 11:q3:271:ASP:HB3  | 11:q3:357:CYS:HA  | 1.46                     | 0.97              |
| 9:o2:164:GLN:OE1   | 11:t3:54:GLN:OE1  | 1.83                     | 0.97              |
| 9:42:238:ARG:NE    | 12:C4:55:ASN:HB2  | 1.79                     | 0.97              |
| 1:E1:294:ARG:O     | 6:U2:66:THR:HG22  | 1.59                     | 0.97              |
| 1:H1:165:PHE:CZ    | 2:B2:147:LEU:CD1  | 2.35                     | 0.97              |
| 1:K1:167:ARG:NE    | 2:A2:244:TYR:C    | 2.22                     | 0.97              |
| 1:T1:294:ARG:HG3   | 6:R2:66:THR:CB    | 1.94                     | 0.97              |
| 1:S1:295:SER:OG    | 6:R2:72:HIS:HA    | 1.63                     | 0.97              |
| 11:x3:271:ASP:HB3  | 11:x3:357:CYS:HA  | 1.46                     | 0.97              |
| 9:12:238:ARG:HH12  | 12:E4:54:GLN:HE22 | 1.02                     | 0.97              |
| 11:b3:271:ASP:HB3  | 11:b3:357:CYS:HA  | 1.46                     | 0.97              |
| 11:c3:271:ASP:HB3  | 11:c3:357:CYS:HA  | 1.46                     | 0.97              |
| 11:i3:271:ASP:HB3  | 11:i3:357:CYS:HA  | 1.46                     | 0.97              |
| 1:B1:165:PHE:CD1   | 2:C2:159:LEU:CD1  | 2.48                     | 0.97              |
| 1:R1:164:LEU:HD11  | 3:F2:174:ARG:CG   | 1.94                     | 0.96              |
| 1:d1:165:PHE:HE2   | 2:D2:144:GLU:CB   | 1.64                     | 0.96              |
| 11:o3:271:ASP:HB3  | 11:o3:357:CYS:HA  | 1.46                     | 0.96              |
| 11:w3:271:ASP:HB3  | 11:w3:357:CYS:HA  | 1.46                     | 0.96              |
| 1:U1:363:THR:CG2   | 6:R2:65:LEU:HD21  | 1.94                     | 0.96              |
| 1:Z1:294:ARG:HG3   | 6:S2:66:THR:HB    | 1.47                     | 0.96              |
| 6:S2:95:LEU:HG     | 8:d2:46:VAL:HG13  | 1.47                     | 0.96              |
| 11:k3:271:ASP:HB3  | 11:k3:357:CYS:HA  | 1.46                     | 0.96              |
| 1:N1:166:VAL:CG2   | 2:A2:162:PRO:N    | 2.28                     | 0.96              |
| 1:c1:297:GLN:CD    | 6:S2:55:ARG:NH2   | 2.23                     | 0.96              |
| 9:z2:237:GLN:HG2   | 12:D4:53:LEU:CD1  | 1.95                     | 0.96              |
| 9:22:23:ALA:CB     | 12:A4:45:LYS:HD2  | 1.96                     | 0.96              |
| 1:h1:125:GLN:HG2   | 4:I2:4:GLU:OE1    | 1.62                     | 0.96              |
| 1:D1:295:SER:HB2   | 6:U2:73:ILE:CD1   | 1.92                     | 0.96              |
| 10:H3:171:ILE:HD12 | 10:J3:88:ALA:HB1  | 1.48                     | 0.96              |
| 11:v3:271:ASP:HB3  | 11:v3:357:CYS:HA  | 1.46                     | 0.96              |
| 9:n2:169:GLN:CD    | 11:y3:53:THR:OG1  | 2.09                     | 0.96              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:I3:171:ILE:HD12 | 10:K3:88:ALA:HB1  | 1.48                     | 0.96              |
| 11:m3:271:ASP:HB3  | 11:m3:357:CYS:HA  | 1.46                     | 0.96              |
| 2:E2:205:MET:HE3   | 4:J2:51:PHE:CE2   | 1.97                     | 0.96              |
| 10:G3:171:ILE:HD12 | 10:I3:88:ALA:HB1  | 1.48                     | 0.96              |
| 11:d3:271:ASP:HB3  | 11:d3:357:CYS:HA  | 1.46                     | 0.96              |
| 1:E1:294:ARG:O     | 6:U2:66:THR:CG2   | 2.05                     | 0.96              |
| 1:T1:165:PHE:HB3   | 3:F2:166:SER:OG   | 1.65                     | 0.96              |
| 10:F3:171:ILE:HD12 | 10:H3:88:ALA:HB1  | 1.47                     | 0.96              |
| 1:T1:294:ARG:HG3   | 6:R2:66:THR:CG2   | 1.96                     | 0.95              |
| 1:B1:165:PHE:CD2   | 2:C2:162:PRO:HA   | 2.00                     | 0.95              |
| 1:R1:165:PHE:O     | 3:F2:257:GLU:OE1  | 1.84                     | 0.95              |
| 1:U1:363:THR:HG23  | 6:R2:65:LEU:CD2   | 1.96                     | 0.95              |
| 1:g1:143:THR:HG23  | 1:h1:154:ARG:HH21 | 1.30                     | 0.95              |
| 10:L3:171:ILE:HD12 | 10:N3:88:ALA:HB1  | 1.48                     | 0.95              |
| 10:M3:171:ILE:HD12 | 10:O3:88:ALA:HB1  | 1.48                     | 0.95              |
| 9:s2:203:GLU:O     | 11:r3:80:GLN:NE2  | 1.99                     | 0.95              |
| 1:E1:167:ARG:CD    | 2:B2:244:TYR:HD2  | 1.78                     | 0.95              |
| 9:z2:237:GLN:HG2   | 12:D4:53:LEU:HD13 | 1.47                     | 0.95              |
| 10:J3:171:ILE:HD12 | 10:L3:88:ALA:HB1  | 1.49                     | 0.95              |
| 1:R1:125:GLN:CG    | 2:E2:230:ASP:CB   | 2.21                     | 0.95              |
| 11:a3:271:ASP:HB3  | 11:a3:357:CYS:HA  | 1.46                     | 0.95              |
| 9:p2:139:ALA:CB    | 11:c3:51:GLN:HE21 | 1.79                     | 0.95              |
| 9:12:238:ARG:NH1   | 12:A4:48:ASP:HB2  | 1.80                     | 0.95              |
| 1:T1:165:PHE:HD1   | 3:F2:167:ASN:H    | 1.05                     | 0.95              |
| 2:E2:205:MET:CE    | 4:J2:51:PHE:CG    | 2.49                     | 0.95              |
| 9:r2:138:PRO:HG2   | 11:m3:54:GLN:NE2  | 1.79                     | 0.95              |
| 10:K3:171:ILE:HD12 | 10:M3:88:ALA:HB1  | 1.49                     | 0.95              |
| 10:N3:171:ILE:HD12 | 10:P3:88:ALA:HB1  | 1.48                     | 0.95              |
| 11:t3:271:ASP:HB3  | 11:t3:357:CYS:HA  | 1.46                     | 0.95              |
| 9:s2:139:ALA:HB2   | 11:q3:53:THR:HG21 | 1.43                     | 0.95              |
| 11:h3:271:ASP:HB3  | 11:h3:357:CYS:HA  | 1.46                     | 0.95              |
| 1:B1:166:VAL:HG22  | 2:C2:162:PRO:CD   | 1.95                     | 0.94              |
| 9:32:29:VAL:HG21   | 12:B4:37:LEU:CD2  | 1.96                     | 0.94              |
| 11:p3:271:ASP:HB3  | 11:p3:357:CYS:HA  | 1.46                     | 0.94              |
| 1:L1:165:PHE:O     | 2:A2:144:GLU:HG2  | 1.13                     | 0.94              |
| 11:r3:271:ASP:HB3  | 11:r3:357:CYS:HA  | 1.46                     | 0.94              |
| 1:T1:167:ARG:NH2   | 2:E2:107:LYS:HG2  | 1.78                     | 0.94              |
| 1:W1:164:LEU:HA    | 2:E2:144:GLU:OE1  | 1.65                     | 0.94              |
| 10:E3:171:ILE:HD12 | 10:G3:88:ALA:HB1  | 1.48                     | 0.94              |
| 11:f3:271:ASP:HB3  | 11:f3:357:CYS:HA  | 1.46                     | 0.94              |
| 11:y3:271:ASP:HB3  | 11:y3:357:CYS:HA  | 1.46                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:R1:167:ARG:HD3   | 3:F2:166:SER:O     | 0.77                     | 0.94              |
| 1:T1:165:PHE:CE1   | 3:F2:167:ASN:HA    | 2.03                     | 0.94              |
| 11:j3:271:ASP:HB3  | 11:j3:357:CYS:HA   | 1.46                     | 0.94              |
| 1:F1:363:THR:CG2   | 6:U2:63:VAL:HG23   | 1.97                     | 0.94              |
| 9:n2:209:ASN:HD21  | 11:z3:114:LYS:HZ1  | 0.95                     | 0.94              |
| 1:W1:164:LEU:HD11  | 2:E2:143:ARG:CB    | 1.98                     | 0.94              |
| 9:z2:237:GLN:CG    | 12:D4:53:LEU:CD1   | 2.45                     | 0.94              |
| 10:T3:171:ILE:HD12 | 10:V3:88:ALA:HB1   | 1.48                     | 0.94              |
| 1:Q1:165:PHE:CZ    | 3:F2:145:TRP:CH2   | 2.56                     | 0.94              |
| 1:a1:167:ARG:CG    | 2:D2:140:ARG:HH22  | 1.79                     | 0.94              |
| 10:O3:171:ILE:HD12 | 10:Q3:88:ALA:HB1   | 1.48                     | 0.94              |
| 11:n3:271:ASP:HB3  | 11:n3:357:CYS:HA   | 1.46                     | 0.94              |
| 10:B3:88:ALA:HB1   | 10:Z3:171:ILE:HD12 | 1.47                     | 0.94              |
| 1:G1:165:PHE:HE2   | 4:H2:88:ILE:HG22   | 1.33                     | 0.93              |
| 1:g1:167:ARG:HG2   | 2:C2:244:TYR:HD2   | 1.06                     | 0.93              |
| 10:S3:171:ILE:HD12 | 10:U3:88:ALA:HB1   | 1.48                     | 0.93              |
| 10:U3:171:ILE:HD12 | 10:W3:88:ALA:HB1   | 1.48                     | 0.93              |
| 1:U1:365:ASN:OD1   | 6:R2:65:LEU:HA     | 1.67                     | 0.93              |
| 2:E2:96:LEU:CG     | 2:E2:236:MET:CE    | 2.46                     | 0.93              |
| 10:W3:171:ILE:HD12 | 10:Y3:88:ALA:HB1   | 1.49                     | 0.93              |
| 11:l3:271:ASP:HB3  | 11:l3:357:CYS:HA   | 1.46                     | 0.93              |
| 9:t2:202:ASN:HB3   | 11:w3:53:THR:HG21  | 1.51                     | 0.93              |
| 9:22:233:MET:SD    | 12:A4:44:LEU:CD1   | 2.48                     | 0.93              |
| 9:j2:6:TRP:CZ3     | 9:j2:9:LYS:HE2     | 2.03                     | 0.93              |
| 10:D3:171:ILE:HD12 | 10:F3:88:ALA:HB1   | 1.49                     | 0.93              |
| 10:X3:171:ILE:HD12 | 10:Z3:88:ALA:HB1   | 1.48                     | 0.93              |
| 10:V3:171:ILE:HD12 | 10:X3:88:ALA:HB1   | 1.49                     | 0.93              |
| 1:R1:143:THR:HG21  | 1:T1:156:HIS:HE1   | 1.33                     | 0.93              |
| 1:W1:164:LEU:CA    | 2:E2:144:GLU:OE2   | 2.17                     | 0.93              |
| 9:q2:139:ALA:O     | 11:h3:54:GLN:NE2   | 2.01                     | 0.93              |
| 11:e3:97:ALA:HB1   | 11:e3:171:ILE:HD13 | 1.52                     | 0.92              |
| 10:R3:171:ILE:HD12 | 10:T3:88:ALA:HB1   | 1.48                     | 0.92              |
| 11:v3:97:ALA:HB1   | 11:v3:171:ILE:HD13 | 1.52                     | 0.92              |
| 1:Y1:167:ARG:HH11  | 2:E2:157:GLY:C     | 1.62                     | 0.92              |
| 9:q2:208:LEU:HD13  | 11:i3:53:THR:HG21  | 1.49                     | 0.92              |
| 9:q2:208:LEU:CD1   | 11:i3:53:THR:HG21  | 1.99                     | 0.92              |
| 10:P3:171:ILE:HD12 | 10:R3:88:ALA:HB1   | 1.49                     | 0.92              |
| 11:u3:97:ALA:HB1   | 11:u3:171:ILE:HD13 | 1.52                     | 0.92              |
| 11:d3:97:ALA:HB1   | 11:d3:171:ILE:HD13 | 1.52                     | 0.92              |
| 10:C3:171:ILE:HD12 | 10:E3:88:ALA:HB1   | 1.48                     | 0.92              |
| 11:f3:97:ALA:HB1   | 11:f3:171:ILE:HD13 | 1.52                     | 0.92              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:z3:97:ALA:HB1   | 11:z3:171:ILE:HD13 | 1.52                     | 0.92              |
| 9:p2:98:LYS:HG3    | 9:12:45:LEU:HD11   | 1.51                     | 0.92              |
| 9:p2:122:VAL:O     | 9:u2:180:ASN:ND2   | 2.02                     | 0.92              |
| 10:A3:171:ILE:HD12 | 10:C3:88:ALA:HB1   | 1.48                     | 0.92              |
| 11:w3:97:ALA:HB1   | 11:w3:171:ILE:HD13 | 1.52                     | 0.92              |
| 11:y3:97:ALA:HB1   | 11:y3:171:ILE:HD13 | 1.52                     | 0.92              |
| 11:h3:97:ALA:HB1   | 11:h3:171:ILE:HD13 | 1.52                     | 0.92              |
| 1:d1:164:LEU:CD1   | 2:D2:148:ALA:CB    | 2.48                     | 0.92              |
| 2:C2:236:MET:HE3   | 2:D2:176:THR:HG21  | 1.50                     | 0.92              |
| 11:a3:97:ALA:HB1   | 11:a3:171:ILE:HD13 | 1.52                     | 0.92              |
| 11:i3:97:ALA:HB1   | 11:i3:171:ILE:HD13 | 1.52                     | 0.92              |
| 11:r3:97:ALA:HB1   | 11:r3:171:ILE:HD13 | 1.52                     | 0.92              |
| 11:t3:97:ALA:HB1   | 11:t3:171:ILE:HD13 | 1.52                     | 0.92              |
| 2:E2:205:MET:HE2   | 4:J2:51:PHE:CE1    | 2.03                     | 0.92              |
| 11:q3:97:ALA:HB1   | 11:q3:171:ILE:HD13 | 1.52                     | 0.92              |
| 9:n2:169:GLN:O     | 11:y3:54:GLN:CD    | 2.13                     | 0.92              |
| 10:Q3:171:ILE:HD12 | 10:S3:88:ALA:HB1   | 1.49                     | 0.92              |
| 11:c3:97:ALA:HB1   | 11:c3:171:ILE:HD13 | 1.52                     | 0.92              |
| 11:g3:97:ALA:HB1   | 11:g3:171:ILE:HD13 | 1.52                     | 0.92              |
| 8:c2:114:THR:HG22  | 8:c2:119:PRO:HB3   | 1.51                     | 0.91              |
| 11:x3:97:ALA:HB1   | 11:x3:171:ILE:HD13 | 1.52                     | 0.91              |
| 1:E1:297:GLN:HE22  | 6:U2:76:GLN:CA     | 1.82                     | 0.91              |
| 11:s3:97:ALA:HB1   | 11:s3:171:ILE:HD13 | 1.52                     | 0.91              |
| 9:i2:44:LEU:HD12   | 9:i2:71:GLY:HA3    | 1.52                     | 0.91              |
| 9:s2:127:GLN:NE2   | 11:p3:78:ASN:HD21  | 1.67                     | 0.91              |
| 11:b3:97:ALA:HB1   | 11:b3:171:ILE:HD13 | 1.52                     | 0.91              |
| 11:j3:97:ALA:HB1   | 11:j3:171:ILE:HD13 | 1.52                     | 0.91              |
| 1:C1:165:PHE:HZ    | 2:C2:145:ALA:CB    | 1.84                     | 0.91              |
| 1:L1:414:ASP:HB3   | 1:M1:431:ASN:HD21  | 1.33                     | 0.91              |
| 1:W1:165:PHE:HE1   | 2:E2:244:TYR:O     | 1.27                     | 0.91              |
| 9:r2:141:THR:HG21  | 11:l3:53:THR:HG22  | 1.51                     | 0.91              |
| 1:N1:125:GLN:HG3   | 3:F2:238:PRO:HG3   | 0.91                     | 0.91              |
| 11:p3:97:ALA:HB1   | 11:p3:171:ILE:HD13 | 1.52                     | 0.91              |
| 1:N1:166:VAL:HG21  | 2:A2:162:PRO:N     | 1.85                     | 0.91              |
| 10:B3:171:ILE:HD12 | 10:D3:88:ALA:HB1   | 1.48                     | 0.91              |
| 11:m3:97:ALA:HB1   | 11:m3:171:ILE:HD13 | 1.52                     | 0.91              |
| 11:n3:97:ALA:HB1   | 11:n3:171:ILE:HD13 | 1.52                     | 0.91              |
| 9:t2:106:MET:HG3   | 11:v3:54:GLN:HE22  | 1.11                     | 0.91              |
| 1:Y1:164:LEU:HD12  | 2:E2:152:ARG:CD    | 2.00                     | 0.91              |
| 11:l3:97:ALA:HB1   | 11:l3:171:ILE:HD13 | 1.52                     | 0.91              |
| 1:N1:125:GLN:HG3   | 3:F2:238:PRO:CD    | 2.00                     | 0.91              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:d1:166:VAL:HB   | 2:D2:162:PRO:HD3   | 1.53                     | 0.91              |
| 9:32:194:GLU:C    | 9:32:195:THR:CA    | 2.44                     | 0.91              |
| 2:B2:96:LEU:HD22  | 2:B2:236:MET:HE1   | 0.91                     | 0.90              |
| 2:D2:115:PRO:HB2  | 2:D2:121:ILE:HD12  | 1.52                     | 0.90              |
| 11:o3:97:ALA:HB1  | 11:o3:171:ILE:HD13 | 1.52                     | 0.90              |
| 11:k3:97:ALA:HB1  | 11:k3:171:ILE:HD13 | 1.52                     | 0.90              |
| 1:T1:167:ARG:HD3  | 2:E2:107:LYS:HE2   | 1.54                     | 0.90              |
| 9:22:237:GLN:NE2  | 12:A4:53:LEU:CD1   | 2.21                     | 0.90              |
| 9:42:44:LEU:HD12  | 9:42:71:GLY:HA3    | 1.51                     | 0.90              |
| 1:T1:165:PHE:CG   | 3:F2:167:ASN:CB    | 2.54                     | 0.90              |
| 1:T1:165:PHE:CB   | 3:F2:166:SER:OG    | 2.19                     | 0.90              |
| 1:g1:167:ARG:NE   | 2:C2:245:SER:C     | 2.25                     | 0.90              |
| 1:R1:164:LEU:CD1  | 3:F2:174:ARG:CD    | 2.50                     | 0.90              |
| 1:a1:365:ASN:OD1  | 6:S2:66:THR:HA     | 1.71                     | 0.90              |
| 9:y2:238:ARG:NH2  | 12:D4:52:PRO:HB3   | 1.87                     | 0.90              |
| 9:h2:44:LEU:HD12  | 9:h2:71:GLY:HA3    | 1.54                     | 0.90              |
| 1:Z1:365:ASN:ND2  | 6:S2:72:HIS:O      | 1.92                     | 0.90              |
| 1:B1:165:PHE:HZ   | 2:C2:165:VAL:N     | 1.67                     | 0.90              |
| 9:o2:161:GLN:NE2  | 11:s3:80:GLN:HE22  | 1.65                     | 0.89              |
| 9:q2:141:THR:OG1  | 11:g3:80:GLN:CD    | 2.13                     | 0.89              |
| 9:22:231:VAL:HG23 | 12:B4:42:ALA:HB2   | 1.53                     | 0.89              |
| 10:H3:166:GLU:HG3 | 10:H3:179:ARG:HG2  | 1.55                     | 0.89              |
| 10:I3:166:GLU:HG3 | 10:I3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:V3:166:GLU:HG3 | 10:V3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:W3:166:GLU:HG3 | 10:W3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:Y3:166:GLU:HG3 | 10:Y3:179:ARG:HG2  | 1.55                     | 0.89              |
| 1:E1:167:ARG:HD3  | 2:B2:244:TYR:HD2   | 1.36                     | 0.89              |
| 10:G3:166:GLU:HG3 | 10:G3:179:ARG:HG2  | 1.55                     | 0.89              |
| 10:L3:166:GLU:HG3 | 10:L3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:U3:166:GLU:HG3 | 10:U3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:X3:166:GLU:HG3 | 10:X3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:Z3:166:GLU:HG3 | 10:Z3:179:ARG:HG2  | 1.55                     | 0.89              |
| 2:B2:115:PRO:HB2  | 2:B2:121:ILE:HD12  | 1.54                     | 0.89              |
| 10:K3:166:GLU:HG3 | 10:K3:179:ARG:HG2  | 1.54                     | 0.89              |
| 1:S1:275:LYS:HB3  | 1:S1:377:MET:HE2   | 1.55                     | 0.89              |
| 1:T1:294:ARG:HG3  | 6:R2:66:THR:HG22   | 1.51                     | 0.89              |
| 10:D3:166:GLU:HG3 | 10:D3:179:ARG:HG2  | 1.55                     | 0.89              |
| 10:M3:166:GLU:HG3 | 10:M3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:A3:88:ALA:HB1  | 10:Y3:171:ILE:HD12 | 1.52                     | 0.89              |
| 10:A3:166:GLU:HG3 | 10:A3:179:ARG:HG2  | 1.54                     | 0.89              |
| 10:C3:166:GLU:HG3 | 10:C3:179:ARG:HG2  | 1.54                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:T3:166:GLU:HG3 | 10:T3:179:ARG:HG2 | 1.54                     | 0.89              |
| 1:X1:165:PHE:CE1  | 2:E2:144:GLU:HB3  | 2.07                     | 0.89              |
| 3:F2:109:SER:HG   | 3:F2:112:THR:HG1  | 1.13                     | 0.89              |
| 10:F3:166:GLU:HG3 | 10:F3:179:ARG:HG2 | 1.54                     | 0.89              |
| 9:k2:44:LEU:HD12  | 9:k2:71:GLY:HA3   | 1.53                     | 0.89              |
| 10:E3:166:GLU:HG3 | 10:E3:179:ARG:HG2 | 1.55                     | 0.89              |
| 1:T1:167:ARG:HH22 | 2:E2:107:LYS:CA   | 1.85                     | 0.89              |
| 10:J3:166:GLU:HG3 | 10:J3:179:ARG:HG2 | 1.55                     | 0.89              |
| 1:E1:167:ARG:CG   | 2:B2:244:TYR:CD2  | 2.55                     | 0.88              |
| 10:B3:166:GLU:HG3 | 10:B3:179:ARG:HG2 | 1.54                     | 0.88              |
| 10:P3:166:GLU:HG3 | 10:P3:179:ARG:HG2 | 1.55                     | 0.88              |
| 10:Q3:166:GLU:HG3 | 10:Q3:179:ARG:HG2 | 1.55                     | 0.88              |
| 10:R3:166:GLU:HG3 | 10:R3:179:ARG:HG2 | 1.54                     | 0.88              |
| 1:N1:165:PHE:HE2  | 2:A2:148:ALA:HB2  | 1.34                     | 0.88              |
| 2:E2:96:LEU:CG    | 2:E2:236:MET:HE1  | 2.03                     | 0.88              |
| 9:q2:141:THR:CB   | 11:g3:80:GLN:OE1  | 2.20                     | 0.88              |
| 9:y2:44:LEU:HD12  | 9:y2:71:GLY:HA3   | 1.52                     | 0.88              |
| 10:N3:166:GLU:HG3 | 10:N3:179:ARG:HG2 | 1.55                     | 0.88              |
| 1:a1:167:ARG:HG3  | 2:D2:140:ARG:NH2  | 1.89                     | 0.88              |
| 1:C1:164:LEU:HD21 | 2:C2:149:LEU:CD1  | 2.03                     | 0.88              |
| 1:G1:166:VAL:HB   | 2:B2:144:GLU:CG   | 2.03                     | 0.88              |
| 1:T1:167:ARG:HH12 | 2:E2:106:ASP:C    | 1.82                     | 0.88              |
| 10:O3:166:GLU:HG3 | 10:O3:179:ARG:HG2 | 1.55                     | 0.88              |
| 11:r3:325:SER:HB3 | 11:r3:330:SER:HB3 | 1.56                     | 0.88              |
| 1:R1:168:GLU:HB3  | 3:F2:261:ASN:CG   | 1.98                     | 0.88              |
| 1:S1:387:VAL:HB   | 1:S1:420:MET:HE2  | 1.55                     | 0.88              |
| 1:d1:164:LEU:HD12 | 2:D2:148:ALA:CB   | 2.01                     | 0.88              |
| 10:S3:166:GLU:HG3 | 10:S3:179:ARG:HG2 | 1.54                     | 0.88              |
| 11:w3:325:SER:HB3 | 11:w3:330:SER:HB3 | 1.56                     | 0.88              |
| 11:y3:325:SER:HB3 | 11:y3:330:SER:HB3 | 1.56                     | 0.88              |
| 1:a1:167:ARG:HD3  | 2:D2:244:TYR:HD2  | 1.05                     | 0.88              |
| 1:F1:297:GLN:HE22 | 6:U2:62:GLY:N     | 1.71                     | 0.88              |
| 9:v2:124:GLN:NE2  | 9:12:196:GLN:O    | 2.06                     | 0.88              |
| 2:C2:236:MET:HE3  | 2:D2:176:THR:CG2  | 2.03                     | 0.88              |
| 9:22:44:LEU:HD12  | 9:22:71:GLY:HA3   | 1.56                     | 0.88              |
| 11:p3:325:SER:HB3 | 11:p3:330:SER:HB3 | 1.56                     | 0.88              |
| 9:y2:231:VAL:CG2  | 12:D4:46:ASN:HD22 | 1.85                     | 0.88              |
| 11:t3:325:SER:HB3 | 11:t3:330:SER:HB3 | 1.56                     | 0.88              |
| 9:k2:6:TRP:CZ3    | 9:k2:9:LYS:HE2    | 2.09                     | 0.87              |
| 1:T1:167:ARG:CZ   | 2:E2:107:LYS:CE   | 2.51                     | 0.87              |
| 11:m3:325:SER:HB3 | 11:m3:330:SER:HB3 | 1.56                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:o3:325:SER:HB3  | 11:o3:330:SER:HB3  | 1.56                     | 0.87              |
| 2:C2:236:MET:CE    | 2:D2:150:PHE:HZ    | 1.87                     | 0.87              |
| 9:n2:209:ASN:ND2   | 11:z3:114:LYS:HZ1  | 1.73                     | 0.87              |
| 11:a3:325:SER:HB3  | 11:a3:330:SER:HB3  | 1.56                     | 0.87              |
| 9:z2:27:ALA:HB2    | 12:D4:45:LYS:HD3   | 1.54                     | 0.87              |
| 1:D1:295:SER:CB    | 6:U2:73:ILE:HD12   | 2.04                     | 0.87              |
| 11:u3:325:SER:HB3  | 11:u3:330:SER:HB3  | 1.56                     | 0.87              |
| 1:W1:164:LEU:HD11  | 2:E2:143:ARG:N     | 1.88                     | 0.87              |
| 1:d1:165:PHE:CD1   | 2:D2:147:LEU:HD12  | 2.10                     | 0.87              |
| 1:g1:167:ARG:HG3   | 2:C2:140:ARG:HH21  | 1.38                     | 0.87              |
| 1:g1:167:ARG:HD2   | 2:C2:245:SER:C     | 1.97                     | 0.87              |
| 9:22:230:LEU:CD1   | 12:A4:62:LEU:HD22  | 2.03                     | 0.87              |
| 11:n3:325:SER:HB3  | 11:n3:330:SER:HB3  | 1.56                     | 0.87              |
| 1:T1:165:PHE:C     | 3:F2:166:SER:OG    | 2.16                     | 0.87              |
| 11:k3:325:SER:HB3  | 11:k3:330:SER:HB3  | 1.56                     | 0.87              |
| 1:R1:125:GLN:CD    | 2:E2:230:ASP:HB3   | 1.96                     | 0.87              |
| 1:R1:125:GLN:CD    | 2:E2:230:ASP:CB    | 2.47                     | 0.87              |
| 11:b3:325:SER:HB3  | 11:b3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:v3:325:SER:HB3  | 11:v3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:z3:325:SER:HB3  | 11:z3:330:SER:HB3  | 1.56                     | 0.86              |
| 1:U1:363:THR:CG2   | 6:R2:65:LEU:CD2    | 2.53                     | 0.86              |
| 1:K1:162:PRO:O     | 4:G2:86:TYR:OH     | 1.93                     | 0.86              |
| 9:q2:141:THR:OG1   | 11:g3:80:GLN:NE2   | 2.07                     | 0.86              |
| 11:a3:141:ILE:HD13 | 11:a3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:c3:325:SER:HB3  | 11:c3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:i3:325:SER:HB3  | 11:i3:330:SER:HB3  | 1.56                     | 0.86              |
| 1:C1:164:LEU:HD21  | 2:C2:149:LEU:HD12  | 1.57                     | 0.86              |
| 1:g1:167:ARG:HG2   | 2:C2:244:TYR:CE2   | 2.10                     | 0.86              |
| 1:h1:275:LYS:HB2   | 1:h1:377:MET:HB2   | 1.55                     | 0.86              |
| 9:x2:127:GLN:OE1   | 9:x2:135:GLN:NE2   | 2.09                     | 0.86              |
| 11:r3:141:ILE:HD13 | 11:r3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:s3:141:ILE:HD13 | 11:s3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:t3:141:ILE:HD13 | 11:t3:165:ILE:HD11 | 1.58                     | 0.86              |
| 1:D1:295:SER:HG    | 6:U2:72:HIS:HA     | 1.04                     | 0.86              |
| 3:F2:123:PRO:HA    | 3:F2:127:ARG:HD3   | 1.58                     | 0.86              |
| 11:q3:141:ILE:HD13 | 11:q3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:u3:141:ILE:HD13 | 11:u3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:x3:141:ILE:HD13 | 11:x3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:y3:141:ILE:HD13 | 11:y3:165:ILE:HD11 | 1.58                     | 0.86              |
| 2:B2:75:ARG:HH12   | 2:B2:85:PRO:HB3    | 1.41                     | 0.86              |
| 11:b3:141:ILE:HD13 | 11:b3:165:ILE:HD11 | 1.58                     | 0.86              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:d3:325:SER:HB3  | 11:d3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:l3:325:SER:HB3  | 11:l3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:v3:141:ILE:HD13 | 11:v3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:z3:141:ILE:HD13 | 11:z3:165:ILE:HD11 | 1.58                     | 0.86              |
| 9:p2:139:ALA:HB3   | 11:c3:51:GLN:NE2   | 1.91                     | 0.86              |
| 11:c3:141:ILE:HD13 | 11:c3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:q3:325:SER:HB3  | 11:q3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:w3:141:ILE:HD13 | 11:w3:165:ILE:HD11 | 1.58                     | 0.86              |
| 11:x3:123:MET:HE1  | 11:x3:136:LEU:HD22 | 1.58                     | 0.86              |
| 11:e3:325:SER:HB3  | 11:e3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:p3:141:ILE:HD13 | 11:p3:165:ILE:HD11 | 1.58                     | 0.86              |
| 1:C1:165:PHE:CZ    | 2:C2:145:ALA:CB    | 2.59                     | 0.86              |
| 1:Y1:164:LEU:CG    | 2:E2:152:ARG:HD2   | 2.05                     | 0.86              |
| 10:N3:82:LEU:HA    | 10:N3:197:SER:HB3  | 1.58                     | 0.86              |
| 10:P3:82:LEU:HA    | 10:P3:197:SER:HB3  | 1.58                     | 0.86              |
| 10:Q3:82:LEU:HA    | 10:Q3:197:SER:HB3  | 1.58                     | 0.86              |
| 11:g3:325:SER:HB3  | 11:g3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:s3:325:SER:HB3  | 11:s3:330:SER:HB3  | 1.56                     | 0.86              |
| 11:y3:123:MET:HE1  | 11:y3:136:LEU:HD22 | 1.58                     | 0.86              |
| 1:G1:128:GLU:OE2   | 4:H2:4:GLU:OE2     | 1.93                     | 0.86              |
| 1:T1:375:THR:HG23  | 1:U1:275:LYS:HZ3   | 1.38                     | 0.86              |
| 9:i2:185:GLU:OE1   | 9:o2:67:GLN:NE2    | 2.09                     | 0.86              |
| 10:L3:82:LEU:HA    | 10:L3:197:SER:HB3  | 1.58                     | 0.86              |
| 10:O3:82:LEU:HA    | 10:O3:197:SER:HB3  | 1.58                     | 0.86              |
| 11:d3:141:ILE:HD13 | 11:d3:165:ILE:HD11 | 1.58                     | 0.86              |
| 1:B1:175:SER:HB2   | 1:h1:197:LEU:HD12  | 1.56                     | 0.85              |
| 10:K3:82:LEU:HA    | 10:K3:197:SER:HB3  | 1.58                     | 0.85              |
| 10:M3:82:LEU:HA    | 10:M3:197:SER:HB3  | 1.58                     | 0.85              |
| 11:w3:123:MET:HE1  | 11:w3:136:LEU:HD22 | 1.58                     | 0.85              |
| 10:R3:82:LEU:HA    | 10:R3:197:SER:HB3  | 1.58                     | 0.85              |
| 11:x3:325:SER:HB3  | 11:x3:330:SER:HB3  | 1.56                     | 0.85              |
| 11:z3:123:MET:HE1  | 11:z3:136:LEU:HD22 | 1.58                     | 0.85              |
| 10:J3:82:LEU:HA    | 10:J3:197:SER:HB3  | 1.58                     | 0.85              |
| 11:e3:123:MET:HE1  | 11:e3:136:LEU:HD22 | 1.58                     | 0.85              |
| 11:f3:123:MET:HE1  | 11:f3:136:LEU:HD22 | 1.58                     | 0.85              |
| 11:f3:325:SER:HB3  | 11:f3:330:SER:HB3  | 1.56                     | 0.85              |
| 11:o3:141:ILE:HD13 | 11:o3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:e3:141:ILE:HD13 | 11:e3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:j3:325:SER:HB3  | 11:j3:330:SER:HB3  | 1.56                     | 0.85              |
| 6:Q2:78:VAL:HG11   | 7:V2:57:GLN:HG3    | 1.58                     | 0.85              |
| 11:r3:32:ARG:NH1   | 11:r3:33:GLU:O     | 2.10                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:s3:32:ARG:NH1   | 11:s3:33:GLU:O     | 2.10                     | 0.85              |
| 11:y3:46:ASP:HA    | 11:z3:161:ASN:HD22 | 1.41                     | 0.85              |
| 10:I3:82:LEU:HA    | 10:I3:197:SER:HB3  | 1.58                     | 0.85              |
| 10:S3:82:LEU:HA    | 10:S3:197:SER:HB3  | 1.58                     | 0.85              |
| 11:c3:32:ARG:NH1   | 11:c3:33:GLU:O     | 2.10                     | 0.85              |
| 11:d3:32:ARG:NH1   | 11:d3:33:GLU:O     | 2.10                     | 0.85              |
| 11:m3:32:ARG:NH1   | 11:m3:33:GLU:O     | 2.10                     | 0.85              |
| 11:z3:32:ARG:NH1   | 11:z3:33:GLU:O     | 2.10                     | 0.85              |
| 1:X1:301:SER:HB3   | 1:X1:359:GLN:HB2   | 1.56                     | 0.85              |
| 11:d3:123:MET:HE1  | 11:d3:136:LEU:HD22 | 1.58                     | 0.85              |
| 11:h3:325:SER:HB3  | 11:h3:330:SER:HB3  | 1.56                     | 0.85              |
| 11:l3:32:ARG:NH1   | 11:l3:33:GLU:O     | 2.10                     | 0.85              |
| 11:l3:141:ILE:HD13 | 11:l3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:m3:141:ILE:HD13 | 11:m3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:n3:32:ARG:NH1   | 11:n3:33:GLU:O     | 2.10                     | 0.85              |
| 11:n3:141:ILE:HD13 | 11:n3:165:ILE:HD11 | 1.58                     | 0.85              |
| 1:c1:420:MET:HE1   | 1:c1:430:LEU:HB2   | 1.56                     | 0.85              |
| 9:v2:189:GLU:OE2   | 9:12:73:ARG:NH2    | 2.10                     | 0.85              |
| 11:g3:32:ARG:NH1   | 11:g3:33:GLU:O     | 2.10                     | 0.85              |
| 11:h3:141:ILE:HD13 | 11:h3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:j3:141:ILE:HD13 | 11:j3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:k3:141:ILE:HD13 | 11:k3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:y3:32:ARG:NH1   | 11:y3:33:GLU:O     | 2.10                     | 0.85              |
| 1:H1:166:VAL:CG1   | 2:B2:160:GLN:O     | 2.24                     | 0.85              |
| 1:f1:164:LEU:HD21  | 2:D2:149:LEU:HB2   | 1.58                     | 0.85              |
| 9:42:237:GLN:HG2   | 12:C4:58:LEU:HD22  | 1.57                     | 0.85              |
| 10:H3:82:LEU:HA    | 10:H3:197:SER:HB3  | 1.58                     | 0.85              |
| 11:a3:123:MET:HE1  | 11:a3:136:LEU:HD22 | 1.58                     | 0.85              |
| 11:i3:141:ILE:HD13 | 11:i3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:t3:32:ARG:NH1   | 11:t3:33:GLU:O     | 2.10                     | 0.85              |
| 9:o2:164:GLN:CB    | 11:s3:78:ASN:ND2   | 2.25                     | 0.85              |
| 11:f3:141:ILE:HD13 | 11:f3:165:ILE:HD11 | 1.58                     | 0.85              |
| 11:v3:123:MET:HE1  | 11:v3:136:LEU:HD22 | 1.58                     | 0.85              |
| 1:g1:167:ARG:HG3   | 2:C2:140:ARG:HH22  | 1.42                     | 0.84              |
| 8:b2:35:ARG:HH21   | 8:b2:101:ARG:HE    | 1.22                     | 0.84              |
| 10:T3:82:LEU:HA    | 10:T3:197:SER:HB3  | 1.58                     | 0.84              |
| 11:g3:123:MET:HE1  | 11:g3:136:LEU:HD22 | 1.58                     | 0.84              |
| 11:q3:32:ARG:NH1   | 11:q3:33:GLU:O     | 2.10                     | 0.84              |
| 9:u2:77:THR:HG23   | 9:z2:66:LEU:HD12   | 1.59                     | 0.84              |
| 11:g3:141:ILE:HD13 | 11:g3:165:ILE:HD11 | 1.58                     | 0.84              |
| 11:h3:32:ARG:NH1   | 11:h3:33:GLU:O     | 2.10                     | 0.84              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:y3:336:ASN:ND2 | 11:z3:318:SER:O    | 2.10                     | 0.84              |
| 1:G1:143:THR:HG22 | 1:H1:154:ARG:HD2   | 1.58                     | 0.84              |
| 1:K1:164:LEU:O    | 2:A2:241:GLN:OE1   | 1.67                     | 0.84              |
| 11:a3:32:ARG:NH1  | 11:a3:33:GLU:O     | 2.10                     | 0.84              |
| 11:v3:32:ARG:NH1  | 11:v3:33:GLU:O     | 2.10                     | 0.84              |
| 1:T1:294:ARG:HG3  | 6:R2:66:THR:HB     | 1.58                     | 0.84              |
| 4:G2:47:MET:HG2   | 4:G2:48:THR:HG23   | 1.59                     | 0.84              |
| 11:e3:32:ARG:NH1  | 11:e3:33:GLU:O     | 2.10                     | 0.84              |
| 11:k3:32:ARG:NH1  | 11:k3:33:GLU:O     | 2.10                     | 0.84              |
| 11:w3:32:ARG:NH1  | 11:w3:33:GLU:O     | 2.10                     | 0.84              |
| 1:R1:125:GLN:CD   | 2:E2:230:ASP:CG    | 2.46                     | 0.84              |
| 1:a1:167:ARG:CD   | 2:D2:244:TYR:HD2   | 1.77                     | 0.84              |
| 1:d1:165:PHE:HD1  | 2:D2:147:LEU:HD12  | 1.43                     | 0.84              |
| 9:v2:44:LEU:HD12  | 9:v2:71:GLY:HA3    | 1.60                     | 0.84              |
| 10:G3:82:LEU:HA   | 10:G3:197:SER:HB3  | 1.58                     | 0.84              |
| 11:o3:32:ARG:NH1  | 11:o3:33:GLU:O     | 2.10                     | 0.84              |
| 11:p3:32:ARG:NH1  | 11:p3:33:GLU:O     | 2.10                     | 0.84              |
| 1:M1:416:THR:HG23 | 1:M1:430:LEU:HD11  | 1.57                     | 0.84              |
| 10:A3:82:LEU:HA   | 10:A3:197:SER:HB3  | 1.58                     | 0.84              |
| 10:U3:82:LEU:HA   | 10:U3:197:SER:HB3  | 1.58                     | 0.84              |
| 10:Y3:82:LEU:HA   | 10:Y3:197:SER:HB3  | 1.58                     | 0.84              |
| 10:Z3:82:LEU:HA   | 10:Z3:197:SER:HB3  | 1.58                     | 0.84              |
| 11:n3:123:MET:HE1 | 11:n3:136:LEU:HD22 | 1.58                     | 0.84              |
| 1:A1:267:THR:HG22 | 1:h1:248:ARG:HH11  | 1.41                     | 0.84              |
| 11:b3:32:ARG:NH1  | 11:b3:33:GLU:O     | 2.10                     | 0.84              |
| 11:c3:123:MET:HE1 | 11:c3:136:LEU:HD22 | 1.58                     | 0.84              |
| 11:f3:32:ARG:NH1  | 11:f3:33:GLU:O     | 2.10                     | 0.84              |
| 11:u3:32:ARG:NH1  | 11:u3:33:GLU:O     | 2.10                     | 0.84              |
| 1:F1:297:GLN:NE2  | 6:U2:62:GLY:N      | 2.25                     | 0.84              |
| 1:L1:275:LYS:HB3  | 1:L1:377:MET:HE2   | 1.60                     | 0.84              |
| 1:g1:191:ILE:HD13 | 1:g1:220:LEU:HB3   | 1.60                     | 0.84              |
| 11:o3:123:MET:HE1 | 11:o3:136:LEU:HD22 | 1.58                     | 0.84              |
| 11:p3:123:MET:HE1 | 11:p3:136:LEU:HD22 | 1.58                     | 0.84              |
| 1:T1:167:ARG:NH1  | 2:E2:106:ASP:C     | 2.36                     | 0.84              |
| 9:n2:98:LYS:O     | 9:n2:212:GLY:HA3   | 1.78                     | 0.84              |
| 10:B3:82:LEU:HA   | 10:B3:197:SER:HB3  | 1.58                     | 0.84              |
| 10:X3:82:LEU:HA   | 10:X3:197:SER:HB3  | 1.58                     | 0.84              |
| 11:b3:123:MET:HE1 | 11:b3:136:LEU:HD22 | 1.58                     | 0.84              |
| 1:H1:275:LYS:HB2  | 1:H1:377:MET:HB2   | 1.59                     | 0.84              |
| 1:Q1:165:PHE:CZ   | 3:F2:145:TRP:CZ3   | 2.66                     | 0.84              |
| 10:F3:82:LEU:HA   | 10:F3:197:SER:HB3  | 1.58                     | 0.84              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:j3:32:ARG:NH1  | 11:j3:33:GLU:O     | 2.10                     | 0.84              |
| 1:T1:165:PHE:CG   | 3:F2:167:ASN:HA    | 2.11                     | 0.83              |
| 9:p2:170:VAL:O    | 11:c3:53:THR:HG21  | 1.78                     | 0.83              |
| 9:z2:233:MET:CE   | 12:D4:58:LEU:CD2   | 2.42                     | 0.83              |
| 11:l3:226:PRO:HG2 | 11:l3:231:SER:HB3  | 1.60                     | 0.83              |
| 11:m3:123:MET:HE1 | 11:m3:136:LEU:HD22 | 1.58                     | 0.83              |
| 11:p3:226:PRO:HG2 | 11:p3:231:SER:HB3  | 1.60                     | 0.83              |
| 11:r3:123:MET:HE1 | 11:r3:136:LEU:HD22 | 1.58                     | 0.83              |
| 2:E2:96:LEU:HD13  | 2:E2:236:MET:HE3   | 1.39                     | 0.83              |
| 9:k2:168:VAL:HG23 | 11:f3:114:LYS:HZ1  | 1.40                     | 0.83              |
| 11:h3:123:MET:HE1 | 11:h3:136:LEU:HD22 | 1.58                     | 0.83              |
| 11:l3:123:MET:HE1 | 11:l3:136:LEU:HD22 | 1.58                     | 0.83              |
| 11:m3:226:PRO:HG2 | 11:m3:231:SER:HB3  | 1.60                     | 0.83              |
| 11:t3:226:PRO:HG2 | 11:t3:231:SER:HB3  | 1.61                     | 0.83              |
| 11:u3:226:PRO:HG2 | 11:u3:231:SER:HB3  | 1.60                     | 0.83              |
| 1:c1:214:ASP:HB3  | 1:c1:218:HIS:HB2   | 1.60                     | 0.83              |
| 9:m2:77:THR:HG23  | 9:r2:66:LEU:HD12   | 1.59                     | 0.83              |
| 10:E3:82:LEU:HA   | 10:E3:197:SER:HB3  | 1.58                     | 0.83              |
| 10:W3:82:LEU:HA   | 10:W3:197:SER:HB3  | 1.58                     | 0.83              |
| 11:k3:123:MET:HE1 | 11:k3:136:LEU:HD22 | 1.58                     | 0.83              |
| 11:o3:226:PRO:HG2 | 11:o3:231:SER:HB3  | 1.60                     | 0.83              |
| 11:q3:123:MET:HE1 | 11:q3:136:LEU:HD22 | 1.58                     | 0.83              |
| 11:q3:226:PRO:HG2 | 11:q3:231:SER:HB3  | 1.60                     | 0.83              |
| 11:s3:123:MET:HE1 | 11:s3:136:LEU:HD22 | 1.58                     | 0.83              |
| 11:x3:32:ARG:NH1  | 11:x3:33:GLU:O     | 2.10                     | 0.83              |
| 1:H1:420:MET:HE1  | 1:H1:430:LEU:HD13  | 1.59                     | 0.83              |
| 2:E2:96:LEU:HD13  | 2:E2:236:MET:HE2   | 1.60                     | 0.83              |
| 10:V3:82:LEU:HA   | 10:V3:197:SER:HB3  | 1.58                     | 0.83              |
| 11:i3:32:ARG:NH1  | 11:i3:33:GLU:O     | 2.10                     | 0.83              |
| 11:j3:123:MET:HE1 | 11:j3:136:LEU:HD22 | 1.58                     | 0.83              |
| 11:s3:226:PRO:HG2 | 11:s3:231:SER:HB3  | 1.61                     | 0.83              |
| 11:u3:123:MET:HE1 | 11:u3:136:LEU:HD22 | 1.58                     | 0.83              |
| 1:R1:143:THR:HG23 | 1:T1:154:ARG:HH21  | 1.42                     | 0.83              |
| 1:T1:165:PHE:CG   | 3:F2:167:ASN:HB2   | 2.14                     | 0.83              |
| 1:T1:167:ARG:NE   | 2:E2:107:LYS:HE2   | 1.87                     | 0.83              |
| 1:g1:190:GLN:HG3  | 1:h1:217:GLY:HA3   | 1.60                     | 0.83              |
| 10:W3:203:ALA:CB  | 10:W3:203:ALA:C    | 2.51                     | 0.83              |
| 1:C1:165:PHE:CZ   | 2:C2:145:ALA:HB2   | 2.12                     | 0.83              |
| 1:a1:179:THR:HA   | 1:a1:215:GLN:HB3   | 1.60                     | 0.83              |
| 10:C3:82:LEU:HA   | 10:C3:197:SER:HB3  | 1.58                     | 0.83              |
| 10:D3:82:LEU:HA   | 10:D3:197:SER:HB3  | 1.58                     | 0.83              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:k3:226:PRO:HG2 | 11:k3:231:SER:HB3  | 1.61                     | 0.83              |
| 1:G1:266:VAL:HG12 | 1:G1:387:VAL:HG22  | 1.60                     | 0.83              |
| 11:n3:226:PRO:HG2 | 11:n3:231:SER:HB3  | 1.61                     | 0.83              |
| 11:r3:226:PRO:HG2 | 11:r3:231:SER:HB3  | 1.61                     | 0.83              |
| 11:v3:226:PRO:HG2 | 11:v3:231:SER:HB3  | 1.61                     | 0.83              |
| 1:F1:297:GLN:CD   | 6:U2:62:GLY:N      | 2.37                     | 0.83              |
| 1:N1:166:VAL:HG21 | 2:A2:162:PRO:CD    | 2.08                     | 0.83              |
| 4:I2:59:PHE:CE1   | 4:J2:14:MET:HG2    | 2.14                     | 0.83              |
| 9:s2:209:ASN:CG   | 11:r3:78:ASN:HD21  | 1.87                     | 0.83              |
| 11:i3:226:PRO:HG2 | 11:i3:231:SER:HB3  | 1.61                     | 0.83              |
| 1:Q1:167:ARG:CD   | 3:F2:156:THR:CG2   | 1.99                     | 0.82              |
| 11:h3:226:PRO:HG2 | 11:h3:231:SER:HB3  | 1.61                     | 0.82              |
| 11:i3:123:MET:HE1 | 11:i3:136:LEU:HD22 | 1.58                     | 0.82              |
| 11:j3:226:PRO:HG2 | 11:j3:231:SER:HB3  | 1.61                     | 0.82              |
| 11:t3:123:MET:HE1 | 11:t3:136:LEU:HD22 | 1.58                     | 0.82              |
| 11:w3:226:PRO:HG2 | 11:w3:231:SER:HB3  | 1.61                     | 0.82              |
| 11:x3:226:PRO:HG2 | 11:x3:231:SER:HB3  | 1.61                     | 0.82              |
| 1:G1:361:ASN:CB   | 6:U2:55:ARG:NH2    | 2.42                     | 0.82              |
| 1:T1:144:ILE:HG21 | 1:T1:153:ALA:HB3   | 1.61                     | 0.82              |
| 1:D1:294:ARG:CZ   | 6:U2:69:SER:OG     | 2.27                     | 0.82              |
| 2:E2:205:MET:HE1  | 4:J2:51:PHE:CG     | 2.13                     | 0.82              |
| 8:d2:181:LEU:HD11 | 8:d2:193:LEU:HD11  | 1.60                     | 0.82              |
| 1:d1:164:LEU:CD1  | 2:D2:148:ALA:HA    | 2.08                     | 0.82              |
| 11:g3:226:PRO:HG2 | 11:g3:231:SER:HB3  | 1.61                     | 0.82              |
| 1:c1:151:LYS:NZ   | 1:c1:180:LEU:O     | 2.11                     | 0.82              |
| 4:H2:46:GLU:HG2   | 4:H2:47:MET:H      | 1.41                     | 0.82              |
| 11:y3:226:PRO:HG2 | 11:y3:231:SER:HB3  | 1.61                     | 0.82              |
| 2:A2:75:ARG:HH11  | 2:A2:81:PRO:HB3    | 1.43                     | 0.82              |
| 9:p2:141:THR:CG2  | 11:c3:54:GLN:NE2   | 2.43                     | 0.82              |
| 9:r2:138:PRO:HB2  | 11:m3:54:GLN:CD    | 2.04                     | 0.82              |
| 1:B1:151:LYS:HZ1  | 1:B1:181:GLU:HA    | 1.42                     | 0.82              |
| 9:g2:122:VAL:O    | 9:l2:180:ASN:ND2   | 2.12                     | 0.82              |
| 9:j2:44:LEU:HD12  | 9:j2:71:GLY:HA3    | 1.61                     | 0.82              |
| 2:C2:92:LEU:HD21  | 2:C2:236:MET:CE    | 2.09                     | 0.82              |
| 9:z2:83:GLN:NE2   | 9:z2:220:GLU:OE2   | 2.13                     | 0.82              |
| 11:r3:319:LEU:CB  | 11:r3:319:LEU:C    | 2.53                     | 0.82              |
| 1:E1:367:GLU:CD   | 6:U2:68:THR:HG21   | 2.04                     | 0.82              |
| 1:Z1:275:LYS:HB3  | 1:Z1:377:MET:HE2   | 1.62                     | 0.82              |
| 9:p2:141:THR:HB   | 11:c3:54:GLN:NE2   | 1.94                     | 0.82              |
| 9:12:238:ARG:NH1  | 12:A4:48:ASP:CB    | 2.42                     | 0.82              |
| 9:42:59:GLN:NE2   | 11:u3:80:GLN:NE2   | 2.27                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:f3:226:PRO:HG2 | 11:f3:231:SER:HB3 | 1.60                     | 0.82              |
| 9:q2:232:ASN:CG   | 9:q2:232:ASN:CA   | 2.52                     | 0.82              |
| 9:t2:106:MET:CG   | 11:v3:54:GLN:NE2  | 2.42                     | 0.82              |
| 9:22:98:LYS:O     | 9:22:212:GLY:HA3  | 1.80                     | 0.82              |
| 11:z3:226:PRO:HG2 | 11:z3:231:SER:HB3 | 1.60                     | 0.82              |
| 1:T1:167:ARG:CZ   | 2:E2:107:LYS:N    | 2.43                     | 0.81              |
| 2:A2:141:GLN:NE2  | 2:A2:243:PHE:O    | 2.12                     | 0.81              |
| 1:B1:166:VAL:CG2  | 2:C2:162:PRO:HD3  | 2.09                     | 0.81              |
| 1:O1:203:ALA:HB1  | 1:Q1:160:PRO:HA   | 1.60                     | 0.81              |
| 8:d2:70:GLN:NE2   | 9:n2:3:SER:O      | 2.12                     | 0.81              |
| 11:c3:226:PRO:HG2 | 11:c3:231:SER:HB3 | 1.60                     | 0.81              |
| 1:A1:277:GLN:OE1  | 1:h1:373:ARG:NH1  | 2.12                     | 0.81              |
| 1:Y1:164:LEU:CD1  | 2:E2:152:ARG:CD   | 2.54                     | 0.81              |
| 1:g1:151:LYS:NZ   | 1:g1:180:LEU:O    | 2.13                     | 0.81              |
| 1:h1:125:GLN:HG3  | 4:I2:4:GLU:CB     | 2.10                     | 0.81              |
| 6:Q2:35:THR:O     | 6:Q2:98:ASN:ND2   | 2.14                     | 0.81              |
| 9:o2:164:GLN:CG   | 11:s3:78:ASN:HD21 | 1.87                     | 0.81              |
| 11:d3:226:PRO:HG2 | 11:d3:231:SER:HB3 | 1.61                     | 0.81              |
| 1:T1:165:PHE:CD1  | 3:F2:167:ASN:HA   | 2.13                     | 0.81              |
| 9:o2:2:ILE:HG13   | 9:o2:3:SER:H      | 1.45                     | 0.81              |
| 9:o2:168:VAL:HG23 | 11:t3:54:GLN:CG   | 2.11                     | 0.81              |
| 11:b3:226:PRO:HG2 | 11:b3:231:SER:HB3 | 1.61                     | 0.81              |
| 11:e3:226:PRO:HG2 | 11:e3:231:SER:HB3 | 1.61                     | 0.81              |
| 1:F1:363:THR:HB   | 6:U2:63:VAL:CG2   | 2.11                     | 0.81              |
| 9:g2:77:THR:HG23  | 9:l2:66:LEU:HB2   | 1.63                     | 0.81              |
| 1:E1:363:THR:HG21 | 6:U2:75:ALA:CB    | 2.07                     | 0.81              |
| 1:R1:164:LEU:HD11 | 3:F2:174:ARG:CD   | 2.10                     | 0.81              |
| 1:h1:164:LEU:HD11 | 2:C2:143:ARG:NE   | 1.96                     | 0.81              |
| 2:E2:96:LEU:HD22  | 2:E2:236:MET:SD   | 2.20                     | 0.81              |
| 9:p2:141:THR:HG22 | 11:c3:54:GLN:NE2  | 1.95                     | 0.81              |
| 1:S1:295:SER:HB3  | 6:R2:73:ILE:HD12  | 1.60                     | 0.81              |
| 6:U2:68:THR:HG22  | 6:U2:69:SER:H     | 1.45                     | 0.81              |
| 11:a3:226:PRO:HG2 | 11:a3:231:SER:HB3 | 1.61                     | 0.81              |
| 9:q2:141:THR:HG21 | 11:g3:80:GLN:OE1  | 1.79                     | 0.81              |
| 1:J1:277:GLN:HB3  | 1:J1:375:THR:HB   | 1.61                     | 0.81              |
| 1:X1:167:ARG:NH2  | 2:E2:158:PRO:C    | 2.38                     | 0.81              |
| 9:u2:238:ARG:NH1  | 9:u2:241:GLU:OE2  | 2.13                     | 0.81              |
| 9:22:231:VAL:HG23 | 12:B4:42:ALA:HB1  | 1.63                     | 0.81              |
| 1:E1:139:GLU:HG2  | 1:G1:154:ARG:HH11 | 1.45                     | 0.81              |
| 8:e2:200:ARG:NH2  | 9:k2:189:GLU:OE1  | 2.14                     | 0.81              |
| 9:s2:89:THR:HG23  | 9:s2:91:ASN:H     | 1.45                     | 0.81              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G1:128:GLU:OE2  | 4:H2:4:GLU:CG      | 2.29                     | 0.80              |
| 1:h1:125:GLN:HG3  | 4:I2:4:GLU:CG      | 2.10                     | 0.80              |
| 2:E2:213:PRO:HD3  | 3:F2:213:ILE:HG21  | 1.63                     | 0.80              |
| 9:o2:168:VAL:CG2  | 11:t3:54:GLN:HG3   | 2.09                     | 0.80              |
| 9:u2:110:GLY:CA   | 11:z3:80:GLN:CD    | 2.48                     | 0.80              |
| 9:u2:202:ASN:HD22 | 11:a3:78:ASN:ND2   | 1.64                     | 0.80              |
| 10:W3:203:ALA:CB  | 10:W3:203:ALA:N    | 2.44                     | 0.80              |
| 1:B1:165:PHE:HZ   | 2:C2:165:VAL:H     | 1.27                     | 0.80              |
| 1:D1:365:ASN:ND2  | 6:U2:73:ILE:HD11   | 1.95                     | 0.80              |
| 1:O1:275:LYS:HB2  | 1:O1:377:MET:HB2   | 1.62                     | 0.80              |
| 1:Y1:161:LYS:HD3  | 1:Y1:162:PRO:HD2   | 1.63                     | 0.80              |
| 9:p2:86:LEU:HD11  | 9:12:45:LEU:HD23   | 1.61                     | 0.80              |
| 9:32:252:GLN:HA   | 9:32:255:GLN:HG2   | 1.61                     | 0.80              |
| 11:a3:266:ARG:HA  | 11:a3:328:LEU:HD22 | 1.64                     | 0.80              |
| 11:z3:266:ARG:HA  | 11:z3:328:LEU:HD22 | 1.64                     | 0.80              |
| 1:M1:363:THR:HG23 | 6:Q2:73:ILE:HD11   | 1.57                     | 0.80              |
| 1:Y1:125:GLN:OE1  | 4:J2:75:ASP:HA     | 1.80                     | 0.80              |
| 1:Y1:295:SER:OG   | 6:S2:72:HIS:HA     | 1.82                     | 0.80              |
| 9:o2:168:VAL:HG21 | 11:t3:54:GLN:HG3   | 1.61                     | 0.80              |
| 9:q2:141:THR:OG1  | 11:g3:80:GLN:OE1   | 1.98                     | 0.80              |
| 11:y3:266:ARG:HA  | 11:y3:328:LEU:HD22 | 1.64                     | 0.80              |
| 1:K1:190:GLN:HG2  | 1:L1:217:GLY:HA3   | 1.62                     | 0.80              |
| 1:W1:164:LEU:C    | 2:E2:144:GLU:OE2   | 2.24                     | 0.80              |
| 1:e1:246:GLN:HE22 | 1:e1:265:GLN:HA    | 1.47                     | 0.80              |
| 10:B3:138:ALA:HB1 | 10:Z3:172:ASN:OD1  | 1.80                     | 0.80              |
| 11:b3:266:ARG:HA  | 11:b3:328:LEU:HD22 | 1.64                     | 0.80              |
| 9:12:238:ARG:HH12 | 12:A4:48:ASP:HB2   | 1.46                     | 0.80              |
| 11:x3:266:ARG:HA  | 11:x3:328:LEU:HD22 | 1.64                     | 0.80              |
| 7:Y2:72:ALA:HB3   | 7:Y2:95:ASN:HD22   | 1.45                     | 0.80              |
| 9:p2:172:GLN:HE21 | 11:d3:54:GLN:HE21  | 1.29                     | 0.80              |
| 1:G1:275:LYS:HB2  | 1:G1:377:MET:HB2   | 1.62                     | 0.80              |
| 6:Q2:92:GLN:OE1   | 7:W2:22:ASN:ND2    | 2.15                     | 0.80              |
| 1:T1:167:ARG:NE   | 2:E2:107:LYS:CD    | 2.31                     | 0.80              |
| 9:h2:122:VAL:O    | 9:m2:180:ASN:ND2   | 2.15                     | 0.80              |
| 1:B1:165:PHE:HE2  | 2:C2:161:GLY:C     | 1.85                     | 0.80              |
| 1:B1:165:PHE:CZ   | 2:C2:161:GLY:O     | 2.35                     | 0.80              |
| 1:G1:166:VAL:H    | 2:B2:144:GLU:CD    | 1.85                     | 0.80              |
| 1:G1:166:VAL:CB   | 2:B2:144:GLU:HG2   | 2.12                     | 0.80              |
| 1:W1:301:SER:HB3  | 1:W1:359:GLN:HB3   | 1.64                     | 0.80              |
| 11:w3:266:ARG:HA  | 11:w3:328:LEU:HD22 | 1.64                     | 0.80              |
| 1:Q1:167:ARG:CG   | 3:F2:156:THR:HG22  | 2.12                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:j2:6:TRP:CE3     | 9:j2:9:LYS:HD3     | 2.17                     | 0.79              |
| 11:c3:266:ARG:HA   | 11:c3:328:LEU:HD22 | 1.64                     | 0.79              |
| 11:r3:336:ASN:ND2  | 11:s3:318:SER:O    | 2.15                     | 0.79              |
| 1:L1:244:ARG:HH22  | 1:M1:239:ASN:HB2   | 1.45                     | 0.79              |
| 6:U2:120:LEU:HD11  | 7:Z2:129:THR:HA    | 1.64                     | 0.79              |
| 9:n2:209:ASN:ND2   | 11:z3:114:LYS:NZ   | 2.29                     | 0.79              |
| 11:p3:266:ARG:HA   | 11:p3:328:LEU:HD22 | 1.64                     | 0.79              |
| 11:q3:266:ARG:HA   | 11:q3:328:LEU:HD22 | 1.64                     | 0.79              |
| 1:d1:417:ARG:HA    | 1:d1:420:MET:HE2   | 1.65                     | 0.79              |
| 9:n2:185:GLU:HB2   | 9:t2:67:GLN:HE22   | 1.46                     | 0.79              |
| 9:y2:238:ARG:HG3   | 12:D4:50:THR:HB    | 1.64                     | 0.79              |
| 10:W3:172:ASN:OD1  | 10:Y3:138:ALA:HB1  | 1.79                     | 0.79              |
| 1:G1:166:VAL:CB    | 2:B2:144:GLU:CG    | 2.61                     | 0.79              |
| 1:R1:167:ARG:CG    | 3:F2:167:ASN:CB    | 2.37                     | 0.79              |
| 1:a1:167:ARG:CG    | 2:D2:140:ARG:NH2   | 2.45                     | 0.79              |
| 1:f1:275:LYS:HB2   | 1:f1:377:MET:HB2   | 1.64                     | 0.79              |
| 1:g1:167:ARG:CG    | 2:C2:140:ARG:NH2   | 2.44                     | 0.79              |
| 3:F2:213:ILE:HG13  | 3:F2:217:GLY:HA3   | 1.65                     | 0.79              |
| 9:m2:241:GLU:HG2   | 9:r2:256:LYS:HD2   | 1.63                     | 0.79              |
| 11:f3:336:ASN:ND2  | 11:g3:318:SER:O    | 2.16                     | 0.79              |
| 11:j3:336:ASN:ND2  | 11:k3:318:SER:O    | 2.16                     | 0.79              |
| 11:r3:266:ARG:HA   | 11:r3:328:LEU:HD22 | 1.64                     | 0.79              |
| 8:f2:76:ARG:NH2    | 8:f2:105:ILE:O     | 2.15                     | 0.79              |
| 11:l3:26:THR:HG21  | 11:l3:187:LEU:HB3  | 1.65                     | 0.79              |
| 11:o3:266:ARG:HA   | 11:o3:328:LEU:HD22 | 1.64                     | 0.79              |
| 1:N1:165:PHE:CE2   | 2:A2:148:ALA:CB    | 2.64                     | 0.79              |
| 2:E2:88:VAL:HG11   | 3:F2:93:ALA:HB2    | 1.64                     | 0.79              |
| 9:k2:127:GLN:OE1   | 9:k2:135:GLN:NE2   | 2.15                     | 0.79              |
| 9:n2:44:LEU:HD12   | 9:n2:71:GLY:HA3    | 1.64                     | 0.79              |
| 9:w2:153:ARG:HH12  | 9:32:189:GLU:HG3   | 1.48                     | 0.79              |
| 9:42:238:ARG:HH11  | 12:C4:55:ASN:HB2   | 1.47                     | 0.79              |
| 11:m3:26:THR:HG21  | 11:m3:187:LEU:HB3  | 1.65                     | 0.79              |
| 11:n3:266:ARG:HA   | 11:n3:328:LEU:HD22 | 1.64                     | 0.79              |
| 11:p3:121:LEU:HD11 | 11:p3:124:THR:HG21 | 1.65                     | 0.79              |
| 11:r3:46:ASP:HA    | 11:s3:161:ASN:HD22 | 1.47                     | 0.79              |
| 11:v3:266:ARG:HA   | 11:v3:328:LEU:HD22 | 1.64                     | 0.79              |
| 1:R1:168:GLU:HB3   | 3:F2:261:ASN:OD1   | 1.82                     | 0.79              |
| 9:j2:156:VAL:HG13  | 9:j2:169:GLN:HE21  | 1.47                     | 0.79              |
| 10:A3:172:ASN:OD1  | 10:C3:138:ALA:HB1  | 1.82                     | 0.79              |
| 11:c3:121:LEU:HD11 | 11:c3:124:THR:HG21 | 1.65                     | 0.79              |
| 11:d3:266:ARG:HA   | 11:d3:328:LEU:HD22 | 1.64                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:m3:266:ARG:HA   | 11:m3:328:LEU:HD22 | 1.64                     | 0.79              |
| 11:s3:266:ARG:HA   | 11:s3:328:LEU:HD22 | 1.64                     | 0.79              |
| 6:Q2:128:LYS:NZ    | 7:V2:133:GLY:O     | 2.16                     | 0.79              |
| 9:s2:209:ASN:OD1   | 11:r3:78:ASN:ND2   | 2.16                     | 0.79              |
| 10:H3:172:ASN:OD1  | 10:J3:138:ALA:HB1  | 1.83                     | 0.79              |
| 10:Y3:51:ILE:HG13  | 11:a3:175:LEU:HD11 | 1.64                     | 0.79              |
| 11:o3:121:LEU:HD11 | 11:o3:124:THR:HG21 | 1.65                     | 0.79              |
| 9:12:117:ASP:OD2   | 9:12:190:ASN:ND2   | 2.16                     | 0.79              |
| 9:22:230:LEU:HD12  | 12:A4:62:LEU:HD22  | 1.64                     | 0.79              |
| 11:a3:121:LEU:HD11 | 11:a3:124:THR:HG21 | 1.65                     | 0.79              |
| 11:d3:121:LEU:HD11 | 11:d3:124:THR:HG21 | 1.65                     | 0.79              |
| 11:k3:26:THR:HG21  | 11:k3:187:LEU:HB3  | 1.65                     | 0.79              |
| 1:G1:128:GLU:OE2   | 4:H2:4:GLU:CD      | 2.26                     | 0.79              |
| 1:c1:125:GLN:NE2   | 4:J2:3:PRO:C       | 2.41                     | 0.79              |
| 1:d1:139:GLU:OE2   | 1:f1:134:ARG:NH1   | 2.15                     | 0.79              |
| 10:B3:172:ASN:OD1  | 10:D3:138:ALA:HB1  | 1.83                     | 0.79              |
| 11:d3:46:ASP:HA    | 11:e3:161:ASN:HD22 | 1.48                     | 0.79              |
| 11:l3:266:ARG:HA   | 11:l3:328:LEU:HD22 | 1.64                     | 0.79              |
| 11:s3:121:LEU:HD11 | 11:s3:124:THR:HG21 | 1.65                     | 0.79              |
| 9:p2:208:LEU:HD11  | 11:e3:54:GLN:NE2   | 1.98                     | 0.78              |
| 9:s2:127:GLN:HE21  | 11:p3:78:ASN:HD21  | 1.29                     | 0.78              |
| 11:b3:121:LEU:HD11 | 11:b3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:g3:121:LEU:HD11 | 11:g3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:l3:121:LEU:HD11 | 11:l3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:m3:121:LEU:HD11 | 11:m3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:q3:26:THR:HG21  | 11:q3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:r3:121:LEU:HD11 | 11:r3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:z3:121:LEU:HD11 | 11:z3:124:THR:HG21 | 1.65                     | 0.78              |
| 1:c1:297:GLN:OE1   | 6:S2:55:ARG:CZ     | 2.31                     | 0.78              |
| 10:E3:172:ASN:OD1  | 10:G3:138:ALA:HB1  | 1.83                     | 0.78              |
| 11:f3:121:LEU:HD11 | 11:f3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:h3:121:LEU:HD11 | 11:h3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:k3:121:LEU:HD11 | 11:k3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:k3:266:ARG:HA   | 11:k3:328:LEU:HD22 | 1.64                     | 0.78              |
| 11:q3:46:ASP:HA    | 11:r3:161:ASN:HD22 | 1.49                     | 0.78              |
| 11:q3:121:LEU:HD11 | 11:q3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:u3:266:ARG:HA   | 11:u3:328:LEU:HD22 | 1.64                     | 0.78              |
| 1:E1:365:ASN:HB2   | 6:U2:66:THR:OG1    | 1.83                     | 0.78              |
| 1:R1:256:ILE:HG21  | 1:R1:412:ILE:HD11  | 1.65                     | 0.78              |
| 10:R3:172:ASN:OD1  | 10:T3:138:ALA:HB1  | 1.83                     | 0.78              |
| 10:S3:172:ASN:OD1  | 10:U3:138:ALA:HB1  | 1.83                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:e3:121:LEU:HD11 | 11:e3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:e3:266:ARG:HA   | 11:e3:328:LEU:HD22 | 1.64                     | 0.78              |
| 11:j3:46:ASP:HA    | 11:k3:161:ASN:HD22 | 1.48                     | 0.78              |
| 11:j3:266:ARG:HA   | 11:j3:328:LEU:HD22 | 1.64                     | 0.78              |
| 11:l3:46:ASP:HA    | 11:m3:161:ASN:HD22 | 1.49                     | 0.78              |
| 11:n3:121:LEU:HD11 | 11:n3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:r3:319:LEU:CB   | 11:r3:319:LEU:N    | 2.46                     | 0.78              |
| 11:t3:266:ARG:HA   | 11:t3:328:LEU:HD22 | 1.64                     | 0.78              |
| 11:u3:121:LEU:HD11 | 11:u3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:z3:26:THR:HG21  | 11:z3:187:LEU:HB3  | 1.65                     | 0.78              |
| 9:n2:169:GLN:N     | 11:x3:78:ASN:HD21  | 1.81                     | 0.78              |
| 9:o2:164:GLN:CG    | 11:s3:78:ASN:ND2   | 2.33                     | 0.78              |
| 11:g3:26:THR:HG21  | 11:g3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:p3:26:THR:HG21  | 11:p3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:x3:121:LEU:HD11 | 11:x3:124:THR:HG21 | 1.65                     | 0.78              |
| 1:B1:165:PHE:CZ    | 2:C2:165:VAL:N     | 2.51                     | 0.78              |
| 2:D2:41:SER:O      | 2:D2:43:GLN:N      | 2.17                     | 0.78              |
| 3:F2:6:SER:HB2     | 3:F2:8:GLN:HG2     | 1.64                     | 0.78              |
| 9:m2:166:ALA:CB    | 11:o3:80:GLN:HE22  | 1.97                     | 0.78              |
| 9:z2:27:ALA:HB2    | 12:D4:45:LYS:CD    | 2.08                     | 0.78              |
| 10:I3:172:ASN:OD1  | 10:K3:138:ALA:HB1  | 1.83                     | 0.78              |
| 10:T3:172:ASN:OD1  | 10:V3:138:ALA:HB1  | 1.83                     | 0.78              |
| 11:h3:26:THR:HG21  | 11:h3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:i3:266:ARG:HA   | 11:i3:328:LEU:HD22 | 1.64                     | 0.78              |
| 1:Y1:151:LYS:NZ    | 1:Y1:180:LEU:O     | 2.16                     | 0.78              |
| 8:d2:116:GLN:NE2   | 9:i2:42:GLU:OE2    | 2.17                     | 0.78              |
| 9:i2:6:TRP:CZ3     | 9:i2:9:LYS:HE3     | 2.19                     | 0.78              |
| 9:12:237:GLN:NE2   | 12:E4:53:LEU:O     | 2.17                     | 0.78              |
| 11:h3:266:ARG:HA   | 11:h3:328:LEU:HD22 | 1.64                     | 0.78              |
| 11:j3:121:LEU:HD11 | 11:j3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:t3:46:ASP:HA    | 11:u3:161:ASN:HD22 | 1.49                     | 0.78              |
| 11:v3:121:LEU:HD11 | 11:v3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:x3:26:THR:HG21  | 11:x3:187:LEU:HB3  | 1.65                     | 0.78              |
| 1:B1:165:PHE:HE2   | 2:C2:162:PRO:C     | 1.91                     | 0.78              |
| 2:A2:115:PRO:HB2   | 2:A2:121:ILE:HD12  | 1.64                     | 0.78              |
| 2:C2:41:SER:OG     | 5:N2:49:GLN:OE1    | 2.00                     | 0.78              |
| 9:u2:200:ALA:CB    | 11:b3:54:GLN:CD    | 2.55                     | 0.78              |
| 9:32:233:MET:HE3   | 12:B4:58:LEU:CD1   | 2.08                     | 0.78              |
| 10:G3:172:ASN:OD1  | 10:I3:138:ALA:HB1  | 1.83                     | 0.78              |
| 10:U3:172:ASN:OD1  | 10:W3:138:ALA:HB1  | 1.83                     | 0.78              |
| 11:n3:26:THR:HG21  | 11:n3:187:LEU:HB3  | 1.65                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:w3:26:THR:HG21  | 11:w3:187:LEU:HB3  | 1.65                     | 0.78              |
| 1:W1:277:GLN:HB3   | 1:W1:375:THR:HB    | 1.66                     | 0.78              |
| 10:C3:172:ASN:OD1  | 10:E3:138:ALA:HB1  | 1.83                     | 0.78              |
| 10:Q3:172:ASN:OD1  | 10:S3:138:ALA:HB1  | 1.84                     | 0.78              |
| 11:f3:26:THR:HG21  | 11:f3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:i3:121:LEU:HD11 | 11:i3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:r3:26:THR:HG21  | 11:r3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:t3:121:LEU:HD11 | 11:t3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:v3:46:ASP:HA    | 11:w3:161:ASN:HD22 | 1.48                     | 0.78              |
| 11:w3:121:LEU:HD11 | 11:w3:124:THR:HG21 | 1.65                     | 0.78              |
| 11:y3:26:THR:HG21  | 11:y3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:y3:121:LEU:HD11 | 11:y3:124:THR:HG21 | 1.65                     | 0.78              |
| 1:N1:144:ILE:HG22  | 1:N1:150:VAL:HG11  | 1.65                     | 0.78              |
| 1:V1:275:LYS:HB2   | 1:V1:377:MET:HB2   | 1.65                     | 0.78              |
| 1:W1:139:GLU:OE2   | 1:X1:154:ARG:NH1   | 2.13                     | 0.78              |
| 1:X1:246:GLN:NE2   | 1:X1:250:GLU:OE2   | 2.17                     | 0.78              |
| 2:C2:92:LEU:HD21   | 2:C2:236:MET:HE2   | 1.64                     | 0.78              |
| 11:a3:26:THR:HG21  | 11:a3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:a3:46:ASP:HA    | 11:b3:161:ASN:HD22 | 1.49                     | 0.78              |
| 11:b3:26:THR:HG21  | 11:b3:187:LEU:HB3  | 1.65                     | 0.78              |
| 11:g3:46:ASP:HA    | 11:h3:161:ASN:HD22 | 1.49                     | 0.78              |
| 11:g3:266:ARG:HA   | 11:g3:328:LEU:HD22 | 1.64                     | 0.78              |
| 11:i3:46:ASP:HA    | 11:j3:161:ASN:HD22 | 1.49                     | 0.78              |
| 11:u3:336:ASN:ND2  | 11:v3:318:SER:O    | 2.17                     | 0.78              |
| 1:T1:294:ARG:CG    | 6:R2:66:THR:HB     | 2.14                     | 0.78              |
| 6:Q2:106:ARG:NH1   | 8:b2:244:ALA:O     | 2.17                     | 0.78              |
| 9:z2:27:ALA:CA     | 12:D4:45:LYS:HD2   | 1.76                     | 0.78              |
| 10:F3:172:ASN:OD1  | 10:H3:138:ALA:HB1  | 1.83                     | 0.78              |
| 11:b3:46:ASP:HA    | 11:c3:161:ASN:HD22 | 1.49                     | 0.78              |
| 11:d3:336:ASN:ND2  | 11:e3:318:SER:O    | 2.16                     | 0.78              |
| 11:i3:336:ASN:ND2  | 11:j3:318:SER:O    | 2.17                     | 0.78              |
| 11:p3:46:ASP:HA    | 11:q3:161:ASN:HD22 | 1.48                     | 0.78              |
| 11:v3:336:ASN:ND2  | 11:w3:318:SER:O    | 2.16                     | 0.78              |
| 1:H1:166:VAL:O     | 1:H1:167:ARG:NE    | 2.16                     | 0.77              |
| 9:r2:138:PRO:HG2   | 11:m3:54:GLN:HE22  | 1.45                     | 0.77              |
| 9:x2:238:ARG:HE    | 9:x2:241:GLU:HG3   | 1.48                     | 0.77              |
| 11:e3:46:ASP:HA    | 11:f3:161:ASN:HD22 | 1.49                     | 0.77              |
| 11:f3:46:ASP:HA    | 11:g3:161:ASN:HD22 | 1.49                     | 0.77              |
| 11:j3:26:THR:HG21  | 11:j3:187:LEU:HB3  | 1.65                     | 0.77              |
| 1:N1:245:ILE:HD11  | 1:N1:420:MET:HA    | 1.66                     | 0.77              |
| 1:T1:165:PHE:CB    | 3:F2:167:ASN:HB2   | 2.13                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:T1:165:PHE:HA   | 3:F2:166:SER:CB    | 2.14                     | 0.77              |
| 1:a1:167:ARG:NH1  | 2:D2:244:TYR:CD1   | 2.53                     | 0.77              |
| 1:a1:167:ARG:HG2  | 2:D2:140:ARG:NH1   | 1.98                     | 0.77              |
| 1:g1:167:ARG:HD3  | 2:C2:245:SER:O     | 1.85                     | 0.77              |
| 2:B2:41:SER:O     | 2:B2:43:GLN:N      | 2.17                     | 0.77              |
| 9:o2:164:GLN:HE22 | 11:s3:80:GLN:HB2   | 1.48                     | 0.77              |
| 11:i3:26:THR:HG21 | 11:i3:187:LEU:HB3  | 1.65                     | 0.77              |
| 11:n3:336:ASN:ND2 | 11:o3:318:SER:O    | 2.17                     | 0.77              |
| 1:K1:246:GLN:NE2  | 1:K1:250:GLU:OE2   | 2.17                     | 0.77              |
| 1:O1:149:PRO:HA   | 1:O1:181:GLU:HG2   | 1.65                     | 0.77              |
| 1:X1:161:LYS:HD2  | 1:X1:162:PRO:HD2   | 1.64                     | 0.77              |
| 10:K3:172:ASN:OD1 | 10:M3:138:ALA:HB1  | 1.83                     | 0.77              |
| 10:N3:172:ASN:OD1 | 10:P3:138:ALA:HB1  | 1.83                     | 0.77              |
| 11:b3:336:ASN:ND2 | 11:c3:318:SER:O    | 2.17                     | 0.77              |
| 11:c3:26:THR:HG21 | 11:c3:187:LEU:HB3  | 1.65                     | 0.77              |
| 11:f3:266:ARG:HA  | 11:f3:328:LEU:HD22 | 1.64                     | 0.77              |
| 11:w3:46:ASP:HA   | 11:x3:161:ASN:HD22 | 1.49                     | 0.77              |
| 12:B4:93:ALA:HB2  | 12:B4:225:LEU:HD21 | 1.66                     | 0.77              |
| 1:H1:216:SER:O    | 1:H1:218:HIS:ND1   | 2.11                     | 0.77              |
| 10:O3:172:ASN:OD1 | 10:Q3:138:ALA:HB1  | 1.83                     | 0.77              |
| 11:n3:46:ASP:HA   | 11:o3:161:ASN:HD22 | 1.49                     | 0.77              |
| 11:o3:46:ASP:HA   | 11:p3:161:ASN:HD22 | 1.49                     | 0.77              |
| 11:u3:26:THR:HG21 | 11:u3:187:LEU:HB3  | 1.65                     | 0.77              |
| 1:N1:275:LYS:HB3  | 1:N1:377:MET:HE2   | 1.66                     | 0.77              |
| 1:U1:365:ASN:OD1  | 6:R2:66:THR:N      | 2.16                     | 0.77              |
| 2:A2:224:MET:HA   | 2:A2:227:VAL:HG12  | 1.67                     | 0.77              |
| 9:j2:238:ARG:NH2  | 9:p2:251:ASP:OD2   | 2.16                     | 0.77              |
| 9:r2:125:ASN:CB   | 11:l3:54:GLN:HE22  | 1.97                     | 0.77              |
| 11:o3:26:THR:HG21 | 11:o3:187:LEU:HB3  | 1.65                     | 0.77              |
| 11:v3:26:THR:HG21 | 11:v3:187:LEU:HB3  | 1.65                     | 0.77              |
| 1:R1:125:GLN:OE1  | 2:E2:230:ASP:OD2   | 2.03                     | 0.77              |
| 1:S1:414:ASP:OD2  | 1:T1:431:ASN:ND2   | 2.16                     | 0.77              |
| 1:U1:246:GLN:NE2  | 1:U1:264:ALA:O     | 2.18                     | 0.77              |
| 9:v2:226:VAL:HG12 | 12:A4:49:PRO:HG2   | 1.65                     | 0.77              |
| 10:L3:172:ASN:OD1 | 10:N3:138:ALA:HB1  | 1.83                     | 0.77              |
| 1:Q1:163:SER:O    | 3:F2:252:ALA:HB1   | 1.85                     | 0.77              |
| 2:B2:199:VAL:HG23 | 4:H2:21:ALA:HB2    | 1.66                     | 0.77              |
| 9:i2:167:PRO:HD3  | 9:t2:196:GLN:HG2   | 1.65                     | 0.77              |
| 10:D3:172:ASN:OD1 | 10:F3:138:ALA:HB1  | 1.84                     | 0.77              |
| 10:J3:172:ASN:OD1 | 10:L3:138:ALA:HB1  | 1.84                     | 0.77              |
| 11:q3:336:ASN:ND2 | 11:r3:318:SER:O    | 2.18                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:s3:26:THR:HG21 | 11:s3:187:LEU:HB3  | 1.65                     | 0.77              |
| 11:w3:336:ASN:ND2 | 11:x3:318:SER:O    | 2.18                     | 0.77              |
| 1:G1:165:PHE:CZ   | 2:B2:143:ARG:CZ    | 2.67                     | 0.77              |
| 1:T1:165:PHE:HA   | 3:F2:166:SER:OG    | 1.85                     | 0.77              |
| 9:q2:116:ARG:NH1  | 9:q2:220:GLU:OE1   | 2.18                     | 0.77              |
| 11:a3:318:SER:O   | 11:z3:336:ASN:ND2  | 2.17                     | 0.77              |
| 11:u3:46:ASP:HA   | 11:v3:161:ASN:HD22 | 1.49                     | 0.77              |
| 1:d1:164:LEU:CD1  | 2:D2:148:ALA:HB2   | 2.11                     | 0.77              |
| 1:g1:414:ASP:OD2  | 1:h1:431:ASN:ND2   | 2.18                     | 0.77              |
| 8:b2:123:GLU:HG3  | 8:b2:160:ARG:HB3   | 1.67                     | 0.77              |
| 9:w2:189:GLU:OE2  | 9:22:73:ARG:NH2    | 2.18                     | 0.77              |
| 11:c3:336:ASN:ND2 | 11:d3:318:SER:O    | 2.17                     | 0.77              |
| 11:g3:336:ASN:ND2 | 11:h3:318:SER:O    | 2.17                     | 0.77              |
| 11:h3:336:ASN:ND2 | 11:i3:318:SER:O    | 2.17                     | 0.77              |
| 11:m3:46:ASP:HA   | 11:n3:161:ASN:HD22 | 1.49                     | 0.77              |
| 1:N1:126:PHE:HA   | 1:N1:129:GLN:HE22  | 1.50                     | 0.77              |
| 11:s3:46:ASP:HA   | 11:t3:161:ASN:HD22 | 1.49                     | 0.77              |
| 1:f1:151:LYS:NZ   | 1:f1:180:LEU:O     | 2.17                     | 0.76              |
| 10:P3:172:ASN:OD1 | 10:R3:138:ALA:HB1  | 1.84                     | 0.76              |
| 11:a3:336:ASN:ND2 | 11:b3:318:SER:O    | 2.17                     | 0.76              |
| 1:E1:174:ALA:O    | 1:E1:210:VAL:HA    | 1.84                     | 0.76              |
| 1:G1:242:GLU:HB2  | 1:G1:266:VAL:HG23  | 1.67                     | 0.76              |
| 1:K1:167:ARG:HD2  | 2:A2:245:SER:O     | 1.80                     | 0.76              |
| 1:W1:275:LYS:HB2  | 1:W1:377:MET:HB2   | 1.68                     | 0.76              |
| 8:d2:80:VAL:HG13  | 8:d2:201:ILE:HG23  | 1.66                     | 0.76              |
| 8:d2:114:THR:HG22 | 8:d2:119:PRO:HB3   | 1.67                     | 0.76              |
| 11:e3:26:THR:HG21 | 11:e3:187:LEU:HB3  | 1.65                     | 0.76              |
| 11:k3:46:ASP:HA   | 11:l3:161:ASN:HD22 | 1.49                     | 0.76              |
| 11:l3:336:ASN:ND2 | 11:m3:318:SER:O    | 2.16                     | 0.76              |
| 11:t3:26:THR:HG21 | 11:t3:187:LEU:HB3  | 1.65                     | 0.76              |
| 1:T1:413:GLU:OE2  | 1:T1:417:ARG:NH1   | 2.18                     | 0.76              |
| 1:W1:164:LEU:CD1  | 2:E2:143:ARG:CB    | 2.59                     | 0.76              |
| 1:X1:275:LYS:HB3  | 1:X1:377:MET:HE2   | 1.68                     | 0.76              |
| 11:d3:26:THR:HG21 | 11:d3:187:LEU:HB3  | 1.65                     | 0.76              |
| 11:e3:336:ASN:ND2 | 11:f3:318:SER:O    | 2.18                     | 0.76              |
| 11:o3:336:ASN:ND2 | 11:p3:318:SER:O    | 2.17                     | 0.76              |
| 1:I1:378:ASN:ND2  | 1:I1:381:ASP:OD1   | 2.19                     | 0.76              |
| 9:s2:139:ALA:CB   | 11:q3:53:THR:CB    | 2.64                     | 0.76              |
| 11:c3:46:ASP:HA   | 11:d3:161:ASN:HD22 | 1.49                     | 0.76              |
| 11:k3:336:ASN:ND2 | 11:l3:318:SER:O    | 2.18                     | 0.76              |
| 1:K1:374:HIS:HB3  | 1:L1:276:GLU:HB3   | 1.68                     | 0.76              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:A2:87:GLN:NE2   | 5:N2:98:GLU:OE2    | 2.19                     | 0.76              |
| 4:G2:46:GLU:HG2   | 4:G2:47:MET:H      | 1.51                     | 0.76              |
| 6:U2:40:ALA:HB2   | 6:U2:100:VAL:HG22  | 1.68                     | 0.76              |
| 9:o2:161:GLN:HE21 | 11:s3:80:GLN:NE2   | 1.83                     | 0.76              |
| 9:o2:168:VAL:HB   | 11:t3:54:GLN:HE22  | 1.49                     | 0.76              |
| 1:D1:294:ARG:NE   | 6:U2:69:SER:OG     | 2.19                     | 0.76              |
| 1:K1:277:GLN:HB3  | 1:K1:375:THR:HB    | 1.68                     | 0.76              |
| 1:L1:203:ALA:HA   | 1:N1:158:ALA:HB1   | 1.67                     | 0.76              |
| 1:N1:165:PHE:CD2  | 2:A2:148:ALA:HB2   | 2.20                     | 0.76              |
| 1:R1:193:ALA:HA   | 1:T1:219:LEU:HG    | 1.66                     | 0.76              |
| 9:u2:109:ASP:O    | 11:z3:80:GLN:NE2   | 2.19                     | 0.76              |
| 10:D3:51:ILE:HG13 | 11:f3:175:LEU:HD11 | 1.68                     | 0.76              |
| 10:V3:172:ASN:OD1 | 10:X3:138:ALA:HB1  | 1.84                     | 0.76              |
| 2:D2:112:ALA:O    | 2:D2:116:PHE:N     | 2.17                     | 0.76              |
| 9:42:238:ARG:NH1  | 12:C4:55:ASN:HB3   | 1.99                     | 0.76              |
| 11:h3:46:ASP:HA   | 11:i3:161:ASN:HD22 | 1.49                     | 0.76              |
| 1:Q1:275:LYS:HB3  | 1:Q1:377:MET:HE2   | 1.67                     | 0.76              |
| 1:Z1:294:ARG:HG2  | 6:S2:68:THR:HG22   | 1.66                     | 0.76              |
| 8:b2:114:THR:HG22 | 8:b2:119:PRO:HB3   | 1.65                     | 0.76              |
| 10:M3:172:ASN:OD1 | 10:O3:138:ALA:HB1  | 1.83                     | 0.76              |
| 11:a3:267:GLU:OE1 | 11:z3:21:ARG:NH1   | 2.18                     | 0.76              |
| 1:G1:164:LEU:CD2  | 2:B2:143:ARG:HG3   | 2.15                     | 0.76              |
| 1:H1:125:GLN:OE1  | 4:H2:3:PRO:HB2     | 1.86                     | 0.76              |
| 1:K1:179:THR:HA   | 1:K1:215:GLN:HB3   | 1.68                     | 0.76              |
| 1:U1:416:THR:HG23 | 1:U1:430:LEU:HD21  | 1.68                     | 0.76              |
| 9:o2:168:VAL:CG2  | 11:t3:54:GLN:CG    | 2.63                     | 0.76              |
| 9:12:115:THR:HB   | 9:12:191:LEU:HG    | 1.66                     | 0.76              |
| 1:D1:297:GLN:HB2  | 6:U2:73:ILE:HG21   | 1.68                     | 0.75              |
| 1:J1:275:LYS:HB2  | 1:J1:377:MET:HB2   | 1.66                     | 0.75              |
| 1:R1:164:LEU:CD1  | 3:F2:174:ARG:HD2   | 2.15                     | 0.75              |
| 1:W1:165:PHE:HZ   | 2:E2:244:TYR:O     | 1.61                     | 0.75              |
| 1:a1:216:SER:O    | 1:a1:218:HIS:ND1   | 2.18                     | 0.75              |
| 9:m2:44:LEU:HD12  | 9:m2:71:GLY:HA3    | 1.66                     | 0.75              |
| 9:q2:77:THR:HG23  | 9:v2:66:LEU:HD12   | 1.68                     | 0.75              |
| 1:S1:294:ARG:HG3  | 6:R2:71:HIS:O      | 1.86                     | 0.75              |
| 6:R2:92:GLN:HE21  | 7:X2:22:ASN:ND2    | 1.83                     | 0.75              |
| 8:f2:35:ARG:NH2   | 8:f2:207:GLU:OE1   | 2.18                     | 0.75              |
| 8:f2:114:THR:HG22 | 8:f2:119:PRO:HB3   | 1.68                     | 0.75              |
| 9:q2:141:THR:CG2  | 11:g3:80:GLN:OE1   | 2.35                     | 0.75              |
| 9:x2:77:THR:HG22  | 9:32:66:LEU:HA     | 1.67                     | 0.75              |
| 10:J3:51:ILE:HG13 | 11:l3:175:LEU:HD11 | 1.68                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:X3:51:ILE:HG13  | 11:z3:175:LEU:HD11 | 1.66                     | 0.75              |
| 11:a3:161:ASN:HD22 | 11:z3:46:ASP:HA    | 1.50                     | 0.75              |
| 1:G1:155:VAL:HG23  | 1:G1:176:VAL:HG22  | 1.66                     | 0.75              |
| 3:F2:6:SER:O       | 3:F2:10:LEU:N      | 2.18                     | 0.75              |
| 9:n2:169:GLN:CD    | 11:y3:53:THR:HG1   | 1.91                     | 0.75              |
| 11:s3:336:ASN:ND2  | 11:t3:318:SER:O    | 2.17                     | 0.75              |
| 1:B1:167:ARG:HB3   | 2:C2:160:GLN:OE1   | 1.86                     | 0.75              |
| 1:H1:174:ALA:HB3   | 1:H1:210:VAL:HG12  | 1.68                     | 0.75              |
| 2:B2:86:ASN:ND2    | 5:N2:102:MET:O     | 2.18                     | 0.75              |
| 2:B2:107:LYS:HE3   | 2:B2:133:PRO:HB3   | 1.67                     | 0.75              |
| 9:s2:209:ASN:CG    | 11:r3:78:ASN:ND2   | 2.45                     | 0.75              |
| 1:K1:129:GLN:O     | 1:K1:133:GLN:NE2   | 2.20                     | 0.75              |
| 1:L1:137:GLU:HG2   | 1:L1:155:VAL:HG13  | 1.67                     | 0.75              |
| 1:T1:375:THR:HG23  | 1:U1:275:LYS:NZ    | 2.01                     | 0.75              |
| 2:A2:87:GLN:HB3    | 2:B2:60:MET:HG3    | 1.68                     | 0.75              |
| 6:Q2:78:VAL:HG11   | 7:V2:57:GLN:CG     | 2.16                     | 0.75              |
| 8:e2:114:THR:HG22  | 8:e2:119:PRO:HB3   | 1.66                     | 0.75              |
| 9:r2:125:ASN:HB2   | 11:l3:54:GLN:HE22  | 1.49                     | 0.75              |
| 11:a3:359:ARG:HB3  | 11:z3:20:GLU:OE2   | 1.87                     | 0.75              |
| 11:z3:117:ARG:NH1  | 11:z3:144:GLY:O    | 2.20                     | 0.75              |
| 1:L1:172:PRO:O     | 1:L1:209:ASN:ND2   | 2.20                     | 0.75              |
| 1:S1:295:SER:CB    | 6:R2:73:ILE:HD12   | 2.12                     | 0.75              |
| 9:p2:141:THR:CB    | 11:c3:54:GLN:HE21  | 2.00                     | 0.75              |
| 10:C3:51:ILE:HG13  | 11:e3:175:LEU:HD11 | 1.69                     | 0.75              |
| 11:c3:117:ARG:NH1  | 11:c3:144:GLY:O    | 2.20                     | 0.75              |
| 11:d3:117:ARG:NH1  | 11:d3:144:GLY:O    | 2.20                     | 0.75              |
| 11:v3:117:ARG:NH1  | 11:v3:144:GLY:O    | 2.20                     | 0.75              |
| 12:C4:84:GLN:HE22  | 12:D4:85:ILE:HG23  | 1.50                     | 0.75              |
| 1:Y1:256:ILE:HG21  | 1:Y1:412:ILE:HD11  | 1.68                     | 0.75              |
| 11:p3:336:ASN:ND2  | 11:q3:318:SER:O    | 2.16                     | 0.75              |
| 11:y3:117:ARG:NH1  | 11:y3:144:GLY:O    | 2.20                     | 0.75              |
| 1:N1:257:VAL:O     | 1:N1:261:ASN:ND2   | 2.20                     | 0.75              |
| 1:R1:167:ARG:NH1   | 3:F2:169:PHE:N     | 2.32                     | 0.75              |
| 1:Y1:203:ALA:HB1   | 1:a1:160:PRO:HA    | 1.69                     | 0.75              |
| 9:p2:141:THR:CB    | 11:c3:54:GLN:NE2   | 2.49                     | 0.75              |
| 9:p2:172:GLN:HB2   | 11:d3:54:GLN:NE2   | 2.01                     | 0.75              |
| 9:p2:230:LEU:HD21  | 9:u2:242:ILE:HD12  | 1.68                     | 0.75              |
| 9:u2:110:GLY:CA    | 11:z3:80:GLN:OE1   | 2.34                     | 0.75              |
| 11:a3:21:ARG:NH1   | 11:b3:267:GLU:OE1  | 2.20                     | 0.75              |
| 11:a3:117:ARG:NH1  | 11:a3:144:GLY:O    | 2.20                     | 0.75              |
| 11:f3:21:ARG:NH1   | 11:g3:267:GLU:OE1  | 2.19                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:U1:139:GLU:HB3  | 1:W1:156:HIS:HE1  | 1.52                     | 0.75              |
| 2:D2:135:ARG:NH2  | 2:D2:165:VAL:O    | 2.20                     | 0.75              |
| 9:s2:127:GLN:HE21 | 11:p3:78:ASN:ND2  | 1.85                     | 0.75              |
| 9:t2:77:THR:HG22  | 9:y2:66:LEU:HA    | 1.67                     | 0.75              |
| 11:b3:117:ARG:NH1 | 11:b3:144:GLY:O   | 2.20                     | 0.75              |
| 1:E1:162:PRO:CB   | 4:H2:86:TYR:OH    | 2.28                     | 0.74              |
| 1:L1:421:GLY:O    | 1:L1:426:ARG:NH2  | 2.20                     | 0.74              |
| 2:B2:84:PRO:HB2   | 2:B2:87:GLN:HB2   | 1.69                     | 0.74              |
| 8:d2:70:GLN:HE21  | 9:n2:7:ILE:HG13   | 1.52                     | 0.74              |
| 9:s2:77:THR:HG23  | 9:x2:66:LEU:HD12  | 1.69                     | 0.74              |
| 11:m3:117:ARG:NH1 | 11:m3:144:GLY:O   | 2.20                     | 0.74              |
| 11:t3:196:MET:HE2 | 11:t3:196:MET:HA  | 1.69                     | 0.74              |
| 11:u3:117:ARG:NH1 | 11:u3:144:GLY:O   | 2.20                     | 0.74              |
| 1:E1:297:GLN:HB2  | 6:U2:65:LEU:HD21  | 1.69                     | 0.74              |
| 1:F1:244:ARG:HH22 | 1:G1:239:ASN:HB2  | 1.52                     | 0.74              |
| 1:T1:165:PHE:CD2  | 3:F2:167:ASN:HB2  | 2.22                     | 0.74              |
| 1:d1:235:LEU:O    | 1:d1:239:ASN:ND2  | 2.20                     | 0.74              |
| 2:D2:185:ILE:HG23 | 4:J2:84:LEU:HD21  | 1.68                     | 0.74              |
| 9:m2:238:ARG:NH1  | 9:s2:255:GLN:OE1  | 2.20                     | 0.74              |
| 9:p2:19:MET:HG2   | 9:u2:253:MET:HE1  | 1.69                     | 0.74              |
| 9:u2:1:MET:HE2    | 9:u2:254:LEU:HD21 | 1.68                     | 0.74              |
| 10:K3:124:MET:HB2 | 10:L3:110:PRO:HG3 | 1.70                     | 0.74              |
| 11:g3:117:ARG:NH1 | 11:g3:144:GLY:O   | 2.20                     | 0.74              |
| 11:p3:117:ARG:NH1 | 11:p3:144:GLY:O   | 2.20                     | 0.74              |
| 11:r3:21:ARG:NH1  | 11:s3:267:GLU:OE1 | 2.20                     | 0.74              |
| 11:s3:196:MET:HE2 | 11:s3:196:MET:HA  | 1.69                     | 0.74              |
| 11:w3:117:ARG:NH1 | 11:w3:144:GLY:O   | 2.20                     | 0.74              |
| 1:a1:167:ARG:HD3  | 2:D2:244:TYR:CG   | 2.15                     | 0.74              |
| 1:e1:275:LYS:HB2  | 1:e1:377:MET:HB2  | 1.69                     | 0.74              |
| 1:h1:125:GLN:HG3  | 4:I2:4:GLU:HB3    | 1.67                     | 0.74              |
| 9:h2:100:GLN:HA   | 9:h2:116:ARG:HH12 | 1.52                     | 0.74              |
| 9:u2:230:LEU:HD21 | 9:z2:242:ILE:HD12 | 1.66                     | 0.74              |
| 9:w2:91:ASN:OD1   | 9:22:38:ARG:NH1   | 2.19                     | 0.74              |
| 10:W3:203:ALA:C   | 10:W3:203:ALA:N   | 2.46                     | 0.74              |
| 11:a3:196:MET:HE2 | 11:a3:196:MET:HA  | 1.69                     | 0.74              |
| 11:b3:196:MET:HE2 | 11:b3:196:MET:HA  | 1.69                     | 0.74              |
| 11:e3:117:ARG:NH1 | 11:e3:144:GLY:O   | 2.20                     | 0.74              |
| 11:l3:117:ARG:NH1 | 11:l3:144:GLY:O   | 2.20                     | 0.74              |
| 11:o3:117:ARG:NH1 | 11:o3:144:GLY:O   | 2.20                     | 0.74              |
| 11:u3:196:MET:HE2 | 11:u3:196:MET:HA  | 1.70                     | 0.74              |
| 11:x3:336:ASN:ND2 | 11:y3:318:SER:O   | 2.21                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:L1:167:ARG:HH21 | 2:A2:245:SER:HB2   | 1.49                     | 0.74              |
| 1:R1:164:LEU:HD13 | 3:F2:174:ARG:CD    | 2.16                     | 0.74              |
| 8:b2:42:ARG:NH1   | 9:g2:64:SER:OG     | 2.19                     | 0.74              |
| 9:w2:195:THR:HG23 | 9:w2:197:SER:H     | 1.51                     | 0.74              |
| 10:E3:51:ILE:HG13 | 11:g3:175:LEU:HD11 | 1.69                     | 0.74              |
| 10:P3:51:ILE:HG13 | 11:r3:175:LEU:HD11 | 1.68                     | 0.74              |
| 11:h3:117:ARG:NH1 | 11:h3:144:GLY:O    | 2.20                     | 0.74              |
| 11:v3:196:MET:HE2 | 11:v3:196:MET:HA   | 1.69                     | 0.74              |
| 11:x3:117:ARG:NH1 | 11:x3:144:GLY:O    | 2.20                     | 0.74              |
| 1:L1:216:SER:O    | 1:L1:218:HIS:ND1   | 2.18                     | 0.74              |
| 1:Q1:139:GLU:O    | 1:R1:154:ARG:NH1   | 2.20                     | 0.74              |
| 9:r2:141:THR:HG23 | 11:l3:53:THR:HG21  | 1.68                     | 0.74              |
| 10:H3:124:MET:HB2 | 10:I3:110:PRO:HG3  | 1.70                     | 0.74              |
| 10:I3:124:MET:HB2 | 10:J3:110:PRO:HG3  | 1.70                     | 0.74              |
| 10:K3:51:ILE:HG13 | 11:m3:175:LEU:HD11 | 1.69                     | 0.74              |
| 10:Q3:124:MET:HB2 | 10:R3:110:PRO:HG3  | 1.70                     | 0.74              |
| 11:c3:196:MET:HE2 | 11:c3:196:MET:HA   | 1.69                     | 0.74              |
| 1:M1:363:THR:CG2  | 6:Q2:73:ILE:HD11   | 2.14                     | 0.74              |
| 1:Y1:164:LEU:CG   | 2:E2:152:ARG:CD    | 2.64                     | 0.74              |
| 1:Y1:413:GLU:OE2  | 1:Y1:417:ARG:NH1   | 2.21                     | 0.74              |
| 2:C2:92:LEU:HD21  | 2:C2:236:MET:SD    | 2.28                     | 0.74              |
| 10:M3:124:MET:HB2 | 10:N3:110:PRO:HG3  | 1.70                     | 0.74              |
| 11:j3:117:ARG:NH1 | 11:j3:144:GLY:O    | 2.20                     | 0.74              |
| 1:f1:389:VAL:HB   | 1:f1:432:VAL:HG12  | 1.70                     | 0.74              |
| 9:j2:185:GLU:OE1  | 9:n2:67:GLN:NE2    | 2.21                     | 0.74              |
| 9:z2:82:SER:HG    | 9:z2:223:ASN:HD22  | 1.35                     | 0.74              |
| 10:L3:124:MET:HB2 | 10:M3:110:PRO:HG3  | 1.70                     | 0.74              |
| 11:m3:196:MET:HE2 | 11:m3:196:MET:HA   | 1.69                     | 0.74              |
| 11:n3:196:MET:HE2 | 11:n3:196:MET:HA   | 1.70                     | 0.74              |
| 11:o3:21:ARG:NH1  | 11:p3:267:GLU:OE1  | 2.21                     | 0.74              |
| 11:r3:117:ARG:NH1 | 11:r3:144:GLY:O    | 2.20                     | 0.74              |
| 11:s3:117:ARG:NH1 | 11:s3:144:GLY:O    | 2.20                     | 0.74              |
| 10:N3:124:MET:HB2 | 10:O3:110:PRO:HG3  | 1.70                     | 0.74              |
| 10:O3:124:MET:HB2 | 10:P3:110:PRO:HG3  | 1.70                     | 0.74              |
| 10:X3:172:ASN:OD1 | 10:Z3:138:ALA:HB1  | 1.86                     | 0.74              |
| 11:f3:117:ARG:NH1 | 11:f3:144:GLY:O    | 2.20                     | 0.74              |
| 11:o3:196:MET:HA  | 11:o3:196:MET:HE2  | 1.69                     | 0.74              |
| 11:z3:196:MET:HA  | 11:z3:196:MET:HE2  | 1.69                     | 0.74              |
| 1:E1:161:LYS:O    | 1:E1:169:GLN:NE2   | 2.21                     | 0.74              |
| 1:G1:256:ILE:HG23 | 1:G1:257:VAL:HG13  | 1.69                     | 0.74              |
| 1:H1:165:PHE:HZ   | 2:B2:147:LEU:HD12  | 1.51                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B2:96:LEU:HD21  | 2:B2:236:MET:HE3   | 1.68                     | 0.74              |
| 9:i2:150:THR:HG21 | 9:y2:54:ALA:HB1    | 1.70                     | 0.74              |
| 11:r3:196:MET:HE2 | 11:r3:196:MET:HA   | 1.70                     | 0.74              |
| 11:w3:196:MET:HA  | 11:w3:196:MET:HE2  | 1.69                     | 0.74              |
| 1:B1:275:LYS:HB3  | 1:B1:377:MET:HE2   | 1.69                     | 0.74              |
| 1:W1:262:VAL:HG12 | 1:W1:391:VAL:HG12  | 1.68                     | 0.74              |
| 1:a1:168:GLU:HG2  | 1:a1:169:GLN:H     | 1.52                     | 0.74              |
| 1:b1:374:HIS:HB3  | 1:c1:276:GLU:HB3   | 1.69                     | 0.74              |
| 1:g1:420:MET:HE3  | 1:g1:422:PHE:HB2   | 1.67                     | 0.74              |
| 9:o2:98:LYS:O     | 9:o2:212:GLY:HA3   | 1.88                     | 0.74              |
| 9:r2:141:THR:HG21 | 11:l3:53:THR:CB    | 2.17                     | 0.74              |
| 11:a3:20:GLU:OE2  | 11:b3:359:ARG:HB3  | 1.88                     | 0.74              |
| 11:i3:117:ARG:NH1 | 11:i3:144:GLY:O    | 2.20                     | 0.74              |
| 11:k3:117:ARG:NH1 | 11:k3:144:GLY:O    | 2.20                     | 0.74              |
| 11:s3:21:ARG:NH1  | 11:t3:267:GLU:OE1  | 2.21                     | 0.74              |
| 1:R1:167:ARG:HG3  | 3:F2:167:ASN:HB3   | 0.76                     | 0.73              |
| 2:A2:68:ILE:HD11  | 5:O2:104:VAL:HG22  | 1.69                     | 0.73              |
| 9:n2:85:ASN:OD1   | 9:z2:47:GLN:NE2    | 2.20                     | 0.73              |
| 10:I3:51:ILE:HG13 | 11:k3:175:LEU:HD11 | 1.69                     | 0.73              |
| 10:O3:51:ILE:HG13 | 11:q3:175:LEU:HD11 | 1.69                     | 0.73              |
| 11:g3:21:ARG:NH1  | 11:h3:267:GLU:OE1  | 2.21                     | 0.73              |
| 11:m3:21:ARG:NH1  | 11:n3:267:GLU:OE1  | 2.21                     | 0.73              |
| 1:I1:180:LEU:HD11 | 1:I1:186:LEU:HG    | 1.71                     | 0.73              |
| 1:W1:165:PHE:CE1  | 2:E2:245:SER:HB2   | 2.23                     | 0.73              |
| 1:d1:244:ARG:HH11 | 1:e1:235:LEU:HD13  | 1.53                     | 0.73              |
| 5:M2:66:ILE:H     | 5:M2:66:ILE:HD12   | 1.52                     | 0.73              |
| 9:r2:2:ILE:HG22   | 9:r2:4:SER:H       | 1.53                     | 0.73              |
| 9:z2:233:MET:HE1  | 12:D4:58:LEU:HD21  | 0.78                     | 0.73              |
| 9:32:29:VAL:HG21  | 12:B4:37:LEU:HD21  | 1.69                     | 0.73              |
| 10:R3:124:MET:HB2 | 10:S3:110:PRO:HG3  | 1.70                     | 0.73              |
| 10:S3:124:MET:HB2 | 10:T3:110:PRO:HG3  | 1.70                     | 0.73              |
| 11:f3:20:GLU:OE2  | 11:g3:359:ARG:HB3  | 1.88                     | 0.73              |
| 1:K1:257:VAL:O    | 1:K1:261:ASN:ND2   | 2.20                     | 0.73              |
| 1:Q1:153:ALA:HA   | 1:Q1:177:THR:O     | 1.87                     | 0.73              |
| 1:a1:164:LEU:C    | 2:D2:241:GLN:OE1   | 2.14                     | 0.73              |
| 1:d1:373:ARG:NH2  | 1:e1:277:GLN:HG2   | 2.03                     | 0.73              |
| 1:h1:125:GLN:NE2  | 4:I2:2:THR:HG23    | 2.03                     | 0.73              |
| 9:12:238:ARG:HH12 | 12:E4:54:GLN:NE2   | 1.81                     | 0.73              |
| 10:E3:124:MET:HB2 | 10:F3:110:PRO:HG3  | 1.69                     | 0.73              |
| 9:12:27:ALA:HB2   | 12:E4:41:VAL:HG21  | 1.69                     | 0.73              |
| 10:B3:51:ILE:HG13 | 11:d3:175:LEU:HD11 | 1.70                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:X3:124:MET:HB2 | 10:Y3:110:PRO:HG3  | 1.68                     | 0.73              |
| 11:l3:196:MET:HA  | 11:l3:196:MET:HE2  | 1.70                     | 0.73              |
| 1:Y1:164:LEU:HG   | 2:E2:152:ARG:CD    | 2.10                     | 0.73              |
| 6:Q2:106:ARG:HH12 | 8:b2:244:ALA:C     | 1.97                     | 0.73              |
| 9:z2:82:SER:OG    | 9:z2:223:ASN:ND2   | 2.19                     | 0.73              |
| 9:32:238:ARG:NH2  | 12:B4:56:ASN:H     | 1.82                     | 0.73              |
| 10:G3:124:MET:HB2 | 10:H3:110:PRO:HG3  | 1.70                     | 0.73              |
| 10:J3:124:MET:HB2 | 10:K3:110:PRO:HG3  | 1.71                     | 0.73              |
| 10:T3:124:MET:HB2 | 10:U3:110:PRO:HG3  | 1.70                     | 0.73              |
| 10:U3:51:ILE:HG13 | 11:w3:175:LEU:HD11 | 1.69                     | 0.73              |
| 11:i3:21:ARG:NH1  | 11:j3:267:GLU:OE1  | 2.21                     | 0.73              |
| 11:n3:117:ARG:NH1 | 11:n3:144:GLY:O    | 2.20                     | 0.73              |
| 11:q3:117:ARG:NH1 | 11:q3:144:GLY:O    | 2.20                     | 0.73              |
| 11:q3:196:MET:HE2 | 11:q3:196:MET:HA   | 1.69                     | 0.73              |
| 11:t3:117:ARG:NH1 | 11:t3:144:GLY:O    | 2.20                     | 0.73              |
| 1:L1:149:PRO:HA   | 1:L1:181:GLU:HG2   | 1.70                     | 0.73              |
| 1:M1:295:SER:HB3  | 6:Q2:65:LEU:HD22   | 1.69                     | 0.73              |
| 1:P1:275:LYS:HB3  | 1:P1:377:MET:HE2   | 1.70                     | 0.73              |
| 7:V2:105:THR:HG21 | 7:a2:118:VAL:HG23  | 1.69                     | 0.73              |
| 9:u2:174:ASN:ND2  | 9:u2:203:GLU:OE2   | 2.21                     | 0.73              |
| 10:V3:51:ILE:HG13 | 11:x3:175:LEU:HD11 | 1.68                     | 0.73              |
| 11:d3:196:MET:HA  | 11:d3:196:MET:HE2  | 1.69                     | 0.73              |
| 11:g3:196:MET:HA  | 11:g3:196:MET:HE2  | 1.69                     | 0.73              |
| 11:h3:196:MET:HE2 | 11:h3:196:MET:HA   | 1.69                     | 0.73              |
| 11:l3:21:ARG:NH1  | 11:m3:267:GLU:OE1  | 2.21                     | 0.73              |
| 11:r3:319:LEU:C   | 11:r3:319:LEU:N    | 2.47                     | 0.73              |
| 1:E1:179:THR:HA   | 1:E1:215:GLN:HB3   | 1.71                     | 0.73              |
| 1:b1:275:LYS:HB3  | 1:b1:377:MET:HE2   | 1.69                     | 0.73              |
| 9:y2:174:ASN:HA   | 9:y2:206:PRO:HD3   | 1.71                     | 0.73              |
| 9:32:238:ARG:CG   | 12:B4:55:ASN:ND2   | 2.51                     | 0.73              |
| 10:P3:124:MET:HB2 | 10:Q3:110:PRO:HG3  | 1.71                     | 0.73              |
| 11:j3:21:ARG:NH1  | 11:k3:267:GLU:OE1  | 2.22                     | 0.73              |
| 11:m3:336:ASN:ND2 | 11:n3:318:SER:O    | 2.17                     | 0.73              |
| 11:x3:196:MET:HE2 | 11:x3:196:MET:HA   | 1.70                     | 0.73              |
| 11:y3:98:ARG:HG3  | 11:z3:188:GLN:HG2  | 1.69                     | 0.73              |
| 1:C1:166:VAL:H    | 2:C2:152:ARG:NE    | 1.85                     | 0.73              |
| 1:C1:420:MET:HE3  | 1:C1:422:PHE:HB2   | 1.71                     | 0.73              |
| 1:Q1:165:PHE:HE2  | 3:F2:145:TRP:CZ3   | 2.05                     | 0.73              |
| 1:X1:165:PHE:HZ   | 2:E2:144:GLU:HB3   | 1.49                     | 0.73              |
| 2:E2:96:LEU:CG    | 2:E2:236:MET:HE3   | 2.15                     | 0.73              |
| 11:p3:196:MET:HE2 | 11:p3:196:MET:HA   | 1.69                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B1:167:ARG:HH12  | 2:C2:164:ALA:HB3   | 1.54                     | 0.73              |
| 1:C1:166:VAL:N     | 2:C2:152:ARG:HE    | 1.86                     | 0.73              |
| 1:T1:165:PHE:CE1   | 3:F2:167:ASN:CA    | 2.69                     | 0.73              |
| 1:X1:197:LEU:HD12  | 1:Y1:175:SER:HB2   | 1.71                     | 0.73              |
| 1:d1:164:LEU:CD1   | 2:D2:148:ALA:CA    | 2.67                     | 0.73              |
| 2:E2:96:LEU:HD22   | 2:E2:236:MET:HE1   | 0.74                     | 0.73              |
| 4:G2:40:ALA:HA     | 4:G2:43:GLN:HA     | 1.71                     | 0.73              |
| 8:d2:86:GLY:O      | 8:d2:101:ARG:NH1   | 2.21                     | 0.73              |
| 11:d3:270:LEU:HD11 | 11:d3:352:MET:HE1  | 1.71                     | 0.73              |
| 11:e3:270:LEU:HD11 | 11:e3:352:MET:HE1  | 1.71                     | 0.73              |
| 11:i3:196:MET:HE2  | 11:i3:196:MET:HA   | 1.69                     | 0.73              |
| 1:a1:233:ALA:HA    | 1:a1:236:LYS:HE2   | 1.70                     | 0.73              |
| 1:a1:259:ASN:OD1   | 1:a1:260:GLY:N     | 2.21                     | 0.73              |
| 1:g1:407:ASP:HA    | 1:g1:410:LYS:HE3   | 1.71                     | 0.73              |
| 7:X2:113:GLN:HB2   | 8:c2:243:ARG:NH1   | 2.04                     | 0.73              |
| 9:m2:189:GLU:HA    | 9:r2:42:GLU:HG2    | 1.71                     | 0.73              |
| 10:M3:51:ILE:HG13  | 11:o3:175:LEU:HD11 | 1.71                     | 0.73              |
| 11:f3:270:LEU:HD11 | 11:f3:352:MET:HE1  | 1.71                     | 0.73              |
| 11:m3:270:LEU:HD11 | 11:m3:352:MET:HE1  | 1.71                     | 0.73              |
| 11:y3:196:MET:HE2  | 11:y3:196:MET:HA   | 1.70                     | 0.73              |
| 1:U1:248:ARG:HH11  | 1:V1:267:THR:HG22  | 1.54                     | 0.72              |
| 1:Z1:252:ILE:HD11  | 1:a1:265:GLN:HB2   | 1.70                     | 0.72              |
| 1:a1:167:ARG:HG2   | 2:D2:140:ARG:HH12  | 1.53                     | 0.72              |
| 6:R2:40:ALA:HB2    | 6:R2:100:VAL:HG22  | 1.70                     | 0.72              |
| 9:p2:175:LEU:HD13  | 9:p2:206:PRO:HG3   | 1.70                     | 0.72              |
| 9:42:180:ASN:ND2   | 9:42:197:SER:O     | 2.21                     | 0.72              |
| 11:f3:196:MET:HE2  | 11:f3:196:MET:HA   | 1.69                     | 0.72              |
| 11:n3:270:LEU:HD11 | 11:n3:352:MET:HE1  | 1.71                     | 0.72              |
| 11:x3:46:ASP:HA    | 11:y3:161:ASN:HD22 | 1.54                     | 0.72              |
| 1:H1:164:LEU:HD22  | 2:B2:148:ALA:HB2   | 1.71                     | 0.72              |
| 1:c1:275:LYS:HB3   | 1:c1:377:MET:HE2   | 1.70                     | 0.72              |
| 9:g2:10:THR:HG21   | 9:g2:71:GLY:HA2    | 1.71                     | 0.72              |
| 9:m2:98:LYS:O      | 9:m2:212:GLY:HA3   | 1.89                     | 0.72              |
| 9:u2:110:GLY:HA3   | 11:z3:80:GLN:OE1   | 1.88                     | 0.72              |
| 9:z2:27:ALA:CB     | 12:D4:45:LYS:HD2   | 2.11                     | 0.72              |
| 10:C3:124:MET:HB2  | 10:D3:110:PRO:HG3  | 1.70                     | 0.72              |
| 10:G3:51:ILE:HG13  | 11:i3:175:LEU:HD11 | 1.70                     | 0.72              |
| 10:U3:124:MET:HB2  | 10:V3:110:PRO:HG3  | 1.70                     | 0.72              |
| 11:c3:270:LEU:HD11 | 11:c3:352:MET:HE1  | 1.71                     | 0.72              |
| 11:l3:270:LEU:HD11 | 11:l3:352:MET:HE1  | 1.71                     | 0.72              |
| 1:E1:375:THR:HG21  | 1:E1:377:MET:HE2   | 1.71                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c2:137:ILE:HD12  | 8:c2:143:ILE:HG12  | 1.71                     | 0.72              |
| 9:42:23:ALA:HA     | 12:C4:41:VAL:HG23  | 1.71                     | 0.72              |
| 10:F3:51:ILE:HG13  | 11:h3:175:LEU:HD11 | 1.71                     | 0.72              |
| 10:N3:51:ILE:HG13  | 11:p3:175:LEU:HD11 | 1.70                     | 0.72              |
| 11:n3:21:ARG:NH1   | 11:o3:267:GLU:OE1  | 2.23                     | 0.72              |
| 11:u3:21:ARG:NH1   | 11:v3:267:GLU:OE1  | 2.21                     | 0.72              |
| 1:C1:166:VAL:N     | 2:C2:152:ARG:NE    | 2.37                     | 0.72              |
| 1:N1:296:ARG:NH2   | 1:O1:366:TYR:OH    | 2.22                     | 0.72              |
| 9:n2:77:THR:HG23   | 9:t2:66:LEU:HD12   | 1.71                     | 0.72              |
| 10:B3:124:MET:HB2  | 10:C3:110:PRO:HG3  | 1.70                     | 0.72              |
| 10:L3:51:ILE:HG13  | 11:n3:175:LEU:HD11 | 1.71                     | 0.72              |
| 10:Q3:51:ILE:HG13  | 11:s3:175:LEU:HD11 | 1.69                     | 0.72              |
| 11:g3:270:LEU:HD11 | 11:g3:352:MET:HE1  | 1.71                     | 0.72              |
| 11:o3:20:GLU:OE2   | 11:p3:359:ARG:HB3  | 1.89                     | 0.72              |
| 1:Y1:253:LEU:HD11  | 1:Y1:412:ILE:HG23  | 1.71                     | 0.72              |
| 1:Y1:405:THR:OG1   | 1:Y1:407:ASP:OD1   | 2.07                     | 0.72              |
| 8:c2:35:ARG:O      | 8:c2:173:ARG:NH2   | 2.22                     | 0.72              |
| 10:F3:124:MET:HB2  | 10:G3:110:PRO:HG3  | 1.71                     | 0.72              |
| 11:g3:20:GLU:OE2   | 11:h3:359:ARG:HB3  | 1.89                     | 0.72              |
| 11:k3:270:LEU:HD11 | 11:k3:352:MET:HE1  | 1.71                     | 0.72              |
| 11:m3:20:GLU:OE2   | 11:n3:359:ARG:HB3  | 1.89                     | 0.72              |
| 11:o3:270:LEU:HD11 | 11:o3:352:MET:HE1  | 1.71                     | 0.72              |
| 11:s3:20:GLU:OE2   | 11:t3:359:ARG:HB3  | 1.89                     | 0.72              |
| 2:E2:205:MET:HE2   | 4:J2:51:PHE:CZ     | 2.24                     | 0.72              |
| 4:J2:46:GLU:HG2    | 4:J2:47:MET:H      | 1.53                     | 0.72              |
| 10:T3:51:ILE:HG13  | 11:v3:175:LEU:HD11 | 1.70                     | 0.72              |
| 10:W3:124:MET:HB2  | 10:X3:110:PRO:HG3  | 1.70                     | 0.72              |
| 11:r3:20:GLU:OE2   | 11:s3:359:ARG:HB3  | 1.89                     | 0.72              |
| 1:O1:378:ASN:ND2   | 1:O1:381:ASP:OD1   | 2.22                     | 0.72              |
| 1:Z1:233:ALA:HA    | 1:Z1:236:LYS:HD3   | 1.70                     | 0.72              |
| 2:E2:71:PHE:HZ     | 2:E2:236:MET:SD    | 2.12                     | 0.72              |
| 9:n2:169:GLN:H     | 11:x3:78:ASN:ND2   | 1.88                     | 0.72              |
| 10:A3:51:ILE:HG13  | 11:c3:175:LEU:HD11 | 1.71                     | 0.72              |
| 11:c3:20:GLU:OE2   | 11:d3:359:ARG:HB3  | 1.89                     | 0.72              |
| 11:h3:270:LEU:HD11 | 11:h3:352:MET:HE1  | 1.71                     | 0.72              |
| 11:t3:336:ASN:ND2  | 11:u3:318:SER:O    | 2.17                     | 0.72              |
| 1:H1:197:LEU:HD12  | 1:I1:175:SER:HB2   | 1.72                     | 0.72              |
| 1:K1:164:LEU:CD1   | 2:A2:241:GLN:O     | 2.33                     | 0.72              |
| 1:N1:167:ARG:HH12  | 2:A2:158:PRO:N     | 1.81                     | 0.72              |
| 1:d1:164:LEU:HD11  | 2:D2:148:ALA:CB    | 2.17                     | 0.72              |
| 11:b3:270:LEU:HD11 | 11:b3:352:MET:HE1  | 1.71                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:c3:21:ARG:NH1   | 11:d3:267:GLU:OE1  | 2.21                     | 0.72              |
| 11:d3:98:ARG:HG3   | 11:e3:188:GLN:HG2  | 1.72                     | 0.72              |
| 11:k3:196:MET:HE2  | 11:k3:196:MET:HA   | 1.70                     | 0.72              |
| 11:u3:270:LEU:HD11 | 11:u3:352:MET:HE1  | 1.71                     | 0.72              |
| 12:D4:134:ASP:OD2  | 12:D4:134:ASP:CB   | 2.38                     | 0.72              |
| 1:E1:367:GLU:OE1   | 6:U2:68:THR:CG2    | 2.38                     | 0.72              |
| 1:E1:389:VAL:HB    | 1:E1:432:VAL:HG22  | 1.71                     | 0.72              |
| 1:a1:378:ASN:ND2   | 1:a1:381:ASP:OD1   | 2.22                     | 0.72              |
| 1:e1:277:GLN:HE22  | 1:e1:279:GLU:HB2   | 1.52                     | 0.72              |
| 9:h2:38:ARG:NH2    | 9:h2:78:GLU:OE1    | 2.20                     | 0.72              |
| 11:p3:270:LEU:HD11 | 11:p3:352:MET:HE1  | 1.71                     | 0.72              |
| 1:T1:165:PHE:CE2   | 3:F2:167:ASN:CG    | 2.68                     | 0.72              |
| 1:X1:142:ARG:HB2   | 1:Y1:154:ARG:HH12  | 1.55                     | 0.72              |
| 1:c1:125:GLN:HG3   | 4:J2:4:GLU:CG      | 2.14                     | 0.72              |
| 9:32:240:TYR:OH    | 12:B4:49:PRO:CB    | 2.37                     | 0.72              |
| 10:A3:124:MET:HB2  | 10:B3:110:PRO:HG3  | 1.70                     | 0.72              |
| 10:D3:124:MET:HB2  | 10:E3:110:PRO:HG3  | 1.71                     | 0.72              |
| 10:S3:51:ILE:HG13  | 11:u3:175:LEU:HD11 | 1.70                     | 0.72              |
| 11:p3:21:ARG:NH1   | 11:q3:267:GLU:OE1  | 2.22                     | 0.72              |
| 11:v3:270:LEU:HD11 | 11:v3:352:MET:HE1  | 1.71                     | 0.72              |
| 11:y3:21:ARG:NH1   | 11:z3:267:GLU:OE1  | 2.22                     | 0.72              |
| 1:B1:166:VAL:HA    | 2:C2:161:GLY:HA2   | 1.72                     | 0.71              |
| 1:F1:373:ARG:NH2   | 1:G1:277:GLN:OE1   | 2.23                     | 0.71              |
| 1:Q1:245:ILE:HD11  | 1:Q1:420:MET:HA    | 1.70                     | 0.71              |
| 1:T1:165:PHE:HB3   | 3:F2:166:SER:C     | 2.14                     | 0.71              |
| 1:Z1:363:THR:CG2   | 6:S2:73:ILE:HG13   | 2.20                     | 0.71              |
| 2:E2:40:LEU:HA     | 3:F2:66:PHE:CZ     | 2.24                     | 0.71              |
| 6:T2:91:ASP:OD1    | 7:Z2:19:LYS:NZ     | 2.23                     | 0.71              |
| 8:e2:146:LEU:HB2   | 8:e2:155:VAL:HG12  | 1.71                     | 0.71              |
| 9:22:237:GLN:HE22  | 12:A4:53:LEU:HD11  | 1.51                     | 0.71              |
| 11:d3:21:ARG:NH1   | 11:e3:267:GLU:OE1  | 2.22                     | 0.71              |
| 11:e3:196:MET:HE2  | 11:e3:196:MET:HA   | 1.69                     | 0.71              |
| 11:j3:270:LEU:HD11 | 11:j3:352:MET:HE1  | 1.71                     | 0.71              |
| 11:l3:20:GLU:OE2   | 11:m3:359:ARG:HB3  | 1.90                     | 0.71              |
| 11:t3:270:LEU:HD11 | 11:t3:352:MET:HE1  | 1.71                     | 0.71              |
| 11:u3:20:GLU:OE2   | 11:v3:359:ARG:HB3  | 1.89                     | 0.71              |
| 11:v3:21:ARG:NH1   | 11:w3:267:GLU:OE1  | 2.22                     | 0.71              |
| 1:U1:365:ASN:CG    | 6:R2:65:LEU:HA     | 2.15                     | 0.71              |
| 1:f1:197:LEU:HD12  | 1:g1:175:SER:HB2   | 1.71                     | 0.71              |
| 2:C2:41:SER:O      | 2:C2:43:GLN:N      | 2.23                     | 0.71              |
| 5:K2:76:GLN:OE1    | 5:P2:91:LYS:NZ     | 2.18                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c2:118:HIS:ND1   | 8:c2:118:HIS:O     | 2.23                     | 0.71              |
| 8:e2:26:LEU:HD21   | 9:j2:242:ILE:HG22  | 1.72                     | 0.71              |
| 9:i2:142:ILE:HD13  | 9:i2:149:ILE:HD13  | 1.70                     | 0.71              |
| 10:H3:51:ILE:HG13  | 11:j3:175:LEU:HD11 | 1.70                     | 0.71              |
| 11:a3:270:LEU:HD11 | 11:a3:352:MET:HE1  | 1.71                     | 0.71              |
| 11:j3:196:MET:HE2  | 11:j3:196:MET:HA   | 1.70                     | 0.71              |
| 12:C4:128:GLU:HB3  | 12:C4:196:GLN:HB3  | 1.72                     | 0.71              |
| 1:U1:245:ILE:HG23  | 1:U1:266:VAL:HG21  | 1.72                     | 0.71              |
| 6:S2:106:ARG:NH1   | 8:d2:244:ALA:O     | 2.23                     | 0.71              |
| 8:b2:165:LYS:O     | 8:b2:189:ARG:NH2   | 2.24                     | 0.71              |
| 9:k2:113:ALA:HB3   | 9:k2:191:LEU:HD23  | 1.71                     | 0.71              |
| 11:v3:98:ARG:HG3   | 11:w3:188:GLN:HG2  | 1.72                     | 0.71              |
| 11:x3:97:ALA:HB1   | 11:x3:171:ILE:CD1  | 2.20                     | 0.71              |
| 11:y3:97:ALA:HB1   | 11:y3:171:ILE:CD1  | 2.20                     | 0.71              |
| 12:A4:140:ILE:HG12 | 12:A4:182:ILE:HG22 | 1.73                     | 0.71              |
| 1:O1:180:LEU:HB2   | 1:O1:215:GLN:HE22  | 1.55                     | 0.71              |
| 9:m2:166:ALA:HB3   | 11:o3:80:GLN:HE22  | 1.55                     | 0.71              |
| 9:p2:145:ASN:O     | 9:p2:162:GLN:NE2   | 2.22                     | 0.71              |
| 9:22:234:ILE:CG2   | 12:A4:55:ASN:ND2   | 2.41                     | 0.71              |
| 10:W3:51:ILE:HG13  | 11:y3:175:LEU:HD11 | 1.71                     | 0.71              |
| 11:i3:20:GLU:OE2   | 11:j3:359:ARG:HB3  | 1.89                     | 0.71              |
| 11:q3:270:LEU:HD11 | 11:q3:352:MET:HE1  | 1.71                     | 0.71              |
| 11:w3:270:LEU:HD11 | 11:w3:352:MET:HE1  | 1.71                     | 0.71              |
| 11:x3:270:LEU:HD11 | 11:x3:352:MET:HE1  | 1.71                     | 0.71              |
| 11:z3:97:ALA:HB1   | 11:z3:171:ILE:CD1  | 2.20                     | 0.71              |
| 1:f1:164:LEU:HD12  | 2:D2:152:ARG:HD2   | 1.72                     | 0.71              |
| 8:c2:225:ARG:NH1   | 8:c2:228:GLU:OE2   | 2.23                     | 0.71              |
| 8:d2:42:ARG:NH1    | 9:i2:64:SER:OG     | 2.21                     | 0.71              |
| 11:y3:270:LEU:HD11 | 11:y3:352:MET:HE1  | 1.71                     | 0.71              |
| 12:D4:134:ASP:CB   | 12:D4:134:ASP:OD1  | 2.38                     | 0.71              |
| 1:E1:167:ARG:HG2   | 2:B2:244:TYR:CG    | 2.23                     | 0.71              |
| 1:E1:277:GLN:HB3   | 1:E1:375:THR:HB    | 1.73                     | 0.71              |
| 1:T1:167:ARG:CZ    | 2:E2:106:ASP:HB3   | 2.20                     | 0.71              |
| 1:b1:360:ARG:NH1   | 1:b1:362:GLU:OE2   | 2.23                     | 0.71              |
| 9:m2:150:THR:HG21  | 9:32:54:ALA:HB1    | 1.73                     | 0.71              |
| 11:i3:270:LEU:HD11 | 11:i3:352:MET:HE1  | 1.71                     | 0.71              |
| 11:n3:97:ALA:HB1   | 11:n3:171:ILE:CD1  | 2.20                     | 0.71              |
| 11:o3:97:ALA:HB1   | 11:o3:171:ILE:CD1  | 2.20                     | 0.71              |
| 11:p3:98:ARG:HG3   | 11:q3:188:GLN:HG2  | 1.71                     | 0.71              |
| 11:s3:270:LEU:HD11 | 11:s3:352:MET:HE1  | 1.71                     | 0.71              |
| 1:B1:165:PHE:HD1   | 2:C2:159:LEU:CD1   | 2.02                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:R1:375:THR:HG23  | 1:S1:275:LYS:HZ3   | 1.54                     | 0.71              |
| 1:Y1:297:GLN:HB2   | 6:S2:73:ILE:CD1    | 2.21                     | 0.71              |
| 1:f1:257:VAL:O     | 1:f1:261:ASN:ND2   | 2.19                     | 0.71              |
| 2:A2:214:PRO:HD2   | 3:F2:120:LEU:HD13  | 1.71                     | 0.71              |
| 3:F2:9:TRP:O       | 3:F2:12:TRP:N      | 2.23                     | 0.71              |
| 9:r2:77:THR:HG23   | 9:w2:66:LEU:HD12   | 1.72                     | 0.71              |
| 9:s2:139:ALA:CB    | 11:q3:53:THR:HB    | 2.21                     | 0.71              |
| 9:s2:232:ASN:OD1   | 9:y2:9:LYS:NZ      | 2.21                     | 0.71              |
| 9:42:244:SER:HB2   | 12:C4:49:PRO:O     | 1.89                     | 0.71              |
| 10:A3:110:PRO:HG3  | 10:Z3:124:MET:HB2  | 1.71                     | 0.71              |
| 11:a3:97:ALA:HB1   | 11:a3:171:ILE:CD1  | 2.20                     | 0.71              |
| 11:b3:21:ARG:NH1   | 11:c3:267:GLU:OE1  | 2.23                     | 0.71              |
| 11:f3:98:ARG:HG3   | 11:g3:188:GLN:HG2  | 1.72                     | 0.71              |
| 11:j3:98:ARG:HG3   | 11:k3:188:GLN:HG2  | 1.71                     | 0.71              |
| 11:p3:97:ALA:HB1   | 11:p3:171:ILE:CD1  | 2.20                     | 0.71              |
| 11:w3:97:ALA:HB1   | 11:w3:171:ILE:CD1  | 2.20                     | 0.71              |
| 1:E1:167:ARG:HD3   | 2:B2:244:TYR:CD2   | 2.17                     | 0.71              |
| 1:S1:404:LEU:HD23  | 1:S1:408:GLN:HG2   | 1.71                     | 0.71              |
| 9:k2:168:VAL:HG23  | 11:f3:114:LYS:CE   | 2.18                     | 0.71              |
| 9:l2:167:PRO:HD3   | 9:w2:196:GLN:HG2   | 1.72                     | 0.71              |
| 11:v3:97:ALA:HB1   | 11:v3:171:ILE:CD1  | 2.20                     | 0.71              |
| 12:A4:229:ARG:HA   | 12:E4:208:LYS:HE2  | 1.70                     | 0.71              |
| 1:H1:143:THR:HG21  | 1:I1:156:HIS:NE2   | 2.06                     | 0.71              |
| 1:T1:167:ARG:HH21  | 2:E2:107:LYS:HG2   | 1.54                     | 0.71              |
| 1:V1:250:GLU:O     | 1:V1:254:SER:OG    | 2.09                     | 0.71              |
| 1:X1:203:ALA:HA    | 1:Y1:158:ALA:HB1   | 1.73                     | 0.71              |
| 1:g1:139:GLU:O     | 1:h1:154:ARG:NH2   | 2.24                     | 0.71              |
| 11:z3:270:LEU:HD11 | 11:z3:352:MET:HE1  | 1.71                     | 0.71              |
| 1:N1:143:THR:HG23  | 1:O1:154:ARG:HH21  | 1.55                     | 0.71              |
| 1:Z1:294:ARG:HE    | 6:S2:68:THR:HB     | 1.54                     | 0.71              |
| 9:l2:98:LYS:HB2    | 9:l2:213:LEU:H     | 1.55                     | 0.71              |
| 9:n2:168:VAL:HG22  | 11:x3:80:GLN:OE1   | 1.91                     | 0.71              |
| 9:12:238:ARG:CZ    | 12:E4:54:GLN:HE22  | 2.03                     | 0.71              |
| 10:A3:138:ALA:HB1  | 10:Y3:172:ASN:OD1  | 1.89                     | 0.71              |
| 10:R3:51:ILE:HG13  | 11:t3:175:LEU:HD11 | 1.71                     | 0.71              |
| 10:V3:124:MET:HB2  | 10:W3:110:PRO:HG3  | 1.71                     | 0.71              |
| 11:h3:21:ARG:NH1   | 11:i3:267:GLU:OE1  | 2.23                     | 0.71              |
| 11:q3:97:ALA:HB1   | 11:q3:171:ILE:CD1  | 2.20                     | 0.71              |
| 11:t3:98:ARG:HG3   | 11:u3:188:GLN:HG2  | 1.73                     | 0.71              |
| 12:E4:133:ALA:HA   | 12:E4:188:ASN:HB2  | 1.72                     | 0.71              |
| 1:M1:360:ARG:NH1   | 1:M1:362:GLU:OE1   | 2.24                     | 0.70              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:Z1:389:VAL:HB    | 1:Z1:432:VAL:HG22 | 1.71                     | 0.70              |
| 8:e2:116:GLN:NE2   | 9:j2:42:GLU:OE2   | 2.24                     | 0.70              |
| 9:v2:241:GLU:HG3   | 9:22:258:THR:HG21 | 1.73                     | 0.70              |
| 9:32:234:ILE:CG2   | 12:B4:55:ASN:HD22 | 2.04                     | 0.70              |
| 11:b3:97:ALA:HB1   | 11:b3:171:ILE:CD1 | 2.20                     | 0.70              |
| 11:b3:98:ARG:HG3   | 11:c3:188:GLN:HG2 | 1.73                     | 0.70              |
| 11:k3:21:ARG:NH1   | 11:l3:267:GLU:OE1 | 2.24                     | 0.70              |
| 11:r3:98:ARG:HG3   | 11:s3:188:GLN:HG2 | 1.72                     | 0.70              |
| 1:Q1:161:LYS:HZ1   | 3:F2:249:ASN:ND2  | 1.73                     | 0.70              |
| 8:b2:118:HIS:ND1   | 8:b2:118:HIS:O    | 2.24                     | 0.70              |
| 9:n2:169:GLN:H     | 11:x3:78:ASN:HD21 | 1.37                     | 0.70              |
| 9:o2:168:VAL:CG2   | 11:t3:54:GLN:HE21 | 2.02                     | 0.70              |
| 9:z2:46:TYR:HA     | 9:z2:69:GLY:HA2   | 1.73                     | 0.70              |
| 9:22:233:MET:SD    | 12:A4:58:LEU:HD11 | 2.31                     | 0.70              |
| 10:Y3:124:MET:HB2  | 10:Z3:110:PRO:HG3 | 1.71                     | 0.70              |
| 11:h3:88:MET:HG2   | 11:h3:110:MET:HG3 | 1.74                     | 0.70              |
| 11:i3:88:MET:HG2   | 11:i3:110:MET:HG3 | 1.74                     | 0.70              |
| 11:m3:88:MET:HG2   | 11:m3:110:MET:HG3 | 1.74                     | 0.70              |
| 11:r3:270:LEU:HD11 | 11:r3:352:MET:HE1 | 1.71                     | 0.70              |
| 1:F1:231:ASN:O     | 1:F1:234:GLN:NE2  | 2.24                     | 0.70              |
| 1:d1:181:GLU:HB3   | 1:d1:184:ARG:HH21 | 1.56                     | 0.70              |
| 7:V2:79:GLU:OE2    | 9:g2:6:TRP:CH2    | 2.43                     | 0.70              |
| 9:w2:2:ILE:HG22    | 9:w2:4:SER:H      | 1.56                     | 0.70              |
| 11:p3:20:GLU:OE2   | 11:q3:359:ARG:HB3 | 1.91                     | 0.70              |
| 11:p3:88:MET:HG2   | 11:p3:110:MET:HG3 | 1.74                     | 0.70              |
| 1:G1:166:VAL:CA    | 2:B2:144:GLU:CG   | 2.69                     | 0.70              |
| 1:K1:244:ARG:NH2   | 1:L1:235:LEU:O    | 2.23                     | 0.70              |
| 1:R1:168:GLU:CB    | 3:F2:261:ASN:OD1  | 2.38                     | 0.70              |
| 1:Z1:257:VAL:O     | 1:Z1:261:ASN:ND2  | 2.24                     | 0.70              |
| 9:n2:169:GLN:O     | 11:y3:54:GLN:OE1  | 2.09                     | 0.70              |
| 9:32:230:LEU:HD13  | 12:B4:62:LEU:HD13 | 1.74                     | 0.70              |
| 11:e3:88:MET:HG2   | 11:e3:110:MET:HG3 | 1.74                     | 0.70              |
| 11:g3:88:MET:HG2   | 11:g3:110:MET:HG3 | 1.73                     | 0.70              |
| 11:h3:98:ARG:HG3   | 11:i3:188:GLN:HG2 | 1.73                     | 0.70              |
| 11:l3:88:MET:HG2   | 11:l3:110:MET:HG3 | 1.74                     | 0.70              |
| 11:n3:88:MET:HG2   | 11:n3:110:MET:HG3 | 1.74                     | 0.70              |
| 11:x3:98:ARG:HG3   | 11:y3:188:GLN:HG2 | 1.72                     | 0.70              |
| 1:E1:143:THR:HG21  | 1:G1:156:HIS:CE1  | 2.26                     | 0.70              |
| 1:U1:165:PHE:CZ    | 2:E2:244:TYR:CE2  | 2.80                     | 0.70              |
| 1:U1:212:LEU:N     | 1:U1:221:THR:OG1  | 2.24                     | 0.70              |
| 1:f1:190:GLN:HG2   | 1:g1:217:GLY:HA3  | 1.73                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:E2:159:LEU:HD13  | 2:E2:165:VAL:HG12  | 1.72                     | 0.70              |
| 11:c3:97:ALA:HB1   | 11:c3:171:ILE:CD1  | 2.20                     | 0.70              |
| 11:e3:97:ALA:HB1   | 11:e3:171:ILE:CD1  | 2.20                     | 0.70              |
| 11:f3:97:ALA:HB1   | 11:f3:171:ILE:CD1  | 2.21                     | 0.70              |
| 11:g3:97:ALA:HB1   | 11:g3:171:ILE:CD1  | 2.21                     | 0.70              |
| 11:h3:97:ALA:HB1   | 11:h3:171:ILE:CD1  | 2.20                     | 0.70              |
| 11:q3:88:MET:HG2   | 11:q3:110:MET:HG3  | 1.74                     | 0.70              |
| 11:r3:97:ALA:HB1   | 11:r3:171:ILE:CD1  | 2.20                     | 0.70              |
| 11:u3:98:ARG:HG3   | 11:v3:188:GLN:HG2  | 1.73                     | 0.70              |
| 1:G1:165:PHE:CE2   | 4:H2:88:ILE:HG22   | 2.23                     | 0.70              |
| 1:H1:248:ARG:HH11  | 1:I1:267:THR:HG22  | 1.57                     | 0.70              |
| 1:L1:275:LYS:HB2   | 1:L1:377:MET:HB2   | 1.73                     | 0.70              |
| 10:B3:136:GLY:HA3  | 10:Z3:213:ILE:HG23 | 1.72                     | 0.70              |
| 10:F3:86:VAL:HB    | 10:F3:142:ASN:OD1  | 1.92                     | 0.70              |
| 10:Y3:86:VAL:HB    | 10:Y3:142:ASN:OD1  | 1.92                     | 0.70              |
| 10:Z3:86:VAL:HB    | 10:Z3:142:ASN:OD1  | 1.92                     | 0.70              |
| 11:d3:20:GLU:OE2   | 11:e3:359:ARG:HB3  | 1.91                     | 0.70              |
| 11:e3:98:ARG:HG3   | 11:f3:188:GLN:HG2  | 1.73                     | 0.70              |
| 11:f3:88:MET:HG2   | 11:f3:110:MET:HG3  | 1.74                     | 0.70              |
| 11:j3:88:MET:HG2   | 11:j3:110:MET:HG3  | 1.74                     | 0.70              |
| 11:u3:97:ALA:HB1   | 11:u3:171:ILE:CD1  | 2.20                     | 0.70              |
| 1:F1:363:THR:HB    | 6:U2:63:VAL:HG21   | 1.72                     | 0.70              |
| 10:S3:86:VAL:HB    | 10:S3:142:ASN:OD1  | 1.92                     | 0.70              |
| 11:d3:88:MET:HG2   | 11:d3:110:MET:HG3  | 1.74                     | 0.70              |
| 11:o3:88:MET:HG2   | 11:o3:110:MET:HG3  | 1.74                     | 0.70              |
| 11:t3:21:ARG:NH1   | 11:u3:267:GLU:OE1  | 2.23                     | 0.70              |
| 1:I1:244:ARG:NH1   | 1:J1:239:ASN:OD1   | 2.24                     | 0.70              |
| 1:U1:160:PRO:HD3   | 1:U1:172:PRO:HB3   | 1.71                     | 0.70              |
| 2:C2:236:MET:CE    | 2:D2:150:PHE:CZ    | 2.74                     | 0.70              |
| 9:w2:122:VAL:O     | 9:22:180:ASN:ND2   | 2.22                     | 0.70              |
| 9:12:46:TYR:HA     | 9:12:69:GLY:HA2    | 1.74                     | 0.70              |
| 9:42:175:LEU:HG    | 9:42:206:PRO:HG3   | 1.74                     | 0.70              |
| 10:A3:86:VAL:HB    | 10:A3:142:ASN:OD1  | 1.92                     | 0.70              |
| 10:G3:86:VAL:HB    | 10:G3:142:ASN:OD1  | 1.92                     | 0.70              |
| 11:c3:88:MET:HG2   | 11:c3:110:MET:HG3  | 1.73                     | 0.70              |
| 11:i3:97:ALA:HB1   | 11:i3:171:ILE:CD1  | 2.20                     | 0.70              |
| 11:k3:88:MET:HG2   | 11:k3:110:MET:HG3  | 1.74                     | 0.70              |
| 11:q3:21:ARG:NH1   | 11:r3:267:GLU:OE1  | 2.24                     | 0.70              |
| 11:x3:345:LEU:HD21 | 11:y3:319:LEU:HD22 | 1.73                     | 0.70              |
| 1:G1:378:ASN:ND2   | 1:G1:381:ASP:OD1   | 2.20                     | 0.70              |
| 1:N1:140:LEU:O     | 1:N1:143:THR:OG1   | 2.08                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:X1:362:GLU:OE2  | 1:X1:364:SER:OG   | 2.10                     | 0.70              |
| 1:h1:125:GLN:HE21 | 4:I2:2:THR:CG2    | 2.04                     | 0.70              |
| 2:D2:118:GLU:OE2  | 6:R2:5:LEU:N      | 2.25                     | 0.70              |
| 3:F2:164:VAL:HA   | 3:F2:258:MET:HE1  | 1.72                     | 0.70              |
| 9:o2:230:LEU:HD21 | 9:s2:242:ILE:HD12 | 1.74                     | 0.70              |
| 9:w2:238:ARG:HH11 | 9:w2:241:GLU:HG3  | 1.56                     | 0.70              |
| 9:42:59:GLN:HE22  | 11:u3:80:GLN:HE21 | 1.39                     | 0.70              |
| 10:E3:86:VAL:HB   | 10:E3:142:ASN:OD1 | 1.92                     | 0.70              |
| 10:K3:86:VAL:HB   | 10:K3:142:ASN:OD1 | 1.92                     | 0.70              |
| 10:L3:86:VAL:HB   | 10:L3:142:ASN:OD1 | 1.92                     | 0.70              |
| 10:M3:86:VAL:HB   | 10:M3:142:ASN:OD1 | 1.92                     | 0.70              |
| 10:O3:86:VAL:HB   | 10:O3:142:ASN:OD1 | 1.92                     | 0.70              |
| 10:P3:86:VAL:HB   | 10:P3:142:ASN:OD1 | 1.92                     | 0.70              |
| 10:X3:86:VAL:HB   | 10:X3:142:ASN:OD1 | 1.92                     | 0.70              |
| 11:r3:88:MET:HG2  | 11:r3:110:MET:HG3 | 1.74                     | 0.70              |
| 12:A4:157:ARG:HD3 | 12:A4:161:HIS:HE1 | 1.57                     | 0.70              |
| 1:L1:414:ASP:HB3  | 1:M1:431:ASN:ND2  | 2.05                     | 0.70              |
| 9:m2:2:ILE:HG23   | 9:m2:3:SER:H      | 1.56                     | 0.70              |
| 9:m2:164:GLN:HG2  | 11:o3:53:THR:OG1  | 1.91                     | 0.70              |
| 9:y2:238:ARG:HH22 | 12:D4:52:PRO:HB3  | 1.55                     | 0.70              |
| 9:32:101:GLY:HA3  | 9:32:175:LEU:HD23 | 1.73                     | 0.70              |
| 11:b3:20:GLU:OE2  | 11:c3:359:ARG:HB3 | 1.92                     | 0.70              |
| 11:d3:97:ALA:HB1  | 11:d3:171:ILE:CD1 | 2.21                     | 0.70              |
| 1:a1:165:PHE:O    | 2:D2:244:TYR:OH   | 2.10                     | 0.69              |
| 1:d1:191:ILE:HG23 | 1:d1:212:LEU:HD23 | 1.74                     | 0.69              |
| 1:g1:195:VAL:HG13 | 1:g1:210:VAL:HB   | 1.74                     | 0.69              |
| 6:U2:92:GLN:HE21  | 7:a2:19:LYS:HG2   | 1.56                     | 0.69              |
| 8:b2:35:ARG:O     | 8:b2:173:ARG:NH2  | 2.24                     | 0.69              |
| 9:p2:172:GLN:HE21 | 11:d3:54:GLN:NE2  | 1.89                     | 0.69              |
| 9:v2:2:ILE:HG22   | 9:v2:4:SER:H      | 1.57                     | 0.69              |
| 9:22:23:ALA:CB    | 12:A4:45:LYS:CD   | 2.65                     | 0.69              |
| 10:R3:86:VAL:HB   | 10:R3:142:ASN:OD1 | 1.92                     | 0.69              |
| 11:c3:98:ARG:HG3  | 11:d3:188:GLN:HG2 | 1.73                     | 0.69              |
| 11:s3:97:ALA:HB1  | 11:s3:171:ILE:CD1 | 2.20                     | 0.69              |
| 11:w3:21:ARG:NH1  | 11:x3:267:GLU:OE1 | 2.24                     | 0.69              |
| 1:B1:165:PHE:CE2  | 2:C2:162:PRO:C    | 2.67                     | 0.69              |
| 1:C1:139:GLU:HG2  | 1:E1:156:HIS:HE1  | 1.57                     | 0.69              |
| 1:E1:375:THR:OG1  | 1:F1:275:LYS:NZ   | 2.24                     | 0.69              |
| 1:X1:139:GLU:OE2  | 1:Y1:154:ARG:NH1  | 2.24                     | 0.69              |
| 1:f1:259:ASN:OD1  | 1:f1:260:GLY:N    | 2.25                     | 0.69              |
| 2:C2:86:ASN:HA    | 2:C2:90:LEU:HD12  | 1.73                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:c2:181:LEU:HD21 | 8:c2:193:LEU:HD11 | 1.74                     | 0.69              |
| 9:i2:98:LYS:HB2   | 9:t2:45:LEU:HD21  | 1.74                     | 0.69              |
| 9:p2:139:ALA:CB   | 11:c3:51:GLN:NE2  | 2.53                     | 0.69              |
| 9:t2:46:TYR:HA    | 9:t2:69:GLY:HA2   | 1.73                     | 0.69              |
| 9:22:238:ARG:CZ   | 12:A4:55:ASN:HD22 | 2.04                     | 0.69              |
| 10:V3:86:VAL:HB   | 10:V3:142:ASN:OD1 | 1.92                     | 0.69              |
| 11:j3:97:ALA:HB1  | 11:j3:171:ILE:CD1 | 2.20                     | 0.69              |
| 11:n3:20:GLU:OE2  | 11:o3:359:ARG:HB3 | 1.92                     | 0.69              |
| 11:s3:98:ARG:HG3  | 11:t3:188:GLN:HG2 | 1.74                     | 0.69              |
| 11:t3:97:ALA:HB1  | 11:t3:171:ILE:CD1 | 2.21                     | 0.69              |
| 1:I1:125:GLN:OE1  | 4:G2:72:LEU:HA    | 1.92                     | 0.69              |
| 1:Q1:190:GLN:HG2  | 1:R1:217:GLY:HA3  | 1.74                     | 0.69              |
| 1:Q1:213:VAL:HG22 | 1:Q1:219:LEU:HD23 | 1.73                     | 0.69              |
| 1:d1:214:ASP:OD1  | 1:d1:215:GLN:N    | 2.25                     | 0.69              |
| 6:U2:95:LEU:HB2   | 8:f2:46:VAL:HG13  | 1.74                     | 0.69              |
| 9:t2:44:LEU:HD12  | 9:t2:71:GLY:HA3   | 1.73                     | 0.69              |
| 10:C3:86:VAL:HB   | 10:C3:142:ASN:OD1 | 1.92                     | 0.69              |
| 10:N3:86:VAL:HB   | 10:N3:142:ASN:OD1 | 1.92                     | 0.69              |
| 11:h3:20:GLU:OE2  | 11:i3:359:ARG:HB3 | 1.92                     | 0.69              |
| 1:L1:409:MET:HE1  | 1:L1:434:ASN:HB2  | 1.74                     | 0.69              |
| 1:h1:394:LYS:HG2  | 1:h1:402:LEU:HB2  | 1.74                     | 0.69              |
| 11:e3:21:ARG:NH1  | 11:f3:267:GLU:OE1 | 2.24                     | 0.69              |
| 11:y3:20:GLU:OE2  | 11:z3:359:ARG:HB3 | 1.93                     | 0.69              |
| 1:B1:214:ASP:OD1  | 1:B1:215:GLN:N    | 2.26                     | 0.69              |
| 1:C1:125:GLN:HB3  | 4:H2:75:ASP:CG    | 2.17                     | 0.69              |
| 1:E1:167:ARG:CG   | 2:B2:244:TYR:HD2  | 1.98                     | 0.69              |
| 1:E1:167:ARG:HB2  | 2:B2:140:ARG:HH12 | 1.56                     | 0.69              |
| 1:d1:296:ARG:NH1  | 1:d1:362:GLU:OE2  | 2.25                     | 0.69              |
| 2:C2:199:VAL:HG23 | 4:I2:21:ALA:HB2   | 1.74                     | 0.69              |
| 2:E2:205:MET:HE1  | 4:J2:51:PHE:CD1   | 2.28                     | 0.69              |
| 9:n2:185:GLU:HB3  | 9:t2:52:PRO:HG2   | 1.74                     | 0.69              |
| 9:y2:38:ARG:HH21  | 9:y2:40:VAL:HG22  | 1.57                     | 0.69              |
| 9:32:240:TYR:OH   | 12:B4:49:PRO:HB3  | 1.92                     | 0.69              |
| 10:B3:86:VAL:HB   | 10:B3:142:ASN:OD1 | 1.92                     | 0.69              |
| 10:H3:86:VAL:HB   | 10:H3:142:ASN:OD1 | 1.92                     | 0.69              |
| 11:a3:88:MET:HG2  | 11:a3:110:MET:HG3 | 1.74                     | 0.69              |
| 11:j3:20:GLU:OE2  | 11:k3:359:ARG:HB3 | 1.91                     | 0.69              |
| 11:k3:97:ALA:HB1  | 11:k3:171:ILE:CD1 | 2.20                     | 0.69              |
| 11:q3:98:ARG:HG3  | 11:r3:188:GLN:HG2 | 1.74                     | 0.69              |
| 11:s3:88:MET:HG2  | 11:s3:110:MET:HG3 | 1.74                     | 0.69              |
| 11:t3:20:GLU:OE2  | 11:u3:359:ARG:HB3 | 1.92                     | 0.69              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:v3:20:GLU:OE2   | 11:w3:359:ARG:HB3 | 1.92                     | 0.69              |
| 11:z3:88:MET:HG2   | 11:z3:110:MET:HG3 | 1.73                     | 0.69              |
| 1:E1:373:ARG:NH1   | 1:F1:277:GLN:OE1  | 2.24                     | 0.69              |
| 1:E1:378:ASN:ND2   | 1:E1:381:ASP:OD1  | 2.24                     | 0.69              |
| 1:U1:139:GLU:HB3   | 1:W1:156:HIS:CE1  | 2.27                     | 0.69              |
| 1:Z1:271:ASP:HB3   | 1:Z1:383:GLU:OE2  | 1.92                     | 0.69              |
| 1:Z1:404:LEU:HD23  | 1:Z1:408:GLN:HG2  | 1.74                     | 0.69              |
| 1:d1:179:THR:HA    | 1:d1:215:GLN:HB3  | 1.74                     | 0.69              |
| 1:h1:164:LEU:HD12  | 2:C2:143:ARG:CD   | 2.22                     | 0.69              |
| 10:W3:86:VAL:HB    | 10:W3:142:ASN:OD1 | 1.92                     | 0.69              |
| 11:t3:88:MET:HG2   | 11:t3:110:MET:HG3 | 1.74                     | 0.69              |
| 11:u3:88:MET:HG2   | 11:u3:110:MET:HG3 | 1.74                     | 0.69              |
| 11:v3:88:MET:HG2   | 11:v3:110:MET:HG3 | 1.73                     | 0.69              |
| 11:w3:98:ARG:HG3   | 11:x3:188:GLN:HG2 | 1.74                     | 0.69              |
| 1:Q1:151:LYS:NZ    | 1:Q1:180:LEU:O    | 2.25                     | 0.69              |
| 1:Q1:151:LYS:HZ1   | 1:Q1:182:PRO:HD3  | 1.57                     | 0.69              |
| 1:Q1:205:LEU:HD12  | 1:Q1:206:PRO:HD2  | 1.73                     | 0.69              |
| 1:R1:164:LEU:HD13  | 3:F2:174:ARG:HD3  | 1.73                     | 0.69              |
| 1:c1:214:ASP:OD1   | 1:c1:215:GLN:N    | 2.26                     | 0.69              |
| 10:A3:213:ILE:HG23 | 10:C3:136:GLY:HA3 | 1.74                     | 0.69              |
| 10:D3:86:VAL:HB    | 10:D3:142:ASN:OD1 | 1.92                     | 0.69              |
| 10:U3:86:VAL:HB    | 10:U3:142:ASN:OD1 | 1.92                     | 0.69              |
| 11:b3:88:MET:HG2   | 11:b3:110:MET:HG3 | 1.74                     | 0.69              |
| 11:g3:98:ARG:HG3   | 11:h3:188:GLN:HG2 | 1.74                     | 0.69              |
| 11:y3:88:MET:HG2   | 11:y3:110:MET:HG3 | 1.73                     | 0.69              |
| 1:I1:182:PRO:O     | 1:I1:184:ARG:NH1  | 2.25                     | 0.69              |
| 1:R1:165:PHE:CE2   | 3:F2:250:LEU:CA   | 2.65                     | 0.69              |
| 1:W1:413:GLU:OE2   | 1:W1:417:ARG:NH1  | 2.26                     | 0.69              |
| 1:X1:167:ARG:HG3   | 2:E2:160:GLN:OE1  | 1.93                     | 0.69              |
| 1:a1:200:SER:OG    | 1:c1:173:SER:OG   | 2.11                     | 0.69              |
| 1:g1:244:ARG:HH11  | 1:h1:239:ASN:HB2  | 1.57                     | 0.69              |
| 1:h1:181:GLU:HB3   | 1:h1:184:ARG:HH21 | 1.58                     | 0.69              |
| 3:F2:108:LEU:O     | 3:F2:121:ASN:ND2  | 2.20                     | 0.69              |
| 7:W2:90:TYR:CZ     | 9:h2:45:LEU:HD22  | 2.27                     | 0.69              |
| 9:h2:143:PRO:HD3   | 9:h2:170:VAL:HG21 | 1.75                     | 0.69              |
| 9:o2:26:LEU:HD22   | 9:s2:242:ILE:HG21 | 1.73                     | 0.69              |
| 9:o2:89:THR:HG23   | 9:o2:91:ASN:H     | 1.58                     | 0.69              |
| 9:o2:168:VAL:HG23  | 11:t3:54:GLN:HG2  | 1.75                     | 0.69              |
| 9:t2:115:THR:HB    | 9:t2:191:LEU:HD23 | 1.75                     | 0.69              |
| 9:z2:51:GLN:HB3    | 9:z2:54:ALA:HB2   | 1.75                     | 0.69              |
| 10:J3:86:VAL:HB    | 10:J3:142:ASN:OD1 | 1.92                     | 0.69              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:i3:98:ARG:HG3   | 11:j3:188:GLN:HG2 | 1.73                     | 0.69              |
| 11:l3:97:ALA:HB1   | 11:l3:171:ILE:CD1 | 2.20                     | 0.69              |
| 11:l3:98:ARG:HG3   | 11:m3:188:GLN:HG2 | 1.73                     | 0.69              |
| 11:q3:20:GLU:OE2   | 11:r3:359:ARG:HB3 | 1.93                     | 0.69              |
| 1:R1:231:ASN:O     | 1:R1:234:GLN:NE2  | 2.26                     | 0.69              |
| 1:c1:275:LYS:HB2   | 1:c1:377:MET:HB2  | 1.73                     | 0.69              |
| 2:A2:39:SER:C      | 2:A2:41:SER:H     | 2.01                     | 0.69              |
| 2:C2:236:MET:CE    | 2:D2:176:THR:CG2  | 2.70                     | 0.69              |
| 6:T2:102:MET:HG3   | 6:T2:106:ARG:HE   | 1.56                     | 0.69              |
| 7:Y2:113:GLN:OE1   | 8:d2:243:ARG:NE   | 2.26                     | 0.69              |
| 9:k2:143:PRO:HG2   | 9:k2:159:VAL:HG21 | 1.74                     | 0.69              |
| 9:n2:169:GLN:C     | 11:y3:54:GLN:CD   | 2.55                     | 0.69              |
| 9:t2:174:ASN:HA    | 9:t2:206:PRO:HD3  | 1.73                     | 0.69              |
| 9:v2:122:VAL:O     | 9:l2:180:ASN:ND2  | 2.26                     | 0.69              |
| 9:y2:79:ARG:NH2    | 9:y2:184:LEU:O    | 2.22                     | 0.69              |
| 10:T3:86:VAL:HB    | 10:T3:142:ASN:OD1 | 1.92                     | 0.69              |
| 11:a3:98:ARG:HG3   | 11:b3:188:GLN:HG2 | 1.74                     | 0.69              |
| 11:n3:258:ARG:NH2  | 11:n3:365:ILE:O   | 2.26                     | 0.69              |
| 11:r3:258:ARG:NH2  | 11:r3:365:ILE:O   | 2.26                     | 0.69              |
| 11:s3:258:ARG:NH2  | 11:s3:365:ILE:O   | 2.26                     | 0.69              |
| 11:w3:88:MET:HG2   | 11:w3:110:MET:HG3 | 1.74                     | 0.69              |
| 11:x3:21:ARG:NH1   | 11:y3:267:GLU:OE1 | 2.24                     | 0.69              |
| 1:X1:199:SER:OG    | 1:X1:205:LEU:O    | 2.08                     | 0.69              |
| 1:b1:392:ASN:OD1   | 1:b1:393:TYR:N    | 2.26                     | 0.69              |
| 6:U2:24:GLU:OE1    | 7:Z2:5:ASN:ND2    | 2.26                     | 0.69              |
| 8:d2:249:SER:OG    | 8:d2:250:MET:SD   | 2.51                     | 0.69              |
| 10:R3:213:ILE:HG23 | 10:T3:136:GLY:HA3 | 1.75                     | 0.69              |
| 11:i3:258:ARG:NH2  | 11:i3:365:ILE:O   | 2.26                     | 0.69              |
| 11:j3:258:ARG:NH2  | 11:j3:365:ILE:O   | 2.26                     | 0.69              |
| 11:k3:258:ARG:NH2  | 11:k3:365:ILE:O   | 2.26                     | 0.69              |
| 11:m3:97:ALA:HB1   | 11:m3:171:ILE:CD1 | 2.20                     | 0.69              |
| 11:o3:98:ARG:HG3   | 11:p3:188:GLN:HG2 | 1.73                     | 0.69              |
| 1:T1:167:ARG:CZ    | 2:E2:106:ASP:CB   | 2.71                     | 0.68              |
| 1:a1:191:ILE:HG23  | 1:a1:212:LEU:HD21 | 1.75                     | 0.68              |
| 1:e1:257:VAL:O     | 1:e1:261:ASN:ND2  | 2.24                     | 0.68              |
| 2:A2:41:SER:O      | 2:A2:43:GLN:N     | 2.26                     | 0.68              |
| 9:32:79:ARG:NH2    | 9:32:184:LEU:O    | 2.25                     | 0.68              |
| 10:B3:82:LEU:HD13  | 10:B3:144:PHE:CD1 | 2.29                     | 0.68              |
| 10:S3:213:ILE:HG23 | 10:U3:136:GLY:HA3 | 1.75                     | 0.68              |
| 11:q3:258:ARG:NH2  | 11:q3:365:ILE:O   | 2.26                     | 0.68              |
| 11:x3:88:MET:HG2   | 11:x3:110:MET:HG3 | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:g1:378:ASN:ND2  | 1:g1:381:ASP:OD1  | 2.22                     | 0.68              |
| 1:h1:362:GLU:OE2  | 1:h1:364:SER:OG   | 2.11                     | 0.68              |
| 2:C2:100:ILE:HG21 | 2:C2:243:PHE:CD2  | 2.28                     | 0.68              |
| 9:z2:2:ILE:HG22   | 9:z2:4:SER:H      | 1.59                     | 0.68              |
| 9:12:233:MET:SD   | 12:E4:44:LEU:HD11 | 2.33                     | 0.68              |
| 9:12:237:GLN:OE1  | 12:E4:57:GLU:OE1  | 2.12                     | 0.68              |
| 10:O3:82:LEU:HD13 | 10:O3:144:PHE:CD1 | 2.29                     | 0.68              |
| 11:e3:20:GLU:OE2  | 11:f3:359:ARG:HB3 | 1.93                     | 0.68              |
| 11:g3:258:ARG:NH2 | 11:g3:365:ILE:O   | 2.26                     | 0.68              |
| 11:n3:98:ARG:HG3  | 11:o3:188:GLN:HG2 | 1.73                     | 0.68              |
| 1:L1:190:GLN:HG2  | 1:N1:217:GLY:HA3  | 1.75                     | 0.68              |
| 1:X1:416:THR:HG23 | 1:X1:430:LEU:HD21 | 1.75                     | 0.68              |
| 2:B2:105:ILE:HG22 | 5:N2:32:VAL:HG21  | 1.75                     | 0.68              |
| 6:U2:98:ASN:OD1   | 6:U2:99:THR:N     | 2.25                     | 0.68              |
| 9:n2:148:SER:HG   | 9:n2:160:THR:HG1  | 1.36                     | 0.68              |
| 9:42:238:ARG:NH1  | 9:42:241:GLU:OE1  | 2.26                     | 0.68              |
| 10:L3:82:LEU:HD13 | 10:L3:144:PHE:CD1 | 2.29                     | 0.68              |
| 10:Q3:86:VAL:HB   | 10:Q3:142:ASN:OD1 | 1.92                     | 0.68              |
| 10:Y3:82:LEU:HD13 | 10:Y3:144:PHE:CD1 | 2.29                     | 0.68              |
| 11:f3:258:ARG:NH2 | 11:f3:365:ILE:O   | 2.26                     | 0.68              |
| 11:k3:98:ARG:HG3  | 11:l3:188:GLN:HG2 | 1.74                     | 0.68              |
| 11:o3:258:ARG:NH2 | 11:o3:365:ILE:O   | 2.26                     | 0.68              |
| 11:v3:258:ARG:NH2 | 11:v3:365:ILE:O   | 2.26                     | 0.68              |
| 1:G1:361:ASN:HB3  | 6:U2:55:ARG:NH2   | 2.08                     | 0.68              |
| 1:H1:155:VAL:HG23 | 1:H1:176:VAL:HG22 | 1.75                     | 0.68              |
| 1:U1:133:GLN:O    | 1:U1:137:GLU:HG2  | 1.92                     | 0.68              |
| 6:T2:14:GLU:OE1   | 6:T2:57:ARG:NH1   | 2.27                     | 0.68              |
| 9:k2:36:ARG:NH2   | 9:k2:229:GLU:OE1  | 2.23                     | 0.68              |
| 9:o2:168:VAL:CA   | 11:t3:54:GLN:HE21 | 2.05                     | 0.68              |
| 9:o2:169:GLN:NE2  | 9:42:55:GLN:OE1   | 2.26                     | 0.68              |
| 9:z2:238:ARG:NE   | 12:E4:48:ASP:HB2  | 2.09                     | 0.68              |
| 10:E3:82:LEU:HD13 | 10:E3:144:PHE:CD1 | 2.29                     | 0.68              |
| 11:l3:258:ARG:NH2 | 11:l3:365:ILE:O   | 2.26                     | 0.68              |
| 11:u3:258:ARG:NH2 | 11:u3:365:ILE:O   | 2.26                     | 0.68              |
| 1:E1:248:ARG:HH11 | 1:F1:267:THR:HG22 | 1.57                     | 0.68              |
| 1:K1:167:ARG:HG2  | 2:A2:244:TYR:CE2  | 2.28                     | 0.68              |
| 1:N1:197:LEU:HD11 | 1:O1:177:THR:HG22 | 1.75                     | 0.68              |
| 1:T1:167:ARG:HH22 | 2:E2:107:LYS:H    | 0.69                     | 0.68              |
| 1:T1:167:ARG:NH1  | 2:E2:107:LYS:CD   | 2.22                     | 0.68              |
| 2:C2:61:MET:HE3   | 2:C2:134:LEU:HD21 | 1.74                     | 0.68              |
| 8:d2:133:SER:HB2  | 8:d2:135:ILE:HG12 | 1.76                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:z2:237:GLN:HG3   | 12:D4:55:ASN:HD21  | 1.56                     | 0.68              |
| 10:I3:86:VAL:HB    | 10:I3:142:ASN:OD1  | 1.92                     | 0.68              |
| 10:Q3:82:LEU:HD13  | 10:Q3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:T3:82:LEU:HD13  | 10:T3:144:PHE:CD1  | 2.29                     | 0.68              |
| 11:d3:258:ARG:NH2  | 11:d3:365:ILE:O    | 2.26                     | 0.68              |
| 11:h3:258:ARG:NH2  | 11:h3:365:ILE:O    | 2.26                     | 0.68              |
| 11:m3:258:ARG:NH2  | 11:m3:365:ILE:O    | 2.26                     | 0.68              |
| 11:p3:258:ARG:NH2  | 11:p3:365:ILE:O    | 2.26                     | 0.68              |
| 1:V1:409:MET:HE1   | 1:V1:434:ASN:HB2   | 1.74                     | 0.68              |
| 9:n2:37:GLN:NE2    | 9:t2:67:GLN:O      | 2.25                     | 0.68              |
| 9:r2:88:GLN:NE2    | 9:r2:90:ASN:OD1    | 2.26                     | 0.68              |
| 9:x2:122:VAL:O     | 9:32:180:ASN:ND2   | 2.27                     | 0.68              |
| 9:y2:145:ASN:HB2   | 9:y2:162:GLN:HB2   | 1.75                     | 0.68              |
| 10:A3:82:LEU:HD13  | 10:A3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:C3:82:LEU:HD13  | 10:C3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:G3:213:ILE:HG23 | 10:I3:136:GLY:HA3  | 1.75                     | 0.68              |
| 10:H3:82:LEU:HD13  | 10:H3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:N3:82:LEU:HD13  | 10:N3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:Q3:213:ILE:HG23 | 10:S3:136:GLY:HA3  | 1.75                     | 0.68              |
| 1:G1:166:VAL:CB    | 2:B2:144:GLU:HG3   | 2.23                     | 0.68              |
| 1:L1:151:LYS:NZ    | 1:L1:180:LEU:O     | 2.22                     | 0.68              |
| 1:O1:191:ILE:HG12  | 1:O1:220:LEU:HD13  | 1.75                     | 0.68              |
| 1:R1:125:GLN:HG2   | 2:E2:234:LEU:CD2   | 2.24                     | 0.68              |
| 1:T1:167:ARG:NH1   | 2:E2:107:LYS:N     | 2.41                     | 0.68              |
| 1:Y1:125:GLN:CB    | 4:J2:75:ASP:OD2    | 2.21                     | 0.68              |
| 2:D2:207:LEU:HD11  | 4:J2:58:VAL:HG11   | 1.75                     | 0.68              |
| 9:s2:36:ARG:HH12   | 9:s2:38:ARG:HB2    | 1.59                     | 0.68              |
| 9:22:92:SER:O      | 9:22:216:GLN:NE2   | 2.22                     | 0.68              |
| 10:K3:82:LEU:HD13  | 10:K3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:W3:82:LEU:HD13  | 10:W3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:Z3:51:ILE:HG13  | 11:b3:175:LEU:HD11 | 1.75                     | 0.68              |
| 11:x3:258:ARG:NH2  | 11:x3:365:ILE:O    | 2.26                     | 0.68              |
| 1:I1:203:ALA:HB1   | 1:K1:160:PRO:HA    | 1.75                     | 0.68              |
| 1:T1:167:ARG:NH1   | 2:E2:106:ASP:HB3   | 2.08                     | 0.68              |
| 1:U1:206:PRO:HG2   | 1:U1:209:ASN:HB2   | 1.74                     | 0.68              |
| 1:d1:389:VAL:HB    | 1:d1:432:VAL:HG12  | 1.75                     | 0.68              |
| 1:f1:165:PHE:CE1   | 2:D2:148:ALA:CB    | 2.76                     | 0.68              |
| 2:C2:75:ARG:HH12   | 2:C2:85:PRO:HB3    | 1.59                     | 0.68              |
| 10:D3:82:LEU:HD13  | 10:D3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:I3:82:LEU:HD13  | 10:I3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:R3:82:LEU:HD13  | 10:R3:144:PHE:CD1  | 2.29                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:V3:82:LEU:HD13  | 10:V3:144:PHE:CD1  | 2.29                     | 0.68              |
| 10:W3:213:ILE:HG23 | 10:Y3:136:GLY:HA3  | 1.75                     | 0.68              |
| 10:Z3:82:LEU:HD13  | 10:Z3:144:PHE:CD1  | 2.29                     | 0.68              |
| 11:b3:89:VAL:HG12  | 11:b3:107:VAL:HG22 | 1.76                     | 0.68              |
| 11:k3:20:GLU:OE2   | 11:l3:359:ARG:HB3  | 1.93                     | 0.68              |
| 11:t3:258:ARG:NH2  | 11:t3:365:ILE:O    | 2.26                     | 0.68              |
| 1:N1:155:VAL:HG23  | 1:N1:176:VAL:HG22  | 1.75                     | 0.68              |
| 1:S1:295:SER:CB    | 6:R2:73:ILE:HD11   | 2.22                     | 0.68              |
| 1:T1:165:PHE:HD2   | 3:F2:167:ASN:CG    | 2.01                     | 0.68              |
| 1:Y1:297:GLN:HB2   | 6:S2:73:ILE:HD11   | 1.76                     | 0.68              |
| 1:a1:133:GLN:O     | 1:a1:137:GLU:HG2   | 1.94                     | 0.68              |
| 7:a2:41:PRO:HB3    | 7:a2:92:LYS:HB3    | 1.75                     | 0.68              |
| 9:g2:75:VAL:O      | 9:l2:51:GLN:NE2    | 2.27                     | 0.68              |
| 9:u2:150:THR:HA    | 9:u2:216:GLN:HE22  | 1.59                     | 0.68              |
| 10:H3:213:ILE:HG23 | 10:J3:136:GLY:HA3  | 1.75                     | 0.68              |
| 10:T3:213:ILE:HG23 | 10:V3:136:GLY:HA3  | 1.75                     | 0.68              |
| 11:a3:258:ARG:NH2  | 11:a3:365:ILE:O    | 2.26                     | 0.68              |
| 11:x3:20:GLU:OE2   | 11:y3:359:ARG:HB3  | 1.93                     | 0.68              |
| 1:D1:416:THR:HG23  | 1:D1:430:LEU:HD11  | 1.76                     | 0.68              |
| 1:F1:404:LEU:HD23  | 1:F1:434:ASN:HD21  | 1.57                     | 0.68              |
| 1:J1:266:VAL:HG22  | 1:J1:387:VAL:HG22  | 1.74                     | 0.68              |
| 1:M1:414:ASP:OD2   | 1:N1:431:ASN:ND2   | 2.27                     | 0.68              |
| 1:Q1:246:GLN:NE2   | 1:Q1:250:GLU:OE2   | 2.27                     | 0.68              |
| 9:p2:189:GLU:HA    | 9:u2:42:GLU:HG2    | 1.75                     | 0.68              |
| 9:s2:127:GLN:NE2   | 11:p3:78:ASN:ND2   | 2.40                     | 0.68              |
| 9:s2:227:ALA:HA    | 9:42:257:LEU:HD21  | 1.76                     | 0.68              |
| 10:F3:82:LEU:HD13  | 10:F3:144:PHE:CD1  | 2.29                     | 0.68              |
| 1:H1:190:GLN:HG2   | 1:I1:217:GLY:HA3   | 1.75                     | 0.67              |
| 1:M1:295:SER:CB    | 6:Q2:65:LEU:HD22   | 2.23                     | 0.67              |
| 1:X1:216:SER:HG    | 1:X1:218:HIS:HE2   | 1.40                     | 0.67              |
| 1:Z1:294:ARG:NE    | 6:S2:68:THR:HB     | 2.08                     | 0.67              |
| 1:a1:200:SER:HG    | 1:c1:173:SER:HG    | 1.42                     | 0.67              |
| 1:a1:362:GLU:OE2   | 1:a1:364:SER:OG    | 2.11                     | 0.67              |
| 2:D2:204:LEU:HD22  | 2:D2:209:MET:HG3   | 1.75                     | 0.67              |
| 7:X2:90:TYR:CZ     | 9:i2:45:LEU:HD22   | 2.30                     | 0.67              |
| 9:n2:99:GLY:O      | 9:n2:116:ARG:NH2   | 2.27                     | 0.67              |
| 10:F3:213:ILE:HG23 | 10:H3:136:GLY:HA3  | 1.75                     | 0.67              |
| 10:J3:82:LEU:HD13  | 10:J3:144:PHE:CD1  | 2.29                     | 0.67              |
| 10:Q3:43:PRO:HD2   | 10:Q3:43:PRO:O     | 1.94                     | 0.67              |
| 11:c3:89:VAL:HG12  | 11:c3:107:VAL:HG22 | 1.76                     | 0.67              |
| 11:y3:258:ARG:NH2  | 11:y3:365:ILE:O    | 2.26                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B1:167:ARG:NH1   | 2:C2:164:ALA:HB3   | 2.07                     | 0.67              |
| 1:E1:174:ALA:HB3   | 1:E1:210:VAL:HG12  | 1.76                     | 0.67              |
| 1:T1:165:PHE:HB3   | 3:F2:166:SER:CB    | 2.24                     | 0.67              |
| 1:W1:233:ALA:HA    | 1:W1:236:LYS:HE2   | 1.74                     | 0.67              |
| 1:X1:151:LYS:NZ    | 1:X1:180:LEU:O     | 2.26                     | 0.67              |
| 1:Z1:297:GLN:HB2   | 6:S2:65:LEU:HD21   | 1.76                     | 0.67              |
| 9:h2:129:VAL:HG21  | 9:r2:63:PRO:HG3    | 1.76                     | 0.67              |
| 10:G3:82:LEU:HD13  | 10:G3:144:PHE:CD1  | 2.29                     | 0.67              |
| 10:U3:43:PRO:O     | 10:U3:43:PRO:HD2   | 1.94                     | 0.67              |
| 11:c3:258:ARG:NH2  | 11:c3:365:ILE:O    | 2.26                     | 0.67              |
| 11:f3:89:VAL:HG12  | 11:f3:107:VAL:HG22 | 1.76                     | 0.67              |
| 11:y3:89:VAL:HG12  | 11:y3:107:VAL:HG22 | 1.76                     | 0.67              |
| 1:C1:275:LYS:HB2   | 1:C1:377:MET:HB2   | 1.76                     | 0.67              |
| 1:D1:249:ILE:HD11  | 1:D1:416:THR:HA    | 1.75                     | 0.67              |
| 1:G1:221:THR:HG22  | 1:G1:223:SER:H     | 1.59                     | 0.67              |
| 1:Q1:179:THR:HA    | 1:Q1:215:GLN:HB3   | 1.77                     | 0.67              |
| 1:R1:375:THR:HG23  | 1:S1:275:LYS:NZ    | 2.09                     | 0.67              |
| 2:A2:185:ILE:HG23  | 4:G2:84:LEU:HD21   | 1.77                     | 0.67              |
| 3:F2:102:ILE:HD11  | 3:F2:187:ALA:HB1   | 1.75                     | 0.67              |
| 8:c2:42:ARG:NH1    | 9:h2:64:SER:OG     | 2.27                     | 0.67              |
| 8:c2:173:ARG:HB3   | 9:h2:67:GLN:HE22   | 1.59                     | 0.67              |
| 9:n2:167:PRO:HG3   | 9:z2:196:GLN:HG2   | 1.76                     | 0.67              |
| 9:32:29:VAL:CG2    | 12:B4:37:LEU:CD2   | 2.72                     | 0.67              |
| 10:G3:43:PRO:O     | 10:G3:43:PRO:HD2   | 1.94                     | 0.67              |
| 10:H3:43:PRO:HD2   | 10:H3:43:PRO:O     | 1.94                     | 0.67              |
| 10:X3:39:PRO:HB3   | 10:Y3:75:GLY:HA3   | 1.77                     | 0.67              |
| 1:U1:165:PHE:CE2   | 2:E2:244:TYR:CE2   | 2.81                     | 0.67              |
| 10:B3:213:ILE:HG23 | 10:D3:136:GLY:HA3  | 1.75                     | 0.67              |
| 10:C3:43:PRO:HD2   | 10:C3:43:PRO:O     | 1.94                     | 0.67              |
| 10:I3:213:ILE:HG23 | 10:K3:136:GLY:HA3  | 1.76                     | 0.67              |
| 10:M3:82:LEU:HD13  | 10:M3:144:PHE:CD1  | 2.29                     | 0.67              |
| 10:S3:82:LEU:HD13  | 10:S3:144:PHE:CD1  | 2.29                     | 0.67              |
| 11:e3:89:VAL:HG12  | 11:e3:107:VAL:HG22 | 1.76                     | 0.67              |
| 11:w3:20:GLU:OE2   | 11:x3:359:ARG:HB3  | 1.93                     | 0.67              |
| 1:G1:199:SER:HA    | 1:G1:205:LEU:HD23  | 1.76                     | 0.67              |
| 1:L1:408:GLN:O     | 1:L1:412:ILE:HG12  | 1.95                     | 0.67              |
| 1:S1:407:ASP:O     | 1:S1:411:GLN:HG2   | 1.95                     | 0.67              |
| 1:T1:167:ARG:HH12  | 2:E2:107:LYS:N     | 1.92                     | 0.67              |
| 1:c1:392:ASN:OD1   | 1:c1:393:TYR:N     | 2.27                     | 0.67              |
| 1:h1:164:LEU:CD1   | 2:C2:143:ARG:HD3   | 2.19                     | 0.67              |
| 8:d2:118:HIS:ND1   | 8:d2:118:HIS:O     | 2.25                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:i2:143:PRO:HD3   | 9:i2:170:VAL:HG21  | 1.76                     | 0.67              |
| 9:n2:168:VAL:CG2   | 11:x3:80:GLN:OE1   | 2.42                     | 0.67              |
| 10:L3:213:ILE:HG23 | 10:N3:136:GLY:HA3  | 1.75                     | 0.67              |
| 10:M3:213:ILE:HG23 | 10:O3:136:GLY:HA3  | 1.75                     | 0.67              |
| 10:U3:82:LEU:HD13  | 10:U3:144:PHE:CD1  | 2.29                     | 0.67              |
| 11:m3:98:ARG:HG3   | 11:n3:188:GLN:HG2  | 1.74                     | 0.67              |
| 11:x3:89:VAL:HG12  | 11:x3:107:VAL:HG22 | 1.76                     | 0.67              |
| 1:M1:295:SER:HB3   | 6:Q2:65:LEU:CD2    | 2.25                     | 0.67              |
| 1:O1:137:GLU:OE1   | 1:O1:155:VAL:HG13  | 1.94                     | 0.67              |
| 1:Q1:143:THR:HG1   | 1:R1:156:HIS:CE1   | 2.13                     | 0.67              |
| 1:T1:165:PHE:HA    | 3:F2:166:SER:HB2   | 1.77                     | 0.67              |
| 1:Y1:275:LYS:HB2   | 1:Y1:377:MET:HB2   | 1.76                     | 0.67              |
| 1:a1:248:ARG:NH1   | 1:b1:267:THR:OG1   | 2.26                     | 0.67              |
| 7:X2:117:GLU:OE1   | 8:d2:248:LEU:HB2   | 1.94                     | 0.67              |
| 8:f2:153:ASN:HA    | 9:q2:196:GLN:HG2   | 1.76                     | 0.67              |
| 9:42:233:MET:HE1   | 12:C4:40:LEU:HD21  | 1.75                     | 0.67              |
| 10:R3:43:PRO:O     | 10:R3:43:PRO:HD2   | 1.94                     | 0.67              |
| 10:T3:43:PRO:HD2   | 10:T3:43:PRO:O     | 1.94                     | 0.67              |
| 10:V3:43:PRO:HD2   | 10:V3:43:PRO:O     | 1.94                     | 0.67              |
| 10:X3:125:GLU:HB3  | 10:Y3:108:THR:HB   | 1.77                     | 0.67              |
| 11:b3:258:ARG:NH2  | 11:b3:365:ILE:O    | 2.26                     | 0.67              |
| 1:J1:360:ARG:NH1   | 1:J1:362:GLU:OE2   | 2.27                     | 0.67              |
| 7:X2:40:GLN:HG3    | 7:X2:41:PRO:HD2    | 1.77                     | 0.67              |
| 10:D3:43:PRO:O     | 10:D3:43:PRO:HD2   | 1.94                     | 0.67              |
| 10:P3:82:LEU:HD13  | 10:P3:144:PHE:CD1  | 2.29                     | 0.67              |
| 10:P3:213:ILE:HG23 | 10:R3:136:GLY:HA3  | 1.76                     | 0.67              |
| 10:U3:213:ILE:HG23 | 10:W3:136:GLY:HA3  | 1.76                     | 0.67              |
| 10:X3:82:LEU:HD13  | 10:X3:144:PHE:CD1  | 2.29                     | 0.67              |
| 11:a3:188:GLN:HG2  | 11:z3:98:ARG:HG3   | 1.75                     | 0.67              |
| 11:e3:258:ARG:NH2  | 11:e3:365:ILE:O    | 2.26                     | 0.67              |
| 11:i3:33:GLU:OE1   | 11:i3:92:SER:OG    | 2.13                     | 0.67              |
| 11:z3:258:ARG:NH2  | 11:z3:365:ILE:O    | 2.26                     | 0.67              |
| 12:D4:90:SER:OG    | 12:E4:92:GLN:NE2   | 2.28                     | 0.67              |
| 1:I1:253:LEU:HD11  | 1:I1:412:ILE:HG23  | 1.75                     | 0.67              |
| 1:T1:166:VAL:HG22  | 1:T1:168:GLU:H     | 1.58                     | 0.67              |
| 2:A2:192:PRO:HA    | 2:A2:195:ILE:HD12  | 1.77                     | 0.67              |
| 4:I2:3:PRO:HA      | 4:I2:6:VAL:HG12    | 1.75                     | 0.67              |
| 4:J2:20:LEU:HD12   | 4:J2:69:MET:HB2    | 1.75                     | 0.67              |
| 9:q2:99:GLY:O      | 9:q2:116:ARG:NH2   | 2.28                     | 0.67              |
| 9:r2:230:LEU:HD12  | 9:32:257:LEU:HG    | 1.75                     | 0.67              |
| 9:y2:16:GLN:HE22   | 9:42:2:ILE:HD12    | 1.60                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:K3:213:ILE:HG23 | 10:M3:136:GLY:HA3  | 1.76                     | 0.67              |
| 10:P3:43:PRO:HD2   | 10:P3:43:PRO:O     | 1.94                     | 0.67              |
| 11:r3:33:GLU:OE1   | 11:r3:92:SER:OG    | 2.13                     | 0.67              |
| 1:C1:155:VAL:HG23  | 1:C1:176:VAL:HG22  | 1.75                     | 0.67              |
| 1:U1:365:ASN:CG    | 6:R2:64:ALA:O      | 2.36                     | 0.67              |
| 5:L2:55:GLN:NE2    | 5:L2:74:ASP:OD1    | 2.26                     | 0.67              |
| 6:R2:90:PRO:HB3    | 6:R2:99:THR:HB     | 1.76                     | 0.67              |
| 9:k2:230:LEU:HD21  | 9:p2:242:ILE:HD12  | 1.76                     | 0.67              |
| 9:y2:26:LEU:HD23   | 9:42:246:ALA:HB2   | 1.77                     | 0.67              |
| 10:B3:43:PRO:O     | 10:B3:43:PRO:HD2   | 1.94                     | 0.67              |
| 11:a3:89:VAL:HG12  | 11:a3:107:VAL:HG22 | 1.76                     | 0.67              |
| 11:o3:89:VAL:HG12  | 11:o3:107:VAL:HG22 | 1.76                     | 0.67              |
| 12:D4:138:ALA:HB1  | 12:D4:182:ILE:HD11 | 1.77                     | 0.67              |
| 1:E1:275:LYS:HB2   | 1:E1:377:MET:HB2   | 1.77                     | 0.67              |
| 1:g1:181:GLU:HB3   | 1:g1:184:ARG:HH21  | 1.60                     | 0.67              |
| 7:Y2:41:PRO:HB3    | 7:Y2:92:LYS:HB3    | 1.77                     | 0.67              |
| 9:g2:44:LEU:HD12   | 9:g2:71:GLY:HA3    | 1.76                     | 0.67              |
| 10:J3:213:ILE:HG23 | 10:L3:136:GLY:HA3  | 1.76                     | 0.67              |
| 10:N3:213:ILE:HG23 | 10:P3:136:GLY:HA3  | 1.75                     | 0.67              |
| 11:h3:33:GLU:OE1   | 11:h3:92:SER:OG    | 2.13                     | 0.67              |
| 11:s3:33:GLU:OE1   | 11:s3:92:SER:OG    | 2.13                     | 0.67              |
| 11:w3:258:ARG:NH2  | 11:w3:365:ILE:O    | 2.26                     | 0.67              |
| 11:z3:89:VAL:HG12  | 11:z3:107:VAL:HG22 | 1.76                     | 0.67              |
| 1:B1:256:ILE:HG21  | 1:B1:412:ILE:HD11  | 1.75                     | 0.66              |
| 1:D1:253:LEU:HD11  | 1:D1:412:ILE:HG23  | 1.77                     | 0.66              |
| 1:g1:182:PRO:O     | 1:g1:184:ARG:NH1   | 2.28                     | 0.66              |
| 6:U2:95:LEU:HD12   | 8:f2:46:VAL:HA     | 1.75                     | 0.66              |
| 9:h2:98:LYS:HG3    | 9:s2:45:LEU:HD11   | 1.77                     | 0.66              |
| 9:o2:151:ILE:HG12  | 9:o2:157:VAL:HG12  | 1.76                     | 0.66              |
| 9:u2:110:GLY:N     | 11:z3:80:GLN:HE22  | 1.91                     | 0.66              |
| 10:F3:43:PRO:HD2   | 10:F3:43:PRO:O     | 1.94                     | 0.66              |
| 10:O3:213:ILE:HG23 | 10:Q3:136:GLY:HA3  | 1.76                     | 0.66              |
| 11:g3:89:VAL:HG12  | 11:g3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:m3:89:VAL:HG12  | 11:m3:107:VAL:HG22 | 1.76                     | 0.66              |
| 1:C1:362:GLU:OE2   | 1:C1:364:SER:OG    | 2.13                     | 0.66              |
| 1:U1:161:LYS:HZ1   | 2:E2:245:SER:C     | 2.03                     | 0.66              |
| 2:A2:228:LEU:HD11  | 4:H2:6:VAL:HG11    | 1.78                     | 0.66              |
| 9:j2:153:ARG:NH2   | 9:p2:189:GLU:OE2   | 2.28                     | 0.66              |
| 9:x2:2:ILE:HG22    | 9:x2:4:SER:H       | 1.60                     | 0.66              |
| 10:A3:39:PRO:HB3   | 10:B3:75:GLY:HA3   | 1.78                     | 0.66              |
| 10:A3:108:THR:HB   | 10:Z3:125:GLU:HB3  | 1.77                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:C3:213:ILE:HG23 | 10:E3:136:GLY:HA3  | 1.76                     | 0.66              |
| 10:E3:213:ILE:HG23 | 10:G3:136:GLY:HA3  | 1.76                     | 0.66              |
| 10:V3:213:ILE:HG23 | 10:X3:136:GLY:HA3  | 1.76                     | 0.66              |
| 10:Y3:43:PRO:HD2   | 10:Y3:43:PRO:O     | 1.94                     | 0.66              |
| 11:d3:33:GLU:OE1   | 11:d3:92:SER:OG    | 2.13                     | 0.66              |
| 11:j3:33:GLU:OE1   | 11:j3:92:SER:OG    | 2.13                     | 0.66              |
| 11:m3:33:GLU:OE1   | 11:m3:92:SER:OG    | 2.13                     | 0.66              |
| 11:n3:33:GLU:OE1   | 11:n3:92:SER:OG    | 2.13                     | 0.66              |
| 11:q3:33:GLU:OE1   | 11:q3:92:SER:OG    | 2.13                     | 0.66              |
| 11:u3:89:VAL:HG12  | 11:u3:107:VAL:HG22 | 1.76                     | 0.66              |
| 1:K1:167:ARG:HD2   | 2:A2:244:TYR:O     | 1.95                     | 0.66              |
| 1:L1:370:ARG:HB3   | 1:M1:280:GLU:OE1   | 1.96                     | 0.66              |
| 1:Y1:295:SER:CB    | 6:S2:72:HIS:HA     | 2.26                     | 0.66              |
| 1:c1:203:ALA:HA    | 1:d1:158:ALA:HB1   | 1.76                     | 0.66              |
| 1:d1:145:GLU:OE2   | 1:d1:153:ALA:N     | 2.27                     | 0.66              |
| 9:22:23:ALA:CB     | 12:A4:45:LYS:HG3   | 2.24                     | 0.66              |
| 10:W3:125:GLU:HB3  | 10:X3:108:THR:HB   | 1.78                     | 0.66              |
| 10:X3:43:PRO:HD2   | 10:X3:43:PRO:O     | 1.94                     | 0.66              |
| 11:j3:345:LEU:HD21 | 11:k3:319:LEU:HD22 | 1.77                     | 0.66              |
| 1:E1:203:ALA:HA    | 1:G1:158:ALA:HB1   | 1.78                     | 0.66              |
| 1:X1:216:SER:OG    | 1:X1:218:HIS:NE2   | 2.28                     | 0.66              |
| 1:c1:246:GLN:NE2   | 1:c1:250:GLU:OE2   | 2.27                     | 0.66              |
| 1:g1:167:ARG:CD    | 2:C2:244:TYR:CD2   | 2.76                     | 0.66              |
| 2:C2:224:MET:HE1   | 4:J2:6:VAL:HG11    | 1.77                     | 0.66              |
| 8:e2:123:GLU:HG3   | 8:e2:160:ARG:HB3   | 1.75                     | 0.66              |
| 9:y2:238:ARG:NH2   | 12:D4:52:PRO:CB    | 2.56                     | 0.66              |
| 10:H3:125:GLU:HB3  | 10:I3:108:THR:HB   | 1.78                     | 0.66              |
| 10:I3:43:PRO:HD2   | 10:I3:43:PRO:O     | 1.94                     | 0.66              |
| 10:U3:125:GLU:HB3  | 10:V3:108:THR:HB   | 1.78                     | 0.66              |
| 11:e3:33:GLU:OE1   | 11:e3:92:SER:OG    | 2.13                     | 0.66              |
| 11:p3:89:VAL:HG12  | 11:p3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:r3:89:VAL:HG12  | 11:r3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:t3:89:VAL:HG12  | 11:t3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:w3:33:GLU:OE1   | 11:w3:92:SER:OG    | 2.13                     | 0.66              |
| 11:x3:33:GLU:OE1   | 11:x3:92:SER:OG    | 2.13                     | 0.66              |
| 1:B1:151:LYS:NZ    | 1:B1:181:GLU:HA    | 2.10                     | 0.66              |
| 1:B1:203:ALA:HA    | 1:C1:158:ALA:HB1   | 1.77                     | 0.66              |
| 1:I1:151:LYS:NZ    | 1:I1:180:LEU:O     | 2.28                     | 0.66              |
| 1:N1:423:SER:OG    | 1:N1:425:LYS:NZ    | 2.28                     | 0.66              |
| 1:R1:179:THR:HA    | 1:R1:215:GLN:HB3   | 1.76                     | 0.66              |
| 1:S1:362:GLU:OE2   | 1:S1:364:SER:OG    | 2.13                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:c1:145:GLU:OE1  | 1:c1:153:ALA:N    | 2.28                     | 0.66              |
| 1:h1:132:TYR:CZ   | 1:h1:136:LEU:HD11 | 2.30                     | 0.66              |
| 6:T2:95:LEU:HG    | 8:e2:46:VAL:HG13  | 1.78                     | 0.66              |
| 8:c2:91:GLN:HB2   | 8:c2:121:ILE:HD11 | 1.77                     | 0.66              |
| 9:q2:98:LYS:O     | 9:q2:212:GLY:HA3  | 1.94                     | 0.66              |
| 10:A3:75:GLY:HA3  | 10:Z3:39:PRO:HB3  | 1.78                     | 0.66              |
| 10:A3:125:GLU:HB3 | 10:B3:108:THR:HB  | 1.77                     | 0.66              |
| 10:E3:125:GLU:HB3 | 10:F3:108:THR:HB  | 1.78                     | 0.66              |
| 10:G3:125:GLU:HB3 | 10:H3:108:THR:HB  | 1.78                     | 0.66              |
| 10:K3:43:PRO:HD2  | 10:K3:43:PRO:O    | 1.94                     | 0.66              |
| 10:K3:125:GLU:HB3 | 10:L3:108:THR:HB  | 1.78                     | 0.66              |
| 10:L3:43:PRO:HD2  | 10:L3:43:PRO:O    | 1.94                     | 0.66              |
| 11:c3:33:GLU:OE1  | 11:c3:92:SER:OG   | 2.13                     | 0.66              |
| 1:E1:167:ARG:HB2  | 2:B2:140:ARG:NH1  | 2.09                     | 0.66              |
| 1:G1:125:GLN:HG2  | 4:H2:8:MET:HA     | 1.77                     | 0.66              |
| 1:N1:394:LYS:HG2  | 1:N1:402:LEU:HB2  | 1.77                     | 0.66              |
| 1:Q1:157:LEU:HD11 | 1:Q1:202:VAL:HG21 | 1.76                     | 0.66              |
| 1:d1:164:LEU:HD13 | 2:D2:148:ALA:HA   | 1.78                     | 0.66              |
| 2:D2:40:LEU:HD12  | 6:R2:130:MET:HE1  | 1.78                     | 0.66              |
| 2:E2:96:LEU:HD11  | 2:E2:236:MET:HE3  | 1.71                     | 0.66              |
| 8:d2:59:ALA:O     | 9:i2:50:ARG:NH2   | 2.28                     | 0.66              |
| 9:z2:44:LEU:HD21  | 9:z2:73:ARG:HB2   | 1.77                     | 0.66              |
| 10:M3:43:PRO:O    | 10:M3:43:PRO:HD2  | 1.94                     | 0.66              |
| 10:S3:125:GLU:HB3 | 10:T3:108:THR:HB  | 1.78                     | 0.66              |
| 11:v3:33:GLU:OE1  | 11:v3:92:SER:OG   | 2.13                     | 0.66              |
| 1:B1:165:PHE:HE2  | 2:C2:162:PRO:N    | 1.93                     | 0.66              |
| 1:C1:378:ASN:ND2  | 1:C1:381:ASP:OD1  | 2.29                     | 0.66              |
| 1:D1:295:SER:HB2  | 6:U2:73:ILE:HD12  | 1.69                     | 0.66              |
| 1:D1:295:SER:HG   | 6:U2:72:HIS:CA    | 1.95                     | 0.66              |
| 1:I1:409:MET:HE3  | 1:I1:434:ASN:HB2  | 1.77                     | 0.66              |
| 1:J1:302:GLU:HG2  | 1:J1:358:THR:HG22 | 1.78                     | 0.66              |
| 1:P1:296:ARG:NH2  | 1:Q1:366:TYR:OH   | 2.28                     | 0.66              |
| 1:U1:275:LYS:HB2  | 1:U1:377:MET:HB2  | 1.78                     | 0.66              |
| 1:Y1:149:PRO:HA   | 1:Y1:181:GLU:HG2  | 1.77                     | 0.66              |
| 1:g1:203:ALA:HA   | 1:h1:158:ALA:HB1  | 1.76                     | 0.66              |
| 2:B2:61:MET:HE2   | 2:B2:171:LEU:HD11 | 1.77                     | 0.66              |
| 6:R2:68:THR:HG22  | 6:R2:69:SER:H     | 1.61                     | 0.66              |
| 9:32:234:ILE:HG23 | 12:B4:55:ASN:HD22 | 1.60                     | 0.66              |
| 10:E3:43:PRO:HD2  | 10:E3:43:PRO:O    | 1.94                     | 0.66              |
| 10:N3:43:PRO:HD2  | 10:N3:43:PRO:O    | 1.94                     | 0.66              |
| 10:O3:125:GLU:HB3 | 10:P3:108:THR:HB  | 1.78                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:T3:125:GLU:HB3  | 10:U3:108:THR:HB   | 1.78                     | 0.66              |
| 11:g3:33:GLU:OE1   | 11:g3:92:SER:OG    | 2.13                     | 0.66              |
| 11:j3:89:VAL:HG12  | 11:j3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:l3:33:GLU:OE1   | 11:l3:92:SER:OG    | 2.13                     | 0.66              |
| 11:o3:33:GLU:OE1   | 11:o3:92:SER:OG    | 2.13                     | 0.66              |
| 1:Q1:139:GLU:HG3   | 1:R1:156:HIS:CE1   | 2.30                     | 0.66              |
| 1:R1:174:ALA:HB3   | 1:R1:210:VAL:HG22  | 1.77                     | 0.66              |
| 1:T1:199:SER:HA    | 1:T1:205:LEU:HD23  | 1.77                     | 0.66              |
| 1:d1:166:VAL:HG23  | 2:D2:161:GLY:CA    | 2.20                     | 0.66              |
| 8:c2:239:GLU:OE1   | 8:c2:243:ARG:NH2   | 2.27                     | 0.66              |
| 9:j2:174:ASN:HA    | 9:j2:206:PRO:HD3   | 1.77                     | 0.66              |
| 9:q2:42:GLU:OE1    | 9:q2:73:ARG:NH1    | 2.29                     | 0.66              |
| 9:u2:44:LEU:HD12   | 9:u2:71:GLY:HA3    | 1.76                     | 0.66              |
| 10:B3:125:GLU:HB3  | 10:C3:108:THR:HB   | 1.78                     | 0.66              |
| 10:D3:213:ILE:HG23 | 10:F3:136:GLY:HA3  | 1.76                     | 0.66              |
| 10:I3:125:GLU:HB3  | 10:J3:108:THR:HB   | 1.78                     | 0.66              |
| 10:L3:125:GLU:HB3  | 10:M3:108:THR:HB   | 1.78                     | 0.66              |
| 11:k3:271:ASP:CB   | 11:k3:357:CYS:HA   | 2.25                     | 0.66              |
| 11:t3:33:GLU:OE1   | 11:t3:92:SER:OG    | 2.13                     | 0.66              |
| 11:y3:46:ASP:OD1   | 11:z3:161:ASN:HB2  | 1.95                     | 0.66              |
| 1:J1:250:GLU:O     | 1:J1:254:SER:OG    | 2.11                     | 0.66              |
| 3:F2:130:ASP:OD1   | 3:F2:131:MET:N     | 2.28                     | 0.66              |
| 4:I2:47:MET:HG2    | 4:I2:48:THR:HG23   | 1.77                     | 0.66              |
| 8:e2:59:ALA:O      | 9:j2:50:ARG:NH2    | 2.26                     | 0.66              |
| 8:f2:152:PRO:HB2   | 9:q2:195:THR:HG22  | 1.78                     | 0.66              |
| 9:k2:167:PRO:HG3   | 9:l2:54:ALA:H      | 1.61                     | 0.66              |
| 9:42:149:ILE:HG12  | 9:42:159:VAL:HG12  | 1.78                     | 0.66              |
| 10:C3:125:GLU:HB3  | 10:D3:108:THR:HB   | 1.78                     | 0.66              |
| 10:M3:125:GLU:HB3  | 10:N3:108:THR:HB   | 1.77                     | 0.66              |
| 10:S3:43:PRO:HD2   | 10:S3:43:PRO:O     | 1.94                     | 0.66              |
| 11:v3:89:VAL:HG12  | 11:v3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:z3:196:MET:HE2  | 11:z3:196:MET:CA   | 2.26                     | 0.66              |
| 1:A1:404:LEU:H     | 1:A1:434:ASN:HD21  | 1.41                     | 0.66              |
| 1:B1:195:VAL:HG13  | 1:B1:210:VAL:HG21  | 1.78                     | 0.66              |
| 1:M1:279:GLU:OE1   | 1:M1:281:HIS:ND1   | 2.29                     | 0.66              |
| 1:R1:277:GLN:HB3   | 1:R1:375:THR:HB    | 1.77                     | 0.66              |
| 8:f2:80:VAL:HG13   | 8:f2:201:ILE:HG23  | 1.77                     | 0.66              |
| 9:42:238:ARG:CD    | 12:C4:55:ASN:HB2   | 2.26                     | 0.66              |
| 11:k3:89:VAL:HG12  | 11:k3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:l3:89:VAL:HG12  | 11:l3:107:VAL:HG22 | 1.76                     | 0.66              |
| 11:q3:89:VAL:HG12  | 11:q3:107:VAL:HG22 | 1.76                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:v3:196:MET:HE2 | 11:v3:196:MET:CA   | 2.26                     | 0.66              |
| 11:x3:196:MET:HE2 | 11:x3:196:MET:CA   | 2.26                     | 0.66              |
| 11:y3:33:GLU:OE1  | 11:y3:92:SER:OG    | 2.13                     | 0.66              |
| 1:N1:365:ASN:OD1  | 6:Q2:66:THR:HG22   | 1.96                     | 0.65              |
| 1:V1:420:MET:HE3  | 1:V1:422:PHE:HB2   | 1.78                     | 0.65              |
| 1:d1:152:SER:HB3  | 1:d1:179:THR:HB    | 1.77                     | 0.65              |
| 1:g1:187:ASP:O    | 1:g1:191:ILE:HG13  | 1.96                     | 0.65              |
| 2:B2:75:ARG:NH1   | 2:B2:85:PRO:HB3    | 2.10                     | 0.65              |
| 6:Q2:95:LEU:HG    | 8:b2:46:VAL:HG23   | 1.78                     | 0.65              |
| 9:l2:175:LEU:HD13 | 9:l2:206:PRO:HG3   | 1.76                     | 0.65              |
| 10:R3:125:GLU:HB3 | 10:S3:108:THR:HB   | 1.78                     | 0.65              |
| 11:b3:33:GLU:OE1  | 11:b3:92:SER:OG    | 2.13                     | 0.65              |
| 11:d3:89:VAL:HG12 | 11:d3:107:VAL:HG22 | 1.76                     | 0.65              |
| 11:f3:33:GLU:OE1  | 11:f3:92:SER:OG    | 2.13                     | 0.65              |
| 11:i3:89:VAL:HG12 | 11:i3:107:VAL:HG22 | 1.76                     | 0.65              |
| 11:t3:196:MET:HE2 | 11:t3:196:MET:CA   | 2.26                     | 0.65              |
| 1:N1:181:GLU:OE1  | 1:N1:184:ARG:NH2   | 2.29                     | 0.65              |
| 1:U1:144:ILE:HG22 | 1:U1:150:VAL:HG11  | 1.78                     | 0.65              |
| 1:U1:370:ARG:HB3  | 1:V1:280:GLU:OE2   | 1.95                     | 0.65              |
| 1:Y1:190:GLN:HG2  | 1:a1:217:GLY:HA3   | 1.78                     | 0.65              |
| 2:A2:212:VAL:HG22 | 2:B2:214:PRO:HG3   | 1.77                     | 0.65              |
| 2:E2:66:ARG:NE    | 2:E2:178:GLU:OE2   | 2.28                     | 0.65              |
| 5:P2:33:SER:O     | 5:P2:36:GLY:N      | 2.24                     | 0.65              |
| 6:U2:35:THR:HG23  | 6:U2:38:TYR:HB2    | 1.79                     | 0.65              |
| 7:Y2:29:ALA:HB1   | 8:d2:57:VAL:HG21   | 1.77                     | 0.65              |
| 8:e2:239:GLU:OE2  | 8:e2:243:ARG:NE    | 2.29                     | 0.65              |
| 10:A3:43:PRO:HD2  | 10:A3:43:PRO:O     | 1.94                     | 0.65              |
| 10:J3:43:PRO:O    | 10:J3:43:PRO:HD2   | 1.94                     | 0.65              |
| 10:Z3:43:PRO:O    | 10:Z3:43:PRO:HD2   | 1.94                     | 0.65              |
| 11:h3:141:ILE:CD1 | 11:h3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:h3:271:ASP:CB  | 11:h3:357:CYS:HA   | 2.25                     | 0.65              |
| 11:k3:33:GLU:OE1  | 11:k3:92:SER:OG    | 2.13                     | 0.65              |
| 11:p3:196:MET:HE2 | 11:p3:196:MET:CA   | 2.26                     | 0.65              |
| 11:r3:89:VAL:HG11 | 11:r3:121:LEU:HD21 | 1.78                     | 0.65              |
| 11:w3:89:VAL:HG12 | 11:w3:107:VAL:HG22 | 1.76                     | 0.65              |
| 1:B1:160:PRO:HA   | 1:h1:203:ALA:HB1   | 1.77                     | 0.65              |
| 1:G1:166:VAL:HG12 | 2:B2:144:GLU:HG3   | 1.77                     | 0.65              |
| 1:H1:165:PHE:HA   | 2:B2:159:LEU:HB2   | 1.77                     | 0.65              |
| 1:H1:245:ILE:HD11 | 1:H1:420:MET:HA    | 1.79                     | 0.65              |
| 1:R1:167:ARG:HH12 | 3:F2:169:PHE:N     | 1.91                     | 0.65              |
| 1:a1:145:GLU:OE2  | 1:a1:153:ALA:N     | 2.28                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:d1:193:ALA:HA    | 1:f1:219:LEU:HD12  | 1.78                     | 0.65              |
| 1:g1:392:ASN:OD1   | 1:g1:393:TYR:N     | 2.30                     | 0.65              |
| 7:W2:121:THR:OG1   | 8:c2:248:LEU:O     | 2.11                     | 0.65              |
| 10:N3:125:GLU:HB3  | 10:O3:108:THR:HB   | 1.78                     | 0.65              |
| 11:n3:89:VAL:HG12  | 11:n3:107:VAL:HG22 | 1.76                     | 0.65              |
| 11:p3:33:GLU:OE1   | 11:p3:92:SER:OG    | 2.13                     | 0.65              |
| 11:r3:196:MET:HE2  | 11:r3:196:MET:CA   | 2.26                     | 0.65              |
| 11:t3:345:LEU:HD21 | 11:u3:319:LEU:HD22 | 1.78                     | 0.65              |
| 11:u3:33:GLU:OE1   | 11:u3:92:SER:OG    | 2.13                     | 0.65              |
| 11:u3:196:MET:HE2  | 11:u3:196:MET:CA   | 2.26                     | 0.65              |
| 1:X1:214:ASP:HB2   | 1:X1:218:HIS:HB2   | 1.77                     | 0.65              |
| 1:X1:279:GLU:OE2   | 1:X1:281:HIS:N     | 2.30                     | 0.65              |
| 6:Q2:13:GLN:HE22   | 6:Q2:57:ARG:HH22   | 1.44                     | 0.65              |
| 7:V2:74:GLU:HA     | 7:V2:95:ASN:HB3    | 1.79                     | 0.65              |
| 8:f2:133:SER:HB2   | 8:f2:135:ILE:HG12  | 1.79                     | 0.65              |
| 10:O3:39:PRO:HB3   | 10:P3:75:GLY:HA3   | 1.79                     | 0.65              |
| 10:Q3:125:GLU:HB3  | 10:R3:108:THR:HB   | 1.78                     | 0.65              |
| 10:W3:43:PRO:O     | 10:W3:43:PRO:HD2   | 1.94                     | 0.65              |
| 11:f3:141:ILE:CD1  | 11:f3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:g3:141:ILE:CD1  | 11:g3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:i3:141:ILE:CD1  | 11:i3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:q3:89:VAL:HG11  | 11:q3:121:LEU:HD21 | 1.78                     | 0.65              |
| 11:s3:89:VAL:HG11  | 11:s3:121:LEU:HD21 | 1.79                     | 0.65              |
| 11:s3:196:MET:HE2  | 11:s3:196:MET:CA   | 2.26                     | 0.65              |
| 12:C4:140:ILE:HG12 | 12:C4:182:ILE:HG22 | 1.78                     | 0.65              |
| 1:E1:392:ASN:OD1   | 1:E1:393:TYR:N     | 2.30                     | 0.65              |
| 1:H1:378:ASN:ND2   | 1:H1:381:ASP:OD1   | 2.24                     | 0.65              |
| 1:N1:137:GLU:HB2   | 1:N1:155:VAL:HG13  | 1.79                     | 0.65              |
| 1:R1:195:VAL:HG22  | 1:R1:212:LEU:HD13  | 1.77                     | 0.65              |
| 1:U1:287:ASP:HB3   | 1:U1:290:LYS:HE3   | 1.78                     | 0.65              |
| 5:K2:70:ASP:OD1    | 6:Q2:13:GLN:NE2    | 2.30                     | 0.65              |
| 6:S2:106:ARG:HH12  | 8:d2:244:ALA:C     | 2.04                     | 0.65              |
| 8:f2:143:ILE:HD11  | 8:f2:161:LEU:HD13  | 1.78                     | 0.65              |
| 9:k2:126:GLY:HA2   | 9:p2:179:MET:HE2   | 1.77                     | 0.65              |
| 9:s2:138:PRO:HB3   | 11:q3:80:GLN:OE1   | 1.96                     | 0.65              |
| 9:x2:230:LEU:HD11  | 9:32:242:ILE:HD12  | 1.77                     | 0.65              |
| 10:M3:39:PRO:HB3   | 10:N3:75:GLY:HA3   | 1.79                     | 0.65              |
| 11:b3:196:MET:HE2  | 11:b3:196:MET:CA   | 2.26                     | 0.65              |
| 11:d3:345:LEU:HD21 | 11:e3:319:LEU:HD22 | 1.77                     | 0.65              |
| 11:p3:141:ILE:CD1  | 11:p3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:q3:141:ILE:CD1  | 11:q3:165:ILE:HD11 | 2.27                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:u3:89:VAL:HG11  | 11:u3:121:LEU:HD21 | 1.78                     | 0.65              |
| 1:O1:200:SER:OG    | 1:Q1:174:ALA:O     | 2.13                     | 0.65              |
| 1:f1:416:THR:HG23  | 1:f1:430:LEU:HD21  | 1.78                     | 0.65              |
| 2:C2:45:LEU:HD22   | 5:N2:82:MET:HE1    | 1.79                     | 0.65              |
| 2:E2:82:SER:O      | 3:F2:97:THR:OG1    | 2.11                     | 0.65              |
| 6:S2:102:MET:O     | 6:S2:106:ARG:HG2   | 1.97                     | 0.65              |
| 7:Z2:26:SER:HB3    | 8:e2:55:THR:HG22   | 1.77                     | 0.65              |
| 10:O3:43:PRO:O     | 10:O3:43:PRO:HD2   | 1.94                     | 0.65              |
| 10:X3:213:ILE:HG23 | 10:Z3:136:GLY:HA3  | 1.78                     | 0.65              |
| 11:a3:196:MET:HE2  | 11:a3:196:MET:CA   | 2.26                     | 0.65              |
| 11:o3:141:ILE:CD1  | 11:o3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:t3:89:VAL:HG11  | 11:t3:121:LEU:HD21 | 1.78                     | 0.65              |
| 11:v3:345:LEU:HD21 | 11:w3:319:LEU:HD22 | 1.77                     | 0.65              |
| 1:G1:392:ASN:OD1   | 1:G1:393:TYR:N     | 2.30                     | 0.65              |
| 1:b1:245:ILE:HG23  | 1:b1:266:VAL:HG21  | 1.78                     | 0.65              |
| 1:b1:275:LYS:HB2   | 1:b1:377:MET:HB2   | 1.79                     | 0.65              |
| 1:f1:164:LEU:HD21  | 2:D2:149:LEU:CB    | 2.26                     | 0.65              |
| 4:H2:40:ALA:HA     | 4:H2:43:GLN:HA     | 1.79                     | 0.65              |
| 7:Z2:18:SER:O      | 7:Z2:22:ASN:ND2    | 2.27                     | 0.65              |
| 9:w2:83:GLN:HE22   | 9:w2:98:LYS:HA     | 1.60                     | 0.65              |
| 11:j3:141:ILE:CD1  | 11:j3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:n3:196:MET:HE2  | 11:n3:196:MET:CA   | 2.26                     | 0.65              |
| 11:o3:166:THR:HG21 | 11:q3:362:LEU:CD2  | 2.27                     | 0.65              |
| 11:q3:196:MET:HE2  | 11:q3:196:MET:CA   | 2.26                     | 0.65              |
| 11:r3:141:ILE:CD1  | 11:r3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:v3:89:VAL:HG11  | 11:v3:121:LEU:HD21 | 1.79                     | 0.65              |
| 11:w3:89:VAL:HG11  | 11:w3:121:LEU:HD21 | 1.78                     | 0.65              |
| 11:w3:196:MET:HE2  | 11:w3:196:MET:CA   | 2.26                     | 0.65              |
| 1:h1:164:LEU:HD12  | 2:C2:143:ARG:HD3   | 1.79                     | 0.65              |
| 9:q2:98:LYS:HD2    | 9:q2:213:LEU:HD12  | 1.77                     | 0.65              |
| 9:t2:237:GLN:O     | 9:t2:241:GLU:HG2   | 1.97                     | 0.65              |
| 9:22:231:VAL:CG2   | 12:B4:42:ALA:HB2   | 2.26                     | 0.65              |
| 9:32:44:LEU:HD12   | 9:32:71:GLY:HA3    | 1.78                     | 0.65              |
| 10:U3:39:PRO:HB3   | 10:V3:75:GLY:HA3   | 1.79                     | 0.65              |
| 10:W3:39:PRO:HB3   | 10:X3:75:GLY:HA3   | 1.79                     | 0.65              |
| 11:c3:196:MET:HE2  | 11:c3:196:MET:CA   | 2.26                     | 0.65              |
| 11:e3:141:ILE:CD1  | 11:e3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:p3:89:VAL:HG11  | 11:p3:121:LEU:HD21 | 1.78                     | 0.65              |
| 11:y3:196:MET:HE2  | 11:y3:196:MET:CA   | 2.26                     | 0.65              |
| 11:z3:33:GLU:OE1   | 11:z3:92:SER:OG    | 2.13                     | 0.65              |
| 1:B1:193:ALA:HA    | 1:C1:219:LEU:HG    | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:191:ILE:HG23  | 1:C1:212:LEU:HD12  | 1.77                     | 0.65              |
| 1:R1:125:GLN:CG    | 2:E2:230:ASP:CG    | 2.70                     | 0.65              |
| 1:X1:413:GLU:OE2   | 1:X1:417:ARG:NH1   | 2.30                     | 0.65              |
| 2:C2:99:PHE:HE1    | 2:D2:154:ALA:HB2   | 1.62                     | 0.65              |
| 3:F2:40:LYS:HD3    | 5:P2:103:GLN:HA    | 1.78                     | 0.65              |
| 6:S2:90:PRO:HB3    | 6:S2:99:THR:HB     | 1.78                     | 0.65              |
| 9:y2:135:GLN:OE1   | 9:y2:137:GLN:NE2   | 2.30                     | 0.65              |
| 10:J3:125:GLU:HB3  | 10:K3:108:THR:HB   | 1.79                     | 0.65              |
| 10:L3:39:PRO:HB3   | 10:M3:75:GLY:HA3   | 1.79                     | 0.65              |
| 11:e3:196:MET:HE2  | 11:e3:196:MET:CA   | 2.26                     | 0.65              |
| 11:h3:345:LEU:HD21 | 11:i3:319:LEU:HD22 | 1.78                     | 0.65              |
| 11:k3:141:ILE:CD1  | 11:k3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:k3:345:LEU:HD21 | 11:l3:319:LEU:HD22 | 1.79                     | 0.65              |
| 11:n3:89:VAL:HG11  | 11:n3:121:LEU:HD21 | 1.78                     | 0.65              |
| 11:n3:141:ILE:CD1  | 11:n3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:s3:89:VAL:HG12  | 11:s3:107:VAL:HG22 | 1.76                     | 0.65              |
| 12:B4:124:PRO:HG2  | 12:B4:200:PHE:HB2  | 1.79                     | 0.65              |
| 12:B4:160:VAL:HG21 | 12:B4:229:ARG:HB3  | 1.79                     | 0.65              |
| 1:E1:294:ARG:HG3   | 6:U2:66:THR:CG2    | 2.26                     | 0.65              |
| 1:G1:128:GLU:OE2   | 4:H2:4:GLU:HG3     | 1.95                     | 0.65              |
| 1:M1:231:ASN:OD1   | 1:M1:232:ASP:N     | 2.30                     | 0.65              |
| 1:T1:157:LEU:HD11  | 1:T1:202:VAL:HG21  | 1.79                     | 0.65              |
| 1:W1:139:GLU:O     | 1:W1:143:THR:HG23  | 1.97                     | 0.65              |
| 2:A2:225:LEU:HD11  | 4:G2:77:VAL:HG21   | 1.79                     | 0.65              |
| 8:d2:70:GLN:NE2    | 9:n2:7:ILE:HG13    | 2.12                     | 0.65              |
| 9:n2:168:VAL:C     | 11:x3:78:ASN:HD21  | 2.05                     | 0.65              |
| 9:o2:109:ASP:OD1   | 9:o2:110:GLY:N     | 2.30                     | 0.65              |
| 9:32:238:ARG:HD2   | 12:C4:46:ASN:O     | 1.96                     | 0.65              |
| 10:C3:39:PRO:HB3   | 10:D3:75:GLY:HA3   | 1.79                     | 0.65              |
| 10:F3:125:GLU:HB3  | 10:G3:108:THR:HB   | 1.79                     | 0.65              |
| 10:N3:39:PRO:HB3   | 10:O3:75:GLY:HA3   | 1.79                     | 0.65              |
| 11:a3:33:GLU:OE1   | 11:a3:92:SER:OG    | 2.13                     | 0.65              |
| 11:a3:141:ILE:CD1  | 11:a3:165:ILE:HD11 | 2.27                     | 0.65              |
| 11:o3:89:VAL:HG11  | 11:o3:121:LEU:HD21 | 1.78                     | 0.65              |
| 12:C4:169:GLN:NE2  | 12:C4:173:THR:OG1  | 2.28                     | 0.65              |
| 1:C1:151:LYS:NZ    | 1:C1:180:LEU:O     | 2.30                     | 0.64              |
| 1:E1:367:GLU:OE1   | 6:U2:68:THR:HG21   | 1.95                     | 0.64              |
| 1:N1:180:LEU:HD13  | 1:N1:185:ALA:HA    | 1.78                     | 0.64              |
| 1:T1:167:ARG:NH2   | 2:E2:107:LYS:CB    | 2.60                     | 0.64              |
| 1:U1:244:ARG:HH11  | 1:V1:239:ASN:HB2   | 1.62                     | 0.64              |
| 1:W1:164:LEU:O     | 2:E2:144:GLU:OE2   | 2.14                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Z1:294:ARG:HG2   | 6:S2:68:THR:CB     | 2.26                     | 0.64              |
| 1:f1:203:ALA:HB1   | 1:g1:160:PRO:HA    | 1.77                     | 0.64              |
| 3:F2:14:HIS:CE1    | 3:F2:64:PRO:HD3    | 2.32                     | 0.64              |
| 9:u2:46:TYR:HA     | 9:u2:69:GLY:HA2    | 1.79                     | 0.64              |
| 9:22:240:TYR:HE1   | 12:A4:49:PRO:O     | 1.80                     | 0.64              |
| 9:42:99:GLY:O      | 9:42:116:ARG:NH2   | 2.26                     | 0.64              |
| 10:B3:39:PRO:HB3   | 10:C3:75:GLY:HA3   | 1.79                     | 0.64              |
| 10:K3:39:PRO:HB3   | 10:L3:75:GLY:HA3   | 1.79                     | 0.64              |
| 11:c3:166:THR:HG21 | 11:e3:362:LEU:CD2  | 2.27                     | 0.64              |
| 11:d3:196:MET:HE2  | 11:d3:196:MET:CA   | 2.26                     | 0.64              |
| 11:g3:196:MET:HE2  | 11:g3:196:MET:CA   | 2.26                     | 0.64              |
| 11:l3:196:MET:HE2  | 11:l3:196:MET:CA   | 2.26                     | 0.64              |
| 11:n3:345:LEU:HD21 | 11:o3:319:LEU:HD22 | 1.78                     | 0.64              |
| 11:y3:79:MET:HE2   | 11:z3:57:PHE:HD2   | 1.62                     | 0.64              |
| 11:y3:141:ILE:CD1  | 11:y3:165:ILE:HD11 | 2.27                     | 0.64              |
| 1:L1:145:GLU:OE2   | 1:L1:153:ALA:N     | 2.29                     | 0.64              |
| 1:g1:279:GLU:OE2   | 1:g1:281:HIS:N     | 2.25                     | 0.64              |
| 8:f2:28:ASN:OD1    | 9:k2:72:VAL:HG12   | 1.97                     | 0.64              |
| 9:m2:237:GLN:NE2   | 9:r2:252:GLN:HG2   | 2.12                     | 0.64              |
| 9:v2:185:GLU:OE1   | 9:12:51:GLN:NE2    | 2.31                     | 0.64              |
| 10:G3:39:PRO:HB3   | 10:H3:75:GLY:HA3   | 1.79                     | 0.64              |
| 10:I3:39:PRO:HB3   | 10:J3:75:GLY:HA3   | 1.79                     | 0.64              |
| 10:V3:125:GLU:HB3  | 10:W3:108:THR:HB   | 1.79                     | 0.64              |
| 11:i3:166:THR:HG21 | 11:k3:362:LEU:CD2  | 2.27                     | 0.64              |
| 11:l3:345:LEU:HD21 | 11:m3:319:LEU:HD22 | 1.79                     | 0.64              |
| 11:s3:141:ILE:CD1  | 11:s3:165:ILE:HD11 | 2.27                     | 0.64              |
| 11:x3:141:ILE:CD1  | 11:x3:165:ILE:HD11 | 2.27                     | 0.64              |
| 11:z3:141:ILE:CD1  | 11:z3:165:ILE:HD11 | 2.27                     | 0.64              |
| 1:I1:373:ARG:HH21  | 1:J1:275:LYS:HE2   | 1.61                     | 0.64              |
| 1:K1:140:LEU:O     | 1:K1:144:ILE:HG13  | 1.97                     | 0.64              |
| 1:R1:153:ALA:HB2   | 1:R1:178:VAL:HG23  | 1.80                     | 0.64              |
| 1:T1:293:LEU:HD13  | 1:T1:296:ARG:HH12  | 1.61                     | 0.64              |
| 1:h1:293:LEU:HD13  | 1:h1:296:ARG:HD2   | 1.80                     | 0.64              |
| 2:C2:96:LEU:O      | 2:C2:100:ILE:HD12  | 1.97                     | 0.64              |
| 2:C2:236:MET:SD    | 2:D2:150:PHE:HZ    | 2.20                     | 0.64              |
| 2:E2:205:MET:HB3   | 4:J2:51:PHE:CE2    | 2.32                     | 0.64              |
| 6:Q2:93:PRO:HB3    | 8:b2:48:GLY:HA3    | 1.78                     | 0.64              |
| 9:m2:19:MET:HB2    | 9:m2:236:VAL:HG11  | 1.78                     | 0.64              |
| 9:y2:46:TYR:HA     | 9:y2:69:GLY:HA2    | 1.79                     | 0.64              |
| 9:z2:195:THR:HG23  | 9:z2:197:SER:H     | 1.62                     | 0.64              |
| 10:Q3:39:PRO:HB3   | 10:R3:75:GLY:HA3   | 1.79                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a3:219:ARG:HD3  | 11:z3:101:GLN:HE22 | 1.62                     | 0.64              |
| 11:h3:89:VAL:HG12  | 11:h3:107:VAL:HG22 | 1.76                     | 0.64              |
| 11:m3:89:VAL:HG11  | 11:m3:121:LEU:HD21 | 1.79                     | 0.64              |
| 11:o3:196:MET:HE2  | 11:o3:196:MET:CA   | 2.26                     | 0.64              |
| 11:p3:345:LEU:HD21 | 11:q3:319:LEU:HD22 | 1.77                     | 0.64              |
| 11:u3:345:LEU:HD21 | 11:v3:319:LEU:HD22 | 1.79                     | 0.64              |
| 1:l1:163:SER:H     | 1:l1:169:GLN:HE22  | 1.42                     | 0.64              |
| 1:Q1:250:GLU:O     | 1:Q1:254:SER:OG    | 2.14                     | 0.64              |
| 1:T1:165:PHE:CB    | 3:F2:167:ASN:N     | 2.59                     | 0.64              |
| 1:T1:167:ARG:HH22  | 2:E2:107:LYS:CB    | 2.11                     | 0.64              |
| 1:a1:276:GLU:OE2   | 1:a1:374:HIS:NE2   | 2.31                     | 0.64              |
| 1:d1:164:LEU:HD11  | 2:D2:148:ALA:HB1   | 1.77                     | 0.64              |
| 1:f1:301:SER:OG    | 1:f1:303:GLN:NE2   | 2.26                     | 0.64              |
| 4:H2:46:GLU:HG2    | 4:H2:47:MET:N      | 2.12                     | 0.64              |
| 8:e2:71:LEU:HD13   | 9:p2:70:THR:HG21   | 1.79                     | 0.64              |
| 9:s2:139:ALA:HB2   | 11:q3:53:THR:CG2   | 2.09                     | 0.64              |
| 9:u2:180:ASN:OD1   | 9:u2:183:GLY:N     | 2.27                     | 0.64              |
| 10:E3:39:PRO:HB3   | 10:F3:75:GLY:HA3   | 1.79                     | 0.64              |
| 10:S3:39:PRO:HB3   | 10:T3:75:GLY:HA3   | 1.79                     | 0.64              |
| 11:b3:141:ILE:CD1  | 11:b3:165:ILE:HD11 | 2.27                     | 0.64              |
| 11:c3:89:VAL:HG11  | 11:c3:121:LEU:HD21 | 1.79                     | 0.64              |
| 11:d3:141:ILE:CD1  | 11:d3:165:ILE:HD11 | 2.27                     | 0.64              |
| 11:h3:196:MET:HE2  | 11:h3:196:MET:CA   | 2.26                     | 0.64              |
| 11:m3:141:ILE:CD1  | 11:m3:165:ILE:HD11 | 2.27                     | 0.64              |
| 11:u3:166:THR:HG21 | 11:w3:362:LEU:CD2  | 2.27                     | 0.64              |
| 11:x3:89:VAL:HG11  | 11:x3:121:LEU:HD21 | 1.79                     | 0.64              |
| 1:G1:257:VAL:O     | 1:G1:261:ASN:ND2   | 2.30                     | 0.64              |
| 2:B2:122:SER:N     | 2:B2:125:GLU:OE2   | 2.27                     | 0.64              |
| 9:i2:75:VAL:O      | 9:o2:51:GLN:NE2    | 2.30                     | 0.64              |
| 9:p2:169:GLN:HG2   | 11:c3:78:ASN:OD1   | 1.95                     | 0.64              |
| 9:32:105:VAL:HB    | 9:32:134:PHE:HB3   | 1.78                     | 0.64              |
| 10:D3:125:GLU:HB3  | 10:E3:108:THR:HB   | 1.79                     | 0.64              |
| 10:H3:39:PRO:HB3   | 10:I3:75:GLY:HA3   | 1.79                     | 0.64              |
| 10:P3:125:GLU:HB3  | 10:Q3:108:THR:HB   | 1.79                     | 0.64              |
| 10:Y3:167:LYS:HD3  | 10:Z3:203:ALA:HB3  | 1.79                     | 0.64              |
| 11:c3:39:TYR:CE1   | 11:c3:61:THR:HG21  | 2.33                     | 0.64              |
| 11:c3:260:GLY:HA2  | 11:c3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:f3:166:THR:HG21 | 11:h3:362:LEU:CD2  | 2.27                     | 0.64              |
| 11:i3:89:VAL:HG11  | 11:i3:121:LEU:HD21 | 1.78                     | 0.64              |
| 11:i3:196:MET:HE2  | 11:i3:196:MET:CA   | 2.26                     | 0.64              |
| 11:l3:141:ILE:CD1  | 11:l3:165:ILE:HD11 | 2.27                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:u3:39:TYR:CE1   | 11:u3:61:THR:HG21  | 2.33                     | 0.64              |
| 11:y3:39:TYR:CE1   | 11:y3:61:THR:HG21  | 2.33                     | 0.64              |
| 12:D4:123:THR:HB   | 12:D4:200:PHE:HB3  | 1.79                     | 0.64              |
| 1:J1:271:ASP:OD2   | 1:J1:381:ASP:N     | 2.30                     | 0.64              |
| 1:L1:248:ARG:NH2   | 1:M1:242:GLU:OE1   | 2.31                     | 0.64              |
| 1:T1:203:ALA:H     | 1:U1:158:ALA:HB1   | 1.63                     | 0.64              |
| 1:f1:407:ASP:HA    | 1:f1:410:LYS:HG2   | 1.79                     | 0.64              |
| 2:C2:38:TRP:HB2    | 2:C2:43:GLN:HG3    | 1.78                     | 0.64              |
| 7:X2:121:THR:OG1   | 8:d2:248:LEU:O     | 2.11                     | 0.64              |
| 9:i2:174:ASN:HA    | 9:i2:206:PRO:HD3   | 1.80                     | 0.64              |
| 9:w2:44:LEU:HD12   | 9:w2:71:GLY:HA3    | 1.78                     | 0.64              |
| 9:42:103:PHE:HB2   | 9:42:115:THR:O     | 1.97                     | 0.64              |
| 10:R3:39:PRO:HB3   | 10:S3:75:GLY:HA3   | 1.79                     | 0.64              |
| 11:a3:89:VAL:HG11  | 11:a3:121:LEU:HD21 | 1.78                     | 0.64              |
| 11:b3:39:TYR:CE1   | 11:b3:61:THR:HG21  | 2.33                     | 0.64              |
| 11:b3:89:VAL:HG11  | 11:b3:121:LEU:HD21 | 1.79                     | 0.64              |
| 11:d3:89:VAL:HG11  | 11:d3:121:LEU:HD21 | 1.79                     | 0.64              |
| 11:l3:271:ASP:CB   | 11:l3:357:CYS:HA   | 2.25                     | 0.64              |
| 11:t3:39:TYR:CE1   | 11:t3:61:THR:HG21  | 2.33                     | 0.64              |
| 11:v3:39:TYR:CE1   | 11:v3:61:THR:HG21  | 2.33                     | 0.64              |
| 4:I2:46:GLU:HG2    | 4:I2:47:MET:H      | 1.63                     | 0.64              |
| 8:c2:80:VAL:HG13   | 8:c2:201:ILE:HG23  | 1.80                     | 0.64              |
| 8:f2:71:LEU:HD23   | 8:f2:205:VAL:HG11  | 1.79                     | 0.64              |
| 9:j2:238:ARG:NH2   | 9:p2:255:GLN:OE1   | 2.31                     | 0.64              |
| 9:12:252:GLN:HA    | 9:12:255:GLN:HG2   | 1.80                     | 0.64              |
| 11:d3:39:TYR:CE1   | 11:d3:61:THR:HG21  | 2.33                     | 0.64              |
| 11:d3:260:GLY:HA2  | 11:d3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:e3:166:THR:HG21 | 11:g3:362:LEU:CD2  | 2.27                     | 0.64              |
| 11:i3:345:LEU:HD21 | 11:j3:319:LEU:HD22 | 1.79                     | 0.64              |
| 11:j3:196:MET:HE2  | 11:j3:196:MET:CA   | 2.26                     | 0.64              |
| 11:p3:260:GLY:HA2  | 11:p3:346:MET:HE1  | 1.80                     | 0.64              |
| 12:A4:198:LEU:HD13 | 12:A4:229:ARG:HE   | 1.63                     | 0.64              |
| 12:E4:128:GLU:OE1  | 12:E4:229:ARG:NH1  | 2.31                     | 0.64              |
| 1:F1:363:THR:CG2   | 6:U2:63:VAL:CG2    | 2.72                     | 0.64              |
| 1:F1:363:THR:CB    | 6:U2:63:VAL:CG2    | 2.75                     | 0.64              |
| 1:F1:393:TYR:HB3   | 1:F1:402:LEU:N     | 2.12                     | 0.64              |
| 1:G1:142:ARG:O     | 1:H1:154:ARG:NH1   | 2.30                     | 0.64              |
| 1:R1:424:ASP:OD1   | 1:R1:425:LYS:NZ    | 2.27                     | 0.64              |
| 5:N2:33:SER:O      | 5:N2:36:GLY:N      | 2.28                     | 0.64              |
| 7:Y2:121:THR:OG1   | 8:e2:248:LEU:O     | 2.07                     | 0.64              |
| 9:u2:2:ILE:HG22    | 9:u2:4:SER:H       | 1.63                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:T3:39:PRO:HB3   | 10:U3:75:GLY:HA3   | 1.79                     | 0.64              |
| 11:a3:39:TYR:CE1   | 11:a3:61:THR:HG21  | 2.33                     | 0.64              |
| 11:c3:141:ILE:CD1  | 11:c3:165:ILE:HD11 | 2.27                     | 0.64              |
| 11:e3:89:VAL:HG11  | 11:e3:121:LEU:HD21 | 1.78                     | 0.64              |
| 11:e3:260:GLY:HA2  | 11:e3:346:MET:HE1  | 1.79                     | 0.64              |
| 11:f3:196:MET:HE2  | 11:f3:196:MET:CA   | 2.26                     | 0.64              |
| 11:f3:345:LEU:HD21 | 11:g3:319:LEU:HD22 | 1.78                     | 0.64              |
| 11:j3:89:VAL:HG11  | 11:j3:121:LEU:HD21 | 1.78                     | 0.64              |
| 11:k3:196:MET:HE2  | 11:k3:196:MET:CA   | 2.26                     | 0.64              |
| 11:m3:101:GLN:HE22 | 11:n3:219:ARG:HD3  | 1.63                     | 0.64              |
| 11:m3:260:GLY:HA2  | 11:m3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:n3:166:THR:HG21 | 11:p3:362:LEU:CD2  | 2.28                     | 0.64              |
| 11:q3:260:GLY:HA2  | 11:q3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:w3:141:ILE:CD1  | 11:w3:165:ILE:HD11 | 2.27                     | 0.64              |
| 1:E1:182:PRO:O     | 1:E1:184:ARG:NH1   | 2.31                     | 0.64              |
| 1:L1:275:LYS:HE3   | 1:L1:275:LYS:HA    | 1.80                     | 0.64              |
| 1:V1:266:VAL:HG22  | 1:V1:387:VAL:HG22  | 1.80                     | 0.64              |
| 3:F2:30:ALA:HB3    | 3:F2:33:LEU:HB2    | 1.80                     | 0.64              |
| 7:Z2:41:PRO:HB3    | 7:Z2:92:LYS:HB3    | 1.79                     | 0.64              |
| 9:h2:167:PRO:HD3   | 9:s2:196:GLN:HG2   | 1.80                     | 0.64              |
| 9:y2:12:LEU:HD22   | 9:y2:243:ASN:HB3   | 1.77                     | 0.64              |
| 11:b3:166:THR:HG21 | 11:d3:362:LEU:CD2  | 2.28                     | 0.64              |
| 11:b3:260:GLY:HA2  | 11:b3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:e3:345:LEU:HD21 | 11:f3:319:LEU:HD22 | 1.79                     | 0.64              |
| 11:k3:89:VAL:HG11  | 11:k3:121:LEU:HD21 | 1.78                     | 0.64              |
| 11:k3:101:GLN:HE22 | 11:l3:219:ARG:HD3  | 1.63                     | 0.64              |
| 11:l3:89:VAL:HG11  | 11:l3:121:LEU:HD21 | 1.79                     | 0.64              |
| 11:s3:101:GLN:HE22 | 11:t3:219:ARG:HD3  | 1.63                     | 0.64              |
| 11:t3:141:ILE:CD1  | 11:t3:165:ILE:HD11 | 2.27                     | 0.64              |
| 11:w3:39:TYR:CE1   | 11:w3:61:THR:HG21  | 2.33                     | 0.64              |
| 11:y3:260:GLY:HA2  | 11:y3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:y3:345:LEU:HD21 | 11:z3:319:LEU:HD22 | 1.80                     | 0.64              |
| 12:A4:214:LEU:HB3  | 12:A4:222:THR:HB   | 1.79                     | 0.64              |
| 1:P1:257:VAL:O     | 1:P1:261:ASN:ND2   | 2.29                     | 0.64              |
| 1:U1:161:LYS:HZ2   | 1:U1:163:SER:HA    | 1.62                     | 0.64              |
| 1:a1:143:THR:HG21  | 1:c1:156:HIS:NE2   | 2.12                     | 0.64              |
| 6:R2:111:ASP:OD2   | 6:R2:115:LYS:NZ    | 2.30                     | 0.64              |
| 8:b2:157:PRO:HD3   | 9:r2:55:GLN:HE22   | 1.63                     | 0.64              |
| 9:p2:175:LEU:HD11  | 9:p2:214:LEU:HD11  | 1.80                     | 0.64              |
| 9:w2:241:GLU:HB3   | 9:32:258:THR:HG21  | 1.80                     | 0.64              |
| 10:F3:39:PRO:HB3   | 10:G3:75:GLY:HA3   | 1.80                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:P3:39:PRO:HB3   | 10:Q3:75:GLY:HA3   | 1.80                     | 0.64              |
| 10:V3:39:PRO:HB3   | 10:W3:75:GLY:HA3   | 1.80                     | 0.64              |
| 11:h3:89:VAL:HG11  | 11:h3:121:LEU:HD21 | 1.79                     | 0.64              |
| 11:m3:196:MET:HE2  | 11:m3:196:MET:CA   | 2.26                     | 0.64              |
| 11:o3:260:GLY:HA2  | 11:o3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:p3:98:ARG:NH1   | 11:q3:220:THR:OG1  | 2.31                     | 0.64              |
| 11:q3:101:GLN:HE22 | 11:r3:219:ARG:HD3  | 1.63                     | 0.64              |
| 11:r3:260:GLY:HA2  | 11:r3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:u3:271:ASP:CB   | 11:u3:357:CYS:HA   | 2.25                     | 0.64              |
| 11:v3:271:ASP:CB   | 11:v3:357:CYS:HA   | 2.25                     | 0.64              |
| 11:w3:345:LEU:HD21 | 11:x3:319:LEU:HD22 | 1.79                     | 0.64              |
| 11:y3:271:ASP:CB   | 11:y3:357:CYS:HA   | 2.25                     | 0.64              |
| 11:z3:89:VAL:HG11  | 11:z3:121:LEU:HD21 | 1.78                     | 0.64              |
| 11:z3:260:GLY:HA2  | 11:z3:346:MET:HE1  | 1.80                     | 0.64              |
| 11:z3:271:ASP:CB   | 11:z3:357:CYS:HA   | 2.25                     | 0.64              |
| 1:E1:151:LYS:NZ    | 1:E1:181:GLU:HA    | 2.14                     | 0.63              |
| 1:G1:373:ARG:NH1   | 1:H1:277:GLN:OE1   | 2.30                     | 0.63              |
| 1:T1:165:PHE:CE1   | 3:F2:167:ASN:N     | 2.58                     | 0.63              |
| 1:V1:296:ARG:NH2   | 1:V1:362:GLU:OE2   | 2.31                     | 0.63              |
| 1:Z1:297:GLN:NE2   | 6:S2:65:LEU:HD21   | 2.08                     | 0.63              |
| 1:f1:304:VAL:HG22  | 1:f1:356:ARG:HG2   | 1.78                     | 0.63              |
| 8:f2:116:GLN:NE2   | 9:k2:42:GLU:OE2    | 2.31                     | 0.63              |
| 9:k2:100:GLN:HA    | 9:k2:116:ARG:HH12  | 1.62                     | 0.63              |
| 9:k2:189:GLU:HA    | 9:p2:42:GLU:HG3    | 1.79                     | 0.63              |
| 9:o2:44:LEU:HD21   | 9:o2:73:ARG:HB2    | 1.80                     | 0.63              |
| 9:u2:238:ARG:NE    | 9:12:255:GLN:OE1   | 2.31                     | 0.63              |
| 9:u2:241:GLU:HG3   | 9:12:258:THR:HG21  | 1.78                     | 0.63              |
| 11:b3:345:LEU:HD21 | 11:c3:319:LEU:HD22 | 1.78                     | 0.63              |
| 11:c3:345:LEU:HD21 | 11:d3:319:LEU:HD22 | 1.79                     | 0.63              |
| 11:h3:166:THR:HG21 | 11:j3:362:LEU:CD2  | 2.28                     | 0.63              |
| 11:l3:260:GLY:HA2  | 11:l3:346:MET:HE1  | 1.80                     | 0.63              |
| 11:n3:260:GLY:HA2  | 11:n3:346:MET:HE1  | 1.80                     | 0.63              |
| 11:t3:166:THR:HG21 | 11:v3:362:LEU:CD2  | 2.28                     | 0.63              |
| 11:v3:98:ARG:NH1   | 11:w3:220:THR:OG1  | 2.31                     | 0.63              |
| 11:w3:101:GLN:HE22 | 11:x3:219:ARG:HD3  | 1.63                     | 0.63              |
| 11:x3:166:THR:HG21 | 11:z3:362:LEU:CD2  | 2.28                     | 0.63              |
| 11:y3:89:VAL:HG11  | 11:y3:121:LEU:HD21 | 1.79                     | 0.63              |
| 1:B1:165:PHE:CE2   | 2:C2:162:PRO:N     | 2.65                     | 0.63              |
| 1:I1:373:ARG:NH1   | 1:J1:277:GLN:OE1   | 2.31                     | 0.63              |
| 1:d1:293:LEU:HD11  | 1:d1:296:ARG:HH21  | 1.63                     | 0.63              |
| 1:f1:231:ASN:OD1   | 1:f1:232:ASP:N     | 2.31                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:V2:113:GLN:CD    | 7:a2:128:LYS:HZ2   | 2.06                     | 0.63              |
| 9:v2:226:VAL:CG1   | 12:A4:49:PRO:HG2   | 2.28                     | 0.63              |
| 9:z2:126:GLY:O     | 9:z2:142:ILE:N     | 2.20                     | 0.63              |
| 9:12:51:GLN:HB3    | 9:12:54:ALA:HB2    | 1.79                     | 0.63              |
| 9:42:55:GLN:NE2    | 9:42:57:SER:O      | 2.31                     | 0.63              |
| 10:Z3:70:ARG:NH2   | 11:y3:72:THR:OG1   | 2.30                     | 0.63              |
| 11:e3:39:TYR:CE1   | 11:e3:61:THR:HG21  | 2.33                     | 0.63              |
| 11:f3:260:GLY:HA2  | 11:f3:346:MET:HE1  | 1.79                     | 0.63              |
| 11:g3:39:TYR:CE1   | 11:g3:61:THR:HG21  | 2.33                     | 0.63              |
| 11:s3:39:TYR:CE1   | 11:s3:61:THR:HG21  | 2.33                     | 0.63              |
| 11:v3:141:ILE:CD1  | 11:v3:165:ILE:HD11 | 2.27                     | 0.63              |
| 1:C1:164:LEU:HD21  | 2:C2:149:LEU:HD13  | 1.78                     | 0.63              |
| 1:C1:392:ASN:OD1   | 1:C1:393:TYR:N     | 2.32                     | 0.63              |
| 1:N1:231:ASN:O     | 1:N1:234:GLN:NE2   | 2.31                     | 0.63              |
| 1:X1:180:LEU:N     | 1:X1:215:GLN:OE1   | 2.27                     | 0.63              |
| 1:d1:167:ARG:HH21  | 2:D2:159:LEU:CG    | 2.04                     | 0.63              |
| 1:f1:283:SER:HB2   | 1:f1:369:ASP:HB2   | 1.80                     | 0.63              |
| 1:h1:125:GLN:O     | 4:I2:4:GLU:OE1     | 2.16                     | 0.63              |
| 2:E2:108:ILE:HG13  | 2:E2:133:PRO:HG2   | 1.80                     | 0.63              |
| 9:w2:230:LEU:HD11  | 9:22:242:ILE:HD12  | 1.80                     | 0.63              |
| 10:J3:39:PRO:HB3   | 10:K3:75:GLY:HA3   | 1.80                     | 0.63              |
| 11:a3:260:GLY:HA2  | 11:a3:346:MET:HE1  | 1.80                     | 0.63              |
| 11:q3:39:TYR:CE1   | 11:q3:61:THR:HG21  | 2.33                     | 0.63              |
| 11:r3:345:LEU:HD21 | 11:s3:319:LEU:HD22 | 1.79                     | 0.63              |
| 11:w3:271:ASP:CB   | 11:w3:357:CYS:HA   | 2.25                     | 0.63              |
| 11:x3:39:TYR:CE1   | 11:x3:61:THR:HG21  | 2.33                     | 0.63              |
| 1:D1:389:VAL:HB    | 1:D1:432:VAL:HG22  | 1.81                     | 0.63              |
| 1:H1:394:LYS:HG2   | 1:H1:402:LEU:HB2   | 1.79                     | 0.63              |
| 1:N1:197:LEU:HD12  | 1:O1:213:VAL:HG21  | 1.79                     | 0.63              |
| 1:P1:407:ASP:OD1   | 1:P1:408:GLN:N     | 2.32                     | 0.63              |
| 1:W1:392:ASN:OD1   | 1:W1:393:TYR:N     | 2.31                     | 0.63              |
| 1:d1:256:ILE:HG21  | 1:d1:412:ILE:HD11  | 1.78                     | 0.63              |
| 7:W2:121:THR:O     | 7:W2:125:MET:HG3   | 1.98                     | 0.63              |
| 9:s2:209:ASN:CB    | 11:s3:54:GLN:HE22  | 2.09                     | 0.63              |
| 9:12:105:VAL:HG11  | 9:12:134:PHE:HB3   | 1.80                     | 0.63              |
| 9:42:46:TYR:HA     | 9:42:69:GLY:HA2    | 1.80                     | 0.63              |
| 11:f3:89:VAL:HG11  | 11:f3:121:LEU:HD21 | 1.78                     | 0.63              |
| 11:g3:89:VAL:HG11  | 11:g3:121:LEU:HD21 | 1.79                     | 0.63              |
| 11:g3:260:GLY:HA2  | 11:g3:346:MET:HE1  | 1.80                     | 0.63              |
| 11:s3:260:GLY:HA2  | 11:s3:346:MET:HE1  | 1.80                     | 0.63              |
| 11:x3:260:GLY:HA2  | 11:x3:346:MET:HE1  | 1.80                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:H1:151:LYS:HZ1   | 1:H1:182:PRO:HD3   | 1.63                     | 0.63              |
| 1:Q1:138:GLY:O     | 1:Q1:142:ARG:HG2   | 1.99                     | 0.63              |
| 1:Y1:407:ASP:OD1   | 1:Y1:408:GLN:N     | 2.32                     | 0.63              |
| 1:b1:231:ASN:O     | 1:b1:234:GLN:NE2   | 2.31                     | 0.63              |
| 2:A2:199:VAL:HG23  | 4:G2:21:ALA:HB2    | 1.80                     | 0.63              |
| 8:d2:131:GLU:HB3   | 9:i2:179:MET:HE2   | 1.80                     | 0.63              |
| 9:h2:150:THR:HG21  | 9:x2:54:ALA:HB1    | 1.80                     | 0.63              |
| 9:l2:77:THR:HG23   | 9:q2:66:LEU:HB2    | 1.81                     | 0.63              |
| 9:y2:240:TYR:CE1   | 9:42:253:MET:HE1   | 2.33                     | 0.63              |
| 10:D3:39:PRO:HB3   | 10:E3:75:GLY:HA3   | 1.80                     | 0.63              |
| 11:a3:271:ASP:CB   | 11:a3:357:CYS:HA   | 2.26                     | 0.63              |
| 11:b3:362:LEU:CD2  | 11:z3:166:THR:HG21 | 2.28                     | 0.63              |
| 11:i3:271:ASP:CB   | 11:i3:357:CYS:HA   | 2.25                     | 0.63              |
| 11:k3:260:GLY:HA2  | 11:k3:346:MET:HE1  | 1.80                     | 0.63              |
| 11:t3:260:GLY:HA2  | 11:t3:346:MET:HE1  | 1.80                     | 0.63              |
| 1:C1:140:LEU:O     | 1:C1:143:THR:OG1   | 2.15                     | 0.63              |
| 1:V1:385:LEU:N     | 1:V1:428:ASP:OD2   | 2.31                     | 0.63              |
| 1:Y1:216:SER:O     | 1:Y1:218:HIS:ND1   | 2.32                     | 0.63              |
| 1:Z1:375:THR:HG23  | 1:a1:275:LYS:NZ    | 2.13                     | 0.63              |
| 1:Z1:392:ASN:OD1   | 1:Z1:393:TYR:N     | 2.30                     | 0.63              |
| 1:d1:133:GLN:HE21  | 1:d1:157:LEU:HB2   | 1.62                     | 0.63              |
| 6:Q2:90:PRO:HB3    | 6:Q2:99:THR:HB     | 1.79                     | 0.63              |
| 9:h2:77:THR:HG22   | 9:m2:66:LEU:HB2    | 1.80                     | 0.63              |
| 9:x2:174:ASN:ND2   | 9:x2:203:GLU:OE2   | 2.31                     | 0.63              |
| 9:z2:98:LYS:O      | 9:z2:212:GLY:HA3   | 1.99                     | 0.63              |
| 9:12:240:TYR:HE2   | 12:E4:49:PRO:HA    | 1.64                     | 0.63              |
| 10:A3:136:GLY:HA3  | 10:Y3:213:ILE:HG23 | 1.80                     | 0.63              |
| 11:u3:101:GLN:HE22 | 11:v3:219:ARG:HD3  | 1.64                     | 0.63              |
| 11:u3:141:ILE:CD1  | 11:u3:165:ILE:HD11 | 2.27                     | 0.63              |
| 11:w3:166:THR:HG21 | 11:y3:362:LEU:CD2  | 2.28                     | 0.63              |
| 11:y3:98:ARG:NH1   | 11:z3:220:THR:OG1  | 2.31                     | 0.63              |
| 11:z3:39:TYR:CE1   | 11:z3:61:THR:HG21  | 2.33                     | 0.63              |
| 12:A4:123:THR:HB   | 12:A4:200:PHE:HB3  | 1.80                     | 0.63              |
| 1:A1:279:GLU:OE2   | 1:A1:281:HIS:N     | 2.32                     | 0.63              |
| 1:B1:161:LYS:NZ    | 1:B1:163:SER:HA    | 2.13                     | 0.63              |
| 1:U1:191:ILE:HG23  | 1:U1:212:LEU:HD23  | 1.79                     | 0.63              |
| 1:f1:165:PHE:HE1   | 2:D2:148:ALA:CB    | 2.12                     | 0.63              |
| 2:A2:75:ARG:NH1    | 2:A2:81:PRO:HB3    | 2.14                     | 0.63              |
| 2:D2:71:PHE:HB3    | 2:D2:89:LEU:HD23   | 1.80                     | 0.63              |
| 2:E2:208:GLY:HA2   | 4:J2:47:MET:SD     | 2.39                     | 0.63              |
| 7:Y2:30:ASN:OD1    | 8:d2:55:THR:OG1    | 2.16                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:b2:83:GLN:HG2    | 8:b2:84:GLN:H      | 1.63                     | 0.63              |
| 9:g2:113:ALA:HB3   | 9:g2:191:LEU:HD23  | 1.80                     | 0.63              |
| 9:j2:190:ASN:N     | 9:n2:42:GLU:OE2    | 2.32                     | 0.63              |
| 9:p2:44:LEU:HB2    | 9:p2:70:THR:O      | 1.98                     | 0.63              |
| 9:r2:124:GLN:NE2   | 9:w2:196:GLN:O     | 2.20                     | 0.63              |
| 9:s2:89:THR:HG21   | 9:s2:94:ASP:HB2    | 1.80                     | 0.63              |
| 11:a3:166:THR:HG21 | 11:c3:362:LEU:CD2  | 2.29                     | 0.63              |
| 11:f3:39:TYR:CE1   | 11:f3:61:THR:HG21  | 2.33                     | 0.63              |
| 11:h3:260:GLY:HA2  | 11:h3:346:MET:HE1  | 1.80                     | 0.63              |
| 11:o3:345:LEU:HD21 | 11:p3:319:LEU:HD22 | 1.79                     | 0.63              |
| 11:u3:260:GLY:HA2  | 11:u3:346:MET:HE1  | 1.80                     | 0.63              |
| 1:E1:167:ARG:CG    | 2:B2:140:ARG:CZ    | 2.71                     | 0.63              |
| 1:T1:133:GLN:O     | 1:T1:137:GLU:HG2   | 1.99                     | 0.63              |
| 1:W1:197:LEU:HG    | 1:X1:175:SER:HB2   | 1.79                     | 0.63              |
| 7:W2:117:GLU:OE1   | 8:c2:248:LEU:HB2   | 1.99                     | 0.63              |
| 7:X2:117:GLU:OE2   | 8:d2:249:SER:N     | 2.32                     | 0.63              |
| 9:g2:98:LYS:HG3    | 9:r2:45:LEU:HD21   | 1.79                     | 0.63              |
| 9:22:140:ILE:HD12  | 9:22:171:GLY:HA3   | 1.80                     | 0.63              |
| 11:q3:345:LEU:HD21 | 11:r3:319:LEU:HD22 | 1.79                     | 0.63              |
| 11:r3:39:TYR:CE1   | 11:r3:61:THR:HG21  | 2.33                     | 0.63              |
| 11:t3:271:ASP:CB   | 11:t3:357:CYS:HA   | 2.25                     | 0.63              |
| 11:x3:271:ASP:CB   | 11:x3:357:CYS:HA   | 2.26                     | 0.63              |
| 12:D4:138:ALA:HB3  | 12:D4:151:LEU:HB2  | 1.80                     | 0.63              |
| 1:M1:363:THR:HG23  | 6:Q2:73:ILE:HD12   | 0.67                     | 0.63              |
| 1:Y1:165:PHE:CE1   | 2:E2:148:ALA:HB2   | 2.34                     | 0.63              |
| 2:A2:52:THR:OG1    | 5:O2:91:LYS:NZ     | 2.25                     | 0.63              |
| 4:G2:36:SER:HA     | 4:G2:39:GLN:HB2    | 1.81                     | 0.63              |
| 9:k2:98:LYS:O      | 9:k2:212:GLY:HA3   | 1.99                     | 0.63              |
| 9:y2:26:LEU:HD21   | 9:42:242:ILE:HG22  | 1.80                     | 0.63              |
| 11:j3:39:TYR:CE1   | 11:j3:61:THR:HG21  | 2.33                     | 0.63              |
| 11:w3:260:GLY:HA2  | 11:w3:346:MET:HE1  | 1.79                     | 0.63              |
| 1:D1:409:MET:HE2   | 1:D1:409:MET:HA    | 1.81                     | 0.62              |
| 1:F1:415:LEU:HD22  | 1:G1:388:ALA:HB1   | 1.81                     | 0.62              |
| 1:N1:275:LYS:HB2   | 1:N1:377:MET:HB2   | 1.81                     | 0.62              |
| 1:V1:256:ILE:HG23  | 1:V1:257:VAL:HG13  | 1.80                     | 0.62              |
| 1:d1:137:GLU:OE1   | 1:d1:155:VAL:HG13  | 1.99                     | 0.62              |
| 1:d1:166:VAL:CG2   | 2:D2:161:GLY:HA2   | 2.22                     | 0.62              |
| 4:G2:7:MET:HA      | 4:G2:7:MET:HE3     | 1.81                     | 0.62              |
| 11:a3:101:GLN:HE22 | 11:b3:219:ARG:HD3  | 1.63                     | 0.62              |
| 11:f3:271:ASP:CB   | 11:f3:357:CYS:HA   | 2.25                     | 0.62              |
| 11:o3:101:GLN:HE22 | 11:p3:219:ARG:HD3  | 1.64                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:p3:39:TYR:CE1   | 11:p3:61:THR:HG21  | 2.33                     | 0.62              |
| 11:v3:260:GLY:HA2  | 11:v3:346:MET:HE1  | 1.79                     | 0.62              |
| 1:F1:244:ARG:NH2   | 1:G1:239:ASN:HB2   | 2.15                     | 0.62              |
| 1:F1:252:ILE:HG23  | 1:F1:253:LEU:HD22  | 1.80                     | 0.62              |
| 1:G1:246:GLN:NE2   | 1:G1:250:GLU:OE2   | 2.32                     | 0.62              |
| 1:O1:203:ALA:HA    | 1:Q1:158:ALA:HB1   | 1.79                     | 0.62              |
| 1:P1:402:LEU:HD12  | 1:P1:403:PRO:HD2   | 1.81                     | 0.62              |
| 1:T1:165:PHE:CE2   | 3:F2:167:ASN:OD1   | 2.51                     | 0.62              |
| 1:a1:424:ASP:OD1   | 1:a1:425:LYS:N     | 2.32                     | 0.62              |
| 1:d1:167:ARG:NH2   | 2:D2:159:LEU:CG    | 2.56                     | 0.62              |
| 6:Q2:37:GLY:N      | 6:Q2:96:ASP:O      | 2.29                     | 0.62              |
| 9:v2:238:ARG:NH1   | 9:22:251:ASP:OD1   | 2.32                     | 0.62              |
| 9:w2:153:ARG:NH1   | 9:32:189:GLU:HG3   | 2.14                     | 0.62              |
| 11:a3:362:LEU:CD2  | 11:y3:166:THR:HG21 | 2.29                     | 0.62              |
| 11:b3:271:ASP:CB   | 11:b3:357:CYS:HA   | 2.25                     | 0.62              |
| 11:g3:101:GLN:HE22 | 11:h3:219:ARG:HD3  | 1.63                     | 0.62              |
| 11:h3:39:TYR:CE1   | 11:h3:61:THR:HG21  | 2.33                     | 0.62              |
| 11:i3:101:GLN:HE22 | 11:j3:219:ARG:HD3  | 1.64                     | 0.62              |
| 11:j3:260:GLY:HA2  | 11:j3:346:MET:HE1  | 1.80                     | 0.62              |
| 11:l3:101:GLN:HE22 | 11:m3:219:ARG:HD3  | 1.65                     | 0.62              |
| 11:n3:39:TYR:CE1   | 11:n3:61:THR:HG21  | 2.33                     | 0.62              |
| 11:s3:98:ARG:NH1   | 11:t3:220:THR:OG1  | 2.33                     | 0.62              |
| 11:s3:345:LEU:HD21 | 11:t3:319:LEU:HD22 | 1.81                     | 0.62              |
| 11:t3:101:GLN:HE22 | 11:u3:219:ARG:HD3  | 1.65                     | 0.62              |
| 1:H1:140:LEU:O     | 1:H1:143:THR:OG1   | 2.17                     | 0.62              |
| 1:H1:303:GLN:NE2   | 1:H1:304:VAL:O     | 2.32                     | 0.62              |
| 1:N1:240:ASP:OD2   | 1:N1:244:ARG:NH2   | 2.32                     | 0.62              |
| 1:W1:375:THR:HG23  | 1:X1:275:LYS:NZ    | 2.14                     | 0.62              |
| 2:A2:135:ARG:HG2   | 2:A2:167:MET:HE1   | 1.81                     | 0.62              |
| 2:E2:128:ASP:OD1   | 2:E2:129:LYS:N     | 2.32                     | 0.62              |
| 4:G2:3:PRO:HA      | 4:G2:6:VAL:HG12    | 1.81                     | 0.62              |
| 9:u2:110:GLY:C     | 11:z3:80:GLN:NE2   | 2.57                     | 0.62              |
| 9:42:174:ASN:HA    | 9:42:206:PRO:HD3   | 1.81                     | 0.62              |
| 11:a3:319:LEU:HD22 | 11:z3:345:LEU:HD21 | 1.81                     | 0.62              |
| 11:k3:39:TYR:CE1   | 11:k3:61:THR:HG21  | 2.33                     | 0.62              |
| 11:k3:166:THR:HG21 | 11:m3:362:LEU:CD2  | 2.29                     | 0.62              |
| 11:l3:39:TYR:CE1   | 11:l3:61:THR:HG21  | 2.33                     | 0.62              |
| 11:l3:166:THR:HG21 | 11:n3:362:LEU:CD2  | 2.28                     | 0.62              |
| 11:m3:39:TYR:CE1   | 11:m3:61:THR:HG21  | 2.33                     | 0.62              |
| 12:A4:176:PRO:O    | 12:A4:180:TYR:OH   | 2.17                     | 0.62              |
| 1:G1:361:ASN:CB    | 6:U2:55:ARG:HH22   | 2.09                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:D2:210:MET:HE1   | 4:H2:47:MET:HE3   | 1.80                     | 0.62              |
| 6:U2:48:GLU:OE2    | 6:U2:84:ASP:N     | 2.32                     | 0.62              |
| 9:i2:26:LEU:HD11   | 9:o2:242:ILE:HG21 | 1.81                     | 0.62              |
| 11:i3:39:TYR:CE1   | 11:i3:61:THR:HG21 | 2.33                     | 0.62              |
| 11:m3:166:THR:HG21 | 11:o3:362:LEU:CD2 | 2.29                     | 0.62              |
| 1:A1:404:LEU:HD23  | 1:A1:408:GLN:HG2  | 1.81                     | 0.62              |
| 1:P1:392:ASN:OD1   | 1:P1:393:TYR:N    | 2.31                     | 0.62              |
| 1:S1:275:LYS:HB2   | 1:S1:377:MET:HB2  | 1.81                     | 0.62              |
| 1:T1:167:ARG:NE    | 2:E2:107:LYS:HE3  | 2.13                     | 0.62              |
| 1:X1:176:VAL:HG13  | 1:X1:212:LEU:HD13 | 1.82                     | 0.62              |
| 1:c1:190:GLN:HE21  | 1:d1:218:HIS:CD2  | 2.17                     | 0.62              |
| 2:D2:121:ILE:HG12  | 2:D2:125:GLU:HG3  | 1.80                     | 0.62              |
| 2:E2:205:MET:SD    | 2:E2:205:MET:CE   | 2.88                     | 0.62              |
| 6:T2:94:SER:OG     | 6:T2:96:ASP:OD1   | 2.16                     | 0.62              |
| 7:Z2:22:ASN:OD1    | 8:e2:54:ARG:NH1   | 2.32                     | 0.62              |
| 9:22:143:PRO:HG2   | 9:22:159:VAL:HG11 | 1.82                     | 0.62              |
| 9:32:12:LEU:HD22   | 9:32:243:ASN:HB3  | 1.81                     | 0.62              |
| 11:i3:260:GLY:HA2  | 11:i3:346:MET:HE1 | 1.80                     | 0.62              |
| 11:n3:101:GLN:HE22 | 11:o3:219:ARG:HD3 | 1.64                     | 0.62              |
| 11:y3:245:ASN:OD1  | 11:y3:245:ASN:N   | 2.33                     | 0.62              |
| 1:M1:248:ARG:NH1   | 1:N1:267:THR:OG1  | 2.33                     | 0.62              |
| 1:T1:275:LYS:HB2   | 1:T1:377:MET:HB2  | 1.81                     | 0.62              |
| 1:a1:140:LEU:O     | 1:a1:144:ILE:HG12 | 1.99                     | 0.62              |
| 9:q2:189:GLU:HA    | 9:v2:42:GLU:HG2   | 1.80                     | 0.62              |
| 9:s2:230:LEU:HD11  | 9:x2:242:ILE:HD12 | 1.82                     | 0.62              |
| 9:22:19:MET:HE1    | 9:22:233:MET:HG3  | 1.82                     | 0.62              |
| 11:p3:166:THR:HG21 | 11:r3:362:LEU:CD2 | 2.30                     | 0.62              |
| 11:q3:166:THR:HG21 | 11:s3:362:LEU:CD2 | 2.29                     | 0.62              |
| 11:r3:101:GLN:HE22 | 11:s3:219:ARG:HD3 | 1.65                     | 0.62              |
| 11:x3:101:GLN:HE22 | 11:y3:219:ARG:HD3 | 1.65                     | 0.62              |
| 1:H1:373:ARG:HH21  | 1:I1:275:LYS:HE2  | 1.65                     | 0.62              |
| 1:H1:404:LEU:HD13  | 1:H1:434:ASN:HD21 | 1.64                     | 0.62              |
| 1:K1:167:ARG:NH2   | 2:A2:244:TYR:N    | 2.42                     | 0.62              |
| 1:Q1:162:PRO:HB2   | 3:F2:253:ASP:CG   | 2.17                     | 0.62              |
| 1:S1:408:GLN:HA    | 1:S1:411:GLN:HE21 | 1.63                     | 0.62              |
| 1:a1:214:ASP:OD1   | 1:a1:215:GLN:N    | 2.32                     | 0.62              |
| 9:32:233:MET:HG3   | 12:B4:44:LEU:HD13 | 1.81                     | 0.62              |
| 11:g3:166:THR:HG21 | 11:i3:362:LEU:CD2 | 2.29                     | 0.62              |
| 11:j3:166:THR:HG21 | 11:l3:362:LEU:CD2 | 2.30                     | 0.62              |
| 11:o3:39:TYR:CE1   | 11:o3:61:THR:HG21 | 2.33                     | 0.62              |
| 12:A4:133:ALA:HA   | 12:A4:188:ASN:HB2 | 1.82                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:D1:374:HIS:HB3   | 1:E1:276:GLU:HB3   | 1.82                     | 0.62              |
| 1:Y1:404:LEU:HB2   | 1:Y1:409:MET:HE3   | 1.82                     | 0.62              |
| 1:a1:167:ARG:HB2   | 2:D2:244:TYR:CD2   | 2.34                     | 0.62              |
| 8:c2:174:SER:OG    | 8:c2:180:ARG:NH1   | 2.33                     | 0.62              |
| 9:h2:85:ASN:OD1    | 9:s2:47:GLN:NE2    | 2.32                     | 0.62              |
| 9:o2:189:GLU:HA    | 9:s2:42:GLU:HG2    | 1.82                     | 0.62              |
| 9:r2:230:LEU:HD21  | 9:w2:242:ILE:HG23  | 1.81                     | 0.62              |
| 9:22:235:GLN:HA    | 12:B4:46:ASN:HD22  | 1.62                     | 0.62              |
| 11:b3:245:ASN:OD1  | 11:b3:245:ASN:N    | 2.33                     | 0.62              |
| 11:d3:166:THR:HG21 | 11:f3:362:LEU:CD2  | 2.29                     | 0.62              |
| 11:e3:101:GLN:HE22 | 11:f3:219:ARG:HD3  | 1.64                     | 0.62              |
| 11:f3:98:ARG:NH1   | 11:g3:220:THR:OG1  | 2.30                     | 0.62              |
| 11:h3:101:GLN:HE22 | 11:i3:219:ARG:HD3  | 1.64                     | 0.62              |
| 11:t3:98:ARG:NH1   | 11:u3:220:THR:OG1  | 2.32                     | 0.62              |
| 1:l1:199:SER:HA    | 1:l1:205:LEU:HD23  | 1.82                     | 0.62              |
| 1:T1:261:ASN:O     | 1:T1:392:ASN:N     | 2.26                     | 0.62              |
| 1:U1:143:THR:HG22  | 1:W1:154:ARG:HE    | 1.63                     | 0.62              |
| 1:Y1:125:GLN:OE1   | 4:J2:75:ASP:CA     | 2.35                     | 0.62              |
| 1:Y1:295:SER:OG    | 6:S2:72:HIS:CA     | 2.39                     | 0.62              |
| 1:Y1:369:ASP:OD1   | 1:Z1:282:TYR:N     | 2.31                     | 0.62              |
| 1:f1:139:GLU:O     | 1:g1:154:ARG:NH1   | 2.32                     | 0.62              |
| 10:Y3:125:GLU:HB3  | 10:Z3:108:THR:HB   | 1.82                     | 0.62              |
| 11:g3:345:LEU:HD21 | 11:h3:319:LEU:HD22 | 1.81                     | 0.62              |
| 11:i3:98:ARG:NH1   | 11:j3:220:THR:OG1  | 2.32                     | 0.62              |
| 11:n3:98:ARG:NH1   | 11:o3:220:THR:OG1  | 2.32                     | 0.62              |
| 11:p3:271:ASP:CB   | 11:p3:357:CYS:HA   | 2.25                     | 0.62              |
| 11:r3:46:ASP:OD1   | 11:s3:161:ASN:HB2  | 2.00                     | 0.62              |
| 11:r3:166:THR:HG21 | 11:t3:362:LEU:CD2  | 2.29                     | 0.62              |
| 11:s3:271:ASP:CB   | 11:s3:357:CYS:HA   | 2.25                     | 0.62              |
| 1:B1:231:ASN:OD1   | 1:B1:232:ASP:N     | 2.31                     | 0.62              |
| 1:G1:361:ASN:HB3   | 6:U2:55:ARG:HH22   | 1.63                     | 0.62              |
| 8:d2:70:GLN:OE1    | 9:n2:3:SER:HA      | 2.00                     | 0.62              |
| 8:f2:144:SER:HA    | 8:f2:157:PRO:HA    | 1.82                     | 0.62              |
| 9:l2:44:LEU:HD22   | 9:l2:71:GLY:HA3    | 1.82                     | 0.62              |
| 9:m2:20:ASP:OD2    | 9:r2:4:SER:OG      | 2.17                     | 0.62              |
| 9:s2:46:TYR:HA     | 9:s2:69:GLY:HA2    | 1.81                     | 0.62              |
| 9:z2:174:ASN:HA    | 9:z2:206:PRO:HD3   | 1.81                     | 0.62              |
| 11:a3:365:ILE:HG23 | 11:z3:164:ARG:NH1  | 2.15                     | 0.62              |
| 11:m3:98:ARG:NH1   | 11:n3:220:THR:OG1  | 2.33                     | 0.62              |
| 11:s3:166:THR:HG21 | 11:u3:362:LEU:CD2  | 2.29                     | 0.62              |
| 12:D4:128:GLU:OE1  | 12:D4:229:ARG:NE   | 2.33                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:E4:53:LEU:O     | 12:E4:56:ASN:ND2   | 2.32                     | 0.62              |
| 1:G1:164:LEU:HD23  | 2:B2:143:ARG:HG3   | 1.82                     | 0.61              |
| 1:K1:375:THR:HG23  | 1:L1:275:LYS:NZ    | 2.15                     | 0.61              |
| 1:L1:139:GLU:HG3   | 1:N1:156:HIS:HE1   | 1.65                     | 0.61              |
| 1:R1:167:ARG:HG3   | 3:F2:167:ASN:CG    | 2.25                     | 0.61              |
| 1:X1:231:ASN:O     | 1:X1:234:GLN:NE2   | 2.33                     | 0.61              |
| 1:Z1:248:ARG:NH1   | 1:a1:267:THR:OG1   | 2.32                     | 0.61              |
| 1:g1:181:GLU:HB3   | 1:g1:184:ARG:NH2   | 2.15                     | 0.61              |
| 4:H2:3:PRO:HA      | 4:H2:6:VAL:HG12    | 1.81                     | 0.61              |
| 9:y2:51:GLN:HB3    | 9:y2:54:ALA:HB2    | 1.81                     | 0.61              |
| 9:12:240:TYR:OH    | 12:E4:49:PRO:HG3   | 2.00                     | 0.61              |
| 11:b3:98:ARG:NH1   | 11:c3:220:THR:OG1  | 2.32                     | 0.61              |
| 11:q3:98:ARG:NH1   | 11:r3:220:THR:OG1  | 2.33                     | 0.61              |
| 12:D4:34:SER:O     | 12:D4:38:THR:OG1   | 2.17                     | 0.61              |
| 1:G1:216:SER:O     | 1:G1:218:HIS:ND1   | 2.34                     | 0.61              |
| 1:J1:415:LEU:HD11  | 1:K1:433:VAL:HG21  | 1.83                     | 0.61              |
| 1:U1:279:GLU:OE2   | 1:U1:281:HIS:N     | 2.28                     | 0.61              |
| 1:Y1:143:THR:HG21  | 1:a1:156:HIS:NE2   | 2.15                     | 0.61              |
| 1:Y1:158:ALA:HB3   | 1:Y1:173:SER:HB3   | 1.82                     | 0.61              |
| 1:a1:167:ARG:CG    | 2:D2:244:TYR:HD2   | 2.13                     | 0.61              |
| 1:a1:167:ARG:HB2   | 2:D2:244:TYR:HD2   | 1.65                     | 0.61              |
| 1:d1:275:LYS:HB2   | 1:d1:377:MET:HB2   | 1.82                     | 0.61              |
| 5:O2:70:ASP:OD1    | 6:U2:17:ASN:ND2    | 2.33                     | 0.61              |
| 7:Z2:93:MET:HE3    | 7:Z2:94:PRO:HD2    | 1.81                     | 0.61              |
| 9:t2:162:GLN:OE1   | 9:y2:210:GLY:N     | 2.33                     | 0.61              |
| 9:42:59:GLN:NE2    | 11:u3:80:GLN:HE22  | 1.95                     | 0.61              |
| 11:c3:271:ASP:CB   | 11:c3:357:CYS:HA   | 2.25                     | 0.61              |
| 11:m3:345:LEU:HD21 | 11:n3:319:LEU:HD22 | 1.81                     | 0.61              |
| 1:N1:166:VAL:HG22  | 2:A2:162:PRO:N     | 2.10                     | 0.61              |
| 1:N1:370:ARG:NH1   | 1:O1:280:GLU:OE2   | 2.33                     | 0.61              |
| 1:Y1:375:THR:HG23  | 1:Z1:275:LYS:HE2   | 1.81                     | 0.61              |
| 1:a1:167:ARG:HG2   | 2:D2:140:ARG:CZ    | 2.30                     | 0.61              |
| 2:B2:137:PHE:HZ    | 2:B2:243:PHE:HE2   | 1.46                     | 0.61              |
| 2:D2:116:PHE:CE1   | 2:D2:123:MET:HG3   | 2.35                     | 0.61              |
| 3:F2:108:LEU:HD13  | 3:F2:124:VAL:HG11  | 1.82                     | 0.61              |
| 6:S2:29:ASN:ND2    | 6:S2:105:GLU:OE1   | 2.24                     | 0.61              |
| 11:a3:345:LEU:HD21 | 11:b3:319:LEU:HD22 | 1.81                     | 0.61              |
| 11:d3:271:ASP:CB   | 11:d3:357:CYS:HA   | 2.26                     | 0.61              |
| 11:o3:123:MET:C    | 11:o3:123:MET:HE3  | 2.26                     | 0.61              |
| 11:q3:271:ASP:CB   | 11:q3:357:CYS:HA   | 2.25                     | 0.61              |
| 12:E4:160:VAL:HG21 | 12:E4:229:ARG:HB3  | 1.82                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M1:240:ASP:OD2   | 1:M1:244:ARG:NH2   | 2.32                     | 0.61              |
| 1:S1:257:VAL:O     | 1:S1:261:ASN:ND2   | 2.33                     | 0.61              |
| 1:U1:275:LYS:HA    | 1:U1:275:LYS:HE3   | 1.82                     | 0.61              |
| 9:q2:19:MET:HB2    | 9:q2:236:VAL:HG11  | 1.82                     | 0.61              |
| 9:x2:58:GLU:HB2    | 9:x2:59:GLN:NE2    | 2.15                     | 0.61              |
| 11:a3:123:MET:HE3  | 11:a3:123:MET:C    | 2.26                     | 0.61              |
| 11:f3:123:MET:HE3  | 11:f3:123:MET:C    | 2.26                     | 0.61              |
| 11:g3:123:MET:C    | 11:g3:123:MET:HE3  | 2.26                     | 0.61              |
| 11:j3:98:ARG:NH1   | 11:k3:220:THR:OG1  | 2.31                     | 0.61              |
| 11:r3:271:ASP:CB   | 11:r3:357:CYS:HA   | 2.25                     | 0.61              |
| 11:v3:101:GLN:HE22 | 11:w3:219:ARG:HD3  | 1.66                     | 0.61              |
| 11:v3:166:THR:HG21 | 11:x3:362:LEU:CD2  | 2.30                     | 0.61              |
| 1:J1:415:LEU:HD22  | 1:K1:388:ALA:HB1   | 1.82                     | 0.61              |
| 2:A2:45:LEU:HG     | 6:U2:133:VAL:HG13  | 1.81                     | 0.61              |
| 7:X2:41:PRO:HB3    | 7:X2:92:LYS:HB3    | 1.82                     | 0.61              |
| 9:32:238:ARG:HG2   | 12:B4:55:ASN:ND2   | 2.15                     | 0.61              |
| 11:e3:123:MET:C    | 11:e3:123:MET:HE3  | 2.26                     | 0.61              |
| 11:j3:101:GLN:HE22 | 11:k3:219:ARG:HD3  | 1.66                     | 0.61              |
| 11:m3:271:ASP:CB   | 11:m3:357:CYS:HA   | 2.26                     | 0.61              |
| 11:n3:123:MET:HE3  | 11:n3:123:MET:C    | 2.26                     | 0.61              |
| 11:p3:123:MET:C    | 11:p3:123:MET:HE3  | 2.26                     | 0.61              |
| 11:r3:123:MET:C    | 11:r3:123:MET:HE3  | 2.26                     | 0.61              |
| 1:I1:246:GLN:NE2   | 1:I1:250:GLU:OE2   | 2.33                     | 0.61              |
| 1:Q1:165:PHE:HZ    | 3:F2:145:TRP:CH2   | 2.10                     | 0.61              |
| 1:X1:394:LYS:HG2   | 1:X1:402:LEU:HB2   | 1.83                     | 0.61              |
| 1:Y1:246:GLN:NE2   | 1:Y1:250:GLU:OE2   | 2.34                     | 0.61              |
| 1:d1:413:GLU:OE1   | 1:d1:417:ARG:NH1   | 2.32                     | 0.61              |
| 2:D2:71:PHE:CE1    | 2:D2:236:MET:SD    | 2.94                     | 0.61              |
| 7:X2:29:ALA:HB1    | 8:c2:57:VAL:HG21   | 1.81                     | 0.61              |
| 7:a2:29:ALA:HB1    | 8:f2:57:VAL:HG21   | 1.80                     | 0.61              |
| 9:h2:241:GLU:HG2   | 9:m2:256:LYS:HG2   | 1.83                     | 0.61              |
| 9:w2:26:LEU:HD11   | 9:22:242:ILE:HG21  | 1.83                     | 0.61              |
| 11:c3:123:MET:HE3  | 11:c3:123:MET:C    | 2.26                     | 0.61              |
| 11:e3:271:ASP:CB   | 11:e3:357:CYS:HA   | 2.25                     | 0.61              |
| 11:i3:353:GLN:HB2  | 11:i3:358:LEU:HD23 | 1.83                     | 0.61              |
| 11:y3:123:MET:HE3  | 11:y3:123:MET:C    | 2.26                     | 0.61              |
| 1:H1:151:LYS:NZ    | 1:H1:180:LEU:O     | 2.33                     | 0.61              |
| 1:N1:297:GLN:NE2   | 6:Q2:77:ALA:HB2    | 2.12                     | 0.61              |
| 1:P1:359:GLN:HE22  | 1:P1:361:ASN:HB2   | 1.65                     | 0.61              |
| 1:Q1:249:ILE:HD11  | 1:Q1:416:THR:HG22  | 1.82                     | 0.61              |
| 1:T1:212:LEU:HG    | 1:T1:220:LEU:HD12  | 1.81                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:T1:253:LEU:HD22 | 1:T1:412:ILE:HG23 | 1.82                     | 0.61              |
| 1:X1:275:LYS:HA   | 1:X1:275:LYS:HE3  | 1.82                     | 0.61              |
| 1:a1:405:THR:OG1  | 1:a1:407:ASP:OD1  | 2.17                     | 0.61              |
| 2:C2:227:VAL:HG11 | 2:D2:187:PHE:CE2  | 2.35                     | 0.61              |
| 8:c2:87:TRP:NE1   | 8:c2:166:ALA:O    | 2.30                     | 0.61              |
| 8:e2:155:VAL:HG21 | 9:u2:54:ALA:H     | 1.65                     | 0.61              |
| 9:h2:35:LYS:NZ    | 9:h2:82:SER:O     | 2.33                     | 0.61              |
| 9:i2:241:GLU:HG2  | 9:o2:256:LYS:HG2  | 1.83                     | 0.61              |
| 9:o2:168:VAL:CG2  | 11:t3:54:GLN:NE2  | 2.62                     | 0.61              |
| 9:z2:44:LEU:HD12  | 9:z2:71:GLY:HA3   | 1.83                     | 0.61              |
| 11:h3:123:MET:HE3 | 11:h3:123:MET:C   | 2.26                     | 0.61              |
| 11:n3:245:ASN:OD1 | 11:n3:245:ASN:N   | 2.33                     | 0.61              |
| 1:A1:275:LYS:HE2  | 1:h1:373:ARG:HH21 | 1.66                     | 0.61              |
| 1:A1:276:GLU:OE2  | 1:A1:374:HIS:NE2  | 2.33                     | 0.61              |
| 1:J1:392:ASN:OD1  | 1:J1:393:TYR:N    | 2.31                     | 0.61              |
| 1:N1:385:LEU:N    | 1:N1:428:ASP:OD2  | 2.32                     | 0.61              |
| 1:Q1:155:VAL:O    | 1:Q1:156:HIS:ND1  | 2.34                     | 0.61              |
| 1:U1:272:PHE:HA   | 1:U1:379:VAL:HG13 | 1.83                     | 0.61              |
| 1:Y1:360:ARG:NH1  | 1:Y1:362:GLU:OE2  | 2.33                     | 0.61              |
| 1:Z1:280:GLU:OE1  | 1:Z1:372:ILE:HG12 | 2.01                     | 0.61              |
| 1:d1:220:LEU:O    | 1:d1:222:GLN:NE2  | 2.33                     | 0.61              |
| 2:D2:121:ILE:HG23 | 2:D2:125:GLU:HG2  | 1.82                     | 0.61              |
| 2:E2:81:PRO:HD2   | 3:F2:119:HIS:NE2  | 2.16                     | 0.61              |
| 9:g2:98:LYS:HD3   | 9:g2:213:LEU:HD12 | 1.83                     | 0.61              |
| 9:k2:168:VAL:HG23 | 11:f3:114:LYS:HZ3 | 0.79                     | 0.61              |
| 9:l2:235:GLN:HG3  | 9:r2:5:LEU:HD23   | 1.83                     | 0.61              |
| 9:u2:174:ASN:HA   | 9:u2:206:PRO:HD3  | 1.81                     | 0.61              |
| 9:y2:230:LEU:HD13 | 12:D4:43:GLN:NE2  | 2.15                     | 0.61              |
| 11:c3:98:ARG:NH1  | 11:d3:220:THR:OG1 | 2.32                     | 0.61              |
| 11:d3:123:MET:HE3 | 11:d3:123:MET:C   | 2.26                     | 0.61              |
| 11:g3:98:ARG:NH1  | 11:h3:220:THR:OG1 | 2.32                     | 0.61              |
| 11:m3:123:MET:C   | 11:m3:123:MET:HE3 | 2.26                     | 0.61              |
| 11:w3:46:ASP:OD1  | 11:x3:161:ASN:HB2 | 2.01                     | 0.61              |
| 1:B1:214:ASP:HB3  | 1:B1:218:HIS:HB2  | 1.83                     | 0.61              |
| 1:D1:404:LEU:HD23 | 1:D1:434:ASN:HD21 | 1.66                     | 0.61              |
| 1:L1:140:LEU:O    | 1:L1:144:ILE:HG12 | 2.01                     | 0.61              |
| 1:V1:374:HIS:HB3  | 1:W1:276:GLU:HB3  | 1.82                     | 0.61              |
| 1:h1:214:ASP:OD1  | 1:h1:215:GLN:N    | 2.34                     | 0.61              |
| 8:c2:202:MET:SD   | 9:o2:73:ARG:NH1   | 2.74                     | 0.61              |
| 8:f2:42:ARG:NH1   | 9:k2:64:SER:OG    | 2.27                     | 0.61              |
| 9:p2:98:LYS:O     | 9:p2:212:GLY:HA3  | 2.00                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:v2:77:THR:HG23   | 9:12:66:LEU:HD12   | 1.82                     | 0.61              |
| 9:v2:153:ARG:NH2   | 9:22:189:GLU:OE2   | 2.31                     | 0.61              |
| 9:22:27:ALA:HB2    | 12:A4:41:VAL:HG11  | 1.83                     | 0.61              |
| 9:22:238:ARG:NE    | 12:A4:55:ASN:HD22  | 1.99                     | 0.61              |
| 9:42:73:ARG:HH21   | 9:42:75:VAL:HG12   | 1.66                     | 0.61              |
| 11:o3:98:ARG:NH1   | 11:p3:220:THR:OG1  | 2.32                     | 0.61              |
| 11:q3:46:ASP:OD1   | 11:r3:161:ASN:HB2  | 2.01                     | 0.61              |
| 11:w3:353:GLN:HB2  | 11:w3:358:LEU:HD23 | 1.83                     | 0.61              |
| 1:E1:300:ILE:HG12  | 1:E1:360:ARG:HG2   | 1.83                     | 0.61              |
| 1:G1:165:PHE:HE2   | 4:H2:88:ILE:CG2    | 2.11                     | 0.61              |
| 1:G1:361:ASN:HB2   | 6:U2:55:ARG:NH2    | 2.16                     | 0.61              |
| 1:Q1:283:SER:HB2   | 1:Q1:369:ASP:HB2   | 1.83                     | 0.61              |
| 1:W1:424:ASP:OD1   | 1:W1:425:LYS:N     | 2.33                     | 0.61              |
| 1:a1:144:ILE:HA    | 1:a1:147:LEU:HD13  | 1.83                     | 0.61              |
| 1:d1:135:ALA:O     | 1:d1:139:GLU:HG2   | 2.00                     | 0.61              |
| 1:d1:284:PRO:O     | 1:d1:290:LYS:NZ    | 2.32                     | 0.61              |
| 1:g1:167:ARG:CG    | 2:C2:140:ARG:HH21  | 2.07                     | 0.61              |
| 2:B2:119:GLN:OE1   | 2:B2:120:LYS:HE3   | 2.00                     | 0.61              |
| 3:F2:51:THR:HA     | 3:F2:54:ILE:HG22   | 1.83                     | 0.61              |
| 8:b2:35:ARG:HH21   | 8:b2:101:ARG:NE    | 1.98                     | 0.61              |
| 9:j2:190:ASN:ND2   | 9:n2:42:GLU:OE1    | 2.34                     | 0.61              |
| 9:12:237:GLN:HE22  | 12:E4:54:GLN:HA    | 1.65                     | 0.61              |
| 9:32:44:LEU:HD21   | 9:32:73:ARG:HB2    | 1.81                     | 0.61              |
| 11:c3:101:GLN:HE22 | 11:d3:219:ARG:HD3  | 1.64                     | 0.61              |
| 11:f3:164:ARG:NH1  | 11:g3:365:ILE:HG23 | 2.16                     | 0.61              |
| 11:g3:353:GLN:HB2  | 11:g3:358:LEU:HD23 | 1.83                     | 0.61              |
| 11:j3:353:GLN:HB2  | 11:j3:358:LEU:HD23 | 1.83                     | 0.61              |
| 11:l3:353:GLN:HB2  | 11:l3:358:LEU:HD23 | 1.83                     | 0.61              |
| 11:o3:164:ARG:NH1  | 11:p3:365:ILE:HG23 | 2.16                     | 0.61              |
| 11:p3:101:GLN:HE22 | 11:q3:219:ARG:HD3  | 1.66                     | 0.61              |
| 11:q3:123:MET:HE3  | 11:q3:123:MET:C    | 2.26                     | 0.61              |
| 11:w3:98:ARG:NH1   | 11:x3:220:THR:OG1  | 2.33                     | 0.61              |
| 11:w3:123:MET:HE3  | 11:w3:123:MET:C    | 2.26                     | 0.61              |
| 11:x3:164:ARG:NH1  | 11:y3:365:ILE:HG23 | 2.15                     | 0.61              |
| 11:x3:353:GLN:HB2  | 11:x3:358:LEU:HD23 | 1.83                     | 0.61              |
| 11:y3:80:GLN:HB3   | 11:z3:54:GLN:HB3   | 1.83                     | 0.61              |
| 1:b1:407:ASP:HA    | 1:b1:410:LYS:HG2   | 1.83                     | 0.60              |
| 1:g1:268:ALA:HB1   | 1:g1:382:ILE:HD11  | 1.83                     | 0.60              |
| 2:D2:188:THR:HG21  | 4:J2:84:LEU:HB2    | 1.83                     | 0.60              |
| 6:Q2:21:GLN:HA     | 6:Q2:24:GLU:OE1    | 2.01                     | 0.60              |
| 7:X2:4:LEU:HG      | 7:X2:5:ASN:H       | 1.64                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:e2:106:GLN:NE2   | 9:j2:78:GLU:OE2    | 2.33                     | 0.60              |
| 9:32:105:VAL:HG12  | 9:32:136:VAL:HG12  | 1.82                     | 0.60              |
| 11:b3:101:GLN:HE22 | 11:c3:219:ARG:HD3  | 1.64                     | 0.60              |
| 11:e3:98:ARG:NH1   | 11:f3:220:THR:OG1  | 2.33                     | 0.60              |
| 11:f3:353:GLN:HB2  | 11:f3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:i3:123:MET:HE3  | 11:i3:123:MET:C    | 2.26                     | 0.60              |
| 11:k3:98:ARG:NH1   | 11:l3:220:THR:OG1  | 2.33                     | 0.60              |
| 11:k3:353:GLN:HB2  | 11:k3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:t3:123:MET:HE3  | 11:t3:123:MET:C    | 2.26                     | 0.60              |
| 11:v3:353:GLN:HB2  | 11:v3:358:LEU:HD23 | 1.83                     | 0.60              |
| 1:G1:193:ALA:HA    | 1:H1:219:LEU:HG    | 1.83                     | 0.60              |
| 1:R1:167:ARG:HH12  | 3:F2:169:PHE:H     | 1.48                     | 0.60              |
| 1:Z1:294:ARG:HG2   | 6:S2:68:THR:HB     | 1.83                     | 0.60              |
| 1:a1:143:THR:HG23  | 1:c1:154:ARG:HH21  | 1.66                     | 0.60              |
| 1:d1:143:THR:HG21  | 1:f1:156:HIS:NE2   | 2.16                     | 0.60              |
| 1:d1:420:MET:HE1   | 1:d1:430:LEU:HB2   | 1.83                     | 0.60              |
| 1:e1:362:GLU:OE2   | 1:e1:364:SER:OG    | 2.17                     | 0.60              |
| 1:h1:125:GLN:NE2   | 4:I2:2:THR:CG2     | 2.62                     | 0.60              |
| 9:m2:26:LEU:HD22   | 9:r2:242:ILE:HG21  | 1.83                     | 0.60              |
| 9:r2:124:GLN:HE22  | 9:22:61:THR:HG21   | 1.65                     | 0.60              |
| 9:s2:44:LEU:HD12   | 9:s2:71:GLY:HA3    | 1.83                     | 0.60              |
| 9:s2:189:GLU:OE2   | 9:x2:73:ARG:NH2    | 2.33                     | 0.60              |
| 9:32:238:ARG:O     | 9:32:242:ILE:HG12  | 2.01                     | 0.60              |
| 11:k3:46:ASP:OD1   | 11:l3:161:ASN:HB2  | 2.01                     | 0.60              |
| 11:l3:123:MET:HE3  | 11:l3:123:MET:C    | 2.26                     | 0.60              |
| 11:u3:123:MET:C    | 11:u3:123:MET:HE3  | 2.26                     | 0.60              |
| 1:A1:378:ASN:ND2   | 1:A1:381:ASP:OD2   | 2.33                     | 0.60              |
| 1:O1:133:GLN:O     | 1:O1:137:GLU:HG2   | 2.01                     | 0.60              |
| 1:X1:257:VAL:O     | 1:X1:261:ASN:ND2   | 2.33                     | 0.60              |
| 1:d1:157:LEU:HD11  | 1:d1:202:VAL:HG21  | 1.84                     | 0.60              |
| 1:f1:404:LEU:H     | 1:f1:434:ASN:ND2   | 1.99                     | 0.60              |
| 1:g1:143:THR:HG23  | 1:h1:154:ARG:NH2   | 2.09                     | 0.60              |
| 2:B2:86:ASN:HA     | 2:B2:90:LEU:HD12   | 1.82                     | 0.60              |
| 2:C2:185:ILE:HD11  | 4:I2:88:ILE:HD11   | 1.82                     | 0.60              |
| 6:U2:42:ASP:OD1    | 6:U2:43:ILE:N      | 2.32                     | 0.60              |
| 8:e2:229:MET:HG3   | 9:k2:258:THR:HG22  | 1.84                     | 0.60              |
| 9:w2:113:ALA:HB3   | 9:w2:191:LEU:HD23  | 1.83                     | 0.60              |
| 9:y2:184:LEU:HB3   | 9:y2:192:TYR:HB3   | 1.81                     | 0.60              |
| 9:y2:238:ARG:NE    | 12:D4:50:THR:O     | 2.32                     | 0.60              |
| 9:22:174:ASN:HA    | 9:22:206:PRO:HD3   | 1.83                     | 0.60              |
| 11:p3:46:ASP:OD1   | 11:q3:161:ASN:HB2  | 2.01                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:s3:123:MET:HE3 | 11:s3:123:MET:C    | 2.26                     | 0.60              |
| 11:u3:164:ARG:NH1 | 11:v3:365:ILE:HG23 | 2.16                     | 0.60              |
| 12:D4:134:ASP:OD2 | 12:D4:134:ASP:OD1  | 2.19                     | 0.60              |
| 1:B1:165:PHE:CD1  | 2:C2:159:LEU:HD12  | 2.36                     | 0.60              |
| 1:E1:259:ASN:OD1  | 1:E1:260:GLY:N     | 2.34                     | 0.60              |
| 1:I1:256:ILE:HG21 | 1:I1:412:ILE:HD11  | 1.83                     | 0.60              |
| 1:K1:275:LYS:HB3  | 1:K1:377:MET:HE2   | 1.83                     | 0.60              |
| 1:Q1:161:LYS:HZ3  | 3:F2:249:ASN:CG    | 2.06                     | 0.60              |
| 1:R1:186:LEU:HD23 | 1:R1:191:ILE:HD13  | 1.83                     | 0.60              |
| 1:R1:245:ILE:O    | 1:R1:249:ILE:HG12  | 2.00                     | 0.60              |
| 1:T1:277:GLN:HB3  | 1:T1:375:THR:HB    | 1.83                     | 0.60              |
| 1:c1:180:LEU:HD13 | 1:c1:185:ALA:HA    | 1.82                     | 0.60              |
| 1:c1:301:SER:HB3  | 1:c1:359:GLN:HB2   | 1.82                     | 0.60              |
| 2:C2:236:MET:HE1  | 2:D2:150:PHE:HZ    | 1.62                     | 0.60              |
| 8:c2:82:LEU:HD21  | 8:c2:88:LEU:HG     | 1.84                     | 0.60              |
| 8:d2:67:THR:O     | 8:d2:210:ASN:ND2   | 2.33                     | 0.60              |
| 8:d2:229:MET:HG3  | 9:j2:258:THR:HG22  | 1.84                     | 0.60              |
| 9:k2:91:ASN:ND2   | 9:p2:78:GLU:OE2    | 2.34                     | 0.60              |
| 9:n2:9:LYS:NZ     | 9:n2:13:ASP:OD2    | 2.35                     | 0.60              |
| 9:y2:95:VAL:O     | 9:y2:118:GLY:HA3   | 2.01                     | 0.60              |
| 11:a3:164:ARG:NH1 | 11:b3:365:ILE:HG23 | 2.16                     | 0.60              |
| 11:c3:164:ARG:NH1 | 11:d3:365:ILE:HG23 | 2.16                     | 0.60              |
| 11:h3:353:GLN:HB2 | 11:h3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:r3:353:GLN:HB2 | 11:r3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:s3:353:GLN:HB2 | 11:s3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:x3:123:MET:C   | 11:x3:123:MET:HE3  | 2.26                     | 0.60              |
| 11:y3:46:ASP:HA   | 11:z3:161:ASN:ND2  | 2.12                     | 0.60              |
| 1:B1:165:PHE:HE1  | 2:C2:159:LEU:HD13  | 1.61                     | 0.60              |
| 1:H1:299:ASN:HB2  | 1:H1:361:ASN:HB2   | 1.83                     | 0.60              |
| 1:U1:192:SER:O    | 1:U1:196:HIS:ND1   | 2.28                     | 0.60              |
| 1:W1:378:ASN:ND2  | 1:W1:381:ASP:OD1   | 2.31                     | 0.60              |
| 6:Q2:40:ALA:HB2   | 6:Q2:100:VAL:HG22  | 1.82                     | 0.60              |
| 7:X2:98:VAL:HB    | 8:c2:229:MET:HE1   | 1.83                     | 0.60              |
| 7:Z2:117:GLU:OE1  | 8:f2:248:LEU:HB2   | 2.02                     | 0.60              |
| 8:b2:80:VAL:HG13  | 8:b2:201:ILE:HG23  | 1.82                     | 0.60              |
| 9:r2:127:GLN:HG2  | 9:r2:141:THR:HG22  | 1.83                     | 0.60              |
| 11:d3:46:ASP:OD1  | 11:e3:161:ASN:HB2  | 2.02                     | 0.60              |
| 11:v3:46:ASP:OD1  | 11:w3:161:ASN:HB2  | 2.01                     | 0.60              |
| 11:v3:123:MET:HE3 | 11:v3:123:MET:C    | 2.26                     | 0.60              |
| 12:B4:128:GLU:HB3 | 12:B4:196:GLN:HB3  | 1.83                     | 0.60              |
| 1:E1:167:ARG:HB2  | 2:B2:140:ARG:NH2   | 2.06                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:a1:275:LYS:HB2  | 1:a1:377:MET:HB2   | 1.84                     | 0.60              |
| 2:C2:209:MET:HA   | 2:D2:205:MET:HE1   | 1.84                     | 0.60              |
| 3:F2:253:ASP:O    | 3:F2:257:GLU:N     | 2.34                     | 0.60              |
| 9:h2:122:VAL:HG23 | 9:m2:180:ASN:HD22  | 1.66                     | 0.60              |
| 9:h2:238:ARG:NH1  | 9:o2:255:GLN:OE1   | 2.35                     | 0.60              |
| 9:r2:174:ASN:ND2  | 9:r2:203:GLU:OE2   | 2.34                     | 0.60              |
| 9:w2:46:TYR:HA    | 9:w2:69:GLY:HA2    | 1.84                     | 0.60              |
| 9:32:241:GLU:OE1  | 12:B4:52:PRO:HD2   | 2.02                     | 0.60              |
| 9:42:35:LYS:HB3   | 9:42:80:LEU:O      | 2.00                     | 0.60              |
| 11:b3:123:MET:C   | 11:b3:123:MET:HE3  | 2.26                     | 0.60              |
| 11:j3:123:MET:C   | 11:j3:123:MET:HE3  | 2.26                     | 0.60              |
| 11:j3:271:ASP:CB  | 11:j3:357:CYS:HA   | 2.25                     | 0.60              |
| 11:k3:89:VAL:HG23 | 11:k3:126:LEU:CD2  | 2.32                     | 0.60              |
| 11:o3:271:ASP:CB  | 11:o3:357:CYS:HA   | 2.25                     | 0.60              |
| 11:x3:98:ARG:NH1  | 11:y3:220:THR:OG1  | 2.31                     | 0.60              |
| 12:B4:54:GLN:OE1  | 12:B4:56:ASN:ND2   | 2.34                     | 0.60              |
| 1:B1:167:ARG:HA   | 2:C2:159:LEU:O     | 2.01                     | 0.60              |
| 1:K1:407:ASP:OD1  | 1:K1:408:GLN:N     | 2.35                     | 0.60              |
| 1:M1:413:GLU:OE1  | 1:M1:417:ARG:NH1   | 2.33                     | 0.60              |
| 1:N1:245:ILE:HG23 | 1:N1:266:VAL:HG21  | 1.84                     | 0.60              |
| 1:R1:151:LYS:NZ   | 1:R1:182:PRO:HD3   | 2.17                     | 0.60              |
| 1:h1:409:MET:HE1  | 1:h1:434:ASN:HB2   | 1.83                     | 0.60              |
| 8:d2:104:ASN:ND2  | 9:i2:78:GLU:OE2    | 2.33                     | 0.60              |
| 9:j2:160:THR:HG21 | 9:z2:51:GLN:HG2    | 1.83                     | 0.60              |
| 9:k2:164:GLN:HG3  | 11:e3:82:LYS:NZ    | 2.16                     | 0.60              |
| 9:m2:115:THR:HB   | 9:m2:191:LEU:HD23  | 1.82                     | 0.60              |
| 9:22:238:ARG:O    | 9:22:242:ILE:HG12  | 2.02                     | 0.60              |
| 9:32:23:ALA:HB1   | 12:B4:45:LYS:HG3   | 1.84                     | 0.60              |
| 9:32:240:TYR:OH   | 12:B4:49:PRO:HA    | 2.02                     | 0.60              |
| 11:b3:46:ASP:OD1  | 11:c3:161:ASN:HB2  | 2.02                     | 0.60              |
| 11:d3:353:GLN:HB2 | 11:d3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:k3:123:MET:HE3 | 11:k3:123:MET:C    | 2.26                     | 0.60              |
| 11:q3:245:ASN:OD1 | 11:q3:245:ASN:N    | 2.32                     | 0.60              |
| 11:s3:164:ARG:NH1 | 11:t3:365:ILE:HG23 | 2.17                     | 0.60              |
| 1:B1:413:GLU:OE2  | 1:B1:417:ARG:NH1   | 2.35                     | 0.60              |
| 1:C1:266:VAL:HG22 | 1:C1:387:VAL:HG22  | 1.83                     | 0.60              |
| 1:I1:128:GLU:N    | 1:I1:128:GLU:OE2   | 2.32                     | 0.60              |
| 1:I1:145:GLU:HA   | 1:I1:150:VAL:HG12  | 1.83                     | 0.60              |
| 1:N1:165:PHE:HE2  | 2:A2:148:ALA:CB    | 2.09                     | 0.60              |
| 1:P1:404:LEU:H    | 1:P1:434:ASN:ND2   | 2.00                     | 0.60              |
| 1:Q1:162:PRO:CB   | 3:F2:253:ASP:CG    | 2.69                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:R1:125:GLN:NE2   | 2:E2:230:ASP:CG    | 2.55                     | 0.60              |
| 1:R1:164:LEU:CD1   | 3:F2:174:ARG:HD3   | 2.30                     | 0.60              |
| 1:T1:165:PHE:HD1   | 3:F2:166:SER:HB2   | 1.65                     | 0.60              |
| 3:F2:12:TRP:HD1    | 5:P2:34:PHE:HZ     | 1.50                     | 0.60              |
| 6:S2:128:LYS:NZ    | 7:X2:133:GLY:O     | 2.35                     | 0.60              |
| 6:U2:106:ARG:NH1   | 8:f2:245:ASN:OD1   | 2.34                     | 0.60              |
| 8:b2:214:VAL:HG22  | 9:h2:9:LYS:HD2     | 1.84                     | 0.60              |
| 9:m2:109:ASP:OD2   | 9:m2:110:GLY:N     | 2.35                     | 0.60              |
| 9:u2:200:ALA:HB3   | 11:b3:54:GLN:OE1   | 2.00                     | 0.60              |
| 9:22:180:ASN:OD1   | 9:22:183:GLY:N     | 2.34                     | 0.60              |
| 10:Y3:82:LEU:HD12  | 10:Y3:146:GLY:CA   | 2.32                     | 0.60              |
| 11:e3:46:ASP:OD1   | 11:f3:161:ASN:HB2  | 2.01                     | 0.60              |
| 11:g3:271:ASP:CB   | 11:g3:357:CYS:HA   | 2.25                     | 0.60              |
| 11:i3:89:VAL:HG23  | 11:i3:126:LEU:CD2  | 2.32                     | 0.60              |
| 11:i3:164:ARG:NH1  | 11:j3:365:ILE:HG23 | 2.16                     | 0.60              |
| 11:j3:245:ASN:OD1  | 11:j3:245:ASN:N    | 2.33                     | 0.60              |
| 11:m3:353:GLN:HB2  | 11:m3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:q3:353:GLN:HB2  | 11:q3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:t3:46:ASP:OD1   | 11:u3:161:ASN:HB2  | 2.02                     | 0.60              |
| 11:t3:353:GLN:HB2  | 11:t3:358:LEU:HD23 | 1.83                     | 0.60              |
| 12:E4:108:ILE:HD11 | 12:E4:125:PHE:HB3  | 1.84                     | 0.60              |
| 1:T1:248:ARG:NH1   | 1:U1:267:THR:OG1   | 2.35                     | 0.60              |
| 1:U1:165:PHE:CE2   | 2:E2:244:TYR:HE2   | 2.19                     | 0.60              |
| 1:W1:144:ILE:HG22  | 1:W1:150:VAL:HG11  | 1.83                     | 0.60              |
| 1:b1:424:ASP:OD1   | 1:b1:425:LYS:N     | 2.35                     | 0.60              |
| 1:c1:407:ASP:OD1   | 1:c1:408:GLN:N     | 2.35                     | 0.60              |
| 2:A2:118:GLU:OE1   | 6:U2:5:LEU:N       | 2.34                     | 0.60              |
| 2:B2:64:PHE:HB2    | 2:B2:97:THR:HG21   | 1.83                     | 0.60              |
| 9:l2:180:ASN:OD1   | 9:l2:183:GLY:N     | 2.33                     | 0.60              |
| 9:42:98:LYS:O      | 9:42:212:GLY:HA3   | 2.02                     | 0.60              |
| 10:A3:82:LEU:HD12  | 10:A3:146:GLY:CA   | 2.32                     | 0.60              |
| 11:a3:353:GLN:HB2  | 11:a3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:b3:353:GLN:HB2  | 11:b3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:b3:362:LEU:HD21 | 11:z3:166:THR:HG21 | 1.84                     | 0.60              |
| 11:e3:353:GLN:HB2  | 11:e3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:f3:101:GLN:HE22 | 11:g3:219:ARG:HD3  | 1.65                     | 0.60              |
| 11:l3:164:ARG:NH1  | 11:m3:365:ILE:HG23 | 2.17                     | 0.60              |
| 11:n3:353:GLN:HB2  | 11:n3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:u3:98:ARG:NH1   | 11:v3:220:THR:OG1  | 2.32                     | 0.60              |
| 11:y3:353:GLN:HB2  | 11:y3:358:LEU:HD23 | 1.83                     | 0.60              |
| 11:z3:123:MET:C    | 11:z3:123:MET:HE3  | 2.26                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C1:157:LEU:HD11 | 1:C1:202:VAL:HG21  | 1.83                     | 0.60              |
| 1:Q1:392:ASN:OD1  | 1:Q1:393:TYR:N     | 2.35                     | 0.60              |
| 1:U1:383:GLU:OE1  | 1:U1:383:GLU:N     | 2.35                     | 0.60              |
| 1:V1:287:ASP:HB2  | 1:V1:290:LYS:NZ    | 2.17                     | 0.60              |
| 1:a1:407:ASP:OD1  | 1:a1:408:GLN:N     | 2.35                     | 0.60              |
| 1:d1:203:ALA:HA   | 1:f1:158:ALA:HB1   | 1.84                     | 0.60              |
| 2:B2:185:ILE:HD11 | 4:H2:88:ILE:HD11   | 1.83                     | 0.60              |
| 8:c2:82:LEU:HD11  | 8:c2:163:LEU:HD22  | 1.84                     | 0.60              |
| 8:d2:226:ARG:O    | 8:d2:230:GLN:HG2   | 2.02                     | 0.60              |
| 9:v2:231:VAL:HG11 | 9:22:9:LYS:HG3     | 1.83                     | 0.60              |
| 10:E3:166:GLU:OE2 | 10:E3:168:GLN:NE2  | 2.27                     | 0.60              |
| 10:W3:82:LEU:HD12 | 10:W3:146:GLY:CA   | 2.32                     | 0.60              |
| 10:Y3:131:SER:OG  | 10:Z3:101:LYS:HG2  | 2.01                     | 0.60              |
| 11:g3:46:ASP:OD1  | 11:h3:161:ASN:HB2  | 2.02                     | 0.60              |
| 11:j3:46:ASP:OD1  | 11:k3:161:ASN:HB2  | 2.01                     | 0.60              |
| 11:l3:98:ARG:NH1  | 11:m3:220:THR:OG1  | 2.31                     | 0.60              |
| 11:n3:89:VAL:HG23 | 11:n3:126:LEU:CD2  | 2.32                     | 0.60              |
| 11:o3:46:ASP:OD1  | 11:p3:161:ASN:HB2  | 2.02                     | 0.60              |
| 11:r3:98:ARG:NH1  | 11:s3:220:THR:OG1  | 2.32                     | 0.60              |
| 5:P2:76:GLN:HG2   | 7:V2:123:LYS:HD3   | 1.84                     | 0.59              |
| 9:m2:230:LEU:HD12 | 9:x2:257:LEU:HG    | 1.84                     | 0.59              |
| 9:p2:141:THR:O    | 11:c3:54:GLN:NE2   | 2.34                     | 0.59              |
| 9:s2:139:ALA:HB3  | 11:q3:53:THR:CB    | 2.29                     | 0.59              |
| 10:C3:82:LEU:HD12 | 10:C3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:J3:82:LEU:HD12 | 10:J3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:Q3:82:LEU:HD12 | 10:Q3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:R3:82:LEU:HD12 | 10:R3:146:GLY:CA   | 2.32                     | 0.59              |
| 11:m3:46:ASP:OD1  | 11:n3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:m3:89:VAL:HG23 | 11:m3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:m3:245:ASN:OD1 | 11:m3:245:ASN:N    | 2.33                     | 0.59              |
| 11:s3:46:ASP:OD1  | 11:t3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:t3:89:VAL:HG23 | 11:t3:126:LEU:HD21 | 1.84                     | 0.59              |
| 11:u3:46:ASP:OD1  | 11:v3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:u3:89:VAL:HG23 | 11:u3:126:LEU:HD21 | 1.84                     | 0.59              |
| 11:u3:353:GLN:HB2 | 11:u3:358:LEU:HD23 | 1.83                     | 0.59              |
| 1:E1:294:ARG:HG2  | 6:U2:68:THR:OG1    | 2.02                     | 0.59              |
| 1:I1:143:THR:HG21 | 1:K1:156:HIS:NE2   | 2.17                     | 0.59              |
| 1:U1:365:ASN:OD1  | 6:R2:65:LEU:O      | 2.18                     | 0.59              |
| 1:X1:234:GLN:HB2  | 1:X1:272:PHE:CZ    | 2.37                     | 0.59              |
| 1:Z1:294:ARG:CG   | 6:S2:66:THR:HB     | 2.27                     | 0.59              |
| 10:I3:82:LEU:HD12 | 10:I3:146:GLY:CA   | 2.32                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:P3:82:LEU:HD12  | 10:P3:146:GLY:CA   | 2.32                     | 0.59              |
| 11:a3:220:THR:OG1  | 11:z3:98:ARG:NH1   | 2.33                     | 0.59              |
| 11:n3:46:ASP:OD1   | 11:o3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:o3:353:GLN:HB2  | 11:o3:358:LEU:HD23 | 1.83                     | 0.59              |
| 11:p3:89:VAL:HG23  | 11:p3:126:LEU:CD2  | 2.32                     | 0.59              |
| 1:B1:142:ARG:HB3   | 1:C1:154:ARG:HH22  | 1.67                     | 0.59              |
| 1:D1:405:THR:HG23  | 1:D1:408:GLN:H     | 1.67                     | 0.59              |
| 1:T1:216:SER:O     | 1:T1:218:HIS:ND1   | 2.35                     | 0.59              |
| 1:W1:143:THR:HG22  | 1:X1:154:ARG:HD3   | 1.84                     | 0.59              |
| 1:b1:301:SER:HB3   | 1:b1:359:GLN:HB3   | 1.83                     | 0.59              |
| 1:h1:393:TYR:CE2   | 1:h1:436:PRO:HD3   | 2.38                     | 0.59              |
| 8:c2:73:TYR:CE1    | 9:o2:74:PRO:HD2    | 2.37                     | 0.59              |
| 8:d2:96:ALA:HB3    | 8:d2:180:ARG:HH21  | 1.68                     | 0.59              |
| 9:j2:143:PRO:HD3   | 9:j2:170:VAL:HG21  | 1.85                     | 0.59              |
| 9:k2:168:VAL:CG2   | 11:f3:114:LYS:CE   | 2.78                     | 0.59              |
| 9:t2:202:ASN:CB    | 11:w3:53:THR:HG21  | 2.30                     | 0.59              |
| 9:x2:19:MET:HE1    | 9:x2:233:MET:HE2   | 1.83                     | 0.59              |
| 9:x2:36:ARG:HH21   | 9:x2:80:LEU:HB2    | 1.65                     | 0.59              |
| 10:D3:58:ILE:HG13  | 10:D3:59:ASN:H     | 1.68                     | 0.59              |
| 10:D3:82:LEU:HD12  | 10:D3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:F3:82:LEU:HD12  | 10:F3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:F3:166:GLU:OE2  | 10:F3:168:GLN:NE2  | 2.27                     | 0.59              |
| 10:K3:131:SER:OG   | 10:L3:101:LYS:HG2  | 2.02                     | 0.59              |
| 10:S3:131:SER:OG   | 10:T3:101:LYS:HG2  | 2.02                     | 0.59              |
| 10:U3:82:LEU:HD12  | 10:U3:146:GLY:CA   | 2.32                     | 0.59              |
| 11:f3:89:VAL:HG23  | 11:f3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:f3:105:VAL:HG22 | 11:f3:165:ILE:HB   | 1.85                     | 0.59              |
| 11:g3:89:VAL:HG23  | 11:g3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:l3:89:VAL:HG23  | 11:l3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:o3:89:VAL:HG23  | 11:o3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:s3:89:VAL:HG23  | 11:s3:126:LEU:HD21 | 1.84                     | 0.59              |
| 11:v3:89:VAL:HG23  | 11:v3:126:LEU:HD21 | 1.84                     | 0.59              |
| 11:w3:89:VAL:HG23  | 11:w3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:w3:89:VAL:HG23  | 11:w3:126:LEU:HD21 | 1.84                     | 0.59              |
| 12:C4:134:ASP:HA   | 12:C4:155:GLU:HA   | 1.83                     | 0.59              |
| 1:I1:140:LEU:O     | 1:I1:144:ILE:HG12  | 2.01                     | 0.59              |
| 1:I1:413:GLU:OE2   | 1:I1:417:ARG:NH1   | 2.35                     | 0.59              |
| 1:K1:138:GLY:O     | 1:K1:142:ARG:HG2   | 2.02                     | 0.59              |
| 1:N1:378:ASN:ND2   | 1:N1:381:ASP:OD1   | 2.36                     | 0.59              |
| 1:P1:245:ILE:O     | 1:P1:249:ILE:HD12  | 2.02                     | 0.59              |
| 1:S1:374:HIS:HB3   | 1:T1:276:GLU:HB2   | 1.82                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Z1:374:HIS:HB3   | 1:a1:276:GLU:HB3   | 1.85                     | 0.59              |
| 1:Z1:388:ALA:HA    | 1:Z1:431:ASN:O     | 2.03                     | 0.59              |
| 2:B2:39:SER:C      | 2:B2:41:SER:H      | 2.11                     | 0.59              |
| 2:E2:39:SER:C      | 2:E2:41:SER:H      | 2.10                     | 0.59              |
| 7:Y2:117:GLU:OE1   | 8:e2:248:LEU:HB2   | 2.03                     | 0.59              |
| 9:m2:122:VAL:O     | 9:r2:180:ASN:ND2   | 2.36                     | 0.59              |
| 9:w2:28:ASN:OD1    | 9:22:72:VAL:HG22   | 2.02                     | 0.59              |
| 9:12:89:THR:HG23   | 9:12:91:ASN:H      | 1.66                     | 0.59              |
| 10:D3:166:GLU:OE2  | 10:D3:168:GLN:NE2  | 2.27                     | 0.59              |
| 10:H3:82:LEU:HD12  | 10:H3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:K3:82:LEU:HD12  | 10:K3:146:GLY:CA   | 2.32                     | 0.59              |
| 11:a3:98:ARG:NH1   | 11:b3:220:THR:OG1  | 2.32                     | 0.59              |
| 11:c3:353:GLN:HB2  | 11:c3:358:LEU:HD23 | 1.83                     | 0.59              |
| 11:d3:101:GLN:HE22 | 11:e3:219:ARG:HD3  | 1.66                     | 0.59              |
| 11:e3:105:VAL:HG22 | 11:e3:165:ILE:HB   | 1.85                     | 0.59              |
| 11:h3:89:VAL:HG23  | 11:h3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:n3:164:ARG:NH1  | 11:o3:365:ILE:HG23 | 2.18                     | 0.59              |
| 11:w3:105:VAL:HG22 | 11:w3:165:ILE:HB   | 1.85                     | 0.59              |
| 11:x3:105:VAL:HG22 | 11:x3:165:ILE:HB   | 1.85                     | 0.59              |
| 1:G1:139:GLU:HG3   | 1:H1:156:HIS:HE1   | 1.67                     | 0.59              |
| 1:J1:298:LEU:HD13  | 1:J1:362:GLU:HB3   | 1.84                     | 0.59              |
| 1:P1:378:ASN:ND2   | 1:P1:381:ASP:OD1   | 2.34                     | 0.59              |
| 1:Y1:374:HIS:HB3   | 1:Z1:276:GLU:HB3   | 1.85                     | 0.59              |
| 6:Q2:88:ARG:NH2    | 6:Q2:105:GLU:OE2   | 2.34                     | 0.59              |
| 9:12:237:GLN:NE2   | 12:E4:54:GLN:HA    | 2.18                     | 0.59              |
| 10:C3:58:ILE:HG13  | 10:C3:59:ASN:H     | 1.68                     | 0.59              |
| 10:O3:58:ILE:HG13  | 10:O3:59:ASN:H     | 1.68                     | 0.59              |
| 10:S3:82:LEU:HD12  | 10:S3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:T3:82:LEU:HD12  | 10:T3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:X3:58:ILE:HG13  | 10:X3:59:ASN:H     | 1.68                     | 0.59              |
| 11:a3:46:ASP:OD1   | 11:b3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:e3:166:THR:HG21 | 11:g3:362:LEU:HD21 | 1.85                     | 0.59              |
| 11:n3:271:ASP:CB   | 11:n3:357:CYS:HA   | 2.26                     | 0.59              |
| 11:r3:325:SER:HB3  | 11:r3:330:SER:CB   | 2.32                     | 0.59              |
| 11:s3:325:SER:HB3  | 11:s3:330:SER:CB   | 2.32                     | 0.59              |
| 11:v3:89:VAL:HG23  | 11:v3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:v3:105:VAL:HG22 | 11:v3:165:ILE:HB   | 1.85                     | 0.59              |
| 11:x3:89:VAL:HG23  | 11:x3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:z3:353:GLN:HB2  | 11:z3:358:LEU:HD23 | 1.83                     | 0.59              |
| 12:D4:176:PRO:O    | 12:D4:180:TYR:OH   | 2.19                     | 0.59              |
| 1:B1:158:ALA:HB1   | 1:h1:203:ALA:HA    | 1.85                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B1:404:LEU:H     | 1:B1:434:ASN:HD21  | 1.50                     | 0.59              |
| 1:N1:203:ALA:HB2   | 1:O1:158:ALA:HB1   | 1.84                     | 0.59              |
| 1:S1:413:GLU:HB3   | 1:S1:432:VAL:HG21  | 1.83                     | 0.59              |
| 1:U1:165:PHE:HZ    | 2:E2:244:TYR:CZ    | 2.21                     | 0.59              |
| 1:b1:248:ARG:NH1   | 1:c1:267:THR:OG1   | 2.36                     | 0.59              |
| 1:g1:256:ILE:HG21  | 1:g1:412:ILE:HD11  | 1.83                     | 0.59              |
| 2:C2:132:GLN:OE1   | 2:C2:135:ARG:NH1   | 2.35                     | 0.59              |
| 2:E2:62:THR:HB     | 2:E2:101:MET:HE2   | 1.83                     | 0.59              |
| 5:N2:66:ILE:H      | 5:N2:66:ILE:HD12   | 1.67                     | 0.59              |
| 6:S2:104:ARG:HE    | 7:Y2:15:ALA:HB2    | 1.68                     | 0.59              |
| 7:X2:22:ASN:OD1    | 8:c2:4:ALA:HB2     | 2.02                     | 0.59              |
| 9:g2:98:LYS:O      | 9:g2:212:GLY:HA3   | 2.03                     | 0.59              |
| 9:j2:25:ASN:ND2    | 9:j2:37:GLN:O      | 2.35                     | 0.59              |
| 9:r2:86:LEU:HD11   | 9:32:45:LEU:HD23   | 1.84                     | 0.59              |
| 10:E3:82:LEU:HD12  | 10:E3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:L3:82:LEU:HD12  | 10:L3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:O3:82:LEU:HD12  | 10:O3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:V3:82:LEU:HD12  | 10:V3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:Y3:58:ILE:HG13  | 10:Y3:59:ASN:H     | 1.68                     | 0.59              |
| 11:a3:26:THR:CG2   | 11:a3:187:LEU:HB3  | 2.33                     | 0.59              |
| 11:a3:161:ASN:HB2  | 11:z3:46:ASP:OD1   | 2.03                     | 0.59              |
| 11:c3:166:THR:HG21 | 11:e3:362:LEU:HD21 | 1.85                     | 0.59              |
| 11:e3:89:VAL:HG23  | 11:e3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:g3:105:VAL:HG22 | 11:g3:165:ILE:HB   | 1.85                     | 0.59              |
| 11:h3:46:ASP:OD1   | 11:i3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:r3:89:VAL:HG23  | 11:r3:126:LEU:HD21 | 1.84                     | 0.59              |
| 11:u3:26:THR:CG2   | 11:u3:187:LEU:HB3  | 2.33                     | 0.59              |
| 11:x3:26:THR:CG2   | 11:x3:187:LEU:HB3  | 2.33                     | 0.59              |
| 11:x3:89:VAL:HG23  | 11:x3:126:LEU:HD21 | 1.84                     | 0.59              |
| 11:y3:89:VAL:HG23  | 11:y3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:z3:26:THR:CG2   | 11:z3:187:LEU:HB3  | 2.33                     | 0.59              |
| 1:C1:143:THR:HG21  | 1:E1:156:HIS:NE2   | 2.18                     | 0.59              |
| 1:F1:363:THR:CB    | 6:U2:63:VAL:HG23   | 2.33                     | 0.59              |
| 1:N1:129:GLN:OE1   | 1:N1:129:GLN:N     | 2.30                     | 0.59              |
| 1:N1:166:VAL:HG22  | 2:A2:162:PRO:CA    | 2.33                     | 0.59              |
| 1:O1:164:LEU:HB2   | 3:F2:141:ASN:ND2   | 2.18                     | 0.59              |
| 1:S1:404:LEU:H     | 1:S1:434:ASN:HD21  | 1.48                     | 0.59              |
| 1:Z1:363:THR:HG23  | 6:S2:73:ILE:CD1    | 2.33                     | 0.59              |
| 1:c1:166:VAL:O     | 2:D2:140:ARG:HA    | 2.03                     | 0.59              |
| 9:g2:167:PRO:HG3   | 9:w2:54:ALA:H      | 1.66                     | 0.59              |
| 9:l2:46:TYR:HA     | 9:l2:69:GLY:HA2    | 1.85                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:s2:209:ASN:OD1   | 11:r3:78:ASN:CG    | 2.45                     | 0.59              |
| 9:u2:28:ASN:OD1    | 9:z2:72:VAL:HG22   | 2.02                     | 0.59              |
| 10:B3:82:LEU:HD12  | 10:B3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:B3:131:SER:OG   | 10:C3:101:LYS:HG2  | 2.03                     | 0.59              |
| 10:G3:166:GLU:OE2  | 10:G3:168:GLN:NE2  | 2.27                     | 0.59              |
| 10:K3:58:ILE:HG13  | 10:K3:59:ASN:H     | 1.68                     | 0.59              |
| 10:L3:58:ILE:HG13  | 10:L3:59:ASN:H     | 1.68                     | 0.59              |
| 10:S3:58:ILE:HG13  | 10:S3:59:ASN:H     | 1.68                     | 0.59              |
| 10:Z3:82:LEU:HD12  | 10:Z3:146:GLY:CA   | 2.32                     | 0.59              |
| 11:d3:89:VAL:HG23  | 11:d3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:d3:98:ARG:NH1   | 11:e3:220:THR:OG1  | 2.31                     | 0.59              |
| 11:d3:105:VAL:HG22 | 11:d3:165:ILE:HB   | 1.85                     | 0.59              |
| 11:g3:245:ASN:OD1  | 11:g3:245:ASN:N    | 2.33                     | 0.59              |
| 11:l3:166:THR:HG21 | 11:n3:362:LEU:HD21 | 1.85                     | 0.59              |
| 11:u3:89:VAL:HG23  | 11:u3:126:LEU:CD2  | 2.32                     | 0.59              |
| 11:v3:26:THR:CG2   | 11:v3:187:LEU:HB3  | 2.33                     | 0.59              |
| 11:v3:164:ARG:NH1  | 11:w3:365:ILE:HG23 | 2.18                     | 0.59              |
| 11:w3:26:THR:CG2   | 11:w3:187:LEU:HB3  | 2.33                     | 0.59              |
| 1:L1:167:ARG:NH2   | 2:A2:245:SER:CB    | 2.57                     | 0.59              |
| 1:R1:125:GLN:NE2   | 2:E2:230:ASP:OD2   | 2.35                     | 0.59              |
| 1:R1:234:GLN:HB2   | 1:R1:272:PHE:CZ    | 2.38                     | 0.59              |
| 1:S1:295:SER:OG    | 6:R2:71:HIS:C      | 2.42                     | 0.59              |
| 1:a1:155:VAL:HG23  | 1:a1:176:VAL:HG22  | 1.82                     | 0.59              |
| 1:a1:167:ARG:HG2   | 2:D2:140:ARG:NH2   | 2.18                     | 0.59              |
| 1:c1:257:VAL:O     | 1:c1:261:ASN:ND2   | 2.36                     | 0.59              |
| 1:f1:248:ARG:NH1   | 1:g1:267:THR:OG1   | 2.36                     | 0.59              |
| 2:B2:137:PHE:HZ    | 2:B2:243:PHE:CE2   | 2.20                     | 0.59              |
| 5:L2:66:ILE:H      | 5:L2:66:ILE:HD12   | 1.67                     | 0.59              |
| 6:S2:103:ASP:OD1   | 7:Y2:112:TYR:OH    | 2.19                     | 0.59              |
| 8:c2:226:ARG:O     | 8:c2:230:GLN:HG2   | 2.03                     | 0.59              |
| 9:h2:185:GLU:OE1   | 9:m2:67:GLN:NE2    | 2.35                     | 0.59              |
| 9:q2:98:LYS:O      | 9:q2:212:GLY:CA    | 2.50                     | 0.59              |
| 9:w2:238:ARG:NH1   | 9:w2:241:GLU:HG3   | 2.17                     | 0.59              |
| 9:y2:240:TYR:CZ    | 9:42:253:MET:HE1   | 2.37                     | 0.59              |
| 9:z2:237:GLN:HE21  | 12:D4:53:LEU:HB2   | 1.68                     | 0.59              |
| 9:12:44:LEU:HD12   | 9:12:71:GLY:HA3    | 1.85                     | 0.59              |
| 9:22:241:GLU:OE1   | 12:A4:52:PRO:HD2   | 2.03                     | 0.59              |
| 9:32:174:ASN:ND2   | 9:32:203:GLU:OE2   | 2.34                     | 0.59              |
| 10:B3:166:GLU:OE2  | 10:B3:168:GLN:NE2  | 2.27                     | 0.59              |
| 10:G3:131:SER:OG   | 10:H3:101:LYS:HG2  | 2.03                     | 0.59              |
| 10:I3:131:SER:OG   | 10:J3:101:LYS:HG2  | 2.03                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:N3:58:ILE:HG13  | 10:N3:59:ASN:H     | 1.68                     | 0.59              |
| 10:T3:131:SER:OG   | 10:U3:101:LYS:HG2  | 2.03                     | 0.59              |
| 10:W3:58:ILE:HG13  | 10:W3:59:ASN:H     | 1.68                     | 0.59              |
| 10:W3:131:SER:OG   | 10:X3:101:LYS:HG2  | 2.02                     | 0.59              |
| 11:f3:166:THR:HG21 | 11:h3:362:LEU:HD21 | 1.84                     | 0.59              |
| 11:h3:166:THR:HG21 | 11:j3:362:LEU:HD21 | 1.85                     | 0.59              |
| 11:i3:46:ASP:OD1   | 11:j3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:l3:46:ASP:OD1   | 11:m3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:p3:353:GLN:HB2  | 11:p3:358:LEU:HD23 | 1.83                     | 0.59              |
| 11:t3:26:THR:CG2   | 11:t3:187:LEU:HB3  | 2.33                     | 0.59              |
| 11:t3:325:SER:HB3  | 11:t3:330:SER:CB   | 2.32                     | 0.59              |
| 11:w3:325:SER:HB3  | 11:w3:330:SER:CB   | 2.32                     | 0.59              |
| 11:y3:26:THR:CG2   | 11:y3:187:LEU:HB3  | 2.33                     | 0.59              |
| 12:D4:169:GLN:HG3  | 12:D4:175:VAL:HG12 | 1.84                     | 0.59              |
| 1:D1:365:ASN:HD22  | 6:U2:73:ILE:CD1    | 2.11                     | 0.59              |
| 1:T1:245:ILE:HD11  | 1:T1:420:MET:HA    | 1.85                     | 0.59              |
| 1:d1:392:ASN:OD1   | 1:d1:393:TYR:N     | 2.35                     | 0.59              |
| 1:d1:420:MET:HE3   | 1:d1:422:PHE:HB2   | 1.84                     | 0.59              |
| 1:e1:408:GLN:HE22  | 1:e1:412:ILE:HD11  | 1.68                     | 0.59              |
| 1:f1:164:LEU:HD21  | 2:D2:149:LEU:CA    | 2.33                     | 0.59              |
| 5:M2:86:ILE:HD11   | 6:R2:133:VAL:HG22  | 1.85                     | 0.59              |
| 6:S2:92:GLN:NE2    | 7:Y2:19:LYS:HA     | 2.18                     | 0.59              |
| 7:V2:113:GLN:OE1   | 7:a2:128:LYS:NZ    | 2.32                     | 0.59              |
| 9:g2:174:ASN:ND2   | 9:g2:203:GLU:OE2   | 2.36                     | 0.59              |
| 9:i2:85:ASN:OD1    | 9:t2:47:GLN:NE2    | 2.36                     | 0.59              |
| 9:k2:174:ASN:HA    | 9:k2:206:PRO:HD3   | 1.85                     | 0.59              |
| 9:p2:171:GLY:HA2   | 11:c3:80:GLN:CD    | 2.27                     | 0.59              |
| 9:s2:139:ALA:HB2   | 11:q3:53:THR:CB    | 2.33                     | 0.59              |
| 9:22:238:ARG:NH2   | 12:A4:55:ASN:O     | 2.12                     | 0.59              |
| 9:42:83:GLN:NE2    | 9:42:84:GLY:O      | 2.35                     | 0.59              |
| 10:A3:131:SER:OG   | 10:B3:101:LYS:HG2  | 2.03                     | 0.59              |
| 10:E3:58:ILE:HG13  | 10:E3:59:ASN:H     | 1.68                     | 0.59              |
| 10:G3:82:LEU:HD12  | 10:G3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:H3:58:ILE:HG13  | 10:H3:59:ASN:H     | 1.68                     | 0.59              |
| 10:I3:58:ILE:HG13  | 10:I3:59:ASN:H     | 1.68                     | 0.59              |
| 10:J3:58:ILE:HG13  | 10:J3:59:ASN:H     | 1.68                     | 0.59              |
| 10:N3:82:LEU:HD12  | 10:N3:146:GLY:CA   | 2.32                     | 0.59              |
| 10:R3:58:ILE:HG13  | 10:R3:59:ASN:H     | 1.68                     | 0.59              |
| 10:T3:58:ILE:HG13  | 10:T3:59:ASN:H     | 1.67                     | 0.59              |
| 10:X3:82:LEU:HD12  | 10:X3:146:GLY:CA   | 2.32                     | 0.59              |
| 11:b3:26:THR:CG2   | 11:b3:187:LEU:HB3  | 2.33                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:c3:105:VAL:HG22 | 11:c3:165:ILE:HB   | 1.85                     | 0.59              |
| 11:f3:46:ASP:OD1   | 11:g3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:h3:164:ARG:NH1  | 11:i3:365:ILE:HG23 | 2.18                     | 0.59              |
| 11:r3:46:ASP:HA    | 11:s3:161:ASN:ND2  | 2.18                     | 0.59              |
| 11:x3:325:SER:HB3  | 11:x3:330:SER:CB   | 2.32                     | 0.59              |
| 11:y3:89:VAL:HG23  | 11:y3:126:LEU:HD21 | 1.84                     | 0.59              |
| 11:z3:89:VAL:HG23  | 11:z3:126:LEU:CD2  | 2.32                     | 0.59              |
| 12:B4:56:ASN:OD1   | 12:B4:57:GLU:N     | 2.36                     | 0.59              |
| 1:B1:167:ARG:HB3   | 2:C2:160:GLN:CD    | 2.28                     | 0.59              |
| 1:W1:186:LEU:HG    | 1:W1:190:GLN:HB2   | 1.84                     | 0.59              |
| 1:h1:165:PHE:HE1   | 2:C2:141:GLN:HE22  | 1.49                     | 0.59              |
| 9:t2:95:VAL:O      | 9:t2:118:GLY:HA3   | 2.03                     | 0.59              |
| 9:w2:142:ILE:HG23  | 9:w2:159:VAL:HG11  | 1.84                     | 0.59              |
| 9:42:238:ARG:O     | 9:42:242:ILE:HG12  | 2.03                     | 0.59              |
| 10:A3:166:GLU:OE2  | 10:A3:168:GLN:NE2  | 2.27                     | 0.59              |
| 11:c3:26:THR:CG2   | 11:c3:187:LEU:HB3  | 2.33                     | 0.59              |
| 11:c3:46:ASP:OD1   | 11:d3:161:ASN:HB2  | 2.02                     | 0.59              |
| 11:m3:164:ARG:NH1  | 11:n3:365:ILE:HG23 | 2.17                     | 0.59              |
| 11:o3:166:THR:HG21 | 11:q3:362:LEU:HD21 | 1.85                     | 0.59              |
| 11:t3:164:ARG:NH1  | 11:u3:365:ILE:HG23 | 2.18                     | 0.59              |
| 11:v3:325:SER:HB3  | 11:v3:330:SER:CB   | 2.32                     | 0.59              |
| 11:y3:105:VAL:HG22 | 11:y3:165:ILE:HB   | 1.85                     | 0.59              |
| 12:E4:149:ARG:NH1  | 12:E4:168:LYS:O    | 2.33                     | 0.59              |
| 1:I1:139:GLU:OE2   | 1:K1:154:ARG:NH1   | 2.35                     | 0.58              |
| 1:L1:293:LEU:HD13  | 1:L1:296:ARG:HE    | 1.68                     | 0.58              |
| 1:Q1:197:LEU:HD12  | 1:R1:175:SER:HB2   | 1.85                     | 0.58              |
| 1:U1:150:VAL:HA    | 1:U1:180:LEU:HA    | 1.84                     | 0.58              |
| 1:X1:250:GLU:O     | 1:X1:254:SER:OG    | 2.20                     | 0.58              |
| 1:a1:250:GLU:O     | 1:a1:254:SER:OG    | 2.16                     | 0.58              |
| 2:A2:75:ARG:HH21   | 5:O2:104:VAL:HB    | 1.68                     | 0.58              |
| 6:U2:106:ARG:HA    | 8:f2:248:LEU:HD21  | 1.85                     | 0.58              |
| 9:g2:228:GLU:OE2   | 9:m2:9:LYS:NZ      | 2.30                     | 0.58              |
| 9:i2:121:GLN:NE2   | 9:s2:64:SER:OG     | 2.36                     | 0.58              |
| 9:u2:200:ALA:HB3   | 11:b3:54:GLN:HE22  | 1.64                     | 0.58              |
| 9:v2:184:LEU:HB3   | 9:v2:192:TYR:HB3   | 1.84                     | 0.58              |
| 9:32:29:VAL:CG2    | 12:B4:37:LEU:HD23  | 2.33                     | 0.58              |
| 10:C3:166:GLU:OE2  | 10:C3:168:GLN:NE2  | 2.27                     | 0.58              |
| 10:M3:131:SER:OG   | 10:N3:101:LYS:HG2  | 2.02                     | 0.58              |
| 11:b3:89:VAL:HG23  | 11:b3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:d3:26:THR:CG2   | 11:d3:187:LEU:HB3  | 2.33                     | 0.58              |
| 11:i3:247:THR:HB   | 11:i3:248:PRO:HD2  | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:k3:105:VAL:HG22 | 11:k3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:q3:89:VAL:HG23  | 11:q3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:q3:325:SER:HB3  | 11:q3:330:SER:CB   | 2.32                     | 0.58              |
| 11:r3:164:ARG:NH1  | 11:s3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:u3:105:VAL:HG22 | 11:u3:165:ILE:HB   | 1.85                     | 0.58              |
| 1:D1:411:GLN:O     | 1:D1:415:LEU:HD23  | 2.03                     | 0.58              |
| 1:E1:294:ARG:HG2   | 6:U2:66:THR:HB     | 1.82                     | 0.58              |
| 1:L1:269:GLN:HB2   | 1:L1:384:ARG:HB3   | 1.85                     | 0.58              |
| 1:U1:187:ASP:OD1   | 1:U1:190:GLN:NE2   | 2.36                     | 0.58              |
| 1:W1:418:GLU:HB3   | 1:X1:388:ALA:HB2   | 1.85                     | 0.58              |
| 1:d1:165:PHE:CE2   | 2:D2:144:GLU:CG    | 2.86                     | 0.58              |
| 2:D2:75:ARG:NH2    | 5:L2:104:VAL:O     | 2.36                     | 0.58              |
| 2:E2:67:ILE:HD13   | 2:E2:96:LEU:HD23   | 1.84                     | 0.58              |
| 4:I2:41:ALA:O      | 4:I2:42:THR:OG1    | 2.19                     | 0.58              |
| 7:Z2:37:PRO:HG3    | 8:e2:45:PRO:HD2    | 1.85                     | 0.58              |
| 9:t2:2:ILE:HG22    | 9:t2:4:SER:H       | 1.68                     | 0.58              |
| 10:A3:101:LYS:HG2  | 10:Z3:131:SER:OG   | 2.03                     | 0.58              |
| 10:A3:160:ASN:HA   | 10:A3:186:PRO:HD3  | 1.86                     | 0.58              |
| 10:B3:58:ILE:HG13  | 10:B3:59:ASN:H     | 1.68                     | 0.58              |
| 10:H3:131:SER:OG   | 10:I3:101:LYS:HG2  | 2.03                     | 0.58              |
| 10:M3:82:LEU:HD12  | 10:M3:146:GLY:CA   | 2.32                     | 0.58              |
| 10:Q3:58:ILE:HG13  | 10:Q3:59:ASN:H     | 1.68                     | 0.58              |
| 10:Y3:39:PRO:HB3   | 10:Z3:75:GLY:HA3   | 1.85                     | 0.58              |
| 11:e3:247:THR:HB   | 11:e3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:g3:164:ARG:NH1  | 11:h3:365:ILE:HG23 | 2.17                     | 0.58              |
| 11:j3:247:THR:HB   | 11:j3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:l3:105:VAL:HG22 | 11:l3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:q3:89:VAL:HG23  | 11:q3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:q3:105:VAL:HG22 | 11:q3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:r3:89:VAL:HG23  | 11:r3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:t3:89:VAL:HG23  | 11:t3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:t3:247:THR:HB   | 11:t3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:u3:247:THR:HB   | 11:u3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:z3:89:VAL:HG23  | 11:z3:126:LEU:HD21 | 1.84                     | 0.58              |
| 12:A4:215:LEU:N    | 12:A4:223:THR:O    | 2.36                     | 0.58              |
| 1:C1:283:SER:HB2   | 1:C1:369:ASP:HB2   | 1.86                     | 0.58              |
| 1:E1:363:THR:CG2   | 6:U2:75:ALA:HB3    | 2.15                     | 0.58              |
| 1:G1:125:GLN:CG    | 4:H2:8:MET:HA      | 2.32                     | 0.58              |
| 1:I1:407:ASP:HA    | 1:I1:410:LYS:HG3   | 1.85                     | 0.58              |
| 1:K1:392:ASN:OD1   | 1:K1:393:TYR:N     | 2.30                     | 0.58              |
| 1:L1:407:ASP:OD1   | 1:L1:408:GLN:N     | 2.37                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:O1:143:THR:HG21  | 1:Q1:156:HIS:NE2   | 2.18                     | 0.58              |
| 1:W1:200:SER:HB3   | 1:X1:175:SER:HB3   | 1.85                     | 0.58              |
| 2:C2:185:ILE:HD12  | 4:I2:84:LEU:HD21   | 1.86                     | 0.58              |
| 6:S2:106:ARG:HE    | 8:d2:248:LEU:HD11  | 1.67                     | 0.58              |
| 9:k2:143:PRO:HD3   | 9:k2:170:VAL:HG21  | 1.84                     | 0.58              |
| 9:l2:164:GLN:HG3   | 11:j3:80:GLN:HE22  | 1.60                     | 0.58              |
| 9:22:23:ALA:CB     | 12:A4:45:LYS:CG    | 2.81                     | 0.58              |
| 9:22:49:ILE:HB     | 9:22:66:LEU:HG     | 1.84                     | 0.58              |
| 9:42:23:ALA:HB1    | 12:C4:41:VAL:HG22  | 1.85                     | 0.58              |
| 10:D3:131:SER:OG   | 10:E3:101:LYS:HG2  | 2.04                     | 0.58              |
| 11:a3:264:MET:HE1  | 11:a3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:b3:105:VAL:HG22 | 11:b3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:f3:264:MET:HE1  | 11:f3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:p3:245:ASN:OD1  | 11:p3:245:ASN:N    | 2.33                     | 0.58              |
| 11:u3:245:ASN:OD1  | 11:u3:245:ASN:N    | 2.33                     | 0.58              |
| 11:v3:247:THR:HB   | 11:v3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:w3:247:THR:HB   | 11:w3:248:PRO:HD2  | 1.85                     | 0.58              |
| 1:H1:407:ASP:OD1   | 1:H1:410:LYS:NZ    | 2.37                     | 0.58              |
| 1:I1:143:THR:HG22  | 1:K1:154:ARG:HD3   | 1.86                     | 0.58              |
| 1:X1:248:ARG:HH11  | 1:Y1:267:THR:HG22  | 1.67                     | 0.58              |
| 4:J2:3:PRO:HA      | 4:J2:6:VAL:HG12    | 1.85                     | 0.58              |
| 9:l2:150:THR:HG21  | 9:22:54:ALA:HB1    | 1.84                     | 0.58              |
| 9:r2:12:LEU:HD22   | 9:r2:243:ASN:HB3   | 1.84                     | 0.58              |
| 9:w2:135:GLN:OE1   | 9:w2:137:GLN:NE2   | 2.34                     | 0.58              |
| 9:y2:93:LYS:HE3    | 9:42:180:ASN:OD1   | 2.04                     | 0.58              |
| 10:B3:160:ASN:HA   | 10:B3:186:PRO:HD3  | 1.86                     | 0.58              |
| 10:G3:72:ARG:N     | 10:G3:76:ASP:OD2   | 2.25                     | 0.58              |
| 10:J3:167:LYS:HD3  | 10:K3:203:ALA:HB3  | 1.86                     | 0.58              |
| 10:Z3:166:GLU:OE2  | 10:Z3:168:GLN:NE2  | 2.27                     | 0.58              |
| 11:a3:89:VAL:HG23  | 11:a3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:b3:264:MET:HE1  | 11:b3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:c3:264:MET:HE1  | 11:c3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:f3:247:THR:HB   | 11:f3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:j3:89:VAL:HG23  | 11:j3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:k3:247:THR:HB   | 11:k3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:k3:264:MET:HE1  | 11:k3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:n3:166:THR:HG21 | 11:p3:362:LEU:HD21 | 1.85                     | 0.58              |
| 11:o3:325:SER:HB3  | 11:o3:330:SER:CB   | 2.32                     | 0.58              |
| 11:p3:89:VAL:HG23  | 11:p3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:r3:105:VAL:HG22 | 11:r3:165:ILE:HB   | 1.85                     | 0.58              |
| 1:A1:267:THR:HG21  | 1:h1:419:ALA:O     | 2.04                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:D1:297:GLN:HB3   | 1:D1:363:THR:HB    | 1.85                     | 0.58              |
| 1:K1:203:ALA:HA    | 1:L1:158:ALA:HB1   | 1.84                     | 0.58              |
| 1:K1:279:GLU:OE2   | 1:K1:281:HIS:N     | 2.34                     | 0.58              |
| 1:N1:166:VAL:HG22  | 2:A2:162:PRO:HA    | 1.86                     | 0.58              |
| 1:N1:297:GLN:HE21  | 6:Q2:77:ALA:CB     | 2.14                     | 0.58              |
| 1:W1:164:LEU:HD13  | 2:E2:143:ARG:CA    | 2.08                     | 0.58              |
| 2:C2:67:ILE:HD12   | 2:C2:97:THR:HG22   | 1.84                     | 0.58              |
| 8:e2:71:LEU:HD23   | 8:e2:205:VAL:HG11  | 1.84                     | 0.58              |
| 9:h2:184:LEU:HB3   | 9:h2:192:TYR:HB3   | 1.84                     | 0.58              |
| 10:C3:72:ARG:N     | 10:C3:76:ASP:OD2   | 2.25                     | 0.58              |
| 10:Q3:131:SER:OG   | 10:R3:101:LYS:HG2  | 2.02                     | 0.58              |
| 10:R3:131:SER:OG   | 10:S3:101:LYS:HG2  | 2.02                     | 0.58              |
| 10:T3:160:ASN:HA   | 10:T3:186:PRO:HD3  | 1.86                     | 0.58              |
| 10:Z3:58:ILE:HG13  | 10:Z3:59:ASN:H     | 1.68                     | 0.58              |
| 10:Z3:160:ASN:HA   | 10:Z3:186:PRO:HD3  | 1.86                     | 0.58              |
| 11:b3:166:THR:HG21 | 11:d3:362:LEU:HD21 | 1.85                     | 0.58              |
| 11:d3:164:ARG:NH1  | 11:e3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:d3:264:MET:HE1  | 11:d3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:h3:105:VAL:HG22 | 11:h3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:h3:264:MET:HE1  | 11:h3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:i3:264:MET:HE1  | 11:i3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:j3:105:VAL:HG22 | 11:j3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:k3:89:VAL:HG23  | 11:k3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:k3:164:ARG:NH1  | 11:l3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:n3:325:SER:HB3  | 11:n3:330:SER:CB   | 2.32                     | 0.58              |
| 11:q3:164:ARG:NH1  | 11:r3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:r3:247:THR:HB   | 11:r3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:w3:164:ARG:NH1  | 11:x3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:y3:101:GLN:HE22 | 11:z3:219:ARG:HD3  | 1.68                     | 0.58              |
| 12:E4:55:ASN:HA    | 12:E4:58:LEU:HB2   | 1.86                     | 0.58              |
| 1:A1:231:ASN:O     | 1:A1:234:GLN:NE2   | 2.36                     | 0.58              |
| 1:M1:392:ASN:OD1   | 1:M1:393:TYR:N     | 2.34                     | 0.58              |
| 1:P1:277:GLN:HB2   | 1:P1:377:MET:HE1   | 1.85                     | 0.58              |
| 1:Q1:405:THR:OG1   | 1:Q1:407:ASP:OD1   | 2.21                     | 0.58              |
| 1:T1:165:PHE:CA    | 3:F2:166:SER:CB    | 2.77                     | 0.58              |
| 1:T1:165:PHE:HB2   | 3:F2:167:ASN:HB2   | 1.84                     | 0.58              |
| 1:U1:365:ASN:ND2   | 6:R2:65:LEU:HA     | 2.18                     | 0.58              |
| 1:V1:299:ASN:HB2   | 1:V1:361:ASN:HB2   | 1.83                     | 0.58              |
| 1:W1:293:LEU:HD13  | 1:W1:296:ARG:HE    | 1.69                     | 0.58              |
| 1:Y1:165:PHE:CD2   | 2:E2:152:ARG:NH2   | 2.72                     | 0.58              |
| 1:c1:233:ALA:HA    | 1:c1:236:LYS:HD3   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:b2:155:VAL:HG21  | 9:r2:54:ALA:H      | 1.68                     | 0.58              |
| 8:f2:225:ARG:NH1   | 9:l2:255:GLN:OE1   | 2.36                     | 0.58              |
| 9:k2:147:LEU:HD21  | 9:k2:162:GLN:HG2   | 1.86                     | 0.58              |
| 9:k2:241:GLU:HG2   | 9:p2:256:LYS:HG2   | 1.84                     | 0.58              |
| 9:q2:230:LEU:HD21  | 9:v2:242:ILE:HG23  | 1.86                     | 0.58              |
| 9:u2:56:SER:HG     | 9:u2:60:THR:HG1    | 1.48                     | 0.58              |
| 10:E3:131:SER:OG   | 10:F3:101:LYS:HG2  | 2.02                     | 0.58              |
| 10:U3:160:ASN:HA   | 10:U3:186:PRO:HD3  | 1.85                     | 0.58              |
| 11:b3:164:ARG:NH1  | 11:c3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:c3:89:VAL:HG23  | 11:c3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:j3:164:ARG:NH1  | 11:k3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:p3:164:ARG:NH1  | 11:q3:365:ILE:HG23 | 2.18                     | 0.58              |
| 11:s3:247:THR:HB   | 11:s3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:y3:325:SER:HB3  | 11:y3:330:SER:CB   | 2.32                     | 0.58              |
| 11:z3:105:VAL:HG22 | 11:z3:165:ILE:HB   | 1.85                     | 0.58              |
| 1:E1:241:VAL:HG22  | 1:F1:235:LEU:HD11  | 1.84                     | 0.58              |
| 1:F1:413:GLU:OE1   | 1:F1:417:ARG:NH1   | 2.33                     | 0.58              |
| 1:L1:139:GLU:O     | 1:L1:143:THR:HG23  | 2.03                     | 0.58              |
| 1:V1:244:ARG:NH2   | 1:W1:235:LEU:HB3   | 2.19                     | 0.58              |
| 1:Z1:275:LYS:HB2   | 1:Z1:377:MET:HB2   | 1.85                     | 0.58              |
| 7:Y2:79:GLU:OE2    | 9:j2:6:TRP:CH2     | 2.56                     | 0.58              |
| 7:Y2:117:GLU:OE2   | 8:e2:249:SER:N     | 2.37                     | 0.58              |
| 8:c2:73:TYR:HE1    | 9:o2:73:ARG:HG3    | 1.68                     | 0.58              |
| 8:f2:34:PHE:O      | 8:f2:35:ARG:NH1    | 2.37                     | 0.58              |
| 9:l2:238:ARG:NH1   | 9:l2:241:GLU:OE2   | 2.35                     | 0.58              |
| 9:u2:99:GLY:O      | 9:u2:116:ARG:NH2   | 2.37                     | 0.58              |
| 9:32:230:LEU:HD13  | 12:B4:62:LEU:CD1   | 2.33                     | 0.58              |
| 9:42:35:LYS:H      | 9:42:79:ARG:NH2    | 2.02                     | 0.58              |
| 10:G3:58:ILE:HG13  | 10:G3:59:ASN:H     | 1.68                     | 0.58              |
| 10:H3:166:GLU:OE2  | 10:H3:168:GLN:NE2  | 2.27                     | 0.58              |
| 10:N3:131:SER:OG   | 10:O3:101:LYS:HG2  | 2.03                     | 0.58              |
| 10:O3:131:SER:OG   | 10:P3:101:LYS:HG2  | 2.03                     | 0.58              |
| 10:U3:58:ILE:HG13  | 10:U3:59:ASN:H     | 1.68                     | 0.58              |
| 11:a3:166:THR:HG21 | 11:c3:362:LEU:HD21 | 1.86                     | 0.58              |
| 11:d3:247:THR:HB   | 11:d3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:h3:89:VAL:HG23  | 11:h3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:h3:98:ARG:NH1   | 11:i3:220:THR:OG1  | 2.32                     | 0.58              |
| 11:j3:89:VAL:HG23  | 11:j3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:l3:89:VAL:HG23  | 11:l3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:m3:105:VAL:HG22 | 11:m3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:m3:166:THR:HG21 | 11:o3:362:LEU:HD21 | 1.86                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:n3:264:MET:HE1  | 11:n3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:p3:105:VAL:HG22 | 11:p3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:u3:325:SER:HB3  | 11:u3:330:SER:CB   | 2.32                     | 0.58              |
| 1:B1:275:LYS:HB2   | 1:B1:377:MET:HB2   | 1.86                     | 0.58              |
| 1:B1:283:SER:HB2   | 1:B1:369:ASP:HB2   | 1.84                     | 0.58              |
| 1:O1:197:LEU:HD22  | 1:Q1:213:VAL:HG21  | 1.85                     | 0.58              |
| 1:V1:392:ASN:OD1   | 1:V1:393:TYR:N     | 2.36                     | 0.58              |
| 1:W1:205:LEU:HD11  | 1:W1:209:ASN:HB2   | 1.85                     | 0.58              |
| 2:A2:185:ILE:O     | 2:A2:189:ILE:HG12  | 2.04                     | 0.58              |
| 2:C2:210:MET:O     | 2:C2:211:MET:HE2   | 2.04                     | 0.58              |
| 2:D2:53:PHE:HD1    | 2:D2:57:ILE:HD12   | 1.67                     | 0.58              |
| 2:E2:75:ARG:NH2    | 5:K2:104:VAL:O     | 2.36                     | 0.58              |
| 2:E2:138:MET:HE3   | 2:E2:170:LEU:HG    | 1.84                     | 0.58              |
| 3:F2:171:ALA:O     | 3:F2:175:ALA:HB2   | 2.03                     | 0.58              |
| 8:b2:87:TRP:NE1    | 8:b2:166:ALA:O     | 2.29                     | 0.58              |
| 9:g2:98:LYS:HE3    | 9:r2:45:LEU:HD23   | 1.86                     | 0.58              |
| 9:n2:35:LYS:NZ     | 9:n2:82:SER:O      | 2.37                     | 0.58              |
| 9:u2:140:ILE:HD13  | 9:u2:157:VAL:HG11  | 1.85                     | 0.58              |
| 10:C3:131:SER:OG   | 10:D3:101:LYS:HG2  | 2.03                     | 0.58              |
| 10:C3:160:ASN:HA   | 10:C3:186:PRO:HD3  | 1.86                     | 0.58              |
| 10:F3:131:SER:OG   | 10:G3:101:LYS:HG2  | 2.04                     | 0.58              |
| 10:S3:160:ASN:HA   | 10:S3:186:PRO:HD3  | 1.86                     | 0.58              |
| 10:Y3:160:ASN:HA   | 10:Y3:186:PRO:HD3  | 1.86                     | 0.58              |
| 11:e3:196:MET:HA   | 11:e3:196:MET:CE   | 2.34                     | 0.58              |
| 11:i3:89:VAL:HG23  | 11:i3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:k3:196:MET:HA   | 11:k3:196:MET:CE   | 2.34                     | 0.58              |
| 11:m3:325:SER:HB3  | 11:m3:330:SER:CB   | 2.32                     | 0.58              |
| 11:o3:264:MET:HE1  | 11:o3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:p3:196:MET:HA   | 11:p3:196:MET:CE   | 2.34                     | 0.58              |
| 11:w3:166:THR:HG21 | 11:y3:362:LEU:HD21 | 1.86                     | 0.58              |
| 11:x3:247:THR:HB   | 11:x3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:x3:264:MET:HE1  | 11:x3:335:LEU:CD1  | 2.34                     | 0.58              |
| 1:K1:299:ASN:HB2   | 1:K1:361:ASN:HB2   | 1.86                     | 0.58              |
| 1:L1:407:ASP:HA    | 1:L1:410:LYS:HG2   | 1.84                     | 0.58              |
| 1:N1:405:THR:OG1   | 1:N1:407:ASP:OD1   | 2.13                     | 0.58              |
| 1:Q1:404:LEU:HD13  | 1:Q1:434:ASN:HD21  | 1.68                     | 0.58              |
| 1:Y1:214:ASP:OD1   | 1:Y1:215:GLN:N     | 2.36                     | 0.58              |
| 2:C2:115:PRO:HB2   | 2:C2:121:ILE:HD12  | 1.84                     | 0.58              |
| 3:F2:44:LEU:HD11   | 5:P2:102:MET:HG3   | 1.85                     | 0.58              |
| 9:g2:44:LEU:HD21   | 9:g2:73:ARG:HG2    | 1.84                     | 0.58              |
| 9:l2:115:THR:HB    | 9:l2:191:LEU:HD23  | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:s2:209:ASN:OD1   | 11:r3:78:ASN:OD1   | 2.21                     | 0.58              |
| 9:32:240:TYR:OH    | 12:B4:49:PRO:CA    | 2.51                     | 0.58              |
| 10:F3:58:ILE:HG13  | 10:F3:59:ASN:H     | 1.68                     | 0.58              |
| 10:K3:167:LYS:HD3  | 10:L3:203:ALA:HB3  | 1.86                     | 0.58              |
| 10:P3:131:SER:OG   | 10:Q3:101:LYS:HG2  | 2.04                     | 0.58              |
| 11:a3:89:VAL:HG23  | 11:a3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:d3:89:VAL:HG23  | 11:d3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:f3:196:MET:HA   | 11:f3:196:MET:CE   | 2.34                     | 0.58              |
| 11:g3:89:VAL:HG23  | 11:g3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:g3:166:THR:HG21 | 11:i3:362:LEU:HD21 | 1.86                     | 0.58              |
| 11:i3:245:ASN:OD1  | 11:i3:245:ASN:N    | 2.33                     | 0.58              |
| 11:m3:264:MET:HE1  | 11:m3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:q3:247:THR:HB   | 11:q3:248:PRO:HD2  | 1.85                     | 0.58              |
| 11:s3:89:VAL:HG23  | 11:s3:126:LEU:CD2  | 2.32                     | 0.58              |
| 11:s3:105:VAL:HG22 | 11:s3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:w3:142:LEU:HD23 | 11:y3:350:GLN:NE2  | 2.18                     | 0.58              |
| 11:y3:247:THR:HB   | 11:y3:248:PRO:HD2  | 1.85                     | 0.58              |
| 1:F1:250:GLU:O     | 1:F1:254:SER:OG    | 2.21                     | 0.58              |
| 1:J1:407:ASP:OD1   | 1:J1:408:GLN:N     | 2.37                     | 0.58              |
| 1:K1:155:VAL:HG23  | 1:K1:176:VAL:HG22  | 1.86                     | 0.58              |
| 1:L1:375:THR:HG23  | 1:M1:275:LYS:HD3   | 1.85                     | 0.58              |
| 1:M1:252:ILE:HD11  | 1:N1:265:GLN:HB2   | 1.86                     | 0.58              |
| 2:E2:84:PRO:HG3    | 3:F2:96:ARG:HD2    | 1.86                     | 0.58              |
| 9:r2:60:THR:HG22   | 9:r2:61:THR:H      | 1.69                     | 0.58              |
| 9:r2:241:GLU:HB3   | 9:x2:258:THR:HG21  | 1.85                     | 0.58              |
| 10:L3:131:SER:OG   | 10:M3:101:LYS:HG2  | 2.03                     | 0.58              |
| 10:P3:58:ILE:HG13  | 10:P3:59:ASN:H     | 1.68                     | 0.58              |
| 11:a3:105:VAL:HG22 | 11:a3:165:ILE:HB   | 1.85                     | 0.58              |
| 11:e3:89:VAL:HG23  | 11:e3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:l3:264:MET:HE1  | 11:l3:335:LEU:CD1  | 2.34                     | 0.58              |
| 11:m3:89:VAL:HG23  | 11:m3:126:LEU:HD21 | 1.84                     | 0.58              |
| 11:z3:264:MET:HE1  | 11:z3:335:LEU:CD1  | 2.34                     | 0.58              |
| 12:D4:46:ASN:OD1   | 12:D4:47:GLN:N     | 2.37                     | 0.58              |
| 1:B1:203:ALA:HB1   | 1:C1:160:PRO:HA    | 1.86                     | 0.57              |
| 1:C1:187:ASP:OD1   | 1:C1:190:GLN:HG2   | 2.04                     | 0.57              |
| 1:H1:374:HIS:HB3   | 1:I1:276:GLU:HB3   | 1.84                     | 0.57              |
| 1:L1:413:GLU:OE1   | 1:L1:417:ARG:NH1   | 2.34                     | 0.57              |
| 1:N1:392:ASN:OD1   | 1:N1:393:TYR:N     | 2.35                     | 0.57              |
| 1:O1:297:GLN:HG2   | 1:P1:363:THR:HG23  | 1.86                     | 0.57              |
| 1:R1:165:PHE:O     | 3:F2:257:GLU:OE2   | 2.22                     | 0.57              |
| 1:T1:407:ASP:HA    | 1:T1:410:LYS:HG2   | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:f1:261:ASN:O     | 1:f1:392:ASN:N     | 2.31                     | 0.57              |
| 1:g1:404:LEU:H     | 1:g1:434:ASN:ND2   | 2.01                     | 0.57              |
| 1:g1:413:GLU:OE2   | 1:g1:417:ARG:NH1   | 2.38                     | 0.57              |
| 2:C2:98:PHE:HE2    | 2:D2:168:ARG:HD2   | 1.67                     | 0.57              |
| 4:G2:59:PHE:HE1    | 4:H2:14:MET:HB3    | 1.70                     | 0.57              |
| 8:b2:173:ARG:HB3   | 9:g2:67:GLN:HE22   | 1.69                     | 0.57              |
| 9:g2:144:ALA:HA    | 9:l2:179:MET:SD    | 2.44                     | 0.57              |
| 10:V3:58:ILE:HG13  | 10:V3:59:ASN:H     | 1.68                     | 0.57              |
| 11:e3:164:ARG:NH1  | 11:f3:365:ILE:HG23 | 2.18                     | 0.57              |
| 11:e3:264:MET:HE1  | 11:e3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:f3:89:VAL:HG23  | 11:f3:126:LEU:HD21 | 1.84                     | 0.57              |
| 11:g3:264:MET:HE1  | 11:g3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:h3:247:THR:HB   | 11:h3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:p3:325:SER:HB3  | 11:p3:330:SER:CB   | 2.32                     | 0.57              |
| 11:z3:247:THR:HB   | 11:z3:248:PRO:HD2  | 1.85                     | 0.57              |
| 1:H1:245:ILE:HG23  | 1:H1:266:VAL:HG21  | 1.86                     | 0.57              |
| 1:N1:407:ASP:OD1   | 1:N1:408:GLN:N     | 2.37                     | 0.57              |
| 1:Y1:389:VAL:HB    | 1:Y1:432:VAL:HG22  | 1.85                     | 0.57              |
| 2:C2:185:ILE:O     | 2:C2:189:ILE:HG12  | 2.04                     | 0.57              |
| 4:I2:62:ILE:HG21   | 4:J2:14:MET:HE1    | 1.85                     | 0.57              |
| 5:N2:99:VAL:HA     | 5:N2:102:MET:HE3   | 1.86                     | 0.57              |
| 8:c2:138:ALA:HB1   | 9:s2:56:SER:O      | 2.04                     | 0.57              |
| 8:f2:82:LEU:HD21   | 8:f2:88:LEU:HG     | 1.86                     | 0.57              |
| 9:l2:230:LEU:HD21  | 9:q2:242:ILE:HD12  | 1.85                     | 0.57              |
| 9:n2:26:LEU:HD21   | 9:t2:242:ILE:HG22  | 1.86                     | 0.57              |
| 9:n2:98:LYS:O      | 9:n2:212:GLY:CA    | 2.51                     | 0.57              |
| 9:r2:36:ARG:HH12   | 9:r2:38:ARG:HB2    | 1.69                     | 0.57              |
| 9:v2:140:ILE:HD13  | 9:v2:157:VAL:HG11  | 1.85                     | 0.57              |
| 9:y2:238:ARG:HH21  | 12:D4:52:PRO:CA    | 2.16                     | 0.57              |
| 10:X3:121:ARG:HA   | 10:Y3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:Y3:80:ILE:HD13  | 10:Y3:195:VAL:HG13 | 1.87                     | 0.57              |
| 11:b3:89:VAL:HG23  | 11:b3:126:LEU:HD21 | 1.84                     | 0.57              |
| 11:c3:89:VAL:HG23  | 11:c3:126:LEU:HD21 | 1.84                     | 0.57              |
| 11:i3:105:VAL:HG22 | 11:i3:165:ILE:HB   | 1.85                     | 0.57              |
| 11:j3:79:MET:HE2   | 11:k3:57:PHE:HD2   | 1.69                     | 0.57              |
| 11:j3:264:MET:HE1  | 11:j3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:k3:26:THR:CG2   | 11:k3:187:LEU:HB3  | 2.33                     | 0.57              |
| 11:n3:89:VAL:HG23  | 11:n3:126:LEU:HD21 | 1.84                     | 0.57              |
| 11:o3:89:VAL:HG23  | 11:o3:126:LEU:HD21 | 1.84                     | 0.57              |
| 11:o3:247:THR:HB   | 11:o3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:t3:166:THR:HG21 | 11:v3:362:LEU:HD21 | 1.85                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:u3:166:THR:HG21 | 11:w3:362:LEU:HD21 | 1.85                     | 0.57              |
| 11:v3:79:MET:HE2   | 11:w3:57:PHE:HD2   | 1.69                     | 0.57              |
| 1:K1:304:VAL:N     | 1:L1:356:ARG:O     | 2.37                     | 0.57              |
| 1:Q1:191:ILE:HG23  | 1:Q1:212:LEU:HD23  | 1.85                     | 0.57              |
| 1:a1:245:ILE:HD11  | 1:a1:420:MET:HA    | 1.86                     | 0.57              |
| 2:E2:233:GLN:HG2   | 3:F2:174:ARG:HB2   | 1.86                     | 0.57              |
| 7:Z2:74:GLU:H      | 7:Z2:95:ASN:HD22   | 1.52                     | 0.57              |
| 7:a2:26:SER:HB3    | 8:f2:55:THR:HG22   | 1.85                     | 0.57              |
| 8:d2:62:PRO:HB3    | 9:i2:62:LEU:HD22   | 1.86                     | 0.57              |
| 8:d2:189:ARG:HH11  | 8:d2:193:LEU:HD23  | 1.68                     | 0.57              |
| 9:m2:117:ASP:OD1   | 9:m2:118:GLY:N     | 2.37                     | 0.57              |
| 10:A3:58:ILE:HG13  | 10:A3:59:ASN:H     | 1.68                     | 0.57              |
| 10:D3:160:ASN:HA   | 10:D3:186:PRO:HD3  | 1.86                     | 0.57              |
| 10:K3:121:ARG:HA   | 10:L3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:Q3:70:ARG:NH2   | 11:p3:72:THR:OG1   | 2.37                     | 0.57              |
| 10:R3:160:ASN:HA   | 10:R3:186:PRO:HD3  | 1.86                     | 0.57              |
| 10:V3:160:ASN:HA   | 10:V3:186:PRO:HD3  | 1.86                     | 0.57              |
| 10:X3:160:ASN:HA   | 10:X3:186:PRO:HD3  | 1.86                     | 0.57              |
| 10:Z3:72:ARG:N     | 10:Z3:76:ASP:OD2   | 2.25                     | 0.57              |
| 10:Z3:80:ILE:HD13  | 10:Z3:195:VAL:HG13 | 1.87                     | 0.57              |
| 11:c3:247:THR:HB   | 11:c3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:f3:245:ASN:OD1  | 11:f3:245:ASN:N    | 2.33                     | 0.57              |
| 11:g3:247:THR:HB   | 11:g3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:i3:166:THR:HG21 | 11:k3:362:LEU:HD21 | 1.85                     | 0.57              |
| 11:j3:26:THR:CG2   | 11:j3:187:LEU:HB3  | 2.33                     | 0.57              |
| 11:l3:325:SER:HB3  | 11:l3:330:SER:CB   | 2.32                     | 0.57              |
| 11:n3:361:LYS:HE2  | 11:n3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:p3:247:THR:HB   | 11:p3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:p3:264:MET:HE1  | 11:p3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:t3:105:VAL:HG22 | 11:t3:165:ILE:HB   | 1.85                     | 0.57              |
| 11:t3:245:ASN:OD1  | 11:t3:245:ASN:N    | 2.33                     | 0.57              |
| 12:D4:44:LEU:HD11  | 12:D4:58:LEU:HG    | 1.86                     | 0.57              |
| 1:C1:160:PRO:HG2   | 1:C1:170:LYS:O     | 2.05                     | 0.57              |
| 1:E1:193:ALA:HA    | 1:G1:219:LEU:HG    | 1.86                     | 0.57              |
| 1:U1:180:LEU:HD21  | 1:U1:186:LEU:HB2   | 1.85                     | 0.57              |
| 1:V1:293:LEU:HD22  | 1:V1:296:ARG:HD2   | 1.87                     | 0.57              |
| 1:h1:157:LEU:HD11  | 1:h1:202:VAL:HG21  | 1.86                     | 0.57              |
| 2:C2:118:GLU:OE2   | 6:S2:5:LEU:N       | 2.38                     | 0.57              |
| 7:W2:76:LEU:H      | 9:h2:47:GLN:HE22   | 1.51                     | 0.57              |
| 9:j2:36:ARG:HH11   | 9:j2:80:LEU:HD12   | 1.67                     | 0.57              |
| 9:s2:51:GLN:HG3    | 9:s2:53:GLY:H      | 1.68                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:F3:70:ARG:NH2   | 11:e3:72:THR:OG1   | 2.37                     | 0.57              |
| 10:G3:160:ASN:HA   | 10:G3:186:PRO:HD3  | 1.86                     | 0.57              |
| 10:L3:72:ARG:N     | 10:L3:76:ASP:OD2   | 2.25                     | 0.57              |
| 10:M3:58:ILE:HG13  | 10:M3:59:ASN:H     | 1.68                     | 0.57              |
| 10:P3:72:ARG:N     | 10:P3:76:ASP:OD2   | 2.24                     | 0.57              |
| 10:Q3:80:ILE:HD13  | 10:Q3:195:VAL:HG13 | 1.87                     | 0.57              |
| 11:k3:166:THR:HG21 | 11:m3:362:LEU:HD21 | 1.86                     | 0.57              |
| 11:k3:361:LYS:HE2  | 11:k3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:q3:264:MET:HE1  | 11:q3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:q3:361:LYS:HE2  | 11:q3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:u3:264:MET:HE1  | 11:u3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:y3:264:MET:HE1  | 11:y3:335:LEU:CD1  | 2.34                     | 0.57              |
| 1:E1:180:LEU:HD11  | 1:E1:186:LEU:HB2   | 1.86                     | 0.57              |
| 1:Q1:165:PHE:HE2   | 3:F2:145:TRP:CE3   | 2.22                     | 0.57              |
| 1:R1:125:GLN:CG    | 2:E2:230:ASP:OD2   | 2.52                     | 0.57              |
| 1:T1:392:ASN:OD1   | 1:T1:393:TYR:N     | 2.37                     | 0.57              |
| 1:Y1:179:THR:HA    | 1:Y1:215:GLN:HB3   | 1.87                     | 0.57              |
| 1:f1:165:PHE:CD1   | 2:D2:152:ARG:NH2   | 2.59                     | 0.57              |
| 2:E2:205:MET:CG    | 4:J2:51:PHE:CZ     | 2.86                     | 0.57              |
| 6:R2:103:ASP:OD1   | 7:X2:14:LEU:HB3    | 2.04                     | 0.57              |
| 6:U2:34:ASP:OD2    | 7:Z2:20:ARG:NH1    | 2.38                     | 0.57              |
| 8:b2:62:PRO:O      | 9:g2:63:PRO:HG2    | 2.05                     | 0.57              |
| 8:b2:137:ILE:HG12  | 8:b2:143:ILE:HG12  | 1.86                     | 0.57              |
| 9:t2:231:VAL:HG11  | 9:z2:9:LYS:HG2     | 1.86                     | 0.57              |
| 9:v2:89:THR:HG23   | 9:v2:91:ASN:H      | 1.70                     | 0.57              |
| 10:A3:80:ILE:HD13  | 10:A3:195:VAL:HG13 | 1.87                     | 0.57              |
| 10:H3:167:LYS:HD3  | 10:I3:203:ALA:HB3  | 1.87                     | 0.57              |
| 10:I3:167:LYS:HD3  | 10:J3:203:ALA:HB3  | 1.87                     | 0.57              |
| 10:P3:80:ILE:HD13  | 10:P3:195:VAL:HG13 | 1.87                     | 0.57              |
| 10:R3:80:ILE:HD13  | 10:R3:195:VAL:HG13 | 1.87                     | 0.57              |
| 11:i3:26:THR:CG2   | 11:i3:187:LEU:HB3  | 2.33                     | 0.57              |
| 11:l3:26:THR:CG2   | 11:l3:187:LEU:HB3  | 2.33                     | 0.57              |
| 11:o3:361:LYS:HE2  | 11:o3:363:GLU:OE2  | 2.05                     | 0.57              |
| 12:B4:140:ILE:HG12 | 12:B4:182:ILE:HG22 | 1.86                     | 0.57              |
| 1:D1:250:GLU:O     | 1:D1:254:SER:OG    | 2.17                     | 0.57              |
| 1:K1:266:VAL:HG22  | 1:K1:387:VAL:HG22  | 1.87                     | 0.57              |
| 1:L1:244:ARG:NH2   | 1:M1:239:ASN:HB2   | 2.19                     | 0.57              |
| 1:T1:158:ALA:O     | 1:T1:172:PRO:HA    | 2.04                     | 0.57              |
| 1:X1:144:ILE:HG22  | 1:X1:150:VAL:HG11  | 1.87                     | 0.57              |
| 1:X1:300:ILE:O     | 1:Y1:359:GLN:NE2   | 2.37                     | 0.57              |
| 1:c1:378:ASN:ND2   | 1:c1:381:ASP:OD1   | 2.35                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:d1:181:GLU:HB3  | 1:d1:184:ARG:NH2   | 2.19                     | 0.57              |
| 1:h1:244:ARG:HH22 | 1:h1:248:ARG:HH22  | 1.52                     | 0.57              |
| 2:D2:185:ILE:O    | 2:D2:189:ILE:HG12  | 2.04                     | 0.57              |
| 6:S2:37:GLY:N     | 6:S2:96:ASP:O      | 2.38                     | 0.57              |
| 6:T2:106:ARG:NH2  | 8:e2:245:ASN:OD1   | 2.36                     | 0.57              |
| 8:d2:33:GLY:O     | 8:d2:35:ARG:NH1    | 2.37                     | 0.57              |
| 9:z2:135:GLN:OE1  | 9:z2:137:GLN:NE2   | 2.30                     | 0.57              |
| 10:H3:160:ASN:HA  | 10:H3:186:PRO:HD3  | 1.86                     | 0.57              |
| 10:K3:80:ILE:HD13 | 10:K3:195:VAL:HG13 | 1.87                     | 0.57              |
| 10:M3:121:ARG:HA  | 10:N3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:N3:121:ARG:HA  | 10:O3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:U3:121:ARG:HA  | 10:V3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:V3:131:SER:OG  | 10:W3:101:LYS:HG2  | 2.04                     | 0.57              |
| 10:Y3:166:GLU:OE2 | 10:Y3:168:GLN:NE2  | 2.27                     | 0.57              |
| 11:l3:42:VAL:O    | 11:l3:84:VAL:HA    | 2.05                     | 0.57              |
| 11:l3:247:THR:HB  | 11:l3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:m3:26:THR:CG2  | 11:m3:187:LEU:HB3  | 2.33                     | 0.57              |
| 11:m3:361:LYS:HE2 | 11:m3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:p3:79:MET:HE2  | 11:q3:57:PHE:HD2   | 1.69                     | 0.57              |
| 11:p3:123:MET:HE3 | 11:p3:123:MET:CA   | 2.35                     | 0.57              |
| 11:p3:361:LYS:HE2 | 11:p3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:s3:123:MET:HE3 | 11:s3:123:MET:CA   | 2.35                     | 0.57              |
| 11:w3:264:MET:HE1 | 11:w3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:x3:164:ARG:HD2 | 11:y3:365:ILE:CG2  | 2.34                     | 0.57              |
| 11:z3:325:SER:HB3 | 11:z3:330:SER:CB   | 2.32                     | 0.57              |
| 1:C1:164:LEU:CD2  | 2:C2:149:LEU:HD13  | 2.35                     | 0.57              |
| 1:G1:166:VAL:CA   | 2:B2:144:GLU:HG3   | 2.34                     | 0.57              |
| 1:H1:165:PHE:CZ   | 2:B2:147:LEU:HD12  | 2.33                     | 0.57              |
| 1:I1:133:GLN:O    | 1:I1:137:GLU:HG2   | 2.04                     | 0.57              |
| 1:J1:297:GLN:OE1  | 1:K1:363:THR:OG1   | 2.10                     | 0.57              |
| 1:N1:141:ALA:O    | 1:N1:144:ILE:N     | 2.37                     | 0.57              |
| 1:R1:176:VAL:HB   | 1:R1:212:LEU:HG    | 1.86                     | 0.57              |
| 1:V1:389:VAL:HB   | 1:V1:432:VAL:HG22  | 1.86                     | 0.57              |
| 1:W1:140:LEU:O    | 1:W1:144:ILE:HG12  | 2.05                     | 0.57              |
| 2:A2:100:ILE:HG21 | 2:A2:243:PHE:CD2   | 2.40                     | 0.57              |
| 9:22:120:PHE:HB3  | 9:22:128:LEU:HD22  | 1.86                     | 0.57              |
| 9:32:188:GLY:O    | 9:32:191:LEU:HD23  | 2.03                     | 0.57              |
| 9:42:26:LEU:HD22  | 9:42:229:GLU:OE2   | 2.04                     | 0.57              |
| 9:42:81:HIS:ND1   | 9:42:181:ASP:O     | 2.38                     | 0.57              |
| 10:H3:121:ARG:HA  | 10:I3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:J3:80:ILE:HD13 | 10:J3:195:VAL:HG13 | 1.87                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L3:80:ILE:HD13  | 10:L3:195:VAL:HG13 | 1.87                     | 0.57              |
| 10:L3:167:LYS:HD3  | 10:M3:203:ALA:HB3  | 1.86                     | 0.57              |
| 11:e3:123:MET:HE3  | 11:e3:123:MET:CA   | 2.35                     | 0.57              |
| 11:k3:42:VAL:O     | 11:k3:84:VAL:HA    | 2.05                     | 0.57              |
| 11:n3:247:THR:HB   | 11:n3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:o3:105:VAL:HG22 | 11:o3:165:ILE:HB   | 1.85                     | 0.57              |
| 11:q3:123:MET:HE3  | 11:q3:123:MET:CA   | 2.35                     | 0.57              |
| 11:r3:123:MET:HE3  | 11:r3:123:MET:CA   | 2.35                     | 0.57              |
| 11:t3:123:MET:HE3  | 11:t3:123:MET:CA   | 2.35                     | 0.57              |
| 11:v3:264:MET:HE1  | 11:v3:335:LEU:CD1  | 2.34                     | 0.57              |
| 1:C1:145:GLU:OE2   | 1:C1:153:ALA:N     | 2.38                     | 0.57              |
| 1:G1:166:VAL:CG1   | 2:B2:144:GLU:HG3   | 2.35                     | 0.57              |
| 1:K1:394:LYS:HE3   | 1:K1:402:LEU:HD13  | 1.87                     | 0.57              |
| 1:N1:193:ALA:HA    | 1:O1:219:LEU:HG    | 1.85                     | 0.57              |
| 1:O1:166:VAL:HA    | 2:A2:152:ARG:HD3   | 1.86                     | 0.57              |
| 1:O1:407:ASP:OD1   | 1:O1:408:GLN:N     | 2.38                     | 0.57              |
| 1:U1:214:ASP:HB3   | 1:U1:218:HIS:HB2   | 1.86                     | 0.57              |
| 1:Y1:245:ILE:HD11  | 1:Y1:420:MET:HA    | 1.86                     | 0.57              |
| 1:c1:421:GLY:O     | 1:c1:426:ARG:NH2   | 2.37                     | 0.57              |
| 1:g1:275:LYS:HB2   | 1:g1:377:MET:HB2   | 1.87                     | 0.57              |
| 2:B2:96:LEU:O      | 2:B2:100:ILE:HG13  | 2.05                     | 0.57              |
| 7:X2:43:ARG:HB3    | 7:X2:69:GLU:OE2    | 2.04                     | 0.57              |
| 8:b2:116:GLN:NE2   | 9:g2:42:GLU:OE2    | 2.37                     | 0.57              |
| 8:c2:160:ARG:NH1   | 9:s2:58:GLU:OE2    | 2.38                     | 0.57              |
| 9:g2:150:THR:HG21  | 9:w2:54:ALA:HB1    | 1.86                     | 0.57              |
| 9:m2:185:GLU:HB3   | 9:r2:52:PRO:HG2    | 1.87                     | 0.57              |
| 9:m2:227:ALA:HA    | 9:x2:257:LEU:HD21  | 1.86                     | 0.57              |
| 9:22:42:GLU:OE1    | 9:22:73:ARG:NE     | 2.37                     | 0.57              |
| 10:E3:80:ILE:HD13  | 10:E3:195:VAL:HG13 | 1.87                     | 0.57              |
| 10:F3:160:ASN:HA   | 10:F3:186:PRO:HD3  | 1.86                     | 0.57              |
| 10:S3:80:ILE:HD13  | 10:S3:195:VAL:HG13 | 1.87                     | 0.57              |
| 10:U3:37:ALA:HB1   | 10:V3:74:ILE:HG22  | 1.87                     | 0.57              |
| 10:W3:121:ARG:HA   | 10:X3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:X3:37:ALA:HB1   | 10:Y3:74:ILE:HG22  | 1.87                     | 0.57              |
| 10:X3:80:ILE:HD13  | 10:X3:195:VAL:HG13 | 1.87                     | 0.57              |
| 11:h3:26:THR:CG2   | 11:h3:187:LEU:HB3  | 2.33                     | 0.57              |
| 11:r3:42:VAL:O     | 11:r3:84:VAL:HA    | 2.05                     | 0.57              |
| 11:r3:264:MET:HE1  | 11:r3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:r3:361:LYS:HE2  | 11:r3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:s3:166:THR:HG21 | 11:u3:362:LEU:HD21 | 1.86                     | 0.57              |
| 11:t3:264:MET:HE1  | 11:t3:335:LEU:CD1  | 2.34                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:t3:361:LYS:HE2 | 11:t3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:u3:123:MET:HE3 | 11:u3:123:MET:CA   | 2.35                     | 0.57              |
| 11:v3:123:MET:HE3 | 11:v3:123:MET:CA   | 2.35                     | 0.57              |
| 1:Z1:297:GLN:O    | 1:Z1:362:GLU:HA    | 2.05                     | 0.57              |
| 1:d1:129:GLN:OE1  | 1:d1:129:GLN:N     | 2.30                     | 0.57              |
| 6:T2:90:PRO:HB3   | 6:T2:99:THR:HB     | 1.85                     | 0.57              |
| 9:i2:254:LEU:O    | 9:i2:258:THR:HG23  | 2.05                     | 0.57              |
| 9:r2:142:ILE:HG23 | 9:r2:159:VAL:HG11  | 1.87                     | 0.57              |
| 9:w2:185:GLU:HB2  | 9:22:52:PRO:HG2    | 1.87                     | 0.57              |
| 9:42:233:MET:SD   | 12:C4:44:LEU:HD11  | 2.44                     | 0.57              |
| 10:I3:121:ARG:HA  | 10:J3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:J3:131:SER:OG  | 10:K3:101:LYS:HG2  | 2.04                     | 0.57              |
| 10:O3:80:ILE:HD13 | 10:O3:195:VAL:HG13 | 1.87                     | 0.57              |
| 10:T3:121:ARG:HA  | 10:U3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:Y3:50:SER:HB3  | 11:z3:99:GLN:NE2   | 2.20                     | 0.57              |
| 11:c3:123:MET:HE3 | 11:c3:123:MET:CA   | 2.35                     | 0.57              |
| 11:c3:245:ASN:OD1 | 11:c3:245:ASN:N    | 2.33                     | 0.57              |
| 11:g3:42:VAL:O    | 11:g3:84:VAL:HA    | 2.05                     | 0.57              |
| 11:m3:42:VAL:O    | 11:m3:84:VAL:HA    | 2.05                     | 0.57              |
| 11:n3:26:THR:CG2  | 11:n3:187:LEU:HB3  | 2.33                     | 0.57              |
| 11:n3:42:VAL:O    | 11:n3:84:VAL:HA    | 2.05                     | 0.57              |
| 11:o3:123:MET:HE3 | 11:o3:123:MET:CA   | 2.35                     | 0.57              |
| 1:B1:167:ARG:CB   | 2:C2:160:GLN:OE1   | 2.52                     | 0.57              |
| 1:H1:145:GLU:HG3  | 1:H1:150:VAL:HG12  | 1.87                     | 0.57              |
| 1:H1:149:PRO:HA   | 1:H1:181:GLU:HG2   | 1.85                     | 0.57              |
| 1:M1:273:ALA:O    | 1:M1:275:LYS:NZ    | 2.35                     | 0.57              |
| 1:P1:250:GLU:O    | 1:P1:254:SER:OG    | 2.20                     | 0.57              |
| 1:Y1:420:MET:SD   | 1:Y1:422:PHE:HB2   | 2.45                     | 0.57              |
| 1:a1:365:ASN:OD1  | 6:S2:66:THR:CA     | 2.51                     | 0.57              |
| 1:d1:200:SER:HB3  | 1:f1:175:SER:HB3   | 1.87                     | 0.57              |
| 1:g1:164:LEU:HD12 | 2:C2:241:GLN:OE1   | 2.05                     | 0.57              |
| 1:g1:408:GLN:O    | 1:g1:412:ILE:HG12  | 2.05                     | 0.57              |
| 8:d2:87:TRP:NE1   | 8:d2:166:ALA:O     | 2.31                     | 0.57              |
| 8:e2:217:MET:SD   | 9:j2:245:LYS:HG2   | 2.45                     | 0.57              |
| 9:k2:6:TRP:CZ3    | 9:k2:9:LYS:CE      | 2.85                     | 0.57              |
| 9:m2:164:GLN:CD   | 11:o3:54:GLN:CG    | 2.72                     | 0.57              |
| 9:n2:28:ASN:HD21  | 9:t2:43:ASP:HB3    | 1.70                     | 0.57              |
| 9:s2:185:GLU:HB2  | 9:x2:52:PRO:HG2    | 1.86                     | 0.57              |
| 9:t2:86:LEU:HD11  | 9:t2:98:LYS:HD3    | 1.85                     | 0.57              |
| 10:B3:121:ARG:HA  | 10:C3:111:ARG:HB2  | 1.86                     | 0.57              |
| 10:E3:167:LYS:HD3 | 10:F3:203:ALA:HB3  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:I3:82:LEU:O    | 10:I3:197:SER:OG   | 2.20                     | 0.57              |
| 10:I3:166:GLU:OE2 | 10:I3:168:GLN:NE2  | 2.27                     | 0.57              |
| 10:L3:121:ARG:HA  | 10:M3:111:ARG:HB2  | 1.87                     | 0.57              |
| 10:Z3:101:LYS:HB2 | 10:Z3:101:LYS:HZ3  | 1.70                     | 0.57              |
| 11:h3:123:MET:HE3 | 11:h3:123:MET:CA   | 2.35                     | 0.57              |
| 11:m3:247:THR:HB  | 11:m3:248:PRO:HD2  | 1.85                     | 0.57              |
| 11:q3:42:VAL:O    | 11:q3:84:VAL:HA    | 2.05                     | 0.57              |
| 11:r3:79:MET:HE2  | 11:s3:57:PHE:HD2   | 1.70                     | 0.57              |
| 11:s3:264:MET:HE1 | 11:s3:335:LEU:CD1  | 2.34                     | 0.57              |
| 11:u3:361:LYS:HE2 | 11:u3:363:GLU:OE2  | 2.05                     | 0.57              |
| 11:w3:123:MET:HE3 | 11:w3:123:MET:CA   | 2.35                     | 0.57              |
| 11:x3:196:MET:HA  | 11:x3:196:MET:CE   | 2.34                     | 0.57              |
| 12:A4:97:ILE:HA   | 12:A4:203:VAL:HB   | 1.86                     | 0.57              |
| 1:B1:155:VAL:HG23 | 1:B1:176:VAL:HG22  | 1.86                     | 0.56              |
| 1:C1:214:ASP:OD1  | 1:C1:215:GLN:N     | 2.38                     | 0.56              |
| 1:K1:214:ASP:OD1  | 1:K1:215:GLN:N     | 2.38                     | 0.56              |
| 1:R1:133:GLN:OE1  | 1:R1:161:LYS:NZ    | 2.37                     | 0.56              |
| 1:T1:167:ARG:HH12 | 2:E2:107:LYS:CA    | 2.18                     | 0.56              |
| 1:U1:140:LEU:O    | 1:U1:144:ILE:HD12  | 2.05                     | 0.56              |
| 1:V1:423:SER:HB2  | 1:W1:384:ARG:NH1   | 2.19                     | 0.56              |
| 1:X1:414:ASP:HB3  | 1:Y1:431:ASN:HD21  | 1.69                     | 0.56              |
| 1:Y1:193:ALA:HA   | 1:a1:219:LEU:HG    | 1.85                     | 0.56              |
| 2:C2:90:LEU:HD13  | 5:M2:100:MET:HA    | 1.87                     | 0.56              |
| 6:Q2:34:ASP:OD2   | 7:V2:20:ARG:NH1    | 2.38                     | 0.56              |
| 8:b2:146:LEU:HB2  | 8:b2:155:VAL:HG12  | 1.87                     | 0.56              |
| 8:e2:226:ARG:O    | 8:e2:230:GLN:HG2   | 2.05                     | 0.56              |
| 9:h2:230:LEU:HD21 | 9:m2:242:ILE:HD12  | 1.86                     | 0.56              |
| 9:l2:98:LYS:O     | 9:l2:212:GLY:CA    | 2.42                     | 0.56              |
| 9:22:120:PHE:HE2  | 9:22:173:LEU:HD21  | 1.69                     | 0.56              |
| 9:22:238:ARG:HG3  | 12:B4:46:ASN:O     | 2.05                     | 0.56              |
| 10:F3:80:ILE:HD13 | 10:F3:195:VAL:HG13 | 1.87                     | 0.56              |
| 10:I3:160:ASN:HA  | 10:I3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:U3:131:SER:OG  | 10:V3:101:LYS:HG2  | 2.03                     | 0.56              |
| 10:W3:72:ARG:N    | 10:W3:76:ASP:OD2   | 2.24                     | 0.56              |
| 10:W3:160:ASN:HA  | 10:W3:186:PRO:HD3  | 1.86                     | 0.56              |
| 11:a3:123:MET:HE3 | 11:a3:123:MET:CA   | 2.35                     | 0.56              |
| 11:a3:247:THR:HB  | 11:a3:248:PRO:HD2  | 1.85                     | 0.56              |
| 11:a3:325:SER:HB3 | 11:a3:330:SER:CB   | 2.32                     | 0.56              |
| 11:b3:123:MET:HE3 | 11:b3:123:MET:CA   | 2.35                     | 0.56              |
| 11:c3:42:VAL:O    | 11:c3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:d3:42:VAL:O    | 11:d3:84:VAL:HA    | 2.05                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:d3:123:MET:HE3  | 11:d3:123:MET:CA   | 2.35                     | 0.56              |
| 11:g3:26:THR:CG2   | 11:g3:187:LEU:HB3  | 2.33                     | 0.56              |
| 11:j3:42:VAL:O     | 11:j3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:j3:361:LYS:HE2  | 11:j3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:n3:105:VAL:HG22 | 11:n3:165:ILE:HB   | 1.85                     | 0.56              |
| 11:n3:123:MET:HE3  | 11:n3:123:MET:CA   | 2.35                     | 0.56              |
| 11:q3:166:THR:HG21 | 11:s3:362:LEU:HD21 | 1.87                     | 0.56              |
| 11:x3:123:MET:HE3  | 11:x3:123:MET:CA   | 2.35                     | 0.56              |
| 11:x3:166:THR:HG21 | 11:z3:362:LEU:HD21 | 1.87                     | 0.56              |
| 11:y3:123:MET:HE3  | 11:y3:123:MET:CA   | 2.35                     | 0.56              |
| 12:E4:104:PRO:HA   | 12:E4:198:LEU:HA   | 1.86                     | 0.56              |
| 1:A1:392:ASN:OD1   | 1:A1:393:TYR:N     | 2.35                     | 0.56              |
| 1:B1:200:SER:HB3   | 1:C1:175:SER:HB3   | 1.86                     | 0.56              |
| 1:J1:404:LEU:H     | 1:J1:434:ASN:ND2   | 2.03                     | 0.56              |
| 1:L1:191:ILE:HG23  | 1:L1:212:LEU:HD23  | 1.87                     | 0.56              |
| 1:O1:199:SER:HA    | 1:O1:205:LEU:HD23  | 1.86                     | 0.56              |
| 1:Q1:256:ILE:HG21  | 1:Q1:412:ILE:HD11  | 1.87                     | 0.56              |
| 1:R1:167:ARG:CD    | 3:F2:167:ASN:CB    | 2.62                     | 0.56              |
| 1:T1:394:LYS:HE2   | 1:T1:402:LEU:HD12  | 1.86                     | 0.56              |
| 1:d1:166:VAL:CB    | 2:D2:162:PRO:HD3   | 2.31                     | 0.56              |
| 1:f1:143:THR:HG23  | 1:g1:154:ARG:HE    | 1.68                     | 0.56              |
| 7:W2:29:ALA:HB1    | 8:b2:57:VAL:HG21   | 1.87                     | 0.56              |
| 7:W2:72:ALA:HB3    | 7:W2:95:ASN:ND2    | 2.20                     | 0.56              |
| 9:g2:256:LYS:O     | 9:g2:259:GLN:HG3   | 2.05                     | 0.56              |
| 9:m2:167:PRO:HG3   | 9:32:54:ALA:H      | 1.68                     | 0.56              |
| 9:w2:174:ASN:HA    | 9:w2:206:PRO:HD3   | 1.87                     | 0.56              |
| 9:32:46:TYR:HA     | 9:32:69:GLY:HA2    | 1.86                     | 0.56              |
| 10:D3:80:ILE:HD13  | 10:D3:195:VAL:HG13 | 1.87                     | 0.56              |
| 10:G3:167:LYS:HD3  | 10:H3:203:ALA:HB3  | 1.87                     | 0.56              |
| 10:M3:160:ASN:HA   | 10:M3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:N3:160:ASN:HA   | 10:N3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:O3:121:ARG:HA   | 10:P3:111:ARG:HB2  | 1.86                     | 0.56              |
| 10:T3:80:ILE:HD13  | 10:T3:195:VAL:HG13 | 1.87                     | 0.56              |
| 11:b3:247:THR:HB   | 11:b3:248:PRO:HD2  | 1.85                     | 0.56              |
| 11:b3:325:SER:HB3  | 11:b3:330:SER:CB   | 2.32                     | 0.56              |
| 11:g3:123:MET:HE3  | 11:g3:123:MET:CA   | 2.35                     | 0.56              |
| 11:i3:42:VAL:O     | 11:i3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:l3:79:MET:HE2   | 11:m3:57:PHE:HD2   | 1.71                     | 0.56              |
| 11:l3:361:LYS:HE2  | 11:l3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:s3:142:LEU:HD23 | 11:u3:350:GLN:NE2  | 2.21                     | 0.56              |
| 12:A4:148:VAL:O    | 12:A4:170:THR:N    | 2.37                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:B1:360:ARG:NH1  | 1:B1:362:GLU:OE1   | 2.35                     | 0.56              |
| 1:F1:424:ASP:OD1  | 1:F1:425:LYS:N     | 2.38                     | 0.56              |
| 1:H1:143:THR:HG21 | 1:I1:156:HIS:CE1   | 2.40                     | 0.56              |
| 1:I1:252:ILE:HB   | 1:J1:265:GLN:HG3   | 1.87                     | 0.56              |
| 1:L1:140:LEU:O    | 1:L1:143:THR:OG1   | 2.16                     | 0.56              |
| 1:U1:283:SER:HB2  | 1:U1:369:ASP:HB2   | 1.88                     | 0.56              |
| 1:V1:277:GLN:HG2  | 1:V1:377:MET:HE1   | 1.85                     | 0.56              |
| 1:W1:140:LEU:O    | 1:W1:143:THR:OG1   | 2.20                     | 0.56              |
| 1:W1:203:ALA:HA   | 1:X1:158:ALA:HB1   | 1.87                     | 0.56              |
| 1:W1:393:TYR:CZ   | 1:W1:436:PRO:HD3   | 2.41                     | 0.56              |
| 1:b1:287:ASP:OD2  | 1:b1:290:LYS:NZ    | 2.37                     | 0.56              |
| 1:d1:162:PRO:HB2  | 1:f1:165:PHE:HD2   | 1.70                     | 0.56              |
| 2:B2:41:SER:HB3   | 5:O2:49:GLN:OE1    | 2.05                     | 0.56              |
| 8:d2:82:LEU:HD11  | 8:d2:163:LEU:HD22  | 1.87                     | 0.56              |
| 9:l2:19:MET:HB2   | 9:l2:236:VAL:HG11  | 1.87                     | 0.56              |
| 9:p2:35:LYS:NZ    | 9:p2:220:GLU:OE2   | 2.35                     | 0.56              |
| 9:t2:239:ALA:HB2  | 9:z2:1:MET:HE1     | 1.87                     | 0.56              |
| 9:v2:105:VAL:HG11 | 9:v2:134:PHE:HB3   | 1.88                     | 0.56              |
| 9:w2:140:ILE:HD11 | 9:w2:157:VAL:HG11  | 1.87                     | 0.56              |
| 9:12:93:LYS:NZ    | 9:12:149:ILE:HD12  | 2.19                     | 0.56              |
| 9:42:103:PHE:O    | 9:42:114:TYR:HA    | 2.04                     | 0.56              |
| 10:E3:121:ARG:HA  | 10:F3:111:ARG:HB2  | 1.86                     | 0.56              |
| 10:E3:160:ASN:HA  | 10:E3:186:PRO:HD3  | 1.85                     | 0.56              |
| 10:F3:167:LYS:HD3 | 10:G3:203:ALA:HB3  | 1.87                     | 0.56              |
| 10:G3:121:ARG:HA  | 10:H3:111:ARG:HB2  | 1.87                     | 0.56              |
| 10:I3:80:ILE:HD13 | 10:I3:195:VAL:HG13 | 1.87                     | 0.56              |
| 10:J3:160:ASN:HA  | 10:J3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:K3:160:ASN:HA  | 10:K3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:L3:160:ASN:HA  | 10:L3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:M3:70:ARG:NH2  | 11:l3:72:THR:OG1   | 2.38                     | 0.56              |
| 10:M3:80:ILE:HD13 | 10:M3:195:VAL:HG13 | 1.87                     | 0.56              |
| 10:O3:160:ASN:HA  | 10:O3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:Q3:160:ASN:HA  | 10:Q3:186:PRO:HD3  | 1.86                     | 0.56              |
| 10:W3:80:ILE:HD13 | 10:W3:195:VAL:HG13 | 1.87                     | 0.56              |
| 11:c3:325:SER:HB3 | 11:c3:330:SER:CB   | 2.32                     | 0.56              |
| 11:d3:192:GLU:OE1 | 11:d3:192:GLU:N    | 2.39                     | 0.56              |
| 11:f3:26:THR:CG2  | 11:f3:187:LEU:HB3  | 2.33                     | 0.56              |
| 11:f3:42:VAL:O    | 11:f3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:g3:361:LYS:HE2 | 11:g3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:h3:192:GLU:OE1 | 11:h3:192:GLU:N    | 2.39                     | 0.56              |
| 11:h3:361:LYS:HE2 | 11:h3:363:GLU:OE2  | 2.05                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:j3:166:THR:HG21 | 11:l3:362:LEU:HD21 | 1.88                     | 0.56              |
| 11:k3:325:SER:HB3  | 11:k3:330:SER:CB   | 2.32                     | 0.56              |
| 11:m3:123:MET:HE3  | 11:m3:123:MET:CA   | 2.35                     | 0.56              |
| 11:o3:26:THR:CG2   | 11:o3:187:LEU:HB3  | 2.33                     | 0.56              |
| 11:o3:42:VAL:O     | 11:o3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:r3:166:THR:HG21 | 11:t3:362:LEU:HD21 | 1.86                     | 0.56              |
| 11:t3:142:LEU:HD23 | 11:v3:350:GLN:NE2  | 2.21                     | 0.56              |
| 11:u3:196:MET:HA   | 11:u3:196:MET:CE   | 2.34                     | 0.56              |
| 11:v3:361:LYS:HE2  | 11:v3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:w3:361:LYS:HE2  | 11:w3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:z3:123:MET:HE3  | 11:z3:123:MET:CA   | 2.35                     | 0.56              |
| 12:A4:95:THR:O     | 12:A4:99:HIS:ND1   | 2.28                     | 0.56              |
| 12:C4:169:GLN:HE21 | 12:C4:173:THR:HG1  | 1.51                     | 0.56              |
| 1:J1:234:GLN:HB3   | 1:J1:272:PHE:CE1   | 2.41                     | 0.56              |
| 1:e1:250:GLU:O     | 1:e1:254:SER:OG    | 2.18                     | 0.56              |
| 5:O2:69:ASN:OD1    | 5:O2:70:ASP:N      | 2.39                     | 0.56              |
| 7:a2:6:ILE:HG21    | 7:a2:122:VAL:HG11  | 1.87                     | 0.56              |
| 8:b2:153:ASN:HA    | 9:m2:196:GLN:HB2   | 1.86                     | 0.56              |
| 9:k2:164:GLN:HG3   | 11:e3:82:LYS:HZ1   | 1.70                     | 0.56              |
| 9:m2:35:LYS:NZ     | 9:m2:220:GLU:OE2   | 2.38                     | 0.56              |
| 9:n2:168:VAL:HA    | 11:x3:78:ASN:CG    | 2.28                     | 0.56              |
| 9:p2:145:ASN:HB3   | 9:p2:162:GLN:HE22  | 1.70                     | 0.56              |
| 9:r2:51:GLN:HG3    | 9:r2:53:GLY:H      | 1.70                     | 0.56              |
| 10:B3:80:ILE:HD13  | 10:B3:195:VAL:HG13 | 1.87                     | 0.56              |
| 10:C3:70:ARG:NH2   | 11:b3:72:THR:OG1   | 2.38                     | 0.56              |
| 10:D3:167:LYS:HD3  | 10:E3:203:ALA:HB3  | 1.86                     | 0.56              |
| 10:V3:121:ARG:HA   | 10:W3:111:ARG:HB2  | 1.87                     | 0.56              |
| 11:f3:123:MET:HE3  | 11:f3:123:MET:CA   | 2.35                     | 0.56              |
| 11:h3:42:VAL:O     | 11:h3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:i3:192:GLU:OE1  | 11:i3:192:GLU:N    | 2.39                     | 0.56              |
| 11:k3:142:LEU:HD23 | 11:m3:350:GLN:NE2  | 2.21                     | 0.56              |
| 11:t3:79:MET:HE2   | 11:u3:57:PHE:HD2   | 1.71                     | 0.56              |
| 11:u3:42:VAL:O     | 11:u3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:y3:83:ASN:ND2   | 11:z3:109:SER:OG   | 2.36                     | 0.56              |
| 12:C4:192:GLN:NE2  | 12:C4:193:LEU:O    | 2.39                     | 0.56              |
| 1:E1:256:ILE:HG23  | 1:E1:257:VAL:HG13  | 1.87                     | 0.56              |
| 1:R1:261:ASN:O     | 1:R1:392:ASN:N     | 2.37                     | 0.56              |
| 1:S1:393:TYR:CE2   | 1:S1:436:PRO:HD3   | 2.41                     | 0.56              |
| 1:Y1:181:GLU:HB3   | 1:Y1:184:ARG:HH21  | 1.70                     | 0.56              |
| 1:a1:191:ILE:HD12  | 1:a1:212:LEU:HD11  | 1.87                     | 0.56              |
| 1:f1:140:LEU:O     | 1:f1:144:ILE:HG12  | 2.06                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:f1:219:LEU:HD23  | 1:f1:221:THR:H     | 1.69                     | 0.56              |
| 9:m2:36:ARG:HB3    | 9:m2:224:VAL:HG22  | 1.87                     | 0.56              |
| 10:C3:121:ARG:HA   | 10:D3:111:ARG:HB2  | 1.87                     | 0.56              |
| 10:G3:80:ILE:HD13  | 10:G3:195:VAL:HG13 | 1.87                     | 0.56              |
| 10:U3:70:ARG:NH2   | 11:t3:72:THR:OG1   | 2.38                     | 0.56              |
| 10:U3:80:ILE:HD13  | 10:U3:195:VAL:HG13 | 1.87                     | 0.56              |
| 11:a3:361:LYS:HE2  | 11:a3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:b3:142:LEU:HD23 | 11:d3:350:GLN:NE2  | 2.21                     | 0.56              |
| 11:d3:325:SER:HB3  | 11:d3:330:SER:CB   | 2.32                     | 0.56              |
| 11:e3:192:GLU:OE1  | 11:e3:192:GLU:N    | 2.39                     | 0.56              |
| 11:f3:361:LYS:HE2  | 11:f3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:i3:361:LYS:HE2  | 11:i3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:l3:123:MET:HE3  | 11:l3:123:MET:CA   | 2.35                     | 0.56              |
| 11:m3:192:GLU:OE1  | 11:m3:192:GLU:N    | 2.39                     | 0.56              |
| 11:n3:79:MET:HE2   | 11:o3:57:PHE:HD2   | 1.71                     | 0.56              |
| 11:u3:192:GLU:N    | 11:u3:192:GLU:OE1  | 2.39                     | 0.56              |
| 11:v3:42:VAL:O     | 11:v3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:v3:192:GLU:OE1  | 11:v3:192:GLU:N    | 2.39                     | 0.56              |
| 12:D4:70:GLY:HA2   | 12:E4:71:ILE:HD13  | 1.86                     | 0.56              |
| 1:D1:248:ARG:NH1   | 1:E1:267:THR:OG1   | 2.39                     | 0.56              |
| 1:E1:297:GLN:CD    | 6:U2:76:GLN:HA     | 2.30                     | 0.56              |
| 1:G1:283:SER:HB2   | 1:G1:369:ASP:HB2   | 1.86                     | 0.56              |
| 1:J1:271:ASP:HB3   | 1:J1:383:GLU:OE2   | 2.06                     | 0.56              |
| 1:L1:413:GLU:HA    | 1:L1:416:THR:HG22  | 1.87                     | 0.56              |
| 1:M1:378:ASN:ND2   | 1:M1:381:ASP:OD1   | 2.34                     | 0.56              |
| 1:d1:407:ASP:OD1   | 1:d1:408:GLN:N     | 2.39                     | 0.56              |
| 2:C2:62:THR:HB     | 2:C2:101:MET:SD    | 2.46                     | 0.56              |
| 9:r2:227:ALA:HA    | 9:32:257:LEU:HD21  | 1.86                     | 0.56              |
| 9:u2:109:ASP:C     | 11:z3:80:GLN:HE22  | 2.14                     | 0.56              |
| 9:32:237:GLN:HE22  | 12:B4:52:PRO:HB2   | 1.71                     | 0.56              |
| 10:J3:37:ALA:HB1   | 10:K3:74:ILE:HG22  | 1.87                     | 0.56              |
| 10:M3:206:GLU:HG2  | 10:M3:208:VAL:HG13 | 1.88                     | 0.56              |
| 10:T3:167:LYS:HD3  | 10:U3:203:ALA:HB3  | 1.87                     | 0.56              |
| 10:U3:167:LYS:HD3  | 10:V3:203:ALA:HB3  | 1.87                     | 0.56              |
| 10:W3:167:LYS:HD3  | 10:X3:203:ALA:HB3  | 1.86                     | 0.56              |
| 10:X3:166:GLU:OE2  | 10:X3:168:GLN:NE2  | 2.27                     | 0.56              |
| 11:c3:192:GLU:OE1  | 11:c3:192:GLU:N    | 2.39                     | 0.56              |
| 11:j3:123:MET:HE3  | 11:j3:123:MET:CA   | 2.35                     | 0.56              |
| 11:k3:123:MET:HE3  | 11:k3:123:MET:CA   | 2.35                     | 0.56              |
| 11:m3:142:LEU:HD23 | 11:o3:350:GLN:NE2  | 2.21                     | 0.56              |
| 11:p3:192:GLU:OE1  | 11:p3:192:GLU:N    | 2.39                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:x3:46:ASP:OD1  | 11:y3:161:ASN:HB2  | 2.05                     | 0.56              |
| 11:y3:42:VAL:O    | 11:y3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:y3:192:GLU:OE1 | 11:y3:192:GLU:N    | 2.39                     | 0.56              |
| 11:z3:42:VAL:O    | 11:z3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:z3:192:GLU:N   | 11:z3:192:GLU:OE1  | 2.39                     | 0.56              |
| 12:A4:89:GLN:NE2  | 12:E4:87:ASN:O     | 2.39                     | 0.56              |
| 1:E1:416:THR:HG23 | 1:E1:430:LEU:HD21  | 1.86                     | 0.56              |
| 1:J1:388:ALA:HA   | 1:J1:431:ASN:O     | 2.05                     | 0.56              |
| 1:K1:143:THR:HG21 | 1:L1:156:HIS:NE2   | 2.20                     | 0.56              |
| 1:M1:303:GLN:HG3  | 1:N1:357:SER:HA    | 1.87                     | 0.56              |
| 1:O1:166:VAL:HG22 | 1:O1:168:GLU:OE1   | 2.06                     | 0.56              |
| 1:O1:262:VAL:O    | 1:O1:263:HIS:ND1   | 2.39                     | 0.56              |
| 1:T1:280:GLU:HG2  | 1:T1:282:TYR:HE2   | 1.71                     | 0.56              |
| 1:X1:245:ILE:O    | 1:X1:249:ILE:HG12  | 2.06                     | 0.56              |
| 1:Y1:275:LYS:HB3  | 1:Y1:377:MET:HE2   | 1.88                     | 0.56              |
| 1:d1:141:ALA:O    | 1:d1:145:GLU:HG2   | 2.05                     | 0.56              |
| 2:B2:128:ASP:OD1  | 2:B2:129:LYS:N     | 2.39                     | 0.56              |
| 2:E2:121:ILE:HG23 | 2:E2:125:GLU:HG2   | 1.87                     | 0.56              |
| 7:Z2:74:GLU:H     | 7:Z2:95:ASN:ND2    | 2.04                     | 0.56              |
| 8:d2:70:GLN:CD    | 9:n2:6:TRP:HB2     | 2.30                     | 0.56              |
| 9:h2:175:LEU:HG   | 9:h2:206:PRO:HG3   | 1.88                     | 0.56              |
| 9:i2:1:MET:HE2    | 9:i2:6:TRP:HB2     | 1.87                     | 0.56              |
| 9:z2:85:ASN:O     | 9:z2:221:THR:OG1   | 2.23                     | 0.56              |
| 9:z2:237:GLN:HE21 | 12:D4:53:LEU:CB    | 2.19                     | 0.56              |
| 10:A3:74:ILE:HG22 | 10:Z3:37:ALA:HB1   | 1.88                     | 0.56              |
| 10:K3:206:GLU:HG2 | 10:K3:208:VAL:HG13 | 1.88                     | 0.56              |
| 10:M3:167:LYS:HD3 | 10:N3:203:ALA:HB3  | 1.87                     | 0.56              |
| 10:N3:80:ILE:HD13 | 10:N3:195:VAL:HG13 | 1.87                     | 0.56              |
| 10:O3:206:GLU:HG2 | 10:O3:208:VAL:HG13 | 1.88                     | 0.56              |
| 10:Q3:72:ARG:N    | 10:Q3:76:ASP:OD2   | 2.24                     | 0.56              |
| 10:S3:37:ALA:HB1  | 10:T3:74:ILE:HG22  | 1.88                     | 0.56              |
| 10:W3:37:ALA:HB1  | 10:X3:74:ILE:HG22  | 1.88                     | 0.56              |
| 11:b3:350:GLN:NE2 | 11:z3:142:LEU:HD23 | 2.20                     | 0.56              |
| 11:e3:325:SER:HB3 | 11:e3:330:SER:CB   | 2.32                     | 0.56              |
| 11:f3:79:MET:HE2  | 11:g3:57:PHE:HD2   | 1.70                     | 0.56              |
| 11:k3:79:MET:HE2  | 11:l3:57:PHE:HD2   | 1.71                     | 0.56              |
| 11:l3:192:GLU:OE1 | 11:l3:192:GLU:N    | 2.39                     | 0.56              |
| 11:n3:192:GLU:OE1 | 11:n3:192:GLU:N    | 2.39                     | 0.56              |
| 11:q3:79:MET:HE2  | 11:r3:57:PHE:HD2   | 1.71                     | 0.56              |
| 11:q3:192:GLU:OE1 | 11:q3:192:GLU:N    | 2.39                     | 0.56              |
| 11:w3:79:MET:HE2  | 11:x3:57:PHE:HD2   | 1.71                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:w3:192:GLU:N    | 11:w3:192:GLU:OE1  | 2.39                     | 0.56              |
| 12:E4:214:LEU:HD22 | 12:E4:224:THR:HG22 | 1.87                     | 0.56              |
| 1:J1:394:LYS:HG2   | 1:J1:402:LEU:HB2   | 1.88                     | 0.56              |
| 1:M1:404:LEU:H     | 1:M1:434:ASN:ND2   | 2.04                     | 0.56              |
| 1:R1:407:ASP:OD1   | 1:R1:408:GLN:N     | 2.39                     | 0.56              |
| 1:S1:275:LYS:CB    | 1:S1:377:MET:HB2   | 2.35                     | 0.56              |
| 1:U1:365:ASN:HD21  | 6:R2:64:ALA:C      | 2.11                     | 0.56              |
| 1:d1:193:ALA:HA    | 1:f1:219:LEU:CD1   | 2.36                     | 0.56              |
| 1:g1:373:ARG:NH2   | 1:h1:275:LYS:HD2   | 2.21                     | 0.56              |
| 2:B2:96:LEU:CD1    | 2:B2:236:MET:HE3   | 2.35                     | 0.56              |
| 6:S2:94:SER:OG     | 6:S2:96:ASP:OD1    | 2.21                     | 0.56              |
| 9:j2:238:ARG:O     | 9:j2:242:ILE:HG12  | 2.06                     | 0.56              |
| 9:r2:125:ASN:CB    | 11:l3:54:GLN:NE2   | 2.68                     | 0.56              |
| 9:v2:72:VAL:O      | 9:v2:72:VAL:HG12   | 2.06                     | 0.56              |
| 9:42:121:GLN:N     | 9:42:129:VAL:O     | 2.34                     | 0.56              |
| 10:B3:37:ALA:HB1   | 10:C3:74:ILE:HG22  | 1.87                     | 0.56              |
| 10:N3:167:LYS:HD3  | 10:O3:203:ALA:HB3  | 1.87                     | 0.56              |
| 10:P3:160:ASN:HA   | 10:P3:186:PRO:HD3  | 1.86                     | 0.56              |
| 11:a3:42:VAL:O     | 11:a3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:q3:26:THR:CG2   | 11:q3:187:LEU:HB3  | 2.33                     | 0.56              |
| 11:r3:45:LEU:HD22  | 11:r3:116:LEU:HA   | 1.88                     | 0.56              |
| 11:s3:42:VAL:O     | 11:s3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:s3:46:ASP:HA    | 11:t3:161:ASN:ND2  | 2.21                     | 0.56              |
| 11:s3:361:LYS:HE2  | 11:s3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:u3:79:MET:HE2   | 11:v3:57:PHE:HD2   | 1.71                     | 0.56              |
| 11:x3:361:LYS:HE2  | 11:x3:363:GLU:OE2  | 2.05                     | 0.56              |
| 1:B1:417:ARG:HG3   | 1:B1:422:PHE:HB3   | 1.88                     | 0.56              |
| 1:D1:360:ARG:NH1   | 1:D1:362:GLU:OE2   | 2.38                     | 0.56              |
| 1:G1:166:VAL:CA    | 2:B2:144:GLU:HG2   | 2.35                     | 0.56              |
| 1:T1:165:PHE:HZ    | 3:F2:170:MET:HG2   | 1.70                     | 0.56              |
| 1:T1:167:ARG:HH12  | 2:E2:107:LYS:HA    | 1.70                     | 0.56              |
| 1:T1:173:SER:HA    | 1:T1:209:ASN:HB3   | 1.88                     | 0.56              |
| 1:X1:369:ASP:OD1   | 1:Y1:282:TYR:N     | 2.37                     | 0.56              |
| 1:a1:241:VAL:HG22  | 1:b1:235:LEU:HD21  | 1.88                     | 0.56              |
| 2:A2:224:MET:HE2   | 2:B2:187:PHE:HB3   | 1.87                     | 0.56              |
| 7:a2:36:GLY:O      | 8:f2:42:ARG:NH2    | 2.36                     | 0.56              |
| 9:h2:190:ASN:ND2   | 9:m2:42:GLU:OE1    | 2.39                     | 0.56              |
| 9:r2:72:VAL:HG12   | 9:r2:72:VAL:O      | 2.05                     | 0.56              |
| 9:v2:161:GLN:HB2   | 9:v2:164:GLN:HB3   | 1.87                     | 0.56              |
| 9:42:107:LEU:HD11  | 9:42:113:ALA:HB2   | 1.87                     | 0.56              |
| 10:B3:167:LYS:HD3  | 10:C3:203:ALA:HB3  | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:Q3:121:ARG:HA   | 10:R3:111:ARG:HB2  | 1.86                     | 0.56              |
| 10:Q3:167:LYS:HD3  | 10:R3:203:ALA:HB3  | 1.86                     | 0.56              |
| 10:R3:70:ARG:NH2   | 11:q3:72:THR:OG1   | 2.37                     | 0.56              |
| 10:S3:121:ARG:HA   | 10:T3:111:ARG:HB2  | 1.86                     | 0.56              |
| 11:b3:42:VAL:O     | 11:b3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:d3:79:MET:HE2   | 11:e3:57:PHE:HD2   | 1.69                     | 0.56              |
| 11:d3:361:LYS:HE2  | 11:d3:363:GLU:OE2  | 2.05                     | 0.56              |
| 11:e3:269:THR:OG1  | 11:e3:359:ARG:HB2  | 2.06                     | 0.56              |
| 11:j3:192:GLU:N    | 11:j3:192:GLU:OE1  | 2.39                     | 0.56              |
| 11:l3:46:ASP:HA    | 11:m3:161:ASN:ND2  | 2.20                     | 0.56              |
| 11:l3:142:LEU:HD23 | 11:n3:350:GLN:NE2  | 2.21                     | 0.56              |
| 11:o3:192:GLU:N    | 11:o3:192:GLU:OE1  | 2.39                     | 0.56              |
| 11:p3:26:THR:CG2   | 11:p3:187:LEU:HB3  | 2.33                     | 0.56              |
| 11:p3:42:VAL:O     | 11:p3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:q3:45:LEU:HD22  | 11:q3:116:LEU:HA   | 1.88                     | 0.56              |
| 11:s3:245:ASN:OD1  | 11:s3:245:ASN:N    | 2.33                     | 0.56              |
| 1:E1:140:LEU:O     | 1:E1:144:ILE:HG12  | 2.06                     | 0.56              |
| 1:E1:284:PRO:O     | 1:E1:290:LYS:NZ    | 2.31                     | 0.56              |
| 1:F1:420:MET:HE3   | 1:F1:422:PHE:HB2   | 1.87                     | 0.56              |
| 1:H1:140:LEU:O     | 1:H1:144:ILE:HG12  | 2.05                     | 0.56              |
| 1:K1:385:LEU:N     | 1:K1:428:ASP:OD2   | 2.38                     | 0.56              |
| 1:X1:193:ALA:HA    | 1:Y1:219:LEU:HG    | 1.86                     | 0.56              |
| 1:Z1:244:ARG:CZ    | 1:a1:235:LEU:HB3   | 2.36                     | 0.56              |
| 1:Z1:294:ARG:HG3   | 6:S2:66:THR:CB     | 2.31                     | 0.56              |
| 1:b1:266:VAL:HG22  | 1:b1:387:VAL:HG22  | 1.88                     | 0.56              |
| 1:d1:267:THR:HB    | 1:d1:386:SER:HB2   | 1.87                     | 0.56              |
| 1:d1:385:LEU:N     | 1:d1:428:ASP:OD2   | 2.35                     | 0.56              |
| 6:T2:22:ARG:HB3    | 6:T2:112:ASN:HD21  | 1.71                     | 0.56              |
| 8:d2:26:LEU:HD21   | 9:i2:242:ILE:HG22  | 1.88                     | 0.56              |
| 9:h2:46:TYR:HA     | 9:h2:69:GLY:HA2    | 1.88                     | 0.56              |
| 9:l2:152:GLY:HA3   | 9:22:56:SER:O      | 2.06                     | 0.56              |
| 9:q2:2:ILE:HG13    | 9:q2:3:SER:H       | 1.71                     | 0.56              |
| 9:s2:209:ASN:ND2   | 11:r3:78:ASN:ND2   | 2.54                     | 0.56              |
| 9:t2:162:GLN:HE22  | 9:y2:208:LEU:HA    | 1.71                     | 0.56              |
| 10:H3:72:ARG:N     | 10:H3:76:ASP:OD2   | 2.25                     | 0.56              |
| 10:I3:206:GLU:HG2  | 10:I3:208:VAL:HG13 | 1.88                     | 0.56              |
| 10:K3:37:ALA:HB1   | 10:L3:74:ILE:HG22  | 1.88                     | 0.56              |
| 10:V3:37:ALA:HB1   | 10:W3:74:ILE:HG22  | 1.87                     | 0.56              |
| 10:Y3:121:ARG:HA   | 10:Z3:111:ARG:HB2  | 1.87                     | 0.56              |
| 11:a3:192:GLU:OE1  | 11:a3:192:GLU:N    | 2.39                     | 0.56              |
| 11:e3:26:THR:CG2   | 11:e3:187:LEU:HB3  | 2.33                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:e3:42:VAL:O     | 11:e3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:f3:325:SER:HB3  | 11:f3:330:SER:CB   | 2.32                     | 0.56              |
| 11:g3:192:GLU:N    | 11:g3:192:GLU:OE1  | 2.39                     | 0.56              |
| 11:h3:269:THR:OG1  | 11:h3:359:ARG:HB2  | 2.06                     | 0.56              |
| 11:j3:325:SER:HB3  | 11:j3:330:SER:CB   | 2.32                     | 0.56              |
| 11:l3:269:THR:OG1  | 11:l3:359:ARG:HB2  | 2.07                     | 0.56              |
| 11:t3:42:VAL:O     | 11:t3:84:VAL:HA    | 2.05                     | 0.56              |
| 11:t3:192:GLU:OE1  | 11:t3:192:GLU:N    | 2.39                     | 0.56              |
| 11:x3:245:ASN:OD1  | 11:x3:245:ASN:N    | 2.33                     | 0.56              |
| 11:y3:361:LYS:HE2  | 11:y3:363:GLU:OE2  | 2.05                     | 0.56              |
| 1:A1:275:LYS:CE    | 1:h1:373:ARG:HH21  | 2.19                     | 0.55              |
| 1:B1:150:VAL:C     | 1:B1:151:LYS:HD3   | 2.30                     | 0.55              |
| 1:E1:161:LYS:HD3   | 1:E1:162:PRO:HD2   | 1.87                     | 0.55              |
| 1:M1:293:LEU:HD21  | 1:M1:296:ARG:HH21  | 1.71                     | 0.55              |
| 1:O1:299:ASN:HB2   | 1:O1:361:ASN:HB2   | 1.88                     | 0.55              |
| 1:U1:237:PHE:HE2   | 1:V1:232:ASP:HA    | 1.70                     | 0.55              |
| 1:X1:275:LYS:CB    | 1:X1:377:MET:HB2   | 2.37                     | 0.55              |
| 1:Y1:172:PRO:HG2   | 1:Y1:205:LEU:HA    | 1.88                     | 0.55              |
| 1:d1:138:GLY:O     | 1:d1:142:ARG:HG2   | 2.05                     | 0.55              |
| 2:E2:96:LEU:CB     | 2:E2:236:MET:HE1   | 2.35                     | 0.55              |
| 2:E2:100:ILE:HD11  | 2:E2:240:ALA:HA    | 1.87                     | 0.55              |
| 6:Q2:114:LEU:HD11  | 7:W2:126:MET:HB2   | 1.88                     | 0.55              |
| 9:g2:230:LEU:HD21  | 9:l2:242:ILE:HD12  | 1.88                     | 0.55              |
| 9:h2:144:ALA:HA    | 9:m2:179:MET:SD    | 2.46                     | 0.55              |
| 9:h2:190:ASN:N     | 9:m2:42:GLU:OE2    | 2.38                     | 0.55              |
| 9:p2:88:GLN:HE22   | 9:p2:90:ASN:CG     | 2.14                     | 0.55              |
| 9:u2:110:GLY:C     | 11:z3:80:GLN:HE22  | 2.06                     | 0.55              |
| 9:u2:200:ALA:CB    | 11:b3:54:GLN:NE2   | 2.54                     | 0.55              |
| 9:v2:151:ILE:N     | 9:v2:216:GLN:OE1   | 2.39                     | 0.55              |
| 9:w2:83:GLN:HE22   | 9:w2:99:GLY:H      | 1.54                     | 0.55              |
| 10:C3:80:ILE:HD13  | 10:C3:195:VAL:HG13 | 1.87                     | 0.55              |
| 10:P3:167:LYS:HD3  | 10:Q3:203:ALA:HB3  | 1.86                     | 0.55              |
| 11:a3:362:LEU:HD21 | 11:y3:166:THR:HG21 | 1.88                     | 0.55              |
| 11:b3:361:LYS:HE2  | 11:b3:363:GLU:OE2  | 2.05                     | 0.55              |
| 11:e3:361:LYS:HE2  | 11:e3:363:GLU:OE2  | 2.05                     | 0.55              |
| 11:g3:142:LEU:HD23 | 11:i3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:h3:79:MET:HE2   | 11:i3:57:PHE:HD2   | 1.71                     | 0.55              |
| 11:i3:123:MET:HE3  | 11:i3:123:MET:CA   | 2.35                     | 0.55              |
| 11:n3:142:LEU:HD23 | 11:p3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:p3:45:LEU:HD22  | 11:p3:116:LEU:HA   | 1.88                     | 0.55              |
| 11:r3:26:THR:CG2   | 11:r3:187:LEU:HB3  | 2.33                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:r3:192:GLU:N    | 11:r3:192:GLU:OE1  | 2.39                     | 0.55              |
| 11:s3:45:LEU:HD22  | 11:s3:116:LEU:HA   | 1.88                     | 0.55              |
| 11:w3:42:VAL:O     | 11:w3:84:VAL:HA    | 2.05                     | 0.55              |
| 11:x3:42:VAL:O     | 11:x3:84:VAL:HA    | 2.05                     | 0.55              |
| 11:z3:123:MET:H    | 11:z3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:z3:361:LYS:HE2  | 11:z3:363:GLU:OE2  | 2.05                     | 0.55              |
| 12:B4:92:GLN:HG3   | 12:C4:92:GLN:HG2   | 1.89                     | 0.55              |
| 12:D4:98:GLY:O     | 12:D4:99:HIS:ND1   | 2.39                     | 0.55              |
| 1:C1:134:ARG:O     | 1:C1:137:GLU:HB3   | 2.06                     | 0.55              |
| 1:E1:166:VAL:N     | 2:B2:244:TYR:HE2   | 1.98                     | 0.55              |
| 1:O1:166:VAL:HA    | 2:A2:152:ARG:NE    | 2.19                     | 0.55              |
| 1:V1:373:ARG:NH1   | 1:W1:277:GLN:OE1   | 2.39                     | 0.55              |
| 1:V1:373:ARG:HH21  | 1:W1:275:LYS:HD2   | 1.70                     | 0.55              |
| 1:b1:287:ASP:HB2   | 1:b1:290:LYS:HG2   | 1.88                     | 0.55              |
| 1:c1:203:ALA:HB1   | 1:d1:160:PRO:HA    | 1.88                     | 0.55              |
| 1:e1:244:ARG:HH11  | 1:f1:239:ASN:HB2   | 1.71                     | 0.55              |
| 1:g1:145:GLU:OE2   | 1:g1:153:ALA:N     | 2.39                     | 0.55              |
| 2:C2:121:ILE:HG23  | 2:C2:126:ALA:HB2   | 1.87                     | 0.55              |
| 2:D2:195:ILE:HD11  | 4:J2:13:ALA:HB1    | 1.88                     | 0.55              |
| 9:l2:98:LYS:HD2    | 9:w2:45:LEU:CD2    | 2.37                     | 0.55              |
| 9:12:82:SER:HB3    | 9:12:223:ASN:HD22  | 1.71                     | 0.55              |
| 10:C3:37:ALA:HB1   | 10:D3:74:ILE:HG22  | 1.87                     | 0.55              |
| 10:C3:167:LYS:HD3  | 10:D3:203:ALA:HB3  | 1.87                     | 0.55              |
| 10:F3:37:ALA:HB1   | 10:G3:74:ILE:HG22  | 1.87                     | 0.55              |
| 10:G3:70:ARG:NH2   | 11:f3:72:THR:OG1   | 2.38                     | 0.55              |
| 10:J3:121:ARG:HA   | 10:K3:111:ARG:HB2  | 1.88                     | 0.55              |
| 10:Q3:206:GLU:HG2  | 10:Q3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:V3:80:ILE:HD13  | 10:V3:195:VAL:HG13 | 1.87                     | 0.55              |
| 10:X3:206:GLU:HG2  | 10:X3:208:VAL:HG13 | 1.88                     | 0.55              |
| 11:g3:325:SER:HB3  | 11:g3:330:SER:CB   | 2.32                     | 0.55              |
| 11:p3:142:LEU:HD23 | 11:r3:350:GLN:NE2  | 2.22                     | 0.55              |
| 11:t3:46:ASP:HA    | 11:u3:161:ASN:ND2  | 2.21                     | 0.55              |
| 1:A1:248:ARG:HH11  | 1:B1:267:THR:HG22  | 1.70                     | 0.55              |
| 1:K1:199:SER:OG    | 1:K1:205:LEU:O     | 2.19                     | 0.55              |
| 1:T1:167:ARG:NH2   | 2:E2:107:LYS:CA    | 2.56                     | 0.55              |
| 1:a1:189:GLY:O     | 1:a1:192:SER:OG    | 2.19                     | 0.55              |
| 6:T2:42:ASP:OD2    | 6:T2:88:ARG:NH2    | 2.37                     | 0.55              |
| 9:g2:185:GLU:OE1   | 9:l2:67:GLN:NE2    | 2.38                     | 0.55              |
| 9:o2:115:THR:HB    | 9:o2:191:LEU:HD23  | 1.88                     | 0.55              |
| 9:s2:36:ARG:NH1    | 9:s2:38:ARG:HB2    | 2.20                     | 0.55              |
| 9:w2:117:ASP:OD2   | 9:w2:190:ASN:ND2   | 2.36                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:22:23:ALA:HB1    | 12:A4:45:LYS:CG    | 2.37                     | 0.55              |
| 10:B3:206:GLU:HG2  | 10:B3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:F3:121:ARG:HA   | 10:G3:111:ARG:HB2  | 1.87                     | 0.55              |
| 10:J3:70:ARG:NH2   | 11:i3:72:THR:OG1   | 2.38                     | 0.55              |
| 10:J3:166:GLU:OE2  | 10:J3:168:GLN:NE2  | 2.27                     | 0.55              |
| 10:T3:72:ARG:N     | 10:T3:76:ASP:OD2   | 2.24                     | 0.55              |
| 10:V3:101:LYS:HZ3  | 10:V3:101:LYS:HB2  | 1.71                     | 0.55              |
| 10:Y3:206:GLU:HG2  | 10:Y3:208:VAL:HG13 | 1.88                     | 0.55              |
| 11:a3:269:THR:OG1  | 11:a3:359:ARG:HB2  | 2.06                     | 0.55              |
| 11:h3:325:SER:HB3  | 11:h3:330:SER:CB   | 2.32                     | 0.55              |
| 11:i3:79:MET:HE2   | 11:j3:57:PHE:HD2   | 1.71                     | 0.55              |
| 11:i3:325:SER:HB3  | 11:i3:330:SER:CB   | 2.32                     | 0.55              |
| 11:k3:192:GLU:OE1  | 11:k3:192:GLU:N    | 2.39                     | 0.55              |
| 11:n3:123:MET:H    | 11:n3:138:GLN:HB2  | 1.72                     | 0.55              |
| 11:o3:45:LEU:HD22  | 11:o3:116:LEU:HA   | 1.88                     | 0.55              |
| 11:o3:123:MET:H    | 11:o3:138:GLN:HB2  | 1.72                     | 0.55              |
| 11:t3:45:LEU:HD22  | 11:t3:116:LEU:HA   | 1.88                     | 0.55              |
| 11:x3:192:GLU:OE1  | 11:x3:192:GLU:N    | 2.39                     | 0.55              |
| 11:y3:123:MET:H    | 11:y3:138:GLN:HB2  | 1.71                     | 0.55              |
| 12:B4:102:MET:HE1  | 12:B4:232:ILE:HG12 | 1.87                     | 0.55              |
| 1:H1:165:PHE:CE1   | 2:B2:147:LEU:HD13  | 2.34                     | 0.55              |
| 1:O1:179:THR:HA    | 1:O1:215:GLN:HB3   | 1.87                     | 0.55              |
| 1:Q1:161:LYS:HZ3   | 3:F2:249:ASN:ND2   | 2.01                     | 0.55              |
| 1:Q1:211:THR:HA    | 1:Q1:221:THR:HG21  | 1.87                     | 0.55              |
| 1:R1:143:THR:CG2   | 1:T1:156:HIS:HE1   | 2.13                     | 0.55              |
| 1:U1:140:LEU:O     | 1:U1:143:THR:OG1   | 2.15                     | 0.55              |
| 1:a1:394:LYS:HE2   | 1:a1:402:LEU:HD22  | 1.89                     | 0.55              |
| 2:A2:62:THR:O      | 2:A2:174:TYR:OH    | 2.24                     | 0.55              |
| 2:C2:101:MET:HE1   | 2:C2:137:PHE:CZ    | 2.41                     | 0.55              |
| 6:S2:30:ILE:HG23   | 6:S2:102:MET:HE1   | 1.87                     | 0.55              |
| 8:d2:42:ARG:HD2    | 9:i2:64:SER:CB     | 2.37                     | 0.55              |
| 9:j2:95:VAL:O      | 9:j2:118:GLY:HA3   | 2.07                     | 0.55              |
| 9:m2:44:LEU:HD21   | 9:m2:73:ARG:HB2    | 1.88                     | 0.55              |
| 9:s2:2:ILE:HG22    | 9:s2:4:SER:H       | 1.71                     | 0.55              |
| 9:v2:46:TYR:HA     | 9:v2:69:GLY:HA2    | 1.88                     | 0.55              |
| 10:A3:206:GLU:HG2  | 10:A3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:R3:167:LYS:HD3  | 10:S3:203:ALA:HB3  | 1.87                     | 0.55              |
| 11:a3:142:LEU:HD23 | 11:c3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:b3:192:GLU:N    | 11:b3:192:GLU:OE1  | 2.39                     | 0.55              |
| 11:d3:269:THR:OG1  | 11:d3:359:ARG:HB2  | 2.07                     | 0.55              |
| 11:e3:123:MET:H    | 11:e3:138:GLN:HB2  | 1.72                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:f3:123:MET:H    | 11:f3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:i3:123:MET:H    | 11:i3:138:GLN:HB2  | 1.72                     | 0.55              |
| 11:j3:142:LEU:HD23 | 11:l3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:k3:269:THR:OG1  | 11:k3:359:ARG:HB2  | 2.07                     | 0.55              |
| 11:l3:123:MET:H    | 11:l3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:p3:166:THR:HG21 | 11:r3:362:LEU:HD21 | 1.88                     | 0.55              |
| 11:r3:196:MET:HA   | 11:r3:196:MET:CE   | 2.34                     | 0.55              |
| 11:t3:123:MET:H    | 11:t3:138:GLN:HB2  | 1.72                     | 0.55              |
| 11:v3:142:LEU:HD23 | 11:x3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:v3:166:THR:HG21 | 11:x3:362:LEU:HD21 | 1.88                     | 0.55              |
| 1:G1:165:PHE:CZ    | 2:B2:143:ARG:NH2   | 2.75                     | 0.55              |
| 1:L1:284:PRO:O     | 1:L1:290:LYS:NZ    | 2.39                     | 0.55              |
| 1:N1:244:ARG:NH1   | 1:O1:239:ASN:OD1   | 2.38                     | 0.55              |
| 1:N1:413:GLU:OE2   | 1:N1:417:ARG:NH1   | 2.40                     | 0.55              |
| 1:T1:203:ALA:N     | 1:U1:158:ALA:HB1   | 2.21                     | 0.55              |
| 1:T1:257:VAL:O     | 1:T1:261:ASN:ND2   | 2.34                     | 0.55              |
| 1:Y1:257:VAL:O     | 1:Y1:261:ASN:ND2   | 2.19                     | 0.55              |
| 1:a1:393:TYR:CE2   | 1:a1:436:PRO:HD3   | 2.41                     | 0.55              |
| 1:f1:165:PHE:CD1   | 2:D2:148:ALA:CB    | 2.89                     | 0.55              |
| 1:h1:219:LEU:HD12  | 1:h1:219:LEU:H     | 1.70                     | 0.55              |
| 4:I2:31:THR:HG21   | 4:I2:57:ALA:HB2    | 1.89                     | 0.55              |
| 5:K2:72:MET:HE3    | 5:P2:84:MET:HE1    | 1.87                     | 0.55              |
| 8:d2:138:ALA:HB1   | 9:t2:56:SER:O      | 2.06                     | 0.55              |
| 8:e2:189:ARG:HH21  | 8:e2:193:LEU:HD23  | 1.71                     | 0.55              |
| 9:w2:26:LEU:HD21   | 9:22:242:ILE:HG22  | 1.87                     | 0.55              |
| 9:x2:44:LEU:HD13   | 9:x2:71:GLY:HA3    | 1.87                     | 0.55              |
| 9:32:82:SER:O      | 9:32:223:ASN:ND2   | 2.39                     | 0.55              |
| 10:C3:206:GLU:HG2  | 10:C3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:D3:72:ARG:N     | 10:D3:76:ASP:OD2   | 2.24                     | 0.55              |
| 10:G3:206:GLU:HG2  | 10:G3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:K3:57:PRO:HB2   | 10:K3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:O3:57:PRO:HB2   | 10:O3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:P3:37:ALA:HB1   | 10:Q3:74:ILE:HG22  | 1.87                     | 0.55              |
| 10:S3:167:LYS:HD3  | 10:T3:203:ALA:HB3  | 1.87                     | 0.55              |
| 10:T3:37:ALA:HB1   | 10:U3:74:ILE:HG22  | 1.88                     | 0.55              |
| 10:W3:206:GLU:HG2  | 10:W3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:Z3:206:GLU:HG2  | 10:Z3:208:VAL:HG13 | 1.88                     | 0.55              |
| 11:c3:361:LYS:HE2  | 11:c3:363:GLU:OE2  | 2.05                     | 0.55              |
| 11:h3:142:LEU:HD23 | 11:j3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:i3:269:THR:OG1  | 11:i3:359:ARG:HB2  | 2.07                     | 0.55              |
| 11:j3:254:VAL:HG13 | 11:j3:365:ILE:HG12 | 1.89                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:p3:269:THR:OG1  | 11:p3:359:ARG:HB2  | 2.06                     | 0.55              |
| 11:s3:26:THR:CG2   | 11:s3:187:LEU:HB3  | 2.33                     | 0.55              |
| 11:u3:45:LEU:HD22  | 11:u3:116:LEU:HA   | 1.88                     | 0.55              |
| 11:z3:269:THR:OG1  | 11:z3:359:ARG:HB2  | 2.06                     | 0.55              |
| 12:A4:60:THR:HG22  | 12:B4:61:GLN:HG2   | 1.87                     | 0.55              |
| 1:B1:166:VAL:HG22  | 2:C2:162:PRO:CG    | 2.36                     | 0.55              |
| 1:E1:164:LEU:O     | 2:B2:241:GLN:HG3   | 2.07                     | 0.55              |
| 1:G1:143:THR:HA    | 1:H1:154:ARG:HH11  | 1.71                     | 0.55              |
| 1:R1:200:SER:HB3   | 1:T1:175:SER:HB3   | 1.88                     | 0.55              |
| 1:Z1:375:THR:HG23  | 1:a1:275:LYS:HZ3   | 1.71                     | 0.55              |
| 1:a1:165:PHE:CE1   | 2:E2:152:ARG:HB3   | 2.42                     | 0.55              |
| 2:A2:119:GLN:HE22  | 2:A2:120:LYS:HZ3   | 1.53                     | 0.55              |
| 7:Z2:121:THR:HG23  | 8:f2:250:MET:HB2   | 1.88                     | 0.55              |
| 8:c2:57:VAL:O      | 8:c2:57:VAL:HG12   | 2.06                     | 0.55              |
| 8:e2:76:ARG:NH1    | 8:e2:79:ASP:OD1    | 2.35                     | 0.55              |
| 9:t2:203:GLU:HG2   | 11:v3:78:ASN:ND2   | 2.18                     | 0.55              |
| 9:42:36:ARG:O      | 9:42:80:LEU:HB3    | 2.06                     | 0.55              |
| 10:A3:82:LEU:O     | 10:A3:197:SER:OG   | 2.20                     | 0.55              |
| 10:D3:37:ALA:HB1   | 10:E3:74:ILE:HG22  | 1.87                     | 0.55              |
| 10:G3:37:ALA:HB1   | 10:H3:74:ILE:HG22  | 1.88                     | 0.55              |
| 10:H3:80:ILE:HD13  | 10:H3:195:VAL:HG13 | 1.87                     | 0.55              |
| 10:K3:70:ARG:NH2   | 11:j3:72:THR:OG1   | 2.37                     | 0.55              |
| 10:L3:57:PRO:HB2   | 10:L3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:N3:37:ALA:HB1   | 10:O3:74:ILE:HG22  | 1.88                     | 0.55              |
| 10:P3:57:PRO:HB2   | 10:P3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:Q3:82:LEU:O     | 10:Q3:197:SER:OG   | 2.20                     | 0.55              |
| 11:b3:79:MET:HE2   | 11:c3:57:PHE:HD2   | 1.71                     | 0.55              |
| 11:b3:196:MET:HA   | 11:b3:196:MET:CE   | 2.34                     | 0.55              |
| 11:e3:245:ASN:OD1  | 11:e3:245:ASN:N    | 2.33                     | 0.55              |
| 11:f3:192:GLU:OE1  | 11:f3:192:GLU:N    | 2.39                     | 0.55              |
| 11:k3:164:ARG:HD2  | 11:l3:365:ILE:CG2  | 2.37                     | 0.55              |
| 11:m3:79:MET:HE2   | 11:n3:57:PHE:HD2   | 1.72                     | 0.55              |
| 11:p3:123:MET:H    | 11:p3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:q3:142:LEU:HD23 | 11:s3:350:GLN:NE2  | 2.22                     | 0.55              |
| 11:r3:142:LEU:HD23 | 11:t3:350:GLN:NE2  | 2.22                     | 0.55              |
| 11:s3:79:MET:HE2   | 11:t3:57:PHE:HD2   | 1.72                     | 0.55              |
| 1:K1:151:LYS:NZ    | 1:K1:180:LEU:O     | 2.40                     | 0.55              |
| 1:Q1:275:LYS:HB2   | 1:Q1:377:MET:HB2   | 1.87                     | 0.55              |
| 1:T1:159:MET:HG3   | 1:T1:172:PRO:HB3   | 1.89                     | 0.55              |
| 1:W1:133:GLN:O     | 1:W1:137:GLU:HG2   | 2.06                     | 0.55              |
| 1:Z1:301:SER:O     | 1:Z1:359:GLN:N     | 2.40                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:d1:151:LYS:HE3   | 1:d1:180:LEU:O     | 2.06                     | 0.55              |
| 1:d1:360:ARG:NH1   | 1:d1:362:GLU:OE1   | 2.40                     | 0.55              |
| 1:f1:420:MET:HE2   | 1:f1:422:PHE:HA    | 1.88                     | 0.55              |
| 2:B2:185:ILE:O     | 2:B2:189:ILE:HG12  | 2.06                     | 0.55              |
| 8:f2:91:GLN:O      | 8:f2:118:HIS:HB2   | 2.07                     | 0.55              |
| 8:f2:140:ASP:O     | 8:f2:160:ARG:NH1   | 2.38                     | 0.55              |
| 9:s2:230:LEU:HD22  | 9:42:257:LEU:HG    | 1.88                     | 0.55              |
| 9:t2:36:ARG:HH21   | 9:t2:80:LEU:HB2    | 1.71                     | 0.55              |
| 9:12:239:ALA:O     | 9:12:242:ILE:HG22  | 2.07                     | 0.55              |
| 9:42:23:ALA:HA     | 12:C4:41:VAL:CG2   | 2.35                     | 0.55              |
| 10:A3:121:ARG:HA   | 10:B3:111:ARG:HB2  | 1.87                     | 0.55              |
| 10:K3:166:GLU:OE2  | 10:K3:168:GLN:NE2  | 2.27                     | 0.55              |
| 10:M3:57:PRO:HB2   | 10:M3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:Q3:50:SER:HB3   | 11:r3:99:GLN:NE2   | 2.22                     | 0.55              |
| 10:Q3:57:PRO:HB2   | 10:Q3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:S3:206:GLU:HG2  | 10:S3:208:VAL:HG13 | 1.88                     | 0.55              |
| 11:a3:123:MET:H    | 11:a3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:d3:123:MET:H    | 11:d3:138:GLN:HB2  | 1.72                     | 0.55              |
| 11:d3:142:LEU:HD23 | 11:f3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:d3:196:MET:HA   | 11:d3:196:MET:CE   | 2.34                     | 0.55              |
| 11:e3:142:LEU:HD23 | 11:g3:350:GLN:NE2  | 2.21                     | 0.55              |
| 11:f3:269:THR:OG1  | 11:f3:359:ARG:HB2  | 2.06                     | 0.55              |
| 11:m3:123:MET:H    | 11:m3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:n3:45:LEU:HD22  | 11:n3:116:LEU:HA   | 1.88                     | 0.55              |
| 11:o3:79:MET:HE2   | 11:p3:57:PHE:HD2   | 1.71                     | 0.55              |
| 11:s3:123:MET:H    | 11:s3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:s3:192:GLU:OE1  | 11:s3:192:GLU:N    | 2.39                     | 0.55              |
| 11:u3:123:MET:H    | 11:u3:138:GLN:HB2  | 1.72                     | 0.55              |
| 11:y3:79:MET:HE2   | 11:z3:57:PHE:CD2   | 2.41                     | 0.55              |
| 1:R1:167:ARG:HD2   | 3:F2:168:ALA:HB2   | 1.87                     | 0.55              |
| 1:X1:203:ALA:HB1   | 1:Y1:160:PRO:HA    | 1.89                     | 0.55              |
| 1:a1:168:GLU:O     | 1:a1:169:GLN:HB2   | 2.07                     | 0.55              |
| 1:d1:374:HIS:HB3   | 1:e1:276:GLU:HB3   | 1.89                     | 0.55              |
| 1:g1:197:LEU:HD12  | 1:h1:213:VAL:HG21  | 1.89                     | 0.55              |
| 2:C2:225:LEU:HD11  | 4:I2:77:VAL:HG21   | 1.88                     | 0.55              |
| 8:e2:64:ALA:HB3    | 8:e2:66:MET:HE2    | 1.88                     | 0.55              |
| 9:n2:238:ARG:NH1   | 9:n2:241:GLU:OE1   | 2.40                     | 0.55              |
| 9:p2:77:THR:HG23   | 9:u2:66:LEU:HD12   | 1.88                     | 0.55              |
| 9:42:23:ALA:O      | 12:C4:41:VAL:HG21  | 2.07                     | 0.55              |
| 10:D3:121:ARG:HA   | 10:E3:111:ARG:HB2  | 1.88                     | 0.55              |
| 10:E3:50:SER:HB3   | 11:f3:99:GLN:NE2   | 2.22                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:I3:37:ALA:HB1   | 10:J3:74:ILE:HG22  | 1.87                     | 0.55              |
| 10:J3:57:PRO:HB2   | 10:J3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:L3:206:GLU:HG2  | 10:L3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:N3:57:PRO:HB2   | 10:N3:60:TYR:HE2   | 1.72                     | 0.55              |
| 11:d3:166:THR:HG21 | 11:f3:362:LEU:HD21 | 1.88                     | 0.55              |
| 11:g3:123:MET:H    | 11:g3:138:GLN:HB2  | 1.72                     | 0.55              |
| 11:g3:269:THR:OG1  | 11:g3:359:ARG:HB2  | 2.06                     | 0.55              |
| 11:m3:269:THR:OG1  | 11:m3:359:ARG:HB2  | 2.07                     | 0.55              |
| 11:n3:254:VAL:HG13 | 11:n3:365:ILE:HG12 | 1.89                     | 0.55              |
| 11:q3:269:THR:OG1  | 11:q3:359:ARG:HB2  | 2.06                     | 0.55              |
| 1:T1:244:ARG:HH11  | 1:U1:239:ASN:HB2   | 1.72                     | 0.55              |
| 1:V1:404:LEU:HD23  | 1:V1:408:GLN:HG2   | 1.89                     | 0.55              |
| 1:W1:186:LEU:HD23  | 1:W1:191:ILE:HD13  | 1.88                     | 0.55              |
| 1:X1:181:GLU:HB3   | 1:X1:184:ARG:NH2   | 2.21                     | 0.55              |
| 1:a1:261:ASN:O     | 1:a1:392:ASN:N     | 2.30                     | 0.55              |
| 1:d1:147:LEU:O     | 1:d1:149:PRO:HD2   | 2.06                     | 0.55              |
| 1:d1:248:ARG:HH11  | 1:e1:267:THR:HG22  | 1.72                     | 0.55              |
| 1:f1:375:THR:HG23  | 1:g1:275:LYS:HZ2   | 1.71                     | 0.55              |
| 2:D2:102:SER:HA    | 2:D2:105:ILE:HG22  | 1.87                     | 0.55              |
| 2:D2:115:PRO:HA    | 2:D2:119:GLN:NE2   | 2.21                     | 0.55              |
| 3:F2:165:ASN:ND2   | 3:F2:262:ASN:OD1   | 2.40                     | 0.55              |
| 6:U2:31:ALA:HB1    | 7:Z2:13:ALA:HB2    | 1.89                     | 0.55              |
| 8:c2:133:SER:HB2   | 8:c2:135:ILE:HG12  | 1.89                     | 0.55              |
| 9:i2:43:ASP:OD1    | 9:i2:43:ASP:N      | 2.40                     | 0.55              |
| 9:j2:238:ARG:CZ    | 9:p2:255:GLN:OE1   | 2.55                     | 0.55              |
| 10:K3:50:SER:HB3   | 11:l3:99:GLN:NE2   | 2.22                     | 0.55              |
| 10:R3:57:PRO:HB2   | 10:R3:60:TYR:HE2   | 1.72                     | 0.55              |
| 10:U3:72:ARG:N     | 10:U3:76:ASP:OD2   | 2.25                     | 0.55              |
| 10:V3:206:GLU:HG2  | 10:V3:208:VAL:HG13 | 1.88                     | 0.55              |
| 11:b3:269:THR:OG1  | 11:b3:359:ARG:HB2  | 2.06                     | 0.55              |
| 11:f3:254:VAL:HG13 | 11:f3:365:ILE:HG12 | 1.89                     | 0.55              |
| 11:g3:254:VAL:HG13 | 11:g3:365:ILE:HG12 | 1.89                     | 0.55              |
| 11:o3:269:THR:OG1  | 11:o3:359:ARG:HB2  | 2.06                     | 0.55              |
| 11:u3:164:ARG:HD2  | 11:v3:365:ILE:CG2  | 2.37                     | 0.55              |
| 11:v3:46:ASP:HA    | 11:w3:161:ASN:ND2  | 2.20                     | 0.55              |
| 1:H1:407:ASP:HA    | 1:H1:410:LYS:HG2   | 1.89                     | 0.55              |
| 1:N1:169:GLN:CD    | 1:N1:170:LYS:H     | 2.15                     | 0.55              |
| 1:W1:165:PHE:CE1   | 2:E2:244:TYR:C     | 2.73                     | 0.55              |
| 1:X1:182:PRO:O     | 1:X1:184:ARG:NH1   | 2.40                     | 0.55              |
| 1:Z1:244:ARG:HH22  | 1:a1:235:LEU:C     | 2.14                     | 0.55              |
| 1:a1:167:ARG:CB    | 2:D2:244:TYR:HD2   | 2.20                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B2:166:PRO:HG2   | 2:B2:169:ILE:HG12  | 1.88                     | 0.55              |
| 2:E2:47:PHE:CZ     | 3:F2:71:LEU:HD13   | 2.42                     | 0.55              |
| 6:S2:106:ARG:NH1   | 8:d2:245:ASN:HA    | 2.22                     | 0.55              |
| 6:T2:102:MET:HG3   | 6:T2:106:ARG:NE    | 2.21                     | 0.55              |
| 7:V2:2:ALA:HB1     | 7:V2:126:MET:HG3   | 1.89                     | 0.55              |
| 7:Z2:43:ARG:NH2    | 7:Z2:70:SER:O      | 2.40                     | 0.55              |
| 9:m2:127:GLN:OE1   | 9:m2:135:GLN:NE2   | 2.40                     | 0.55              |
| 9:w2:238:ARG:O     | 9:w2:242:ILE:HG12  | 2.07                     | 0.55              |
| 9:22:98:LYS:O      | 9:22:212:GLY:CA    | 2.53                     | 0.55              |
| 10:D3:206:GLU:HG2  | 10:D3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:J3:72:ARG:N     | 10:J3:76:ASP:OD2   | 2.25                     | 0.55              |
| 10:J3:206:GLU:HG2  | 10:J3:208:VAL:HG13 | 1.88                     | 0.55              |
| 10:O3:167:LYS:HD3  | 10:P3:203:ALA:HB3  | 1.87                     | 0.55              |
| 10:P3:121:ARG:HA   | 10:Q3:111:ARG:HB2  | 1.88                     | 0.55              |
| 10:Q3:37:ALA:HB1   | 10:R3:74:ILE:HG22  | 1.88                     | 0.55              |
| 10:R3:72:ARG:N     | 10:R3:76:ASP:OD2   | 2.24                     | 0.55              |
| 10:R3:121:ARG:HA   | 10:S3:111:ARG:HB2  | 1.87                     | 0.55              |
| 11:j3:123:MET:H    | 11:j3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:m3:254:VAL:HG13 | 11:m3:365:ILE:HG12 | 1.89                     | 0.55              |
| 11:u3:46:ASP:HA    | 11:v3:161:ASN:ND2  | 2.20                     | 0.55              |
| 11:w3:123:MET:H    | 11:w3:138:GLN:HB2  | 1.71                     | 0.55              |
| 11:w3:164:ARG:HD2  | 11:x3:365:ILE:CG2  | 2.37                     | 0.55              |
| 1:E1:248:ARG:NH1   | 1:F1:267:THR:HG22  | 2.22                     | 0.54              |
| 1:E1:367:GLU:OE2   | 6:U2:68:THR:HG21   | 2.07                     | 0.54              |
| 1:R1:151:LYS:HZ1   | 1:R1:182:PRO:HD3   | 1.70                     | 0.54              |
| 1:X1:195:VAL:HG13  | 1:X1:210:VAL:HB    | 1.89                     | 0.54              |
| 1:f1:164:LEU:CD1   | 2:D2:152:ARG:HD2   | 2.37                     | 0.54              |
| 2:D2:123:MET:HA    | 2:D2:126:ALA:HB3   | 1.89                     | 0.54              |
| 2:E2:71:PHE:CZ     | 2:E2:236:MET:SD    | 2.98                     | 0.54              |
| 8:c2:133:SER:OG    | 8:c2:134:GLU:N     | 2.40                     | 0.54              |
| 8:d2:137:ILE:HG12  | 8:d2:143:ILE:HG12  | 1.88                     | 0.54              |
| 9:g2:152:GLY:HA3   | 9:w2:56:SER:O      | 2.08                     | 0.54              |
| 9:z2:52:PRO:HA     | 9:z2:65:GLY:H      | 1.72                     | 0.54              |
| 9:22:46:TYR:HA     | 9:22:69:GLY:HA2    | 1.88                     | 0.54              |
| 10:H3:37:ALA:HB1   | 10:I3:74:ILE:HG22  | 1.87                     | 0.54              |
| 10:N3:206:GLU:HG2  | 10:N3:208:VAL:HG13 | 1.88                     | 0.54              |
| 10:S3:57:PRO:HB2   | 10:S3:60:TYR:HE2   | 1.72                     | 0.54              |
| 11:f3:46:ASP:HA    | 11:g3:161:ASN:ND2  | 2.20                     | 0.54              |
| 11:i3:45:LEU:HD22  | 11:i3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:j3:45:LEU:HD22  | 11:j3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:v3:123:MET:H    | 11:v3:138:GLN:HB2  | 1.71                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:D1:394:LYS:HG2   | 1:D1:402:LEU:HB2   | 1.89                     | 0.54              |
| 1:F1:420:MET:HE1   | 1:F1:430:LEU:HB2   | 1.89                     | 0.54              |
| 1:H1:125:GLN:HG3   | 4:G2:67:PRO:HB3    | 1.83                     | 0.54              |
| 1:O1:147:LEU:O     | 1:O1:149:PRO:HD2   | 2.08                     | 0.54              |
| 1:U1:392:ASN:OD1   | 1:U1:393:TYR:N     | 2.40                     | 0.54              |
| 1:Z1:280:GLU:OE2   | 1:Z1:370:ARG:HD2   | 2.07                     | 0.54              |
| 1:a1:270:LEU:HD23  | 1:a1:382:ILE:HA    | 1.89                     | 0.54              |
| 1:c1:393:TYR:CE2   | 1:c1:436:PRO:HD3   | 2.42                     | 0.54              |
| 1:d1:167:ARG:N     | 2:D2:160:GLN:O     | 2.41                     | 0.54              |
| 5:M2:53:ARG:O      | 5:M2:57:GLU:HG2    | 2.06                     | 0.54              |
| 8:d2:69:GLY:N      | 8:d2:207:GLU:OE2   | 2.41                     | 0.54              |
| 8:f2:57:VAL:O      | 8:f2:57:VAL:HG12   | 2.06                     | 0.54              |
| 9:k2:95:VAL:O      | 9:k2:118:GLY:HA3   | 2.08                     | 0.54              |
| 9:l2:85:ASN:OD1    | 9:w2:47:GLN:NE2    | 2.40                     | 0.54              |
| 9:r2:86:LEU:HD12   | 9:32:44:LEU:HD13   | 1.88                     | 0.54              |
| 9:x2:95:VAL:O      | 9:x2:118:GLY:HA3   | 2.07                     | 0.54              |
| 9:z2:72:VAL:HG12   | 9:z2:72:VAL:O      | 2.08                     | 0.54              |
| 10:U3:206:GLU:HG2  | 10:U3:208:VAL:HG13 | 1.88                     | 0.54              |
| 11:g3:46:ASP:HA    | 11:h3:161:ASN:ND2  | 2.20                     | 0.54              |
| 11:g3:79:MET:HE2   | 11:h3:57:PHE:HD2   | 1.72                     | 0.54              |
| 11:h3:45:LEU:HD22  | 11:h3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:h3:123:MET:H    | 11:h3:138:GLN:HB2  | 1.71                     | 0.54              |
| 11:u3:269:THR:OG1  | 11:u3:359:ARG:HB2  | 2.07                     | 0.54              |
| 11:v3:45:LEU:HD22  | 11:v3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:v3:269:THR:OG1  | 11:v3:359:ARG:HB2  | 2.07                     | 0.54              |
| 11:x3:123:MET:H    | 11:x3:138:GLN:HB2  | 1.71                     | 0.54              |
| 12:A4:122:THR:HG21 | 12:A4:165:TRP:HB3  | 1.90                     | 0.54              |
| 12:C4:108:ILE:HD11 | 12:C4:125:PHE:HB3  | 1.89                     | 0.54              |
| 1:L1:165:PHE:O     | 2:A2:144:GLU:HG3   | 1.68                     | 0.54              |
| 1:Q1:394:LYS:HE2   | 1:Q1:402:LEU:HD22  | 1.89                     | 0.54              |
| 1:R1:125:GLN:HG3   | 2:E2:230:ASP:HB3   | 0.60                     | 0.54              |
| 1:W1:287:ASP:HB3   | 1:W1:290:LYS:HG2   | 1.88                     | 0.54              |
| 1:X1:138:GLY:O     | 1:X1:142:ARG:HG2   | 2.06                     | 0.54              |
| 1:b1:367:GLU:HG3   | 1:c1:368:VAL:HG11  | 1.89                     | 0.54              |
| 1:c1:191:ILE:HD13  | 1:c1:220:LEU:HB3   | 1.89                     | 0.54              |
| 2:B2:62:THR:HB     | 2:B2:101:MET:SD    | 2.48                     | 0.54              |
| 9:i2:6:TRP:CZ3     | 9:i2:9:LYS:CE      | 2.89                     | 0.54              |
| 9:i2:6:TRP:CE3     | 9:i2:9:LYS:HD3     | 2.43                     | 0.54              |
| 9:k2:23:ALA:HB3    | 9:p2:7:ILE:HD11    | 1.89                     | 0.54              |
| 9:22:3:SER:O       | 9:22:7:ILE:HG13    | 2.07                     | 0.54              |
| 9:22:241:GLU:OE2   | 12:A4:52:PRO:HB2   | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A3:167:LYS:HD3  | 10:B3:203:ALA:HB3  | 1.88                     | 0.54              |
| 10:I3:57:PRO:HB2   | 10:I3:60:TYR:HE2   | 1.72                     | 0.54              |
| 10:N3:70:ARG:NH2   | 11:m3:72:THR:OG1   | 2.39                     | 0.54              |
| 10:O3:37:ALA:HB1   | 10:P3:74:ILE:HG22  | 1.87                     | 0.54              |
| 10:O3:109:VAL:HG21 | 10:O3:117:PHE:O    | 2.08                     | 0.54              |
| 10:R3:37:ALA:HB1   | 10:S3:74:ILE:HG22  | 1.89                     | 0.54              |
| 11:c3:254:VAL:HG13 | 11:c3:365:ILE:HG12 | 1.89                     | 0.54              |
| 11:k3:45:LEU:HD22  | 11:k3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:k3:254:VAL:HG13 | 11:k3:365:ILE:HG12 | 1.89                     | 0.54              |
| 11:m3:46:ASP:HA    | 11:n3:161:ASN:ND2  | 2.20                     | 0.54              |
| 11:m3:164:ARG:HD2  | 11:n3:365:ILE:CG2  | 2.38                     | 0.54              |
| 11:n3:164:ARG:HD2  | 11:o3:365:ILE:CG2  | 2.38                     | 0.54              |
| 12:A4:157:ARG:HD3  | 12:A4:161:HIS:CE1  | 2.41                     | 0.54              |
| 12:B4:217:LEU:HB2  | 12:B4:220:TYR:HB2  | 1.89                     | 0.54              |
| 1:M1:404:LEU:HD23  | 1:M1:434:ASN:HD21  | 1.73                     | 0.54              |
| 1:Y1:177:THR:HG22  | 1:Y1:213:VAL:HB    | 1.89                     | 0.54              |
| 1:d1:165:PHE:CE2   | 2:D2:144:GLU:CA    | 2.41                     | 0.54              |
| 2:D2:100:ILE:HG21  | 2:D2:243:PHE:CD2   | 2.42                     | 0.54              |
| 2:E2:99:PHE:CE2    | 3:F2:170:MET:HE2   | 2.42                     | 0.54              |
| 6:T2:37:GLY:N      | 6:T2:96:ASP:O      | 2.41                     | 0.54              |
| 6:U2:93:PRO:O      | 8:f2:54:ARG:NH1    | 2.40                     | 0.54              |
| 8:d2:175:ASP:HA    | 9:i2:46:TYR:HB2    | 1.89                     | 0.54              |
| 9:n2:98:LYS:HD2    | 9:n2:213:LEU:HD12  | 1.89                     | 0.54              |
| 10:D3:70:ARG:NH2   | 11:c3:72:THR:OG1   | 2.38                     | 0.54              |
| 10:E3:37:ALA:HB1   | 10:F3:74:ILE:HG22  | 1.88                     | 0.54              |
| 10:E3:206:GLU:HG2  | 10:E3:208:VAL:HG13 | 1.88                     | 0.54              |
| 10:N3:109:VAL:HG21 | 10:N3:117:PHE:O    | 2.08                     | 0.54              |
| 10:P3:109:VAL:HG21 | 10:P3:117:PHE:O    | 2.08                     | 0.54              |
| 10:V3:70:ARG:NH2   | 11:u3:72:THR:OG1   | 2.38                     | 0.54              |
| 10:W3:166:GLU:OE2  | 10:W3:168:GLN:NE2  | 2.27                     | 0.54              |
| 11:a3:196:MET:HA   | 11:a3:196:MET:CE   | 2.34                     | 0.54              |
| 11:a3:353:GLN:HG3  | 11:a3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:d3:45:LEU:HD22  | 11:d3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:e3:79:MET:HE2   | 11:f3:57:PHE:HD2   | 1.71                     | 0.54              |
| 11:e3:228:GLY:O    | 11:e3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:f3:142:LEU:HD23 | 11:h3:350:GLN:NE2  | 2.22                     | 0.54              |
| 11:f3:284:VAL:HG21 | 11:f3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:i3:254:VAL:HG13 | 11:i3:365:ILE:HG12 | 1.89                     | 0.54              |
| 11:m3:45:LEU:HD22  | 11:m3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:u3:142:LEU:HD23 | 11:w3:350:GLN:NE2  | 2.23                     | 0.54              |
| 11:y3:284:VAL:HG21 | 11:y3:316:GLY:HA2  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B1:375:THR:HG23  | 1:C1:275:LYS:HE3   | 1.88                     | 0.54              |
| 1:Q1:216:SER:O     | 1:Q1:218:HIS:ND1   | 2.40                     | 0.54              |
| 1:Z1:283:SER:HB2   | 1:Z1:369:ASP:HB2   | 1.89                     | 0.54              |
| 1:b1:413:GLU:OE1   | 1:b1:417:ARG:NH1   | 2.20                     | 0.54              |
| 1:d1:373:ARG:HH22  | 1:e1:277:GLN:HG2   | 1.72                     | 0.54              |
| 2:C2:225:LEU:HD21  | 4:I2:77:VAL:HG21   | 1.89                     | 0.54              |
| 5:P2:56:ALA:O      | 5:P2:60:THR:HG22   | 2.06                     | 0.54              |
| 6:S2:40:ALA:HB2    | 6:S2:100:VAL:HG22  | 1.90                     | 0.54              |
| 8:f2:98:GLY:HA3    | 8:f2:178:LEU:HD23  | 1.90                     | 0.54              |
| 9:m2:235:GLN:HG3   | 9:s2:5:LEU:HD23    | 1.90                     | 0.54              |
| 9:w2:238:ARG:HH21  | 9:32:255:GLN:HE22  | 1.54                     | 0.54              |
| 10:F3:109:VAL:HG21 | 10:F3:117:PHE:O    | 2.08                     | 0.54              |
| 10:G3:109:VAL:HG21 | 10:G3:117:PHE:O    | 2.08                     | 0.54              |
| 10:M3:37:ALA:HB1   | 10:N3:74:ILE:HG22  | 1.88                     | 0.54              |
| 10:P3:206:GLU:HG2  | 10:P3:208:VAL:HG13 | 1.88                     | 0.54              |
| 10:T3:57:PRO:HB2   | 10:T3:60:TYR:HE2   | 1.72                     | 0.54              |
| 11:c3:269:THR:OG1  | 11:c3:359:ARG:HB2  | 2.06                     | 0.54              |
| 11:d3:46:ASP:HA    | 11:e3:161:ASN:ND2  | 2.20                     | 0.54              |
| 11:e3:164:ARG:HD2  | 11:f3:365:ILE:CG2  | 2.37                     | 0.54              |
| 11:g3:45:LEU:HD22  | 11:g3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:h3:228:GLY:O    | 11:h3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:r3:254:VAL:HG13 | 11:r3:365:ILE:HG12 | 1.89                     | 0.54              |
| 11:s3:269:THR:OG1  | 11:s3:359:ARG:HB2  | 2.07                     | 0.54              |
| 11:x3:269:THR:OG1  | 11:x3:359:ARG:HB2  | 2.06                     | 0.54              |
| 11:y3:269:THR:OG1  | 11:y3:359:ARG:HB2  | 2.06                     | 0.54              |
| 1:E1:252:ILE:O     | 1:E1:255:PRO:HD2   | 2.08                     | 0.54              |
| 1:H1:199:SER:HA    | 1:H1:205:LEU:HD22  | 1.89                     | 0.54              |
| 1:I1:181:GLU:OE1   | 1:I1:184:ARG:NH2   | 2.41                     | 0.54              |
| 1:I1:200:SER:OG    | 1:K1:173:SER:OG    | 2.21                     | 0.54              |
| 1:V1:417:ARG:HA    | 1:V1:420:MET:HE2   | 1.89                     | 0.54              |
| 1:X1:404:LEU:H     | 1:X1:434:ASN:ND2   | 2.05                     | 0.54              |
| 1:b1:234:GLN:HB2   | 1:b1:272:PHE:CZ    | 2.42                     | 0.54              |
| 2:D2:135:ARG:HG2   | 2:D2:167:MET:HE2   | 1.89                     | 0.54              |
| 2:E2:40:LEU:HD13   | 3:F2:66:PHE:CE2    | 2.43                     | 0.54              |
| 7:W2:76:LEU:N      | 9:h2:47:GLN:HE22   | 2.04                     | 0.54              |
| 7:a2:38:ASP:N      | 7:a2:38:ASP:OD1    | 2.39                     | 0.54              |
| 8:f2:71:LEU:HD21   | 9:q2:45:LEU:HD23   | 1.89                     | 0.54              |
| 9:l2:18:ASN:O      | 9:l2:22:ILE:HG12   | 2.07                     | 0.54              |
| 10:E3:109:VAL:HG21 | 10:E3:117:PHE:O    | 2.08                     | 0.54              |
| 10:L3:166:GLU:OE2  | 10:L3:168:GLN:NE2  | 2.27                     | 0.54              |
| 10:T3:206:GLU:HG2  | 10:T3:208:VAL:HG13 | 1.88                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:X3:131:SER:OG   | 10:Y3:101:LYS:HG2  | 2.06                     | 0.54              |
| 11:b3:228:GLY:O    | 11:b3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:b3:353:GLN:HG3  | 11:b3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:c3:45:LEU:HD22  | 11:c3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:c3:284:VAL:HG21 | 11:c3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:h3:46:ASP:HA    | 11:i3:161:ASN:ND2  | 2.20                     | 0.54              |
| 11:j3:80:GLN:HB3   | 11:k3:54:GLN:HB3   | 1.90                     | 0.54              |
| 11:j3:269:THR:OG1  | 11:j3:359:ARG:HB2  | 2.07                     | 0.54              |
| 11:l3:45:LEU:HD22  | 11:l3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:o3:196:MET:HA   | 11:o3:196:MET:CE   | 2.34                     | 0.54              |
| 11:q3:123:MET:H    | 11:q3:138:GLN:HB2  | 1.72                     | 0.54              |
| 11:s3:196:MET:HA   | 11:s3:196:MET:CE   | 2.34                     | 0.54              |
| 11:u3:284:VAL:HG21 | 11:u3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:v3:284:VAL:HG21 | 11:v3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:w3:245:ASN:OD1  | 11:w3:245:ASN:N    | 2.33                     | 0.54              |
| 11:w3:269:THR:OG1  | 11:w3:359:ARG:HB2  | 2.06                     | 0.54              |
| 11:x3:353:GLN:HG3  | 11:x3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:y3:164:ARG:NH1  | 11:z3:365:ILE:HG23 | 2.22                     | 0.54              |
| 1:A1:424:ASP:OD2   | 1:A1:425:LYS:N     | 2.40                     | 0.54              |
| 1:I1:163:SER:N     | 1:I1:169:GLN:HE22  | 2.06                     | 0.54              |
| 1:K1:234:GLN:OE1   | 1:K1:234:GLN:N     | 2.39                     | 0.54              |
| 1:R1:143:THR:HG21  | 1:T1:156:HIS:CE1   | 2.26                     | 0.54              |
| 1:T1:153:ALA:HA    | 1:T1:177:THR:O     | 2.08                     | 0.54              |
| 1:U1:165:PHE:HE2   | 2:E2:244:TYR:HE2   | 1.54                     | 0.54              |
| 1:X1:133:GLN:O     | 1:X1:137:GLU:HG2   | 2.07                     | 0.54              |
| 1:Y1:417:ARG:HA    | 1:Y1:420:MET:SD    | 2.47                     | 0.54              |
| 1:e1:394:LYS:HG2   | 1:e1:402:LEU:HB2   | 1.88                     | 0.54              |
| 2:B2:125:GLU:H     | 2:B2:125:GLU:CD    | 2.16                     | 0.54              |
| 2:C2:236:MET:HE1   | 2:D2:150:PHE:CZ    | 2.40                     | 0.54              |
| 6:R2:88:ARG:NH1    | 6:R2:105:GLU:OE2   | 2.40                     | 0.54              |
| 8:b2:136:THR:OG1   | 8:b2:144:SER:OG    | 2.24                     | 0.54              |
| 8:c2:175:ASP:HA    | 9:h2:46:TYR:HB2    | 1.90                     | 0.54              |
| 9:w2:238:ARG:HD2   | 9:32:254:LEU:HB3   | 1.89                     | 0.54              |
| 10:A3:111:ARG:HB2  | 10:Z3:121:ARG:HA   | 1.88                     | 0.54              |
| 10:C3:109:VAL:HG21 | 10:C3:117:PHE:O    | 2.08                     | 0.54              |
| 10:F3:206:GLU:HG2  | 10:F3:208:VAL:HG13 | 1.88                     | 0.54              |
| 10:H3:50:SER:HB3   | 11:i3:99:GLN:NE2   | 2.23                     | 0.54              |
| 10:J3:109:VAL:HG21 | 10:J3:117:PHE:O    | 2.08                     | 0.54              |
| 10:M3:109:VAL:HG21 | 10:M3:117:PHE:O    | 2.08                     | 0.54              |
| 10:Q3:109:VAL:HG21 | 10:Q3:117:PHE:O    | 2.08                     | 0.54              |
| 10:Y3:37:ALA:HB1   | 10:Z3:74:ILE:HG22  | 1.88                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:b3:45:LEU:HD22  | 11:b3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:c3:123:MET:H    | 11:c3:138:GLN:HB2  | 1.72                     | 0.54              |
| 11:c3:164:ARG:HD2  | 11:d3:365:ILE:CG2  | 2.37                     | 0.54              |
| 11:c3:228:GLY:O    | 11:c3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:f3:45:LEU:HD22  | 11:f3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:g3:284:VAL:HG21 | 11:g3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:i3:228:GLY:O    | 11:i3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:k3:284:VAL:HG21 | 11:k3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:o3:164:ARG:HD2  | 11:p3:365:ILE:CG2  | 2.37                     | 0.54              |
| 11:o3:254:VAL:HG13 | 11:o3:365:ILE:HG12 | 1.89                     | 0.54              |
| 11:r3:80:GLN:HB3   | 11:s3:54:GLN:HB3   | 1.90                     | 0.54              |
| 11:t3:164:ARG:HD2  | 11:u3:365:ILE:CG2  | 2.38                     | 0.54              |
| 11:t3:269:THR:OG1  | 11:t3:359:ARG:HB2  | 2.06                     | 0.54              |
| 12:C4:157:ARG:HG3  | 12:C4:161:HIS:HE1  | 1.73                     | 0.54              |
| 1:B1:198:VAL:HG13  | 1:B1:210:VAL:HG11  | 1.90                     | 0.54              |
| 1:H1:257:VAL:O     | 1:H1:261:ASN:ND2   | 2.30                     | 0.54              |
| 1:I1:275:LYS:HB3   | 1:I1:377:MET:HE2   | 1.90                     | 0.54              |
| 1:N1:214:ASP:OD2   | 1:N1:216:SER:N     | 2.40                     | 0.54              |
| 1:Q1:394:LYS:HE3   | 1:Q1:402:LEU:HD13  | 1.88                     | 0.54              |
| 1:U1:159:MET:HE2   | 1:U1:172:PRO:HB2   | 1.90                     | 0.54              |
| 1:V1:411:GLN:O     | 1:V1:415:LEU:HD23  | 2.07                     | 0.54              |
| 1:c1:374:HIS:HB3   | 1:d1:276:GLU:HB3   | 1.90                     | 0.54              |
| 1:c1:394:LYS:HG2   | 1:c1:402:LEU:HB2   | 1.90                     | 0.54              |
| 1:f1:375:THR:HG23  | 1:g1:275:LYS:NZ    | 2.23                     | 0.54              |
| 7:Z2:22:ASN:OD1    | 8:e2:4:ALA:HB2     | 2.08                     | 0.54              |
| 7:Z2:77:VAL:HB     | 9:k2:6:TRP:NE1     | 2.22                     | 0.54              |
| 9:r2:184:LEU:HB3   | 9:r2:192:TYR:HB3   | 1.89                     | 0.54              |
| 9:t2:184:LEU:HB3   | 9:t2:192:TYR:HB3   | 1.90                     | 0.54              |
| 9:x2:46:TYR:HA     | 9:x2:69:GLY:HA2    | 1.90                     | 0.54              |
| 9:42:184:LEU:HB3   | 9:42:192:TYR:HB3   | 1.89                     | 0.54              |
| 10:A3:37:ALA:HB1   | 10:B3:74:ILE:HG22  | 1.89                     | 0.54              |
| 10:D3:109:VAL:HG21 | 10:D3:117:PHE:O    | 2.08                     | 0.54              |
| 10:H3:57:PRO:HB2   | 10:H3:60:TYR:HE2   | 1.72                     | 0.54              |
| 10:H3:109:VAL:HG21 | 10:H3:117:PHE:O    | 2.08                     | 0.54              |
| 10:H3:206:GLU:HG2  | 10:H3:208:VAL:HG13 | 1.88                     | 0.54              |
| 10:L3:37:ALA:HB1   | 10:M3:74:ILE:HG22  | 1.87                     | 0.54              |
| 10:R3:206:GLU:HG2  | 10:R3:208:VAL:HG13 | 1.88                     | 0.54              |
| 10:S3:109:VAL:HG21 | 10:S3:117:PHE:O    | 2.08                     | 0.54              |
| 10:U3:57:PRO:HB2   | 10:U3:60:TYR:HE2   | 1.72                     | 0.54              |
| 11:a3:228:GLY:O    | 11:a3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:b3:123:MET:H    | 11:b3:138:GLN:HB2  | 1.72                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:c3:79:MET:HE2   | 11:d3:57:PHE:HD2   | 1.71                     | 0.54              |
| 11:c3:353:GLN:HG3  | 11:c3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:j3:228:GLY:O    | 11:j3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:j3:284:VAL:HG21 | 11:j3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:k3:123:MET:H    | 11:k3:138:GLN:HB2  | 1.72                     | 0.54              |
| 11:q3:164:ARG:HD2  | 11:r3:365:ILE:CG2  | 2.37                     | 0.54              |
| 11:r3:123:MET:H    | 11:r3:138:GLN:HB2  | 1.72                     | 0.54              |
| 11:w3:45:LEU:HD22  | 11:w3:116:LEU:HA   | 1.88                     | 0.54              |
| 12:C4:133:ALA:HB2  | 12:C4:193:LEU:HD12 | 1.89                     | 0.54              |
| 12:E4:141:THR:HG22 | 12:E4:147:VAL:HA   | 1.89                     | 0.54              |
| 1:J1:378:ASN:ND2   | 1:J1:381:ASP:OD1   | 2.35                     | 0.54              |
| 1:U1:248:ARG:NH1   | 1:V1:267:THR:HG22  | 2.22                     | 0.54              |
| 1:V1:410:LYS:NZ    | 1:V1:414:ASP:OD2   | 2.40                     | 0.54              |
| 1:Z1:372:ILE:O     | 1:a1:277:GLN:HA    | 2.07                     | 0.54              |
| 1:a1:404:LEU:H     | 1:a1:434:ASN:ND2   | 2.06                     | 0.54              |
| 1:f1:165:PHE:CD1   | 2:D2:148:ALA:HB1   | 2.43                     | 0.54              |
| 2:A2:213:PRO:HA    | 3:F2:120:LEU:HD13  | 1.90                     | 0.54              |
| 2:C2:93:ALA:O      | 2:C2:97:THR:HG23   | 2.08                     | 0.54              |
| 8:e2:35:ARG:O      | 8:e2:173:ARG:NH2   | 2.41                     | 0.54              |
| 8:e2:72:ASP:OD2    | 9:p2:9:LYS:NZ      | 2.28                     | 0.54              |
| 8:f2:117:GLY:O     | 8:f2:118:HIS:CD2   | 2.61                     | 0.54              |
| 9:g2:94:ASP:OD1    | 9:g2:95:VAL:N      | 2.41                     | 0.54              |
| 9:t2:57:SER:N      | 9:t2:60:THR:OG1    | 2.35                     | 0.54              |
| 9:y2:10:THR:OG1    | 9:y2:71:GLY:HA2    | 2.08                     | 0.54              |
| 9:y2:143:PRO:HD2   | 9:y2:159:VAL:HG11  | 1.89                     | 0.54              |
| 9:z2:33:GLY:N      | 9:z2:220:GLU:O     | 2.39                     | 0.54              |
| 9:42:72:VAL:HG12   | 9:42:72:VAL:O      | 2.07                     | 0.54              |
| 10:M3:72:ARG:N     | 10:M3:76:ASP:OD2   | 2.24                     | 0.54              |
| 10:N3:50:SER:HB3   | 11:o3:99:GLN:NE2   | 2.23                     | 0.54              |
| 10:W3:50:SER:HB3   | 11:x3:99:GLN:NE2   | 2.22                     | 0.54              |
| 11:b3:254:VAL:HG13 | 11:b3:365:ILE:HG12 | 1.90                     | 0.54              |
| 11:b3:284:VAL:HG21 | 11:b3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:i3:142:LEU:HD23 | 11:k3:350:GLN:NE2  | 2.23                     | 0.54              |
| 11:i3:164:ARG:HD2  | 11:j3:365:ILE:CG2  | 2.37                     | 0.54              |
| 11:i3:284:VAL:HG21 | 11:i3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:j3:46:ASP:HA    | 11:k3:161:ASN:ND2  | 2.20                     | 0.54              |
| 11:k3:228:GLY:O    | 11:k3:232:GLN:HG3  | 2.08                     | 0.54              |
| 11:t3:284:VAL:HG21 | 11:t3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:v3:353:GLN:HG3  | 11:v3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:w3:353:GLN:HG3  | 11:w3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:z3:284:VAL:HG21 | 11:z3:316:GLY:HA2  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:z3:353:GLN:HG3  | 11:z3:362:LEU:HD22 | 1.90                     | 0.54              |
| 12:D4:56:ASN:O     | 12:D4:56:ASN:ND2   | 2.40                     | 0.54              |
| 1:A1:266:VAL:HG22  | 1:A1:387:VAL:HG22  | 1.89                     | 0.54              |
| 1:K1:197:LEU:HD12  | 1:L1:175:SER:HB2   | 1.89                     | 0.54              |
| 1:Q1:407:ASP:HA    | 1:Q1:410:LYS:HG3   | 1.89                     | 0.54              |
| 1:R1:164:LEU:HD13  | 3:F2:174:ARG:HD2   | 1.86                     | 0.54              |
| 1:V1:287:ASP:HB2   | 1:V1:290:LYS:HZ3   | 1.71                     | 0.54              |
| 1:Y1:181:GLU:HB3   | 1:Y1:184:ARG:NH2   | 2.23                     | 0.54              |
| 1:g1:283:SER:HB2   | 1:g1:369:ASP:HB2   | 1.90                     | 0.54              |
| 7:W2:75:LYS:HA     | 9:h2:47:GLN:HE22   | 1.72                     | 0.54              |
| 7:X2:19:LYS:HD3    | 7:X2:64:VAL:HG11   | 1.89                     | 0.54              |
| 8:e2:117:GLY:O     | 8:e2:118:HIS:CD2   | 2.61                     | 0.54              |
| 9:r2:209:ASN:OD1   | 11:n3:53:THR:OG1   | 2.24                     | 0.54              |
| 9:t2:203:GLU:H     | 11:w3:54:GLN:NE2   | 2.05                     | 0.54              |
| 10:C3:50:SER:HB3   | 11:d3:99:GLN:NE2   | 2.23                     | 0.54              |
| 10:I3:109:VAL:HG21 | 10:I3:117:PHE:O    | 2.08                     | 0.54              |
| 10:L3:70:ARG:NH2   | 11:k3:72:THR:OG1   | 2.37                     | 0.54              |
| 10:L3:109:VAL:HG21 | 10:L3:117:PHE:O    | 2.08                     | 0.54              |
| 10:T3:101:LYS:HB2  | 10:T3:101:LYS:HZ3  | 1.73                     | 0.54              |
| 11:b3:164:ARG:HD2  | 11:c3:365:ILE:CG2  | 2.38                     | 0.54              |
| 11:d3:353:GLN:HG3  | 11:d3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:e3:45:LEU:HD22  | 11:e3:116:LEU:HA   | 1.88                     | 0.54              |
| 11:e3:353:GLN:HG3  | 11:e3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:f3:80:GLN:HB3   | 11:g3:54:GLN:HB3   | 1.90                     | 0.54              |
| 11:g3:164:ARG:HD2  | 11:h3:365:ILE:CG2  | 2.38                     | 0.54              |
| 11:h3:254:VAL:HG13 | 11:h3:365:ILE:HG12 | 1.89                     | 0.54              |
| 11:j3:196:MET:HA   | 11:j3:196:MET:CE   | 2.34                     | 0.54              |
| 11:p3:164:ARG:HD2  | 11:q3:365:ILE:CG2  | 2.38                     | 0.54              |
| 11:p3:284:VAL:HG21 | 11:p3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:s3:164:ARG:HD2  | 11:t3:365:ILE:CG2  | 2.38                     | 0.54              |
| 11:v3:80:GLN:HB3   | 11:w3:54:GLN:HB3   | 1.90                     | 0.54              |
| 11:x3:284:VAL:HG21 | 11:x3:316:GLY:HA2  | 1.90                     | 0.54              |
| 11:y3:353:GLN:HG3  | 11:y3:362:LEU:HD22 | 1.90                     | 0.54              |
| 11:z3:228:GLY:O    | 11:z3:232:GLN:HG3  | 2.08                     | 0.54              |
| 1:B1:156:HIS:CD2   | 1:h1:143:THR:HG21  | 2.43                     | 0.53              |
| 1:B1:167:ARG:HD3   | 2:C2:160:GLN:CD    | 2.33                     | 0.53              |
| 1:G1:279:GLU:OE2   | 1:G1:281:HIS:HB2   | 2.08                     | 0.53              |
| 1:H1:276:GLU:OE2   | 1:H1:374:HIS:NE2   | 2.34                     | 0.53              |
| 1:K1:212:LEU:HG    | 1:K1:220:LEU:HD12  | 1.89                     | 0.53              |
| 1:R1:137:GLU:OE2   | 1:R1:157:LEU:N     | 2.31                     | 0.53              |
| 1:T1:165:PHE:CB    | 3:F2:166:SER:CB    | 2.82                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:g1:194:VAL:HG21  | 1:g1:212:LEU:HD22  | 1.90                     | 0.53              |
| 2:E2:121:ILE:HG12  | 2:E2:125:GLU:HG3   | 1.90                     | 0.53              |
| 8:e2:87:TRP:NE1    | 8:e2:166:ALA:O     | 2.40                     | 0.53              |
| 9:h2:156:VAL:HG13  | 9:h2:169:GLN:HG3   | 1.91                     | 0.53              |
| 9:l2:98:LYS:HD2    | 9:w2:45:LEU:HD21   | 1.90                     | 0.53              |
| 9:y2:238:ARG:HH21  | 12:D4:52:PRO:CB    | 2.21                     | 0.53              |
| 9:22:105:VAL:CG1   | 9:22:134:PHE:HB3   | 2.38                     | 0.53              |
| 10:V3:166:GLU:OE2  | 10:V3:168:GLN:NE2  | 2.27                     | 0.53              |
| 10:W3:70:ARG:NH2   | 11:v3:72:THR:OG1   | 2.37                     | 0.53              |
| 11:a3:164:ARG:HD2  | 11:b3:365:ILE:CG2  | 2.38                     | 0.53              |
| 11:d3:228:GLY:O    | 11:d3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:d3:254:VAL:HG13 | 11:d3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:e3:284:VAL:HG21 | 11:e3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:f3:353:GLN:HG3  | 11:f3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:g3:114:LYS:O    | 11:g3:160:LEU:HD13 | 2.08                     | 0.53              |
| 11:n3:269:THR:OG1  | 11:n3:359:ARG:HB2  | 2.07                     | 0.53              |
| 11:o3:284:VAL:HG21 | 11:o3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:q3:254:VAL:HG13 | 11:q3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:r3:269:THR:OG1  | 11:r3:359:ARG:HB2  | 2.07                     | 0.53              |
| 12:C4:100:GLY:N    | 12:C4:232:ILE:OXT  | 2.36                     | 0.53              |
| 1:S1:411:GLN:O     | 1:S1:415:LEU:HD23  | 2.08                     | 0.53              |
| 1:T1:140:LEU:O     | 1:U1:154:ARG:NH1   | 2.41                     | 0.53              |
| 1:V1:245:ILE:HG23  | 1:V1:266:VAL:HG21  | 1.89                     | 0.53              |
| 1:X1:139:GLU:HG3   | 1:Y1:156:HIS:HE1   | 1.73                     | 0.53              |
| 1:X1:142:ARG:HB2   | 1:Y1:154:ARG:NH1   | 2.22                     | 0.53              |
| 1:X1:297:GLN:HB3   | 1:X1:363:THR:HB    | 1.89                     | 0.53              |
| 1:Z1:245:ILE:HG23  | 1:Z1:266:VAL:HG21  | 1.89                     | 0.53              |
| 1:a1:182:PRO:O     | 1:a1:184:ARG:NH1   | 2.41                     | 0.53              |
| 1:d1:405:THR:OG1   | 1:d1:407:ASP:OD1   | 2.23                     | 0.53              |
| 1:e1:392:ASN:OD1   | 1:e1:393:TYR:N     | 2.36                     | 0.53              |
| 1:f1:155:VAL:HG23  | 1:f1:176:VAL:HG22  | 1.90                     | 0.53              |
| 1:h1:182:PRO:O     | 1:h1:184:ARG:NH1   | 2.42                     | 0.53              |
| 2:C2:87:GLN:HB3    | 2:D2:60:MET:HG3    | 1.90                     | 0.53              |
| 8:b2:73:TYR:CE1    | 9:m2:73:ARG:HG3    | 2.43                     | 0.53              |
| 8:e2:89:VAL:HG13   | 8:e2:97:GLU:HB3    | 1.90                     | 0.53              |
| 9:h2:28:ASN:ND2    | 9:m2:43:ASP:HB3    | 2.24                     | 0.53              |
| 9:m2:27:ALA:C      | 9:r2:72:VAL:HG21   | 2.32                     | 0.53              |
| 9:o2:161:GLN:HE22  | 11:s3:80:GLN:NE2   | 2.02                     | 0.53              |
| 9:42:35:LYS:NZ     | 9:42:82:SER:O      | 2.39                     | 0.53              |
| 10:D3:50:SER:HB3   | 11:e3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:E3:101:LYS:HZ3  | 10:E3:101:LYS:HB2  | 1.73                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:I3:50:SER:HB3   | 11:j3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:O3:70:ARG:NH2   | 11:n3:72:THR:OG1   | 2.38                     | 0.53              |
| 10:T3:50:SER:HB3   | 11:u3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:T3:109:VAL:HG21 | 10:T3:117:PHE:O    | 2.08                     | 0.53              |
| 10:Y3:51:ILE:CG1   | 11:a3:175:LEU:HD11 | 2.36                     | 0.53              |
| 10:Z3:109:VAL:HG21 | 10:Z3:117:PHE:O    | 2.08                     | 0.53              |
| 11:a3:45:LEU:HD22  | 11:a3:116:LEU:HA   | 1.88                     | 0.53              |
| 11:a3:79:MET:HE2   | 11:b3:57:PHE:HD2   | 1.73                     | 0.53              |
| 11:d3:80:GLN:HB3   | 11:e3:54:GLN:HB3   | 1.90                     | 0.53              |
| 11:d3:114:LYS:O    | 11:d3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:e3:254:VAL:HG13 | 11:e3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:g3:196:MET:HA   | 11:g3:196:MET:CE   | 2.34                     | 0.53              |
| 11:i3:46:ASP:HA    | 11:j3:161:ASN:ND2  | 2.21                     | 0.53              |
| 11:l3:228:GLY:O    | 11:l3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:n3:46:ASP:HA    | 11:o3:161:ASN:ND2  | 2.21                     | 0.53              |
| 11:o3:142:LEU:HD23 | 11:q3:350:GLN:NE2  | 2.23                     | 0.53              |
| 11:s3:254:VAL:HG13 | 11:s3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:x3:114:LYS:O    | 11:x3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:y3:228:GLY:O    | 11:y3:232:GLN:HG3  | 2.08                     | 0.53              |
| 12:D4:59:THR:HG22  | 12:E4:39:LEU:HD23  | 1.90                     | 0.53              |
| 12:E4:93:ALA:HA    | 12:E4:206:VAL:HG11 | 1.90                     | 0.53              |
| 1:B1:234:GLN:HB3   | 1:B1:272:PHE:CE1   | 2.43                     | 0.53              |
| 1:D1:392:ASN:OD1   | 1:D1:393:TYR:N     | 2.37                     | 0.53              |
| 1:L1:188:GLU:HA    | 1:L1:191:ILE:HD12  | 1.90                     | 0.53              |
| 1:S1:392:ASN:OD1   | 1:S1:393:TYR:N     | 2.42                     | 0.53              |
| 1:U1:161:LYS:NZ    | 2:E2:245:SER:C     | 2.65                     | 0.53              |
| 1:W1:189:GLY:O     | 1:W1:192:SER:OG    | 2.23                     | 0.53              |
| 1:Z1:297:GLN:HB2   | 6:S2:65:LEU:CD2    | 2.37                     | 0.53              |
| 1:Z1:304:VAL:HG22  | 1:Z1:356:ARG:HG2   | 1.90                     | 0.53              |
| 1:a1:165:PHE:HE1   | 2:E2:152:ARG:HB3   | 1.72                     | 0.53              |
| 1:a1:199:SER:HA    | 1:a1:205:LEU:HD23  | 1.89                     | 0.53              |
| 1:g1:301:SER:HB3   | 1:g1:359:GLN:HB2   | 1.90                     | 0.53              |
| 9:i2:2:ILE:HD11    | 9:i2:250:THR:HG23  | 1.89                     | 0.53              |
| 10:A3:203:ALA:HB3  | 10:Z3:167:LYS:HD3  | 1.89                     | 0.53              |
| 10:B3:69:ARG:HG3   | 10:B3:69:ARG:O     | 2.09                     | 0.53              |
| 10:B3:101:LYS:HZ3  | 10:B3:101:LYS:HB2  | 1.72                     | 0.53              |
| 10:Y3:69:ARG:HG3   | 10:Y3:69:ARG:O     | 2.09                     | 0.53              |
| 11:a3:245:ASN:OD1  | 11:a3:245:ASN:N    | 2.33                     | 0.53              |
| 11:f3:228:GLY:O    | 11:f3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:g3:228:GLY:O    | 11:g3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:g3:353:GLN:HG3  | 11:g3:362:LEU:HD22 | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:h3:164:ARG:HD2  | 11:i3:365:ILE:CG2  | 2.38                     | 0.53              |
| 11:l3:254:VAL:HG13 | 11:l3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:q3:284:VAL:HG21 | 11:q3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:r3:114:LYS:O    | 11:r3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:u3:114:LYS:O    | 11:u3:160:LEU:HD13 | 2.09                     | 0.53              |
| 12:C4:48:ASP:OD1   | 12:C4:50:THR:OG1   | 2.26                     | 0.53              |
| 1:A1:404:LEU:H     | 1:A1:434:ASN:ND2   | 2.07                     | 0.53              |
| 1:E1:155:VAL:HG23  | 1:E1:176:VAL:HG22  | 1.89                     | 0.53              |
| 1:N1:145:GLU:OE2   | 1:N1:153:ALA:N     | 2.40                     | 0.53              |
| 1:Q1:416:THR:OG1   | 1:Q1:430:LEU:HD21  | 2.09                     | 0.53              |
| 1:R1:147:LEU:HG    | 1:T1:216:SER:HA    | 1.90                     | 0.53              |
| 1:U1:389:VAL:HB    | 1:U1:432:VAL:HG13  | 1.90                     | 0.53              |
| 1:c1:141:ALA:O     | 1:c1:145:GLU:HG2   | 2.09                     | 0.53              |
| 1:h1:231:ASN:O     | 1:h1:234:GLN:NE2   | 2.39                     | 0.53              |
| 2:A2:119:GLN:HE22  | 2:A2:120:LYS:NZ    | 2.06                     | 0.53              |
| 2:E2:223:LEU:HD11  | 3:F2:101:PHE:CD2   | 2.43                     | 0.53              |
| 5:P2:30:SER:OG     | 5:P2:31:THR:N      | 2.41                     | 0.53              |
| 5:P2:84:MET:HE2    | 5:P2:84:MET:HA     | 1.90                     | 0.53              |
| 6:Q2:49:LEU:O      | 6:Q2:53:MET:HG2    | 2.09                     | 0.53              |
| 6:U2:92:GLN:HE21   | 7:a2:19:LYS:CG     | 2.20                     | 0.53              |
| 7:X2:28:LEU:HD13   | 7:X2:101:GLU:HB2   | 1.91                     | 0.53              |
| 9:j2:184:LEU:HB3   | 9:j2:192:TYR:HB3   | 1.90                     | 0.53              |
| 9:m2:151:ILE:HG12  | 9:m2:157:VAL:HG23  | 1.90                     | 0.53              |
| 9:p2:19:MET:HB2    | 9:p2:236:VAL:HG11  | 1.89                     | 0.53              |
| 9:p2:143:PRO:HA    | 11:b3:78:ASN:HD21  | 1.74                     | 0.53              |
| 9:q2:162:GLN:NE2   | 9:v2:207:GLY:O     | 2.40                     | 0.53              |
| 9:s2:98:LYS:HB3    | 9:s2:213:LEU:HB2   | 1.90                     | 0.53              |
| 9:22:72:VAL:O      | 9:22:72:VAL:HG12   | 2.08                     | 0.53              |
| 9:42:51:GLN:HB3    | 9:42:54:ALA:HB2    | 1.91                     | 0.53              |
| 10:A3:72:ARG:N     | 10:A3:76:ASP:OD2   | 2.24                     | 0.53              |
| 10:B3:57:PRO:HB2   | 10:B3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:C3:101:LYS:HZ3  | 10:C3:101:LYS:HB2  | 1.74                     | 0.53              |
| 10:G3:57:PRO:HB2   | 10:G3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:V3:57:PRO:HB2   | 10:V3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:V3:109:VAL:HG21 | 10:V3:117:PHE:O    | 2.08                     | 0.53              |
| 11:a3:114:LYS:O    | 11:a3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:a3:365:ILE:CG2  | 11:z3:164:ARG:HD2  | 2.38                     | 0.53              |
| 11:h3:172:GLU:HA   | 11:h3:172:GLU:OE1  | 2.09                     | 0.53              |
| 11:l3:284:VAL:HG21 | 11:l3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:s3:114:LYS:O    | 11:s3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:z3:45:LEU:HD22  | 11:z3:116:LEU:HA   | 1.89                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:203:ALA:HA    | 1:E1:158:ALA:HB1   | 1.90                     | 0.53              |
| 1:D1:294:ARG:NE    | 6:U2:69:SER:HG     | 2.05                     | 0.53              |
| 1:L1:245:ILE:HG23  | 1:L1:266:VAL:HG21  | 1.90                     | 0.53              |
| 1:L1:280:GLU:HG2   | 1:L1:282:TYR:HE2   | 1.74                     | 0.53              |
| 1:U1:372:ILE:HG22  | 1:V1:278:THR:HB    | 1.90                     | 0.53              |
| 1:a1:126:PHE:HA    | 1:a1:129:GLN:NE2   | 2.24                     | 0.53              |
| 1:e1:371:THR:HG22  | 1:f1:279:GLU:HG2   | 1.89                     | 0.53              |
| 1:h1:179:THR:HA    | 1:h1:215:GLN:HB3   | 1.91                     | 0.53              |
| 2:A2:67:ILE:HD13   | 2:A2:96:LEU:HD23   | 1.90                     | 0.53              |
| 3:F2:210:GLN:HG3   | 4:G2:45:ASN:ND2    | 2.24                     | 0.53              |
| 6:T2:35:THR:HG22   | 7:Y2:49:PHE:HB3    | 1.91                     | 0.53              |
| 9:q2:95:VAL:O      | 9:q2:118:GLY:HA3   | 2.09                     | 0.53              |
| 9:t2:35:LYS:NZ     | 9:t2:220:GLU:OE2   | 2.37                     | 0.53              |
| 9:32:38:ARG:NE     | 9:32:78:GLU:OE2    | 2.28                     | 0.53              |
| 9:32:180:ASN:HB3   | 9:32:198:SER:HA    | 1.91                     | 0.53              |
| 10:A3:57:PRO:HB2   | 10:A3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:D3:57:PRO:HB2   | 10:D3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:E3:70:ARG:NH2   | 11:d3:72:THR:OG1   | 2.37                     | 0.53              |
| 10:L3:50:SER:HB3   | 11:m3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:O3:50:SER:HB3   | 11:p3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:U3:50:SER:HB3   | 11:v3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:U3:69:ARG:HG3   | 10:U3:69:ARG:O     | 2.09                     | 0.53              |
| 10:U3:109:VAL:HG21 | 10:U3:117:PHE:O    | 2.08                     | 0.53              |
| 10:V3:50:SER:HB3   | 11:w3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:W3:109:VAL:HG21 | 10:W3:117:PHE:O    | 2.08                     | 0.53              |
| 10:X3:69:ARG:HG3   | 10:X3:69:ARG:O     | 2.09                     | 0.53              |
| 10:Y3:70:ARG:NH2   | 11:x3:72:THR:OG1   | 2.40                     | 0.53              |
| 10:Y3:109:VAL:HG21 | 10:Y3:117:PHE:O    | 2.08                     | 0.53              |
| 11:c3:114:LYS:O    | 11:c3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:e3:172:GLU:OE1  | 11:e3:172:GLU:HA   | 2.09                     | 0.53              |
| 11:o3:114:LYS:O    | 11:o3:160:LEU:HD13 | 2.08                     | 0.53              |
| 11:t3:193:ASP:HB3  | 11:t3:196:MET:HB2  | 1.91                     | 0.53              |
| 11:x3:228:GLY:O    | 11:x3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:x3:254:VAL:HG13 | 11:x3:365:ILE:HG12 | 1.89                     | 0.53              |
| 1:B1:166:VAL:HG13  | 2:C2:161:GLY:HA2   | 1.89                     | 0.53              |
| 1:C1:409:MET:HE2   | 1:C1:434:ASN:HB2   | 1.91                     | 0.53              |
| 1:O1:253:LEU:HD22  | 1:O1:412:ILE:HG23  | 1.91                     | 0.53              |
| 1:Q1:161:LYS:HE2   | 3:F2:249:ASN:HD21  | 1.38                     | 0.53              |
| 1:T1:275:LYS:HG3   | 1:T1:377:MET:HE2   | 1.91                     | 0.53              |
| 2:E2:80:THR:HG23   | 3:F2:104:LEU:HD11  | 1.89                     | 0.53              |
| 3:F2:233:MET:HB3   | 4:G2:11:THR:HG22   | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:H2:70:LEU:HD22   | 4:I2:7:MET:HE3     | 1.91                     | 0.53              |
| 7:X2:30:ASN:ND2    | 8:c2:57:VAL:HG22   | 2.24                     | 0.53              |
| 7:X2:42:TYR:O      | 7:X2:94:PRO:HB3    | 2.09                     | 0.53              |
| 8:e2:80:VAL:HG13   | 8:e2:201:ILE:HG23  | 1.91                     | 0.53              |
| 8:f2:70:GLN:CD     | 9:q2:3:SER:HB2     | 2.34                     | 0.53              |
| 9:n2:89:THR:HG23   | 9:n2:91:ASN:H      | 1.73                     | 0.53              |
| 9:o2:77:THR:HG23   | 9:s2:66:LEU:HD12   | 1.91                     | 0.53              |
| 10:A3:109:VAL:HG21 | 10:A3:117:PHE:O    | 2.08                     | 0.53              |
| 10:B3:50:SER:HB3   | 11:c3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:E3:57:PRO:HB2   | 10:E3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:P3:50:SER:HB3   | 11:q3:99:GLN:NE2   | 2.23                     | 0.53              |
| 10:X3:109:VAL:HG21 | 10:X3:117:PHE:O    | 2.08                     | 0.53              |
| 11:g3:172:GLU:OE1  | 11:g3:172:GLU:HA   | 2.09                     | 0.53              |
| 11:k3:353:GLN:HG3  | 11:k3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:l3:164:ARG:HD2  | 11:m3:365:ILE:CG2  | 2.38                     | 0.53              |
| 11:l3:353:GLN:HG3  | 11:l3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:u3:172:GLU:OE1  | 11:u3:172:GLU:HA   | 2.09                     | 0.53              |
| 11:v3:114:LYS:O    | 11:v3:160:LEU:HD13 | 2.08                     | 0.53              |
| 11:w3:254:VAL:HG13 | 11:w3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:x3:45:LEU:HD22  | 11:x3:116:LEU:HA   | 1.88                     | 0.53              |
| 11:y3:45:LEU:HD22  | 11:y3:116:LEU:HA   | 1.89                     | 0.53              |
| 11:y3:172:GLU:OE1  | 11:y3:172:GLU:HA   | 2.09                     | 0.53              |
| 11:z3:114:LYS:O    | 11:z3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:z3:196:MET:HA   | 11:z3:196:MET:CE   | 2.34                     | 0.53              |
| 12:E4:226:ASP:OD1  | 12:E4:227:GLU:N    | 2.42                     | 0.53              |
| 1:H1:250:GLU:O     | 1:H1:254:SER:OG    | 2.23                     | 0.53              |
| 1:K1:167:ARG:CD    | 2:A2:244:TYR:O     | 2.55                     | 0.53              |
| 1:R1:283:SER:HB2   | 1:R1:369:ASP:HB2   | 1.91                     | 0.53              |
| 1:U1:142:ARG:HG3   | 1:W1:154:ARG:HH12  | 1.74                     | 0.53              |
| 1:U1:420:MET:HE2   | 1:U1:430:LEU:HD22  | 1.91                     | 0.53              |
| 1:W1:143:THR:HG21  | 1:X1:156:HIS:NE2   | 2.24                     | 0.53              |
| 1:Y1:234:GLN:HG3   | 1:Y1:272:PHE:CE1   | 2.44                     | 0.53              |
| 1:d1:420:MET:HE3   | 1:d1:422:PHE:HD1   | 1.72                     | 0.53              |
| 2:C2:119:GLN:HE22  | 2:C2:120:LYS:HZ2   | 1.57                     | 0.53              |
| 8:b2:30:SER:OG     | 9:g2:235:GLN:NE2   | 2.32                     | 0.53              |
| 8:f2:70:GLN:OE1    | 9:q2:3:SER:HB2     | 2.08                     | 0.53              |
| 8:f2:182:THR:C     | 8:f2:184:GLU:H     | 2.16                     | 0.53              |
| 9:r2:46:TYR:HA     | 9:r2:69:GLY:HA2    | 1.91                     | 0.53              |
| 9:22:36:ARG:HH21   | 9:22:80:LEU:HD22   | 1.73                     | 0.53              |
| 10:C3:57:PRO:HB2   | 10:C3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:J3:50:SER:HB3   | 11:k3:99:GLN:NE2   | 2.23                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:K3:109:VAL:HG21 | 10:K3:117:PHE:O    | 2.08                     | 0.53              |
| 10:R3:109:VAL:HG21 | 10:R3:117:PHE:O    | 2.08                     | 0.53              |
| 10:S3:70:ARG:NH2   | 11:r3:72:THR:OG1   | 2.38                     | 0.53              |
| 10:U3:166:GLU:OE2  | 10:U3:168:GLN:NE2  | 2.27                     | 0.53              |
| 10:V3:72:ARG:N     | 10:V3:76:ASP:OD2   | 2.25                     | 0.53              |
| 10:X3:57:PRO:HB2   | 10:X3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:Y3:57:PRO:HB2   | 10:Y3:60:TYR:HE2   | 1.72                     | 0.53              |
| 10:Z3:57:PRO:HB2   | 10:Z3:60:TYR:HE2   | 1.72                     | 0.53              |
| 11:a3:46:ASP:HA    | 11:b3:161:ASN:ND2  | 2.21                     | 0.53              |
| 11:a3:254:VAL:HG13 | 11:a3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:b3:46:ASP:HA    | 11:c3:161:ASN:ND2  | 2.21                     | 0.53              |
| 11:c3:142:LEU:HD23 | 11:e3:350:GLN:NE2  | 2.23                     | 0.53              |
| 11:d3:284:VAL:HG21 | 11:d3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:f3:114:LYS:O    | 11:f3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:h3:284:VAL:HG21 | 11:h3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:l3:80:GLN:HB3   | 11:m3:54:GLN:HB3   | 1.91                     | 0.53              |
| 11:m3:353:GLN:HG3  | 11:m3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:s3:193:ASP:HB3  | 11:s3:196:MET:HB2  | 1.91                     | 0.53              |
| 11:u3:193:ASP:HB3  | 11:u3:196:MET:HB2  | 1.91                     | 0.53              |
| 11:u3:254:VAL:HG13 | 11:u3:365:ILE:HG12 | 1.89                     | 0.53              |
| 11:v3:164:ARG:HD2  | 11:w3:365:ILE:CG2  | 2.38                     | 0.53              |
| 11:x3:172:GLU:HA   | 11:x3:172:GLU:OE1  | 2.09                     | 0.53              |
| 1:C1:190:GLN:OE1   | 1:E1:217:GLY:HA3   | 2.09                     | 0.53              |
| 1:Q1:407:ASP:OD1   | 1:Q1:408:GLN:N     | 2.41                     | 0.53              |
| 1:S1:294:ARG:HG2   | 6:R2:71:HIS:HB2    | 1.90                     | 0.53              |
| 1:T1:165:PHE:HB3   | 3:F2:167:ASN:N     | 2.23                     | 0.53              |
| 1:c1:259:ASN:OD1   | 1:c1:260:GLY:N     | 2.41                     | 0.53              |
| 2:A2:175:VAL:HG21  | 3:F2:49:MET:HE1    | 1.91                     | 0.53              |
| 2:B2:71:PHE:CE1    | 2:B2:236:MET:SD    | 2.98                     | 0.53              |
| 8:c2:77:PRO:O      | 8:c2:203:SER:OG    | 2.27                     | 0.53              |
| 9:q2:227:ALA:HA    | 9:22:257:LEU:HD21  | 1.91                     | 0.53              |
| 9:t2:203:GLU:H     | 11:w3:54:GLN:HE22  | 1.57                     | 0.53              |
| 9:x2:105:VAL:CG1   | 9:x2:134:PHE:HB3   | 2.39                     | 0.53              |
| 10:C3:69:ARG:O     | 10:C3:69:ARG:HG3   | 2.09                     | 0.53              |
| 10:F3:50:SER:HB3   | 11:g3:99:GLN:NE2   | 2.24                     | 0.53              |
| 10:F3:69:ARG:O     | 10:F3:69:ARG:HG3   | 2.09                     | 0.53              |
| 10:X3:167:LYS:HD3  | 10:Y3:203:ALA:HB3  | 1.90                     | 0.53              |
| 11:a3:172:GLU:OE1  | 11:a3:172:GLU:HA   | 2.09                     | 0.53              |
| 11:a3:269:THR:HG22 | 11:a3:326:ALA:O    | 2.09                     | 0.53              |
| 11:b3:172:GLU:OE1  | 11:b3:172:GLU:HA   | 2.09                     | 0.53              |
| 11:i3:172:GLU:OE1  | 11:i3:172:GLU:HA   | 2.09                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:n3:228:GLY:O    | 11:n3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:p3:80:GLN:HB3   | 11:q3:54:GLN:HB3   | 1.90                     | 0.53              |
| 11:r3:193:ASP:HB3  | 11:r3:196:MET:HB2  | 1.91                     | 0.53              |
| 11:r3:228:GLY:O    | 11:r3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:t3:269:THR:HG22 | 11:t3:326:ALA:O    | 2.09                     | 0.53              |
| 11:u3:353:GLN:HG3  | 11:u3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:v3:269:THR:HG22 | 11:v3:326:ALA:O    | 2.09                     | 0.53              |
| 11:w3:284:VAL:HG21 | 11:w3:316:GLY:HA2  | 1.90                     | 0.53              |
| 12:D4:40:LEU:HD22  | 12:D4:61:GLN:HB2   | 1.89                     | 0.53              |
| 1:D1:295:SER:HB2   | 6:U2:71:HIS:O      | 2.09                     | 0.53              |
| 1:D1:298:LEU:HD13  | 1:D1:362:GLU:HB3   | 1.89                     | 0.53              |
| 1:O1:132:TYR:HE2   | 1:Q1:130:VAL:HG13  | 1.74                     | 0.53              |
| 1:Y1:272:PHE:HA    | 1:Y1:379:VAL:HG13  | 1.90                     | 0.53              |
| 1:Z1:294:ARG:CD    | 6:S2:68:THR:HB     | 2.39                     | 0.53              |
| 1:g1:304:VAL:HB    | 1:h1:356:ARG:H     | 1.74                     | 0.53              |
| 5:K2:86:ILE:HD11   | 5:P2:99:VAL:HG12   | 1.90                     | 0.53              |
| 7:W2:76:LEU:HD23   | 7:W2:90:TYR:HB3    | 1.90                     | 0.53              |
| 8:c2:143:ILE:HD11  | 8:c2:161:LEU:HD13  | 1.91                     | 0.53              |
| 8:c2:173:ARG:HB3   | 9:h2:67:GLN:NE2    | 2.24                     | 0.53              |
| 10:D3:69:ARG:HG3   | 10:D3:69:ARG:O     | 2.09                     | 0.53              |
| 10:E3:69:ARG:HG3   | 10:E3:69:ARG:O     | 2.09                     | 0.53              |
| 10:M3:166:GLU:OE2  | 10:M3:168:GLN:NE2  | 2.27                     | 0.53              |
| 10:V3:69:ARG:O     | 10:V3:69:ARG:HG3   | 2.09                     | 0.53              |
| 10:W3:57:PRO:HB2   | 10:W3:60:TYR:HE2   | 1.72                     | 0.53              |
| 11:d3:164:ARG:HD2  | 11:e3:365:ILE:CG2  | 2.38                     | 0.53              |
| 11:f3:96:PHE:O     | 11:g3:219:ARG:HD2  | 2.09                     | 0.53              |
| 11:i3:196:MET:HA   | 11:i3:196:MET:CE   | 2.34                     | 0.53              |
| 11:l3:196:MET:HA   | 11:l3:196:MET:CE   | 2.34                     | 0.53              |
| 11:o3:228:GLY:O    | 11:o3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:o3:269:THR:HG22 | 11:o3:326:ALA:O    | 2.09                     | 0.53              |
| 11:s3:228:GLY:O    | 11:s3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:t3:353:GLN:HG3  | 11:t3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:v3:193:ASP:HB3  | 11:v3:196:MET:HB2  | 1.91                     | 0.53              |
| 11:x3:79:MET:HE2   | 11:y3:57:PHE:HD2   | 1.74                     | 0.53              |
| 11:z3:172:GLU:OE1  | 11:z3:172:GLU:HA   | 2.09                     | 0.53              |
| 1:J1:420:MET:HE1   | 1:J1:429:THR:O     | 2.09                     | 0.53              |
| 1:N1:167:ARG:HH12  | 2:A2:158:PRO:CD    | 2.22                     | 0.53              |
| 1:Q1:125:GLN:HG3   | 3:F2:181:LEU:HD11  | 1.91                     | 0.53              |
| 1:T1:179:THR:HA    | 1:T1:215:GLN:HB3   | 1.91                     | 0.53              |
| 1:U1:189:GLY:O     | 1:U1:192:SER:OG    | 2.23                     | 0.53              |
| 1:g1:294:ARG:NE    | 1:g1:367:GLU:OE1   | 2.42                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:h1:165:PHE:HA    | 2:C2:142:THR:O     | 2.09                     | 0.53              |
| 2:B2:207:LEU:HD12  | 4:H2:58:VAL:HG21   | 1.91                     | 0.53              |
| 4:G2:59:PHE:CE1    | 4:H2:14:MET:HB3    | 2.44                     | 0.53              |
| 7:V2:117:GLU:C     | 7:V2:117:GLU:CD    | 2.77                     | 0.53              |
| 8:b2:74:THR:HG23   | 8:b2:76:ARG:H      | 1.74                     | 0.53              |
| 8:e2:134:GLU:HB3   | 8:e2:146:LEU:O     | 2.08                     | 0.53              |
| 9:r2:104:GLN:HG3   | 9:r2:114:TYR:CE1   | 2.44                     | 0.53              |
| 9:u2:95:VAL:O      | 9:u2:118:GLY:HA3   | 2.09                     | 0.53              |
| 9:w2:83:GLN:NE2    | 9:w2:98:LYS:HA     | 2.23                     | 0.53              |
| 9:32:120:PHE:O     | 9:32:121:GLN:NE2   | 2.38                     | 0.53              |
| 9:32:233:MET:HG3   | 12:B4:44:LEU:CD1   | 2.39                     | 0.53              |
| 10:N3:80:ILE:HD13  | 10:N3:195:VAL:CG1  | 2.39                     | 0.53              |
| 10:Q3:101:LYS:HB2  | 10:Q3:101:LYS:HZ3  | 1.74                     | 0.53              |
| 10:R3:50:SER:HB3   | 11:s3:99:GLN:NE2   | 2.24                     | 0.53              |
| 10:S3:72:ARG:N     | 10:S3:76:ASP:OD2   | 2.25                     | 0.53              |
| 10:U3:80:ILE:HD13  | 10:U3:195:VAL:CG1  | 2.39                     | 0.53              |
| 10:V3:80:ILE:HD13  | 10:V3:195:VAL:CG1  | 2.39                     | 0.53              |
| 11:a3:57:PHE:HD2   | 11:z3:79:MET:HE2   | 1.74                     | 0.53              |
| 11:a3:219:ARG:HD3  | 11:z3:101:GLN:NE2  | 2.24                     | 0.53              |
| 11:c3:46:ASP:HA    | 11:d3:161:ASN:ND2  | 2.21                     | 0.53              |
| 11:c3:269:THR:HG22 | 11:c3:326:ALA:O    | 2.09                     | 0.53              |
| 11:d3:172:GLU:OE1  | 11:d3:172:GLU:HA   | 2.09                     | 0.53              |
| 11:f3:164:ARG:HD2  | 11:g3:365:ILE:CG2  | 2.38                     | 0.53              |
| 11:h3:114:LYS:O    | 11:h3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:h3:353:GLN:HG3  | 11:h3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:j3:114:LYS:O    | 11:j3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:k3:114:LYS:O    | 11:k3:160:LEU:HD13 | 2.09                     | 0.53              |
| 11:m3:228:GLY:O    | 11:m3:232:GLN:HG3  | 2.08                     | 0.53              |
| 11:n3:114:LYS:O    | 11:n3:160:LEU:HD13 | 2.08                     | 0.53              |
| 11:n3:284:VAL:HG21 | 11:n3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:n3:353:GLN:HG3  | 11:n3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:q3:101:GLN:NE2  | 11:r3:219:ARG:HD3  | 2.24                     | 0.53              |
| 11:q3:269:THR:HG22 | 11:q3:326:ALA:O    | 2.09                     | 0.53              |
| 11:r3:284:VAL:HG21 | 11:r3:316:GLY:HA2  | 1.90                     | 0.53              |
| 11:s3:353:GLN:HG3  | 11:s3:362:LEU:HD22 | 1.90                     | 0.53              |
| 11:y3:269:THR:HG22 | 11:y3:326:ALA:O    | 2.09                     | 0.53              |
| 1:B1:154:ARG:HH22  | 1:h1:143:THR:N     | 2.06                     | 0.52              |
| 1:G1:294:ARG:NE    | 1:G1:367:GLU:OE1   | 2.37                     | 0.52              |
| 1:H1:125:GLN:OE1   | 4:H2:3:PRO:CB      | 2.55                     | 0.52              |
| 1:L1:287:ASP:OD1   | 1:L1:289:SER:N     | 2.30                     | 0.52              |
| 1:W1:142:ARG:HG3   | 1:X1:154:ARG:HH22  | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:W1:151:LYS:NZ    | 1:W1:180:LEU:O     | 2.43                     | 0.52              |
| 1:W1:163:SER:OG    | 1:W1:164:LEU:N     | 2.41                     | 0.52              |
| 1:X1:203:ALA:O     | 1:Y1:170:LYS:NZ    | 2.42                     | 0.52              |
| 1:X1:266:VAL:HG22  | 1:X1:387:VAL:HG22  | 1.90                     | 0.52              |
| 1:Z1:294:ARG:HG2   | 6:S2:68:THR:HG21   | 1.88                     | 0.52              |
| 1:a1:186:LEU:HD23  | 1:a1:191:ILE:HD13  | 1.91                     | 0.52              |
| 1:f1:392:ASN:OD1   | 1:f1:393:TYR:N     | 2.42                     | 0.52              |
| 1:g1:253:LEU:HD11  | 1:g1:412:ILE:HG23  | 1.90                     | 0.52              |
| 1:g1:420:MET:HE1   | 1:g1:430:LEU:HB2   | 1.91                     | 0.52              |
| 1:h1:188:GLU:OE2   | 1:h1:188:GLU:N     | 2.39                     | 0.52              |
| 2:E2:140:ARG:HH12  | 2:E2:244:TYR:HB2   | 1.74                     | 0.52              |
| 9:j2:6:TRP:CE3     | 9:j2:9:LYS:CD      | 2.91                     | 0.52              |
| 9:n2:46:TYR:HA     | 9:n2:69:GLY:HA2    | 1.91                     | 0.52              |
| 9:o2:140:ILE:HG21  | 9:o2:157:VAL:HG21  | 1.91                     | 0.52              |
| 9:y2:36:ARG:HH21   | 9:y2:80:LEU:HB2    | 1.75                     | 0.52              |
| 9:12:42:GLU:OE1    | 9:12:73:ARG:NE     | 2.42                     | 0.52              |
| 10:F3:57:PRO:HB2   | 10:F3:60:TYR:HE2   | 1.72                     | 0.52              |
| 10:I3:72:ARG:N     | 10:I3:76:ASP:OD2   | 2.25                     | 0.52              |
| 10:Q3:80:ILE:HD13  | 10:Q3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:W3:80:ILE:HD13  | 10:W3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:Y3:80:ILE:HD13  | 10:Y3:195:VAL:CG1  | 2.39                     | 0.52              |
| 11:a3:161:ASN:ND2  | 11:z3:46:ASP:HA    | 2.21                     | 0.52              |
| 11:a3:284:VAL:HG21 | 11:a3:316:GLY:HA2  | 1.90                     | 0.52              |
| 11:e3:101:GLN:NE2  | 11:f3:219:ARG:HD3  | 2.24                     | 0.52              |
| 11:j3:172:GLU:OE1  | 11:j3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:j3:353:GLN:HG3  | 11:j3:362:LEU:HD22 | 1.90                     | 0.52              |
| 11:k3:46:ASP:HA    | 11:l3:161:ASN:ND2  | 2.21                     | 0.52              |
| 11:l3:114:LYS:O    | 11:l3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:m3:269:THR:HG22 | 11:m3:326:ALA:O    | 2.09                     | 0.52              |
| 11:o3:353:GLN:HG3  | 11:o3:362:LEU:HD22 | 1.90                     | 0.52              |
| 11:p3:114:LYS:O    | 11:p3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:p3:172:GLU:HA   | 11:p3:172:GLU:OE1  | 2.09                     | 0.52              |
| 11:q3:193:ASP:HB3  | 11:q3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:t3:228:GLY:O    | 11:t3:232:GLN:HG3  | 2.08                     | 0.52              |
| 11:u3:228:GLY:O    | 11:u3:232:GLN:HG3  | 2.08                     | 0.52              |
| 11:v3:254:VAL:HG13 | 11:v3:365:ILE:HG12 | 1.89                     | 0.52              |
| 11:w3:193:ASP:HB3  | 11:w3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:x3:193:ASP:HB3  | 11:x3:196:MET:HB2  | 1.91                     | 0.52              |
| 12:D4:149:ARG:HG2  | 12:D4:165:TRP:HE1  | 1.73                     | 0.52              |
| 12:D4:226:ASP:OD1  | 12:D4:227:GLU:N    | 2.42                     | 0.52              |
| 12:E4:140:ILE:HB   | 12:E4:149:ARG:HB3  | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B1:143:THR:HG21  | 1:C1:156:HIS:CD2   | 2.44                     | 0.52              |
| 1:N1:139:GLU:O     | 1:O1:154:ARG:NH2   | 2.43                     | 0.52              |
| 1:Q1:149:PRO:O     | 1:Q1:180:LEU:HD13  | 2.09                     | 0.52              |
| 1:Q1:181:GLU:OE1   | 1:Q1:184:ARG:NH2   | 2.43                     | 0.52              |
| 1:S1:252:ILE:HD11  | 1:T1:265:GLN:HB2   | 1.91                     | 0.52              |
| 1:a1:375:THR:HG23  | 1:b1:275:LYS:HE3   | 1.90                     | 0.52              |
| 1:c1:155:VAL:HG23  | 1:c1:176:VAL:HG22  | 1.90                     | 0.52              |
| 1:c1:409:MET:HE3   | 1:c1:434:ASN:HB2   | 1.92                     | 0.52              |
| 1:h1:279:GLU:OE2   | 1:h1:281:HIS:N     | 2.41                     | 0.52              |
| 2:C2:220:PRO:HB3   | 2:D2:190:PHE:HD2   | 1.74                     | 0.52              |
| 2:E2:80:THR:HG21   | 3:F2:104:LEU:HD21  | 1.91                     | 0.52              |
| 7:Y2:30:ASN:ND2    | 8:d2:57:VAL:HG22   | 2.25                     | 0.52              |
| 7:Z2:83:PRO:HG2    | 9:j2:62:LEU:HD23   | 1.91                     | 0.52              |
| 8:b2:82:LEU:HD21   | 8:b2:88:LEU:HG     | 1.91                     | 0.52              |
| 9:o2:19:MET:HB2    | 9:o2:236:VAL:HG11  | 1.91                     | 0.52              |
| 9:u2:36:ARG:HH21   | 9:u2:80:LEU:HD22   | 1.74                     | 0.52              |
| 9:w2:51:GLN:HB3    | 9:w2:54:ALA:HB2    | 1.92                     | 0.52              |
| 10:A3:69:ARG:HG3   | 10:A3:69:ARG:O     | 2.09                     | 0.52              |
| 10:B3:109:VAL:HG21 | 10:B3:117:PHE:O    | 2.08                     | 0.52              |
| 10:J3:51:ILE:CG1   | 11:l3:175:LEU:HD11 | 2.39                     | 0.52              |
| 10:O3:80:ILE:HD13  | 10:O3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:R3:80:ILE:HD13  | 10:R3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:S3:80:ILE:HD13  | 10:S3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:Z3:80:ILE:HD13  | 10:Z3:195:VAL:CG1  | 2.39                     | 0.52              |
| 11:e3:114:LYS:O    | 11:e3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:f3:280:LEU:HD11 | 11:f3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:g3:280:LEU:HD11 | 11:g3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:h3:196:MET:HA   | 11:h3:196:MET:CE   | 2.34                     | 0.52              |
| 11:j3:164:ARG:HD2  | 11:k3:365:ILE:CG2  | 2.38                     | 0.52              |
| 11:p3:254:VAL:HG13 | 11:p3:365:ILE:HG12 | 1.89                     | 0.52              |
| 11:q3:172:GLU:OE1  | 11:q3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:q3:228:GLY:O    | 11:q3:232:GLN:HG3  | 2.08                     | 0.52              |
| 11:r3:216:LEU:HD11 | 11:r3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:s3:284:VAL:HG21 | 11:s3:316:GLY:HA2  | 1.90                     | 0.52              |
| 11:w3:114:LYS:O    | 11:w3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:x3:269:THR:HG22 | 11:x3:326:ALA:O    | 2.09                     | 0.52              |
| 11:y3:193:ASP:HB3  | 11:y3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:y3:254:VAL:HG13 | 11:y3:365:ILE:HG12 | 1.89                     | 0.52              |
| 11:z3:254:VAL:HG13 | 11:z3:365:ILE:HG12 | 1.89                     | 0.52              |
| 12:D4:203:VAL:HA   | 12:D4:217:LEU:HD23 | 1.92                     | 0.52              |
| 1:J1:413:GLU:OE1   | 1:J1:432:VAL:HB    | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:K1:167:ARG:CD    | 2:A2:244:TYR:C     | 2.81                     | 0.52              |
| 1:L1:193:ALA:HA    | 1:N1:219:LEU:HG    | 1.91                     | 0.52              |
| 1:R1:151:LYS:NZ    | 1:R1:180:LEU:O     | 2.42                     | 0.52              |
| 1:S1:404:LEU:H     | 1:S1:434:ASN:ND2   | 2.07                     | 0.52              |
| 1:Y1:176:VAL:HB    | 1:Y1:212:LEU:HD23  | 1.91                     | 0.52              |
| 1:a1:197:LEU:HG    | 1:c1:213:VAL:HG21  | 1.91                     | 0.52              |
| 1:h1:125:GLN:NE2   | 4:I2:5:SER:OG      | 2.17                     | 0.52              |
| 1:h1:144:ILE:HA    | 1:h1:147:LEU:HD23  | 1.92                     | 0.52              |
| 2:A2:159:LEU:HD13  | 2:A2:165:VAL:HG12  | 1.92                     | 0.52              |
| 2:C2:128:ASP:O     | 2:C2:132:GLN:HG2   | 2.09                     | 0.52              |
| 2:E2:62:THR:O      | 2:E2:174:TYR:OH    | 2.15                     | 0.52              |
| 6:U2:123:LEU:HD23  | 7:Z2:132:LEU:HD21  | 1.92                     | 0.52              |
| 7:V2:26:SER:O      | 7:V2:30:ASN:ND2    | 2.29                     | 0.52              |
| 8:c2:22:THR:O      | 8:c2:26:LEU:N      | 2.42                     | 0.52              |
| 8:f2:202:MET:SD    | 9:q2:45:LEU:HD22   | 2.49                     | 0.52              |
| 9:j2:6:TRP:CZ3     | 9:j2:9:LYS:CE      | 2.85                     | 0.52              |
| 9:t2:203:GLU:N     | 11:w3:54:GLN:HE22  | 2.07                     | 0.52              |
| 9:u2:202:ASN:HD21  | 11:a3:78:ASN:HD22  | 1.43                     | 0.52              |
| 9:y2:16:GLN:NE2    | 9:42:2:ILE:HD12    | 2.25                     | 0.52              |
| 10:M3:80:ILE:HD13  | 10:M3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:P3:51:ILE:CG1   | 11:r3:175:LEU:HD11 | 2.39                     | 0.52              |
| 10:P3:80:ILE:HD13  | 10:P3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:T3:69:ARG:HG3   | 10:T3:69:ARG:O     | 2.09                     | 0.52              |
| 10:Z3:69:ARG:HG3   | 10:Z3:69:ARG:O     | 2.09                     | 0.52              |
| 11:b3:114:LYS:O    | 11:b3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:c3:280:LEU:HD11 | 11:c3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:d3:280:LEU:HD11 | 11:d3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:h3:280:LEU:HD11 | 11:h3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:j3:280:LEU:HD11 | 11:j3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:k3:172:GLU:OE1  | 11:k3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:p3:193:ASP:HB3  | 11:p3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:q3:114:LYS:O    | 11:q3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:q3:216:LEU:HD11 | 11:q3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:r3:164:ARG:HD2  | 11:s3:365:ILE:CG2  | 2.40                     | 0.52              |
| 11:v3:172:GLU:OE1  | 11:v3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:w3:46:ASP:HA    | 11:x3:161:ASN:ND2  | 2.21                     | 0.52              |
| 11:w3:216:LEU:HD11 | 11:w3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:y3:114:LYS:O    | 11:y3:160:LEU:HD13 | 2.09                     | 0.52              |
| 12:C4:141:THR:HG22 | 12:C4:147:VAL:HA   | 1.91                     | 0.52              |
| 12:D4:38:THR:HA    | 12:D4:41:VAL:HG22  | 1.90                     | 0.52              |
| 1:B1:217:GLY:HA3   | 1:h1:190:GLN:HG2   | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:K1:375:THR:HG23  | 1:L1:275:LYS:HZ1   | 1.75                     | 0.52              |
| 1:K1:375:THR:HA    | 1:L1:275:LYS:HZ2   | 1.75                     | 0.52              |
| 1:N1:393:TYR:CE2   | 1:N1:436:PRO:HD3   | 2.44                     | 0.52              |
| 1:O1:176:VAL:HB    | 1:O1:212:LEU:HD13  | 1.91                     | 0.52              |
| 1:S1:267:THR:OG1   | 1:S1:386:SER:HB2   | 2.09                     | 0.52              |
| 1:S1:295:SER:HB2   | 6:R2:73:ILE:HD11   | 1.91                     | 0.52              |
| 1:U1:151:LYS:NZ    | 1:U1:180:LEU:O     | 2.28                     | 0.52              |
| 1:W1:165:PHE:HE1   | 2:E2:244:TYR:C     | 2.11                     | 0.52              |
| 1:X1:165:PHE:CZ    | 2:E2:144:GLU:CB    | 2.82                     | 0.52              |
| 1:d1:420:MET:HE3   | 1:d1:422:PHE:CD1   | 2.45                     | 0.52              |
| 1:e1:253:LEU:HD11  | 1:e1:416:THR:HG22  | 1.91                     | 0.52              |
| 2:D2:199:VAL:HG23  | 4:J2:21:ALA:HB2    | 1.91                     | 0.52              |
| 6:R2:11:PHE:HD1    | 6:R2:53:MET:SD     | 2.32                     | 0.52              |
| 8:f2:62:PRO:O      | 9:k2:63:PRO:HG2    | 2.09                     | 0.52              |
| 9:u2:104:GLN:HG3   | 9:u2:114:TYR:CE1   | 2.45                     | 0.52              |
| 9:u2:184:LEU:HB3   | 9:u2:192:TYR:HB3   | 1.92                     | 0.52              |
| 9:u2:238:ARG:O     | 9:u2:241:GLU:HB3   | 2.10                     | 0.52              |
| 9:12:252:GLN:O     | 9:12:255:GLN:HB2   | 2.10                     | 0.52              |
| 10:G3:50:SER:HB3   | 11:h3:99:GLN:NE2   | 2.24                     | 0.52              |
| 10:H3:70:ARG:NH2   | 11:g3:72:THR:OG1   | 2.39                     | 0.52              |
| 10:M3:50:SER:HB3   | 11:n3:99:GLN:NE2   | 2.24                     | 0.52              |
| 10:S3:50:SER:HB3   | 11:t3:99:GLN:NE2   | 2.24                     | 0.52              |
| 11:b3:80:GLN:HB3   | 11:c3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:c3:101:GLN:NE2  | 11:d3:219:ARG:HD3  | 2.25                     | 0.52              |
| 11:e3:46:ASP:HA    | 11:f3:161:ASN:ND2  | 2.20                     | 0.52              |
| 11:e3:280:LEU:HD11 | 11:e3:340:ALA:HB2  | 1.92                     | 0.52              |
| 11:f3:172:GLU:OE1  | 11:f3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:i3:80:GLN:HB3   | 11:j3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:i3:280:LEU:HD11 | 11:i3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:n3:80:GLN:HB3   | 11:o3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:o3:193:ASP:HB3  | 11:o3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:s3:101:GLN:NE2  | 11:t3:219:ARG:HD3  | 2.24                     | 0.52              |
| 11:s3:269:THR:HG22 | 11:s3:326:ALA:O    | 2.09                     | 0.52              |
| 11:t3:254:VAL:HG13 | 11:t3:365:ILE:HG12 | 1.89                     | 0.52              |
| 11:v3:216:LEU:HD11 | 11:v3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:z3:193:ASP:HB3  | 11:z3:196:MET:HB2  | 1.91                     | 0.52              |
| 1:I1:203:ALA:HA    | 1:K1:158:ALA:HB1   | 1.91                     | 0.52              |
| 1:R1:125:GLN:HG2   | 2:E2:234:LEU:HD23  | 1.90                     | 0.52              |
| 1:R1:143:THR:HG23  | 1:T1:154:ARG:NH2   | 2.19                     | 0.52              |
| 1:T1:167:ARG:CZ    | 2:E2:106:ASP:C     | 2.82                     | 0.52              |
| 1:U1:139:GLU:O     | 1:U1:143:THR:HG23  | 2.09                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:U1:360:ARG:NH1   | 1:U1:362:GLU:OE1  | 2.42                     | 0.52              |
| 1:Y1:267:THR:OG1   | 1:Y1:386:SER:HB2  | 2.10                     | 0.52              |
| 1:Y1:393:TYR:HB3   | 1:Y1:402:LEU:N    | 2.23                     | 0.52              |
| 1:Z1:386:SER:HA    | 1:Z1:429:THR:O    | 2.10                     | 0.52              |
| 1:g1:148:GLY:O     | 1:g1:150:VAL:N    | 2.41                     | 0.52              |
| 2:C2:193:PHE:HB3   | 2:C2:222:LYS:HD3  | 1.92                     | 0.52              |
| 5:P2:87:GLN:HE22   | 7:V2:134:GLN:NE2  | 2.07                     | 0.52              |
| 9:g2:140:ILE:HD13  | 9:g2:157:VAL:HG11 | 1.92                     | 0.52              |
| 10:K3:80:ILE:HD13  | 10:K3:195:VAL:CG1 | 2.39                     | 0.52              |
| 10:P3:82:LEU:O     | 10:P3:197:SER:OG  | 2.20                     | 0.52              |
| 10:R3:69:ARG:HG3   | 10:R3:69:ARG:O    | 2.09                     | 0.52              |
| 10:S3:69:ARG:O     | 10:S3:69:ARG:HG3  | 2.09                     | 0.52              |
| 10:T3:80:ILE:HD13  | 10:T3:195:VAL:CG1 | 2.39                     | 0.52              |
| 11:a3:101:GLN:NE2  | 11:b3:219:ARG:HD3 | 2.25                     | 0.52              |
| 11:b3:280:LEU:HD11 | 11:b3:340:ALA:HB2 | 1.91                     | 0.52              |
| 11:d3:245:ASN:OD1  | 11:d3:245:ASN:N   | 2.33                     | 0.52              |
| 11:e3:89:VAL:HG11  | 11:e3:121:LEU:CD2 | 2.40                     | 0.52              |
| 11:e3:269:THR:HG22 | 11:e3:326:ALA:O   | 2.09                     | 0.52              |
| 11:h3:80:GLN:HB3   | 11:i3:54:GLN:HB3  | 1.92                     | 0.52              |
| 11:k3:269:THR:HG22 | 11:k3:326:ALA:O   | 2.09                     | 0.52              |
| 11:k3:280:LEU:HD11 | 11:k3:340:ALA:HB2 | 1.91                     | 0.52              |
| 11:l3:172:GLU:OE1  | 11:l3:172:GLU:HA  | 2.09                     | 0.52              |
| 11:m3:80:GLN:HB3   | 11:n3:54:GLN:HB3  | 1.92                     | 0.52              |
| 11:m3:280:LEU:HD11 | 11:m3:340:ALA:HB2 | 1.91                     | 0.52              |
| 11:r3:172:GLU:OE1  | 11:r3:172:GLU:HA  | 2.09                     | 0.52              |
| 11:r3:269:THR:HG22 | 11:r3:326:ALA:O   | 2.09                     | 0.52              |
| 11:y3:101:GLN:NE2  | 11:z3:188:GLN:HB3 | 2.23                     | 0.52              |
| 1:E1:404:LEU:H     | 1:E1:434:ASN:ND2  | 2.08                     | 0.52              |
| 1:I1:393:TYR:CE2   | 1:I1:436:PRO:HD3  | 2.45                     | 0.52              |
| 1:L1:369:ASP:OD1   | 1:M1:282:TYR:N    | 2.43                     | 0.52              |
| 1:W1:129:GLN:O     | 1:W1:133:GLN:HG2  | 2.09                     | 0.52              |
| 1:W1:256:ILE:HD11  | 1:X1:390:VAL:HG21 | 1.92                     | 0.52              |
| 1:X1:392:ASN:OD1   | 1:X1:393:TYR:N    | 2.42                     | 0.52              |
| 1:c1:405:THR:OG1   | 1:c1:407:ASP:OD1  | 2.24                     | 0.52              |
| 4:H2:59:PHE:CD1    | 4:I2:14:MET:HE2   | 2.45                     | 0.52              |
| 7:V2:102:MET:HG3   | 9:g2:257:LEU:HD11 | 1.90                     | 0.52              |
| 9:h2:77:THR:HG21   | 9:m2:67:GLN:H     | 1.74                     | 0.52              |
| 9:l2:101:GLY:HA3   | 9:l2:175:LEU:HD23 | 1.90                     | 0.52              |
| 9:o2:98:LYS:O      | 9:o2:212:GLY:CA   | 2.57                     | 0.52              |
| 9:q2:35:LYS:NZ     | 9:q2:82:SER:O     | 2.37                     | 0.52              |
| 9:r2:141:THR:CG2   | 11:l3:53:THR:HG22 | 2.24                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:v2:142:ILE:HG23  | 9:v2:159:VAL:HG11  | 1.91                     | 0.52              |
| 9:w2:140:ILE:CD1   | 9:w2:157:VAL:HG11  | 2.39                     | 0.52              |
| 9:w2:180:ASN:OD1   | 9:w2:182:THR:OG1   | 2.21                     | 0.52              |
| 10:B3:80:ILE:HD13  | 10:B3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:H3:68:ASP:O     | 10:H3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:K3:68:ASP:O     | 10:K3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:K3:69:ARG:O     | 10:K3:69:ARG:HG3   | 2.09                     | 0.52              |
| 10:L3:101:LYS:HB2  | 10:L3:101:LYS:HZ3  | 1.75                     | 0.52              |
| 10:N3:101:LYS:HZ3  | 10:N3:101:LYS:HB2  | 1.75                     | 0.52              |
| 10:X3:68:ASP:O     | 10:X3:69:ARG:HG2   | 2.10                     | 0.52              |
| 11:a3:89:VAL:HG11  | 11:a3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:f3:89:VAL:HG11  | 11:f3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:h3:89:VAL:HG11  | 11:h3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:i3:89:VAL:HG11  | 11:i3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:i3:353:GLN:HG3  | 11:i3:362:LEU:HD22 | 1.90                     | 0.52              |
| 11:m3:114:LYS:O    | 11:m3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:n3:193:ASP:HB3  | 11:n3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:p3:46:ASP:HA    | 11:q3:161:ASN:ND2  | 2.20                     | 0.52              |
| 11:s3:80:GLN:HB3   | 11:t3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:t3:114:LYS:O    | 11:t3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:t3:172:GLU:OE1  | 11:t3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:u3:80:GLN:HB3   | 11:v3:54:GLN:HB3   | 1.91                     | 0.52              |
| 11:w3:172:GLU:OE1  | 11:w3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:w3:269:THR:HG22 | 11:w3:326:ALA:O    | 2.09                     | 0.52              |
| 11:x3:216:LEU:HD11 | 11:x3:222:GLN:HB2  | 1.92                     | 0.52              |
| 12:A4:97:ILE:HD11  | 12:A4:206:VAL:HG23 | 1.92                     | 0.52              |
| 12:A4:230:GLN:NE2  | 12:E4:207:THR:HG22 | 2.25                     | 0.52              |
| 1:B1:165:PHE:O     | 2:C2:159:LEU:HB2   | 2.10                     | 0.52              |
| 1:G1:169:GLN:HE22  | 1:H1:161:LYS:HZ3   | 1.56                     | 0.52              |
| 1:J1:385:LEU:N     | 1:J1:428:ASP:OD2   | 2.42                     | 0.52              |
| 1:L1:258:GLY:HA3   | 1:L1:261:ASN:HD22  | 1.75                     | 0.52              |
| 1:R1:407:ASP:HA    | 1:R1:410:LYS:HG2   | 1.92                     | 0.52              |
| 1:T1:187:ASP:O     | 1:T1:191:ILE:HG12  | 2.10                     | 0.52              |
| 1:a1:187:ASP:O     | 1:a1:191:ILE:HG12  | 2.08                     | 0.52              |
| 1:a1:199:SER:OG    | 1:a1:205:LEU:O     | 2.21                     | 0.52              |
| 1:c1:268:ALA:HB1   | 1:c1:382:ILE:HD11  | 1.90                     | 0.52              |
| 1:h1:392:ASN:OD1   | 1:h1:393:TYR:N     | 2.43                     | 0.52              |
| 2:D2:184:GLN:HA    | 2:D2:187:PHE:HD2   | 1.74                     | 0.52              |
| 7:a2:29:ALA:HB1    | 8:f2:11:ALA:HB2    | 1.92                     | 0.52              |
| 8:d2:165:LYS:O     | 8:d2:189:ARG:NH1   | 2.42                     | 0.52              |
| 8:e2:138:ALA:HB1   | 9:u2:56:SER:O      | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:p2:4:SER:HA      | 9:p2:7:ILE:HG12    | 1.92                     | 0.52              |
| 9:v2:36:ARG:NH2    | 9:v2:80:LEU:HD22   | 2.25                     | 0.52              |
| 9:w2:241:GLU:CD    | 9:22:256:LYS:HD2   | 2.34                     | 0.52              |
| 9:z2:184:LEU:HB3   | 9:z2:192:TYR:HB3   | 1.92                     | 0.52              |
| 10:D3:51:ILE:CG1   | 11:f3:175:LEU:HD11 | 2.39                     | 0.52              |
| 10:I3:68:ASP:O     | 10:I3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:J3:68:ASP:O     | 10:J3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:Q3:69:ARG:HG3   | 10:Q3:69:ARG:O     | 2.09                     | 0.52              |
| 10:X3:80:ILE:HD13  | 10:X3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:Y3:68:ASP:O     | 10:Y3:69:ARG:HG2   | 2.10                     | 0.52              |
| 11:a3:280:LEU:HD11 | 11:a3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:b3:89:VAL:HG11  | 11:b3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:c3:89:VAL:HG11  | 11:c3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:d3:89:VAL:HG11  | 11:d3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:g3:80:GLN:HB3   | 11:h3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:g3:89:VAL:HG11  | 11:g3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:g3:269:THR:HG22 | 11:g3:326:ALA:O    | 2.09                     | 0.52              |
| 11:i3:269:THR:HG22 | 11:i3:326:ALA:O    | 2.09                     | 0.52              |
| 11:j3:89:VAL:HG11  | 11:j3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:l3:280:LEU:HD11 | 11:l3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:m3:216:LEU:HD11 | 11:m3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:o3:46:ASP:HA    | 11:p3:161:ASN:ND2  | 2.21                     | 0.52              |
| 11:o3:80:GLN:HB3   | 11:p3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:o3:280:LEU:HD11 | 11:o3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:r3:353:GLN:HG3  | 11:r3:362:LEU:HD22 | 1.90                     | 0.52              |
| 11:t3:80:GLN:HB3   | 11:u3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:v3:228:GLY:O    | 11:v3:232:GLN:HG3  | 2.08                     | 0.52              |
| 11:w3:80:GLN:HB3   | 11:x3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:x3:254:VAL:CG2  | 11:y3:355:ALA:HB2  | 2.39                     | 0.52              |
| 11:z3:89:VAL:HG11  | 11:z3:121:LEU:CD2  | 2.40                     | 0.52              |
| 1:B1:237:PHE:HE1   | 1:C1:232:ASP:HA    | 1.74                     | 0.52              |
| 1:C1:257:VAL:O     | 1:C1:261:ASN:ND2   | 2.32                     | 0.52              |
| 1:D1:237:PHE:HE1   | 1:E1:232:ASP:HA    | 1.75                     | 0.52              |
| 1:H1:203:ALA:HA    | 1:I1:158:ALA:HB1   | 1.92                     | 0.52              |
| 1:I1:151:LYS:HZ3   | 1:I1:182:PRO:HD3   | 1.75                     | 0.52              |
| 1:K1:187:ASP:O     | 1:K1:191:ILE:HG12  | 2.10                     | 0.52              |
| 1:Q1:182:PRO:O     | 1:Q1:184:ARG:NH1   | 2.42                     | 0.52              |
| 1:Q1:297:GLN:OE1   | 1:R1:363:THR:OG1   | 2.18                     | 0.52              |
| 1:S1:389:VAL:HB    | 1:S1:432:VAL:HG12  | 1.92                     | 0.52              |
| 1:W1:407:ASP:OD1   | 1:W1:408:GLN:N     | 2.43                     | 0.52              |
| 1:e1:378:ASN:ND2   | 1:e1:381:ASP:OD1   | 2.37                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:C2:140:ARG:HH22  | 2:C2:244:TYR:HB2   | 1.75                     | 0.52              |
| 2:E2:41:SER:HB3    | 5:L2:49:GLN:CD     | 2.34                     | 0.52              |
| 3:F2:140:PHE:HB3   | 3:F2:141:ASN:HB2   | 1.91                     | 0.52              |
| 7:X2:76:LEU:HD12   | 9:i2:45:LEU:HD11   | 1.90                     | 0.52              |
| 7:Z2:102:MET:HE1   | 8:e2:232:LYS:HD3   | 1.92                     | 0.52              |
| 8:e2:89:VAL:HG12   | 8:e2:121:ILE:HB    | 1.92                     | 0.52              |
| 9:g2:147:LEU:HD11  | 9:g2:162:GLN:HG2   | 1.92                     | 0.52              |
| 9:p2:235:GLN:HG2   | 9:v2:5:LEU:HD23    | 1.91                     | 0.52              |
| 9:r2:234:ILE:HD11  | 9:32:260:LEU:HD21  | 1.90                     | 0.52              |
| 9:u2:105:VAL:HG11  | 9:u2:134:PHE:HB3   | 1.92                     | 0.52              |
| 9:22:235:GLN:HA    | 12:B4:46:ASN:ND2   | 2.24                     | 0.52              |
| 10:A3:50:SER:HB3   | 11:b3:99:GLN:NE2   | 2.25                     | 0.52              |
| 10:H3:101:LYS:HZ3  | 10:H3:101:LYS:HB2  | 1.74                     | 0.52              |
| 10:I3:80:ILE:HD13  | 10:I3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:N3:69:ARG:O     | 10:N3:69:ARG:HG3   | 2.09                     | 0.52              |
| 10:T3:166:GLU:OE2  | 10:T3:168:GLN:NE2  | 2.27                     | 0.52              |
| 10:Z3:68:ASP:O     | 10:Z3:69:ARG:HG2   | 2.10                     | 0.52              |
| 11:c3:80:GLN:HB3   | 11:d3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:d3:275:VAL:HG21 | 11:d3:338:LEU:HD21 | 1.92                     | 0.52              |
| 11:m3:193:ASP:HB3  | 11:m3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:m3:284:VAL:HG21 | 11:m3:316:GLY:HA2  | 1.90                     | 0.52              |
| 11:n3:280:LEU:HD11 | 11:n3:340:ALA:HB2  | 1.91                     | 0.52              |
| 11:p3:228:GLY:O    | 11:p3:232:GLN:HG3  | 2.08                     | 0.52              |
| 11:s3:216:LEU:HD11 | 11:s3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:v3:245:ASN:OD1  | 11:v3:245:ASN:N    | 2.33                     | 0.52              |
| 1:B1:146:THR:O     | 1:B1:147:LEU:HD23  | 2.10                     | 0.52              |
| 1:G1:160:PRO:O     | 1:G1:161:LYS:HG2   | 2.09                     | 0.52              |
| 1:G1:169:GLN:HE22  | 1:H1:161:LYS:NZ    | 2.06                     | 0.52              |
| 1:K1:170:LYS:HD2   | 1:K1:171:SER:O     | 2.10                     | 0.52              |
| 1:M1:415:LEU:HD22  | 1:N1:431:ASN:ND2   | 2.25                     | 0.52              |
| 1:Q1:389:VAL:HB    | 1:Q1:432:VAL:HG22  | 1.92                     | 0.52              |
| 1:V1:369:ASP:OD1   | 1:W1:282:TYR:N     | 2.39                     | 0.52              |
| 3:F2:48:ILE:O      | 3:F2:51:THR:HG22   | 2.10                     | 0.52              |
| 8:d2:82:LEU:HD21   | 8:d2:88:LEU:HG     | 1.92                     | 0.52              |
| 9:o2:129:VAL:HG21  | 9:x2:63:PRO:HG3    | 1.91                     | 0.52              |
| 9:q2:163:GLY:HA2   | 9:22:111:THR:HG21  | 1.91                     | 0.52              |
| 9:r2:60:THR:HG22   | 9:r2:61:THR:N      | 2.24                     | 0.52              |
| 9:22:106:MET:HE3   | 9:22:110:GLY:HA2   | 1.92                     | 0.52              |
| 10:K3:72:ARG:N     | 10:K3:76:ASP:OD2   | 2.25                     | 0.52              |
| 10:N3:72:ARG:N     | 10:N3:76:ASP:OD2   | 2.24                     | 0.52              |
| 10:R3:68:ASP:O     | 10:R3:69:ARG:HG2   | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:U3:68:ASP:O     | 10:U3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:W3:69:ARG:HG3   | 10:W3:69:ARG:O     | 2.09                     | 0.52              |
| 10:X3:72:ARG:N     | 10:X3:76:ASP:OD2   | 2.25                     | 0.52              |
| 11:a3:193:ASP:HB3  | 11:a3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:b3:101:GLN:NE2  | 11:c3:219:ARG:HD3  | 2.25                     | 0.52              |
| 11:c3:275:VAL:HG21 | 11:c3:338:LEU:HD21 | 1.92                     | 0.52              |
| 11:d3:193:ASP:HB3  | 11:d3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:d3:269:THR:HG22 | 11:d3:326:ALA:O    | 2.09                     | 0.52              |
| 11:i3:114:LYS:O    | 11:i3:160:LEU:HD13 | 2.09                     | 0.52              |
| 11:k3:101:GLN:NE2  | 11:l3:219:ARG:HD3  | 2.24                     | 0.52              |
| 11:l3:216:LEU:HD11 | 11:l3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:o3:172:GLU:OE1  | 11:o3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:p3:216:LEU:HD11 | 11:p3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:p3:353:GLN:HG3  | 11:p3:362:LEU:HD22 | 1.90                     | 0.52              |
| 11:s3:172:GLU:OE1  | 11:s3:172:GLU:HA   | 2.09                     | 0.52              |
| 1:B1:157:LEU:HD11  | 1:B1:202:VAL:HG11  | 1.91                     | 0.52              |
| 1:D1:416:THR:HG21  | 1:D1:432:VAL:HG21  | 1.92                     | 0.52              |
| 1:G1:165:PHE:HZ    | 2:B2:143:ARG:NH1   | 2.08                     | 0.52              |
| 1:N1:297:GLN:HE21  | 6:Q2:77:ALA:HB2    | 1.74                     | 0.52              |
| 1:R1:416:THR:HG23  | 1:R1:430:LEU:HD21  | 1.92                     | 0.52              |
| 1:T1:125:GLN:N     | 1:T1:128:GLU:OE1   | 2.43                     | 0.52              |
| 1:T1:195:VAL:HG13  | 1:T1:210:VAL:HB    | 1.92                     | 0.52              |
| 1:U1:195:VAL:HG13  | 1:U1:210:VAL:HB    | 1.91                     | 0.52              |
| 1:g1:248:ARG:NH2   | 1:h1:242:GLU:OE1   | 2.42                     | 0.52              |
| 6:T2:92:GLN:HE22   | 7:Z2:22:ASN:ND2    | 2.07                     | 0.52              |
| 9:l2:238:ARG:O     | 9:l2:242:ILE:HG12  | 2.10                     | 0.52              |
| 9:t2:144:ALA:HB2   | 9:y2:179:MET:HE1   | 1.91                     | 0.52              |
| 9:w2:83:GLN:NE2    | 9:w2:99:GLY:H      | 2.07                     | 0.52              |
| 9:w2:95:VAL:O      | 9:w2:118:GLY:HA3   | 2.10                     | 0.52              |
| 9:w2:95:VAL:HG12   | 9:w2:216:GLN:HA    | 1.92                     | 0.52              |
| 10:A3:68:ASP:O     | 10:A3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:A3:80:ILE:HD13  | 10:A3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:D3:80:ILE:HD13  | 10:D3:195:VAL:CG1  | 2.39                     | 0.52              |
| 10:E3:68:ASP:O     | 10:E3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:G3:69:ARG:HG3   | 10:G3:69:ARG:O     | 2.09                     | 0.52              |
| 10:O3:69:ARG:HG3   | 10:O3:69:ARG:O     | 2.09                     | 0.52              |
| 10:Q3:68:ASP:O     | 10:Q3:69:ARG:HG2   | 2.10                     | 0.52              |
| 10:S3:68:ASP:O     | 10:S3:69:ARG:HG2   | 2.10                     | 0.52              |
| 11:a3:80:GLN:HB3   | 11:b3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:b3:269:THR:HG22 | 11:b3:326:ALA:O    | 2.09                     | 0.52              |
| 11:b3:275:VAL:HG21 | 11:b3:338:LEU:HD21 | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:c3:193:ASP:HB3  | 11:c3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:e3:193:ASP:HB3  | 11:e3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:j3:193:ASP:HB3  | 11:j3:196:MET:HB2  | 1.91                     | 0.52              |
| 11:k3:80:GLN:HB3   | 11:l3:54:GLN:HB3   | 1.92                     | 0.52              |
| 11:k3:89:VAL:HG11  | 11:k3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:l3:275:VAL:HG21 | 11:l3:338:LEU:CD2  | 2.40                     | 0.52              |
| 11:n3:172:GLU:OE1  | 11:n3:172:GLU:HA   | 2.09                     | 0.52              |
| 11:p3:269:THR:HG22 | 11:p3:326:ALA:O    | 2.09                     | 0.52              |
| 11:u3:216:LEU:HD11 | 11:u3:222:GLN:HB2  | 1.92                     | 0.52              |
| 11:y3:89:VAL:HG11  | 11:y3:121:LEU:CD2  | 2.40                     | 0.52              |
| 11:z3:269:THR:HG22 | 11:z3:326:ALA:O    | 2.09                     | 0.52              |
| 11:z3:280:LEU:HD11 | 11:z3:340:ALA:HB2  | 1.91                     | 0.52              |
| 12:D4:148:VAL:HB   | 12:D4:169:GLN:HG2  | 1.92                     | 0.52              |
| 1:G1:413:GLU:OE2   | 1:G1:417:ARG:NH1   | 2.43                     | 0.51              |
| 1:H1:165:PHE:HA    | 2:B2:159:LEU:CB    | 2.40                     | 0.51              |
| 1:H1:246:GLN:O     | 1:H1:250:GLU:HG2   | 2.10                     | 0.51              |
| 1:M1:363:THR:HG22  | 6:Q2:73:ILE:CD1    | 2.29                     | 0.51              |
| 1:M1:365:ASN:OD1   | 6:Q2:72:HIS:CA     | 2.19                     | 0.51              |
| 1:M1:369:ASP:OD1   | 1:N1:282:TYR:N     | 2.43                     | 0.51              |
| 1:O1:153:ALA:HA    | 1:O1:177:THR:O     | 2.09                     | 0.51              |
| 1:W1:279:GLU:OE2   | 1:W1:281:HIS:HB2   | 2.10                     | 0.51              |
| 1:X1:301:SER:HB2   | 1:Y1:359:GLN:HE22  | 1.75                     | 0.51              |
| 1:Y1:283:SER:HB2   | 1:Y1:369:ASP:HB2   | 1.92                     | 0.51              |
| 1:b1:250:GLU:O     | 1:b1:254:SER:OG    | 2.26                     | 0.51              |
| 1:b1:301:SER:O     | 1:b1:359:GLN:N     | 2.32                     | 0.51              |
| 1:h1:245:ILE:O     | 1:h1:249:ILE:HG13  | 2.10                     | 0.51              |
| 2:D2:74:LEU:HD22   | 2:D2:235:LEU:HD22  | 1.92                     | 0.51              |
| 3:F2:6:SER:HA      | 5:K2:75:MET:HE1    | 1.92                     | 0.51              |
| 6:U2:93:PRO:HB3    | 8:f2:48:GLY:HA3    | 1.93                     | 0.51              |
| 7:X2:83:PRO:O      | 7:X2:84:LEU:HB2    | 2.10                     | 0.51              |
| 8:e2:107:VAL:HG12  | 8:e2:113:LEU:HD23  | 1.93                     | 0.51              |
| 9:l2:252:GLN:O     | 9:l2:255:GLN:HB2   | 2.10                     | 0.51              |
| 9:22:105:VAL:HG11  | 9:22:134:PHE:HB3   | 1.91                     | 0.51              |
| 10:E3:72:ARG:N     | 10:E3:76:ASP:OD2   | 2.25                     | 0.51              |
| 10:I3:51:ILE:CG1   | 11:k3:175:LEU:HD11 | 2.40                     | 0.51              |
| 10:I3:69:ARG:HG3   | 10:I3:69:ARG:O     | 2.09                     | 0.51              |
| 10:L3:68:ASP:O     | 10:L3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:L3:80:ILE:HD13  | 10:L3:195:VAL:CG1  | 2.39                     | 0.51              |
| 10:P3:68:ASP:O     | 10:P3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:P3:70:ARG:NH2   | 11:o3:72:THR:OG1   | 2.38                     | 0.51              |
| 10:X3:50:SER:HB3   | 11:y3:99:GLN:NE2   | 2.24                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:c3:172:GLU:OE1  | 11:c3:172:GLU:HA   | 2.09                     | 0.51              |
| 11:e3:80:GLN:HB3   | 11:f3:54:GLN:HB3   | 1.92                     | 0.51              |
| 11:e3:275:VAL:HG21 | 11:e3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:f3:269:THR:HG22 | 11:f3:326:ALA:O    | 2.09                     | 0.51              |
| 11:l3:193:ASP:HB3  | 11:l3:196:MET:HB2  | 1.91                     | 0.51              |
| 11:p3:275:VAL:HG21 | 11:p3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:w3:275:VAL:HG21 | 11:w3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:x3:89:VAL:HG11  | 11:x3:121:LEU:CD2  | 2.40                     | 0.51              |
| 11:x3:96:PHE:O     | 11:y3:219:ARG:HD2  | 2.11                     | 0.51              |
| 11:z3:275:VAL:HG21 | 11:z3:338:LEU:CD2  | 2.41                     | 0.51              |
| 12:D4:134:ASP:HA   | 12:D4:155:GLU:HG2  | 1.91                     | 0.51              |
| 12:D4:141:THR:HG22 | 12:D4:147:VAL:HG22 | 1.92                     | 0.51              |
| 1:C1:164:LEU:O     | 2:C2:148:ALA:HB1   | 2.11                     | 0.51              |
| 1:D1:279:GLU:OE2   | 1:D1:281:HIS:N     | 2.40                     | 0.51              |
| 1:I1:369:ASP:OD1   | 1:J1:282:TYR:N     | 2.42                     | 0.51              |
| 1:N1:125:GLN:CB    | 3:F2:238:PRO:CG    | 2.87                     | 0.51              |
| 1:Q1:297:GLN:HB3   | 1:Q1:363:THR:HB    | 1.92                     | 0.51              |
| 1:U1:199:SER:OG    | 1:U1:205:LEU:O     | 2.20                     | 0.51              |
| 1:d1:181:GLU:N     | 1:d1:181:GLU:OE1   | 2.43                     | 0.51              |
| 1:f1:200:SER:HB3   | 1:g1:175:SER:HB3   | 1.91                     | 0.51              |
| 6:R2:114:LEU:HD11  | 7:X2:126:MET:HB2   | 1.91                     | 0.51              |
| 8:d2:216:ALA:O     | 8:d2:220:MET:HG3   | 2.10                     | 0.51              |
| 9:n2:128:LEU:O     | 9:n2:136:VAL:HG12  | 2.11                     | 0.51              |
| 9:p2:2:ILE:HG12    | 9:p2:254:LEU:HD21  | 1.92                     | 0.51              |
| 9:p2:169:GLN:CG    | 11:c3:78:ASN:OD1   | 2.57                     | 0.51              |
| 9:r2:36:ARG:HH21   | 9:r2:80:LEU:HD22   | 1.76                     | 0.51              |
| 9:z2:174:ASN:ND2   | 9:z2:203:GLU:OE2   | 2.43                     | 0.51              |
| 9:12:149:ILE:HG12  | 9:12:159:VAL:HG12  | 1.92                     | 0.51              |
| 10:B3:68:ASP:O     | 10:B3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:G3:68:ASP:O     | 10:G3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:N3:166:GLU:OE2  | 10:N3:168:GLN:NE2  | 2.27                     | 0.51              |
| 10:O3:51:ILE:CG1   | 11:q3:175:LEU:HD11 | 2.40                     | 0.51              |
| 11:b3:193:ASP:HB3  | 11:b3:196:MET:HB2  | 1.91                     | 0.51              |
| 11:b3:216:LEU:HD11 | 11:b3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:i3:193:ASP:HB3  | 11:i3:196:MET:HB2  | 1.91                     | 0.51              |
| 11:j3:280:LEU:CD1  | 11:j3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:k3:193:ASP:HB3  | 11:k3:196:MET:HB2  | 1.91                     | 0.51              |
| 11:p3:280:LEU:HD11 | 11:p3:340:ALA:HB2  | 1.91                     | 0.51              |
| 11:q3:353:GLN:HG3  | 11:q3:362:LEU:HD22 | 1.90                     | 0.51              |
| 11:s3:141:ILE:HD13 | 11:s3:165:ILE:CD1  | 2.37                     | 0.51              |
| 11:s3:275:VAL:HG21 | 11:s3:338:LEU:CD2  | 2.40                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:s3:275:VAL:HG21 | 11:s3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:t3:275:VAL:HG21 | 11:t3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:t3:275:VAL:HG21 | 11:t3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:u3:269:THR:HG22 | 11:u3:326:ALA:O    | 2.09                     | 0.51              |
| 11:u3:275:VAL:HG21 | 11:u3:338:LEU:CD2  | 2.40                     | 0.51              |
| 1:A1:283:SER:HB2   | 1:A1:369:ASP:HB2   | 1.91                     | 0.51              |
| 1:F1:301:SER:HB2   | 1:G1:359:GLN:OE1   | 2.10                     | 0.51              |
| 1:M1:374:HIS:HB3   | 1:N1:276:GLU:HB3   | 1.92                     | 0.51              |
| 1:P1:394:LYS:HG2   | 1:P1:402:LEU:HB3   | 1.91                     | 0.51              |
| 1:X1:423:SER:OG    | 1:X1:425:LYS:NZ    | 2.29                     | 0.51              |
| 1:Y1:195:VAL:HA    | 1:Y1:210:VAL:HG11  | 1.93                     | 0.51              |
| 1:b1:420:MET:SD    | 1:b1:422:PHE:HD1   | 2.33                     | 0.51              |
| 1:c1:125:GLN:NE2   | 4:J2:6:VAL:N       | 2.53                     | 0.51              |
| 1:d1:190:GLN:CD    | 1:f1:217:GLY:HA2   | 2.36                     | 0.51              |
| 1:f1:246:GLN:NE2   | 1:f1:250:GLU:OE2   | 2.43                     | 0.51              |
| 7:Z2:29:ALA:HB1    | 8:e2:57:VAL:HG21   | 1.91                     | 0.51              |
| 8:e2:133:SER:OG    | 8:e2:134:GLU:N     | 2.44                     | 0.51              |
| 9:h2:86:LEU:HD12   | 9:s2:44:LEU:HD13   | 1.91                     | 0.51              |
| 9:i2:129:VAL:HG21  | 9:s2:63:PRO:HG3    | 1.91                     | 0.51              |
| 9:r2:122:VAL:O     | 9:w2:180:ASN:ND2   | 2.43                     | 0.51              |
| 9:v2:238:ARG:O     | 9:v2:241:GLU:HB3   | 2.10                     | 0.51              |
| 9:32:233:MET:SD    | 12:B4:44:LEU:CD1   | 2.82                     | 0.51              |
| 9:42:178:PHE:CE2   | 9:42:184:LEU:HD21  | 2.46                     | 0.51              |
| 10:D3:68:ASP:O     | 10:D3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:L3:69:ARG:HG3   | 10:L3:69:ARG:O     | 2.09                     | 0.51              |
| 10:O3:101:LYS:HB2  | 10:O3:101:LYS:HZ3  | 1.74                     | 0.51              |
| 10:Z3:50:SER:HB3   | 11:a3:99:GLN:NE2   | 2.25                     | 0.51              |
| 11:a3:141:ILE:HD13 | 11:a3:165:ILE:CD1  | 2.37                     | 0.51              |
| 11:f3:275:VAL:HG21 | 11:f3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:l3:89:VAL:HG11  | 11:l3:121:LEU:CD2  | 2.40                     | 0.51              |
| 11:n3:216:LEU:HD11 | 11:n3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:o3:275:VAL:HG21 | 11:o3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:o3:275:VAL:HG21 | 11:o3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:p3:275:VAL:HG21 | 11:p3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:q3:80:GLN:HB3   | 11:r3:54:GLN:HB3   | 1.92                     | 0.51              |
| 11:q3:275:VAL:HG21 | 11:q3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:r3:275:VAL:HG21 | 11:r3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:t3:101:GLN:NE2  | 11:u3:219:ARG:HD3  | 2.25                     | 0.51              |
| 11:u3:98:ARG:HA    | 11:u3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:v3:275:VAL:HG21 | 11:v3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:w3:228:GLY:O    | 11:w3:232:GLN:HG3  | 2.08                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:x3:280:LEU:CD1  | 11:x3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:y3:98:ARG:HA    | 11:y3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:y3:208:ARG:HH21 | 11:y3:238:ASP:HB2  | 1.76                     | 0.51              |
| 12:E4:132:PRO:HD3  | 12:E4:158:ALA:HB2  | 1.93                     | 0.51              |
| 1:C1:143:THR:O     | 1:C1:146:THR:OG1   | 2.27                     | 0.51              |
| 1:C1:420:MET:HE1   | 1:C1:430:LEU:HB2   | 1.92                     | 0.51              |
| 1:F1:389:VAL:HB    | 1:F1:432:VAL:HG13  | 1.93                     | 0.51              |
| 1:K1:303:GLN:HG3   | 1:L1:357:SER:HB2   | 1.92                     | 0.51              |
| 1:L1:392:ASN:OD1   | 1:L1:393:TYR:N     | 2.43                     | 0.51              |
| 1:Q1:147:LEU:O     | 1:Q1:149:PRO:HD2   | 2.10                     | 0.51              |
| 1:U1:214:ASP:OD1   | 1:U1:216:SER:N     | 2.37                     | 0.51              |
| 2:A2:230:ASP:OD2   | 2:A2:233:GLN:HB2   | 2.10                     | 0.51              |
| 2:E2:38:TRP:NE1    | 5:L2:43:ASP:OD1    | 2.23                     | 0.51              |
| 2:E2:207:LEU:O     | 3:F2:206:ARG:NH1   | 2.43                     | 0.51              |
| 7:V2:77:VAL:HG13   | 7:V2:93:MET:HG3    | 1.93                     | 0.51              |
| 8:d2:35:ARG:HE     | 8:d2:210:ASN:ND2   | 2.07                     | 0.51              |
| 9:g2:46:TYR:HA     | 9:g2:69:GLY:HA2    | 1.91                     | 0.51              |
| 9:22:238:ARG:CZ    | 12:A4:55:ASN:ND2   | 2.23                     | 0.51              |
| 9:42:142:ILE:HG23  | 9:42:159:VAL:HG11  | 1.93                     | 0.51              |
| 10:F3:80:ILE:HD13  | 10:F3:195:VAL:CG1  | 2.39                     | 0.51              |
| 10:G3:80:ILE:HD13  | 10:G3:195:VAL:CG1  | 2.39                     | 0.51              |
| 10:J3:69:ARG:HG3   | 10:J3:69:ARG:O     | 2.09                     | 0.51              |
| 10:K3:51:ILE:CG1   | 11:m3:175:LEU:HD11 | 2.40                     | 0.51              |
| 10:N3:68:ASP:O     | 10:N3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:P3:112:TYR:CE1  | 10:P3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:S3:82:LEU:O     | 10:S3:197:SER:OG   | 2.20                     | 0.51              |
| 10:T3:68:ASP:O     | 10:T3:69:ARG:HG2   | 2.10                     | 0.51              |
| 11:a3:54:GLN:HB3   | 11:z3:80:GLN:HB3   | 1.92                     | 0.51              |
| 11:a3:208:ARG:HH21 | 11:a3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:b3:208:ARG:HH21 | 11:b3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:c3:216:LEU:HD11 | 11:c3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:c3:280:LEU:CD1  | 11:c3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:f3:280:LEU:CD1  | 11:f3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:h3:280:LEU:CD1  | 11:h3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:j3:275:VAL:HG21 | 11:j3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:o3:280:LEU:CD1  | 11:o3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:q3:196:MET:HA   | 11:q3:196:MET:CE   | 2.34                     | 0.51              |
| 11:q3:275:VAL:HG21 | 11:q3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:u3:101:GLN:NE2  | 11:v3:219:ARG:HD3  | 2.25                     | 0.51              |
| 11:u3:208:ARG:HH21 | 11:u3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:v3:208:ARG:HH21 | 11:v3:238:ASP:HB2  | 1.76                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:v3:280:LEU:CD1  | 11:v3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:w3:89:VAL:HG11  | 11:w3:121:LEU:CD2  | 2.40                     | 0.51              |
| 11:x3:275:VAL:HG21 | 11:x3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:y3:196:MET:HA   | 11:y3:196:MET:CE   | 2.34                     | 0.51              |
| 11:y3:216:LEU:HD11 | 11:y3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:y3:280:LEU:HD11 | 11:y3:340:ALA:HB2  | 1.91                     | 0.51              |
| 1:A1:234:GLN:HG2   | 1:A1:272:PHE:CD2   | 2.45                     | 0.51              |
| 1:C1:163:SER:O     | 1:C1:169:GLN:NE2   | 2.34                     | 0.51              |
| 1:F1:294:ARG:NH1   | 1:G1:368:VAL:HG22  | 2.26                     | 0.51              |
| 1:G1:173:SER:HA    | 1:G1:209:ASN:HB3   | 1.92                     | 0.51              |
| 1:T1:165:PHE:HD2   | 3:F2:167:ASN:ND2   | 2.08                     | 0.51              |
| 1:V1:394:LYS:HG2   | 1:V1:402:LEU:HB2   | 1.92                     | 0.51              |
| 1:f1:287:ASP:OD2   | 1:f1:290:LYS:NZ    | 2.32                     | 0.51              |
| 1:g1:188:GLU:HA    | 1:g1:191:ILE:HD12  | 1.92                     | 0.51              |
| 1:h1:246:GLN:O     | 1:h1:250:GLU:HG2   | 2.10                     | 0.51              |
| 2:D2:115:PRO:O     | 2:D2:121:ILE:HB    | 2.11                     | 0.51              |
| 2:E2:41:SER:O      | 2:E2:43:GLN:N      | 2.43                     | 0.51              |
| 4:J2:45:ASN:HA     | 4:J2:49:LEU:HD12   | 1.92                     | 0.51              |
| 8:f2:228:GLU:HG2   | 9:k2:256:LYS:HG3   | 1.91                     | 0.51              |
| 9:g2:95:VAL:O      | 9:g2:118:GLY:HA3   | 2.10                     | 0.51              |
| 9:j2:94:ASP:OD1    | 9:j2:95:VAL:N      | 2.43                     | 0.51              |
| 9:l2:241:GLU:HG2   | 9:q2:256:LYS:HG2   | 1.90                     | 0.51              |
| 9:o2:189:GLU:HA    | 9:s2:42:GLU:CG     | 2.39                     | 0.51              |
| 10:E3:51:ILE:CG1   | 11:g3:175:LEU:HD11 | 2.40                     | 0.51              |
| 10:O3:68:ASP:O     | 10:O3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:W3:68:ASP:O     | 10:W3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:X3:51:ILE:CG1   | 11:z3:175:LEU:HD11 | 2.37                     | 0.51              |
| 11:a3:216:LEU:HD11 | 11:a3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:a3:219:ARG:HD2  | 11:z3:96:PHE:O     | 2.11                     | 0.51              |
| 11:a3:275:VAL:HG21 | 11:a3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:b3:275:VAL:HG21 | 11:b3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:h3:98:ARG:HA    | 11:h3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:i3:275:VAL:HG21 | 11:i3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:k3:216:LEU:HD11 | 11:k3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:m3:98:ARG:HA    | 11:m3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:n3:275:VAL:HG21 | 11:n3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:n3:275:VAL:HG21 | 11:n3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:q3:280:LEU:HD11 | 11:q3:340:ALA:HB2  | 1.92                     | 0.51              |
| 11:r3:275:VAL:HG21 | 11:r3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:w3:208:ARG:HH21 | 11:w3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:w3:280:LEU:CD1  | 11:w3:340:ALA:HB2  | 2.41                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:x3:208:ARG:HH21 | 11:x3:238:ASP:HB2 | 1.76                     | 0.51              |
| 11:z3:208:ARG:HH21 | 11:z3:238:ASP:HB2 | 1.76                     | 0.51              |
| 1:A1:267:THR:OG1   | 1:A1:386:SER:HB2  | 2.09                     | 0.51              |
| 1:E1:188:GLU:HA    | 1:E1:191:ILE:HD12 | 1.92                     | 0.51              |
| 1:H1:294:ARG:NH1   | 1:I1:366:TYR:O    | 2.44                     | 0.51              |
| 1:L1:376:LYS:C     | 1:L1:376:LYS:HD3  | 2.36                     | 0.51              |
| 1:M1:394:LYS:HG2   | 1:M1:402:LEU:HB3  | 1.92                     | 0.51              |
| 1:M1:410:LYS:O     | 1:M1:413:GLU:HG3  | 2.10                     | 0.51              |
| 1:P1:283:SER:HB2   | 1:P1:369:ASP:HB3  | 1.93                     | 0.51              |
| 1:T1:152:SER:O     | 1:T1:178:VAL:HA   | 2.09                     | 0.51              |
| 1:Y1:164:LEU:HD11  | 2:E2:152:ARG:HD2  | 1.79                     | 0.51              |
| 1:c1:420:MET:HE3   | 1:c1:422:PHE:HD1  | 1.76                     | 0.51              |
| 2:C2:236:MET:SD    | 2:D2:150:PHE:CZ   | 3.03                     | 0.51              |
| 9:k2:89:THR:HG23   | 9:k2:91:ASN:H     | 1.75                     | 0.51              |
| 9:t2:91:ASN:ND2    | 9:y2:80:LEU:HD13  | 2.26                     | 0.51              |
| 9:y2:12:LEU:HD12   | 9:y2:240:TYR:CZ   | 2.46                     | 0.51              |
| 9:y2:159:VAL:HG13  | 9:y2:170:VAL:HG11 | 1.91                     | 0.51              |
| 9:y2:240:TYR:CD1   | 9:42:253:MET:HE1  | 2.46                     | 0.51              |
| 9:y2:248:SER:OG    | 9:42:260:LEU:HD12 | 2.10                     | 0.51              |
| 9:12:127:GLN:HG2   | 9:12:135:GLN:HE22 | 1.76                     | 0.51              |
| 10:B3:112:TYR:CE1  | 10:B3:113:LEU:HG  | 2.46                     | 0.51              |
| 10:H3:69:ARG:HG3   | 10:H3:69:ARG:O    | 2.09                     | 0.51              |
| 10:V3:68:ASP:O     | 10:V3:69:ARG:HG2  | 2.10                     | 0.51              |
| 10:Z3:112:TYR:CE1  | 10:Z3:113:LEU:HG  | 2.46                     | 0.51              |
| 11:a3:280:LEU:CD1  | 11:a3:340:ALA:HB2 | 2.41                     | 0.51              |
| 11:b3:141:ILE:HD13 | 11:b3:165:ILE:CD1 | 2.38                     | 0.51              |
| 11:c3:98:ARG:HA    | 11:c3:174:GLU:OE2 | 2.11                     | 0.51              |
| 11:c3:208:ARG:HH21 | 11:c3:238:ASP:HB2 | 1.76                     | 0.51              |
| 11:d3:96:PHE:O     | 11:e3:219:ARG:HD2 | 2.11                     | 0.51              |
| 11:f3:193:ASP:HB3  | 11:f3:196:MET:HB2 | 1.91                     | 0.51              |
| 11:g3:275:VAL:HG21 | 11:g3:338:LEU:CD2 | 2.40                     | 0.51              |
| 11:h3:193:ASP:HB3  | 11:h3:196:MET:HB2 | 1.91                     | 0.51              |
| 11:h3:269:THR:HG22 | 11:h3:326:ALA:O   | 2.09                     | 0.51              |
| 11:j3:269:THR:HG22 | 11:j3:326:ALA:O   | 2.09                     | 0.51              |
| 11:l3:280:LEU:CD1  | 11:l3:340:ALA:HB2 | 2.41                     | 0.51              |
| 11:m3:89:VAL:HG11  | 11:m3:121:LEU:CD2 | 2.40                     | 0.51              |
| 11:m3:275:VAL:HG21 | 11:m3:338:LEU:CD2 | 2.40                     | 0.51              |
| 11:n3:269:THR:HG22 | 11:n3:326:ALA:O   | 2.09                     | 0.51              |
| 11:p3:98:ARG:HA    | 11:p3:174:GLU:OE2 | 2.11                     | 0.51              |
| 11:p3:280:LEU:CD1  | 11:p3:340:ALA:HB2 | 2.41                     | 0.51              |
| 11:q3:98:ARG:HA    | 11:q3:174:GLU:OE2 | 2.11                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:t3:98:ARG:HA    | 11:t3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:t3:208:ARG:HH21 | 11:t3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:t3:216:LEU:HD11 | 11:t3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:t3:280:LEU:HD11 | 11:t3:340:ALA:HB2  | 1.91                     | 0.51              |
| 11:u3:275:VAL:HG21 | 11:u3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:v3:96:PHE:O     | 11:w3:219:ARG:HD2  | 2.11                     | 0.51              |
| 11:y3:141:ILE:HD13 | 11:y3:165:ILE:CD1  | 2.37                     | 0.51              |
| 11:y3:275:VAL:HG21 | 11:y3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:z3:141:ILE:HD13 | 11:z3:165:ILE:CD1  | 2.38                     | 0.51              |
| 12:C4:215:LEU:HD11 | 12:C4:225:LEU:HD23 | 1.93                     | 0.51              |
| 12:D4:153:ILE:HG23 | 12:D4:163:PHE:HE2  | 1.76                     | 0.51              |
| 1:C1:252:ILE:HG12  | 1:D1:265:GLN:HG3   | 1.93                     | 0.51              |
| 1:E1:253:LEU:HD11  | 1:E1:412:ILE:HG23  | 1.92                     | 0.51              |
| 1:H1:205:LEU:HD21  | 1:H1:210:VAL:HG13  | 1.91                     | 0.51              |
| 1:M1:363:THR:HG21  | 6:Q2:73:ILE:HD12   | 1.75                     | 0.51              |
| 1:N1:166:VAL:CG2   | 2:A2:162:PRO:CA    | 2.89                     | 0.51              |
| 1:O1:166:VAL:HA    | 2:A2:152:ARG:CD    | 2.40                     | 0.51              |
| 1:P1:299:ASN:HB2   | 1:P1:361:ASN:HB3   | 1.93                     | 0.51              |
| 1:T1:138:GLY:O     | 1:T1:142:ARG:HG3   | 2.10                     | 0.51              |
| 1:Y1:214:ASP:HB3   | 1:Y1:218:HIS:HB2   | 1.92                     | 0.51              |
| 1:c1:388:ALA:HA    | 1:c1:431:ASN:O     | 2.10                     | 0.51              |
| 1:h1:140:LEU:O     | 1:h1:143:THR:OG1   | 2.25                     | 0.51              |
| 2:C2:181:THR:O     | 2:C2:185:ILE:HG12  | 2.10                     | 0.51              |
| 3:F2:254:ILE:HA    | 3:F2:257:GLU:HB3   | 1.93                     | 0.51              |
| 5:K2:83:GLN:HG2    | 5:P2:98:GLU:OE2    | 2.11                     | 0.51              |
| 6:Q2:42:ASP:HB2    | 6:Q2:88:ARG:HE     | 1.76                     | 0.51              |
| 8:b2:164:VAL:HG11  | 8:b2:193:LEU:HD13  | 1.93                     | 0.51              |
| 8:e2:82:LEU:HD21   | 8:e2:88:LEU:HG     | 1.93                     | 0.51              |
| 9:g2:140:ILE:HD12  | 9:g2:173:LEU:HD13  | 1.93                     | 0.51              |
| 9:j2:98:LYS:HE3    | 9:u2:45:LEU:HD23   | 1.92                     | 0.51              |
| 9:l2:35:LYS:NZ     | 9:l2:220:GLU:OE2   | 2.44                     | 0.51              |
| 9:x2:26:LEU:HD23   | 9:32:246:ALA:HB2   | 1.92                     | 0.51              |
| 9:x2:238:ARG:O     | 9:x2:242:ILE:HG12  | 2.10                     | 0.51              |
| 9:42:233:MET:HE3   | 12:C4:58:LEU:HD11  | 1.92                     | 0.51              |
| 10:G3:101:LYS:HB2  | 10:G3:101:LYS:HZ3  | 1.75                     | 0.51              |
| 10:K3:101:LYS:HZ3  | 10:K3:101:LYS:HB2  | 1.76                     | 0.51              |
| 11:b3:98:ARG:HA    | 11:b3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:c3:141:ILE:HD13 | 11:c3:165:ILE:CD1  | 2.38                     | 0.51              |
| 11:d3:208:ARG:HH21 | 11:d3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:d3:254:VAL:CG2  | 11:e3:355:ALA:HB2  | 2.41                     | 0.51              |
| 11:e3:98:ARG:HA    | 11:e3:174:GLU:OE2  | 2.11                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:e3:280:LEU:CD1  | 11:e3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:g3:101:GLN:NE2  | 11:h3:219:ARG:HD3  | 2.24                     | 0.51              |
| 11:g3:275:VAL:HG21 | 11:g3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:i3:101:GLN:NE2  | 11:j3:219:ARG:HD3  | 2.25                     | 0.51              |
| 11:j3:98:ARG:HA    | 11:j3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:j3:216:LEU:HD11 | 11:j3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:k3:275:VAL:HG21 | 11:k3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:n3:280:LEU:CD1  | 11:n3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:o3:101:GLN:NE2  | 11:p3:219:ARG:HD3  | 2.25                     | 0.51              |
| 11:s3:280:LEU:HD11 | 11:s3:340:ALA:HB2  | 1.91                     | 0.51              |
| 11:x3:280:LEU:HD11 | 11:x3:340:ALA:HB2  | 1.91                     | 0.51              |
| 11:y3:280:LEU:CD1  | 11:y3:340:ALA:HB2  | 2.41                     | 0.51              |
| 12:A4:108:ILE:HD11 | 12:A4:125:PHE:HB3  | 1.93                     | 0.51              |
| 1:H1:193:ALA:HA    | 1:I1:219:LEU:HD21  | 1.93                     | 0.51              |
| 1:P1:389:VAL:HB    | 1:P1:432:VAL:HG13  | 1.92                     | 0.51              |
| 1:S1:420:MET:HE1   | 1:S1:430:LEU:HB2   | 1.93                     | 0.51              |
| 1:U1:407:ASP:O     | 1:U1:410:LYS:HG3   | 2.11                     | 0.51              |
| 1:W1:213:VAL:HG22  | 1:W1:219:LEU:HD23  | 1.92                     | 0.51              |
| 1:X1:414:ASP:HB3   | 1:Y1:431:ASN:ND2   | 2.24                     | 0.51              |
| 1:g1:287:ASP:HB3   | 1:g1:290:LYS:HG2   | 1.93                     | 0.51              |
| 1:g1:407:ASP:OD1   | 1:g1:408:GLN:N     | 2.44                     | 0.51              |
| 2:A2:57:ILE:HG22   | 2:A2:58:LEU:HD22   | 1.93                     | 0.51              |
| 2:C2:100:ILE:HG21  | 2:C2:243:PHE:HD2   | 1.76                     | 0.51              |
| 2:E2:213:PRO:CD    | 3:F2:213:ILE:HD13  | 2.41                     | 0.51              |
| 3:F2:216:ILE:HD11  | 4:G2:33:LEU:HA     | 1.93                     | 0.51              |
| 7:V2:43:ARG:NE     | 7:V2:74:GLU:OE2    | 2.44                     | 0.51              |
| 7:a2:6:ILE:HD13    | 7:a2:122:VAL:HG21  | 1.93                     | 0.51              |
| 8:b2:152:PRO:HB3   | 9:r2:51:GLN:NE2    | 2.26                     | 0.51              |
| 9:l2:36:ARG:HB3    | 9:l2:224:VAL:HG22  | 1.91                     | 0.51              |
| 9:m2:98:LYS:HB2    | 9:m2:213:LEU:HB2   | 1.92                     | 0.51              |
| 9:n2:12:LEU:HD12   | 9:n2:243:ASN:HB3   | 1.92                     | 0.51              |
| 9:n2:227:ALA:HA    | 9:z2:257:LEU:HD21  | 1.92                     | 0.51              |
| 9:q2:115:THR:HB    | 9:q2:191:LEU:HD23  | 1.92                     | 0.51              |
| 9:s2:36:ARG:HH21   | 9:s2:80:LEU:HB2    | 1.76                     | 0.51              |
| 9:22:50:ARG:HG3    | 9:22:66:LEU:HB3    | 1.92                     | 0.51              |
| 10:C3:51:ILE:CG1   | 11:e3:175:LEU:HD11 | 2.40                     | 0.51              |
| 10:C3:68:ASP:O     | 10:C3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:F3:68:ASP:O     | 10:F3:69:ARG:HG2   | 2.10                     | 0.51              |
| 10:H3:80:ILE:HD13  | 10:H3:195:VAL:CG1  | 2.39                     | 0.51              |
| 10:N3:112:TYR:CE1  | 10:N3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:Q3:112:TYR:CE1  | 10:Q3:113:LEU:HG   | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:W3:112:TYR:CE1  | 10:W3:113:LEU:HG   | 2.46                     | 0.51              |
| 11:d3:280:LEU:CD1  | 11:d3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:j3:42:VAL:CG1   | 11:j3:119:GLY:HA3  | 2.41                     | 0.51              |
| 11:k3:98:ARG:HA    | 11:k3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:m3:101:GLN:NE2  | 11:n3:219:ARG:HD3  | 2.24                     | 0.51              |
| 11:m3:275:VAL:HG21 | 11:m3:338:LEU:HD21 | 1.92                     | 0.51              |
| 11:n3:89:VAL:HG11  | 11:n3:121:LEU:CD2  | 2.40                     | 0.51              |
| 11:r3:208:ARG:HH21 | 11:r3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:r3:280:LEU:HD11 | 11:r3:340:ALA:HB2  | 1.91                     | 0.51              |
| 11:s3:208:ARG:HH21 | 11:s3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:t3:280:LEU:CD1  | 11:t3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:u3:280:LEU:HD11 | 11:u3:340:ALA:HB2  | 1.91                     | 0.51              |
| 11:u3:280:LEU:CD1  | 11:u3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:v3:254:VAL:CG2  | 11:w3:355:ALA:HB2  | 2.41                     | 0.51              |
| 11:w3:101:GLN:NE2  | 11:x3:219:ARG:HD3  | 2.24                     | 0.51              |
| 11:x3:98:ARG:HA    | 11:x3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:x3:141:ILE:HD13 | 11:x3:165:ILE:CD1  | 2.37                     | 0.51              |
| 1:E1:162:PRO:HB2   | 4:H2:86:TYR:HH     | 1.66                     | 0.51              |
| 1:G1:190:GLN:HG2   | 1:H1:217:GLY:HA3   | 1.92                     | 0.51              |
| 1:G1:252:ILE:O     | 1:G1:255:PRO:HD2   | 2.10                     | 0.51              |
| 1:I1:139:GLU:HG3   | 1:K1:156:HIS:HE1   | 1.76                     | 0.51              |
| 1:N1:393:TYR:CZ    | 1:N1:436:PRO:HD3   | 2.46                     | 0.51              |
| 1:T1:373:ARG:HH21  | 1:U1:275:LYS:HE2   | 1.76                     | 0.51              |
| 1:W1:199:SER:HA    | 1:W1:205:LEU:HD23  | 1.93                     | 0.51              |
| 1:Z1:249:ILE:HD12  | 1:Z1:416:THR:HG23  | 1.91                     | 0.51              |
| 1:c1:149:PRO:HA    | 1:c1:181:GLU:HG2   | 1.93                     | 0.51              |
| 1:h1:271:ASP:OD1   | 1:h1:381:ASP:N     | 2.40                     | 0.51              |
| 2:C2:37:SER:HA     | 2:C2:124:GLN:OE1   | 2.10                     | 0.51              |
| 2:C2:227:VAL:HG11  | 2:D2:187:PHE:HE2   | 1.76                     | 0.51              |
| 2:D2:150:PHE:CZ    | 2:D2:172:PRO:HB2   | 2.46                     | 0.51              |
| 2:E2:114:GLN:HB2   | 2:E2:115:PRO:HD3   | 1.92                     | 0.51              |
| 6:Q2:61:GLY:O      | 6:Q2:79:SER:HA     | 2.10                     | 0.51              |
| 7:a2:110:ARG:NH2   | 9:g2:255:GLN:OE1   | 2.44                     | 0.51              |
| 9:l2:44:LEU:HB2    | 9:l2:70:THR:O      | 2.10                     | 0.51              |
| 9:o2:127:GLN:NE2   | 9:o2:141:THR:OG1   | 2.43                     | 0.51              |
| 9:o2:185:GLU:HB2   | 9:s2:52:PRO:HG2    | 1.92                     | 0.51              |
| 9:o2:238:ARG:NH1   | 9:o2:241:GLU:OE1   | 2.42                     | 0.51              |
| 9:r2:174:ASN:HA    | 9:r2:206:PRO:HD3   | 1.92                     | 0.51              |
| 9:s2:141:THR:HG21  | 11:p3:78:ASN:HD22  | 1.75                     | 0.51              |
| 9:x2:142:ILE:HG23  | 9:x2:159:VAL:HG11  | 1.92                     | 0.51              |
| 10:D3:112:TYR:CE1  | 10:D3:113:LEU:HG   | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:H3:112:TYR:CE1  | 10:H3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:I3:112:TYR:CE1  | 10:I3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:J3:112:TYR:CE1  | 10:J3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:M3:69:ARG:HG3   | 10:M3:69:ARG:O     | 2.09                     | 0.51              |
| 10:M3:112:TYR:CE1  | 10:M3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:P3:69:ARG:HG3   | 10:P3:69:ARG:O     | 2.09                     | 0.51              |
| 10:P3:166:GLU:OE2  | 10:P3:168:GLN:NE2  | 2.27                     | 0.51              |
| 10:Q3:51:ILE:CG1   | 11:s3:175:LEU:HD11 | 2.41                     | 0.51              |
| 10:R3:112:TYR:CE1  | 10:R3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:S3:112:TYR:CE1  | 10:S3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:S3:166:GLU:OE2  | 10:S3:168:GLN:NE2  | 2.27                     | 0.51              |
| 10:Y3:112:TYR:CE1  | 10:Y3:113:LEU:HG   | 2.46                     | 0.51              |
| 11:d3:216:LEU:HD11 | 11:d3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:f3:98:ARG:HA    | 11:f3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:l3:42:VAL:CG1   | 11:l3:119:GLY:HA3  | 2.41                     | 0.51              |
| 11:l3:245:ASN:OD1  | 11:l3:245:ASN:N    | 2.33                     | 0.51              |
| 11:l3:269:THR:HG22 | 11:l3:326:ALA:O    | 2.09                     | 0.51              |
| 11:m3:280:LEU:CD1  | 11:m3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:o3:216:LEU:HD11 | 11:o3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:p3:254:VAL:CG2  | 11:q3:355:ALA:HB2  | 2.41                     | 0.51              |
| 11:q3:42:VAL:CG1   | 11:q3:119:GLY:HA3  | 2.41                     | 0.51              |
| 11:q3:280:LEU:CD1  | 11:q3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:v3:89:VAL:HG11  | 11:v3:121:LEU:CD2  | 2.40                     | 0.51              |
| 11:x3:42:VAL:CG1   | 11:x3:119:GLY:HA3  | 2.41                     | 0.51              |
| 11:y3:94:PRO:HB2   | 11:z3:219:ARG:NH2  | 2.25                     | 0.51              |
| 11:z3:245:ASN:OD1  | 11:z3:245:ASN:N    | 2.33                     | 0.51              |
| 12:A4:128:GLU:HG3  | 12:A4:160:VAL:HG22 | 1.93                     | 0.51              |
| 12:A4:141:THR:HG22 | 12:A4:147:VAL:HA   | 1.91                     | 0.51              |
| 12:C4:149:ARG:NH1  | 12:C4:168:LYS:O    | 2.34                     | 0.51              |
| 1:A1:275:LYS:HB2   | 1:A1:377:MET:HB2   | 1.91                     | 0.51              |
| 1:H1:139:GLU:O     | 1:H1:143:THR:HG23  | 2.11                     | 0.51              |
| 1:I1:281:HIS:CE1   | 1:I1:282:TYR:O     | 2.64                     | 0.51              |
| 1:L1:378:ASN:ND2   | 1:L1:381:ASP:OD1   | 2.38                     | 0.51              |
| 1:O1:139:GLU:CD    | 1:Q1:154:ARG:HH11  | 2.19                     | 0.51              |
| 1:R1:269:GLN:HG3   | 1:R1:384:ARG:CZ    | 2.40                     | 0.51              |
| 1:T1:294:ARG:CG    | 6:R2:66:THR:HG22   | 2.32                     | 0.51              |
| 1:U1:159:MET:CE    | 1:U1:172:PRO:HB2   | 2.40                     | 0.51              |
| 1:U1:363:THR:CG2   | 6:R2:65:LEU:HD23   | 2.38                     | 0.51              |
| 1:d1:164:LEU:HD12  | 2:D2:148:ALA:CA    | 2.36                     | 0.51              |
| 1:h1:165:PHE:C     | 1:h1:167:ARG:HH12  | 2.19                     | 0.51              |
| 2:A2:62:THR:HB     | 2:A2:101:MET:HE3   | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B2:49:THR:O      | 2:B2:52:THR:HG22   | 2.11                     | 0.51              |
| 2:E2:42:VAL:HG13   | 5:L2:42:LEU:HD12   | 1.93                     | 0.51              |
| 2:E2:110:VAL:HA    | 2:E2:114:GLN:OE1   | 2.11                     | 0.51              |
| 7:X2:113:GLN:CD    | 8:c2:243:ARG:HH11  | 2.19                     | 0.51              |
| 8:d2:133:SER:OG    | 8:d2:134:GLU:N     | 2.44                     | 0.51              |
| 8:f2:133:SER:OG    | 8:f2:134:GLU:N     | 2.44                     | 0.51              |
| 9:p2:149:ILE:HG13  | 9:p2:159:VAL:HG12  | 1.93                     | 0.51              |
| 9:q2:121:GLN:NE2   | 9:12:64:SER:OG     | 2.43                     | 0.51              |
| 10:G3:112:TYR:CE1  | 10:G3:113:LEU:HG   | 2.46                     | 0.51              |
| 10:O3:166:GLU:OE2  | 10:O3:168:GLN:NE2  | 2.27                     | 0.51              |
| 10:Q3:166:GLU:OE2  | 10:Q3:168:GLN:NE2  | 2.27                     | 0.51              |
| 10:U3:51:ILE:CG1   | 11:w3:175:LEU:HD11 | 2.40                     | 0.51              |
| 11:a3:96:PHE:O     | 11:b3:219:ARG:HD2  | 2.11                     | 0.51              |
| 11:a3:275:VAL:HG21 | 11:a3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:c3:275:VAL:HG21 | 11:c3:338:LEU:CD2  | 2.40                     | 0.51              |
| 11:e3:251:ALA:HB1  | 11:e3:360:ALA:HB2  | 1.93                     | 0.51              |
| 11:g3:280:LEU:CD1  | 11:g3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:h3:28:VAL:HB    | 11:h3:31:VAL:HG23  | 1.93                     | 0.51              |
| 11:h3:216:LEU:HD11 | 11:h3:222:GLN:HB2  | 1.92                     | 0.51              |
| 11:m3:251:ALA:HB1  | 11:m3:360:ALA:HB2  | 1.93                     | 0.51              |
| 11:n3:208:ARG:HH21 | 11:n3:238:ASP:HB2  | 1.76                     | 0.51              |
| 11:o3:98:ARG:HA    | 11:o3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:p3:89:VAL:HG11  | 11:p3:121:LEU:CD2  | 2.40                     | 0.51              |
| 11:r3:98:ARG:HA    | 11:r3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:r3:280:LEU:CD1  | 11:r3:340:ALA:HB2  | 2.41                     | 0.51              |
| 11:v3:42:VAL:CG1   | 11:v3:119:GLY:HA3  | 2.41                     | 0.51              |
| 11:v3:98:ARG:HA    | 11:v3:174:GLU:OE2  | 2.11                     | 0.51              |
| 11:v3:280:LEU:HD11 | 11:v3:340:ALA:HB2  | 1.91                     | 0.51              |
| 11:w3:93:TYR:OH    | 11:w3:173:ARG:O    | 2.25                     | 0.51              |
| 11:z3:28:VAL:HB    | 11:z3:31:VAL:HG23  | 1.94                     | 0.51              |
| 11:z3:216:LEU:HD11 | 11:z3:222:GLN:HB2  | 1.92                     | 0.51              |
| 12:D4:140:ILE:HG12 | 12:D4:182:ILE:HD13 | 1.93                     | 0.51              |
| 12:E4:169:GLN:HB3  | 12:E4:175:VAL:HG12 | 1.93                     | 0.51              |
| 1:H1:299:ASN:N     | 1:H1:361:ASN:O     | 2.39                     | 0.50              |
| 1:I1:303:GLN:HB2   | 1:I1:357:SER:H     | 1.75                     | 0.50              |
| 1:L1:287:ASP:OD1   | 1:L1:288:ALA:N     | 2.44                     | 0.50              |
| 1:N1:196:HIS:HB2   | 1:O1:219:LEU:HD21  | 1.94                     | 0.50              |
| 1:R1:233:ALA:HA    | 1:R1:236:LYS:HE2   | 1.92                     | 0.50              |
| 1:T1:282:TYR:CZ    | 1:T1:370:ARG:HD3   | 2.45                     | 0.50              |
| 1:Z1:276:GLU:OE2   | 1:Z1:374:HIS:NE2   | 2.44                     | 0.50              |
| 1:h1:194:VAL:HG21  | 1:h1:212:LEU:HD22  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:C2:60:MET:HG3    | 2:C2:65:THR:HG22   | 1.92                     | 0.50              |
| 2:C2:92:LEU:CD2    | 2:C2:236:MET:CE    | 2.87                     | 0.50              |
| 5:M2:82:MET:O      | 5:M2:86:ILE:HG12   | 2.12                     | 0.50              |
| 6:Q2:31:ALA:HB1    | 7:V2:13:ALA:HB2    | 1.93                     | 0.50              |
| 7:V2:3:LEU:O       | 7:V2:6:ILE:HG22    | 2.10                     | 0.50              |
| 7:a2:113:GLN:OE1   | 8:f2:243:ARG:NH1   | 2.45                     | 0.50              |
| 8:b2:218:THR:HG23  | 9:h2:9:LYS:HE3     | 1.93                     | 0.50              |
| 9:h2:95:VAL:O      | 9:h2:118:GLY:HA3   | 2.11                     | 0.50              |
| 9:o2:27:ALA:C      | 9:s2:72:VAL:HG21   | 2.35                     | 0.50              |
| 9:r2:138:PRO:HG3   | 11:m3:54:GLN:HE21  | 1.65                     | 0.50              |
| 9:12:42:GLU:HB2    | 9:12:75:VAL:HB     | 1.93                     | 0.50              |
| 10:B3:70:ARG:NH2   | 11:a3:72:THR:OG1   | 2.40                     | 0.50              |
| 10:C3:80:ILE:HD13  | 10:C3:195:VAL:CG1  | 2.39                     | 0.50              |
| 10:E3:80:ILE:HD13  | 10:E3:195:VAL:CG1  | 2.39                     | 0.50              |
| 10:T3:112:TYR:CE1  | 10:T3:113:LEU:HG   | 2.46                     | 0.50              |
| 11:b3:28:VAL:HB    | 11:b3:31:VAL:HG23  | 1.93                     | 0.50              |
| 11:d3:101:GLN:NE2  | 11:e3:219:ARG:HD3  | 2.26                     | 0.50              |
| 11:e3:208:ARG:HH21 | 11:e3:238:ASP:HB2  | 1.76                     | 0.50              |
| 11:e3:275:VAL:HG21 | 11:e3:338:LEU:CD2  | 2.40                     | 0.50              |
| 11:f3:28:VAL:HB    | 11:f3:31:VAL:HG23  | 1.94                     | 0.50              |
| 11:f3:216:LEU:HD11 | 11:f3:222:GLN:HB2  | 1.92                     | 0.50              |
| 11:f3:251:ALA:HB1  | 11:f3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:f3:254:VAL:CG2  | 11:g3:355:ALA:HB2  | 2.41                     | 0.50              |
| 11:g3:28:VAL:HB    | 11:g3:31:VAL:HG23  | 1.94                     | 0.50              |
| 11:l3:275:VAL:HG21 | 11:l3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:m3:208:ARG:HH21 | 11:m3:238:ASP:HB2  | 1.76                     | 0.50              |
| 11:n3:101:GLN:NE2  | 11:o3:219:ARG:HD3  | 2.25                     | 0.50              |
| 11:n3:251:ALA:HB1  | 11:n3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:o3:42:VAL:CG1   | 11:o3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:o3:96:PHE:O     | 11:p3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:r3:101:GLN:NE2  | 11:s3:219:ARG:HD3  | 2.26                     | 0.50              |
| 11:t3:42:VAL:CG1   | 11:t3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:t3:141:ILE:HD13 | 11:t3:165:ILE:CD1  | 2.38                     | 0.50              |
| 11:u3:89:VAL:HG11  | 11:u3:121:LEU:CD2  | 2.40                     | 0.50              |
| 11:x3:101:GLN:NE2  | 11:y3:219:ARG:HD3  | 2.25                     | 0.50              |
| 11:y3:28:VAL:HB    | 11:y3:31:VAL:HG23  | 1.94                     | 0.50              |
| 11:z3:98:ARG:HA    | 11:z3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:z3:280:LEU:CD1  | 11:z3:340:ALA:HB2  | 2.41                     | 0.50              |
| 12:A4:106:THR:HG22 | 12:A4:197:PRO:HG2  | 1.93                     | 0.50              |
| 12:E4:57:GLU:HA    | 12:E4:61:GLN:HG2   | 1.93                     | 0.50              |
| 1:H1:252:ILE:HB    | 1:I1:265:GLN:HG3   | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:I1:294:ARG:NE    | 1:I1:367:GLU:OE1   | 2.37                     | 0.50              |
| 1:L1:257:VAL:O     | 1:L1:261:ASN:ND2   | 2.40                     | 0.50              |
| 1:L1:393:TYR:HB3   | 1:L1:402:LEU:N     | 2.26                     | 0.50              |
| 1:d1:199:SER:HA    | 1:d1:205:LEU:HD23  | 1.92                     | 0.50              |
| 1:e1:240:ASP:OD2   | 1:e1:244:ARG:NH2   | 2.44                     | 0.50              |
| 1:f1:165:PHE:HE1   | 2:D2:148:ALA:HB3   | 1.75                     | 0.50              |
| 1:f1:418:GLU:HB3   | 1:g1:388:ALA:HB2   | 1.93                     | 0.50              |
| 1:f1:424:ASP:OD2   | 1:f1:424:ASP:N     | 2.41                     | 0.50              |
| 5:K2:79:SER:O      | 5:K2:83:GLN:HG3    | 2.11                     | 0.50              |
| 6:S2:88:ARG:NH1    | 6:S2:105:GLU:OE2   | 2.45                     | 0.50              |
| 9:p2:254:LEU:O     | 9:p2:258:THR:HG23  | 2.12                     | 0.50              |
| 9:t2:106:MET:HG3   | 11:v3:54:GLN:HE21  | 1.63                     | 0.50              |
| 9:u2:56:SER:OG     | 9:u2:60:THR:OG1    | 2.19                     | 0.50              |
| 10:K3:112:TYR:CE1  | 10:K3:113:LEU:HG   | 2.46                     | 0.50              |
| 10:M3:68:ASP:O     | 10:M3:69:ARG:HG2   | 2.10                     | 0.50              |
| 10:O3:72:ARG:N     | 10:O3:76:ASP:OD2   | 2.24                     | 0.50              |
| 10:O3:112:TYR:CE1  | 10:O3:113:LEU:HG   | 2.46                     | 0.50              |
| 10:U3:112:TYR:CE1  | 10:U3:113:LEU:HG   | 2.46                     | 0.50              |
| 10:X3:70:ARG:NH2   | 11:w3:72:THR:OG1   | 2.37                     | 0.50              |
| 11:a3:28:VAL:HB    | 11:a3:31:VAL:HG23  | 1.94                     | 0.50              |
| 11:d3:251:ALA:HB1  | 11:d3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:e3:28:VAL:HB    | 11:e3:31:VAL:HG23  | 1.94                     | 0.50              |
| 11:e3:216:LEU:HD11 | 11:e3:222:GLN:HB2  | 1.92                     | 0.50              |
| 11:h3:42:VAL:CG1   | 11:h3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:i3:96:PHE:O     | 11:j3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:i3:251:ALA:HB1  | 11:i3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:j3:96:PHE:O     | 11:k3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:j3:251:ALA:HB1  | 11:j3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:l3:96:PHE:O     | 11:m3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:l3:251:ALA:HB1  | 11:l3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:n3:42:VAL:CG1   | 11:n3:119:GLY:HA3  | 2.42                     | 0.50              |
| 11:o3:89:VAL:HG11  | 11:o3:121:LEU:CD2  | 2.40                     | 0.50              |
| 11:o3:208:ARG:HH21 | 11:o3:238:ASP:HB2  | 1.76                     | 0.50              |
| 11:s3:42:VAL:CG1   | 11:s3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:s3:98:ARG:HA    | 11:s3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:v3:275:VAL:HG21 | 11:v3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:w3:28:VAL:HB    | 11:w3:31:VAL:HG23  | 1.93                     | 0.50              |
| 11:w3:141:ILE:HD13 | 11:w3:165:ILE:CD1  | 2.38                     | 0.50              |
| 11:z3:275:VAL:HG21 | 11:z3:338:LEU:HD21 | 1.92                     | 0.50              |
| 1:C1:394:LYS:HE3   | 1:C1:402:LEU:HD13  | 1.92                     | 0.50              |
| 1:F1:374:HIS:HB3   | 1:G1:276:GLU:HB3   | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G1:374:HIS:HB3   | 1:H1:276:GLU:HB3   | 1.94                     | 0.50              |
| 1:I1:147:LEU:O     | 1:I1:149:PRO:HD2   | 2.11                     | 0.50              |
| 1:I1:301:SER:HB3   | 1:I1:359:GLN:HB3   | 1.92                     | 0.50              |
| 1:M1:409:MET:CE    | 1:M1:434:ASN:HB2   | 2.41                     | 0.50              |
| 1:N1:370:ARG:HG2   | 1:N1:371:THR:N     | 2.26                     | 0.50              |
| 1:O1:155:VAL:HG23  | 1:O1:176:VAL:HG22  | 1.93                     | 0.50              |
| 1:Q1:252:ILE:HD11  | 1:R1:265:GLN:HB2   | 1.93                     | 0.50              |
| 1:S1:385:LEU:HB2   | 1:S1:428:ASP:OD2   | 2.10                     | 0.50              |
| 1:Y1:404:LEU:H     | 1:Y1:434:ASN:ND2   | 2.09                     | 0.50              |
| 1:a1:137:GLU:OE1   | 1:a1:155:VAL:HG13  | 2.12                     | 0.50              |
| 1:a1:382:ILE:HD12  | 1:a1:382:ILE:H     | 1.75                     | 0.50              |
| 1:b1:283:SER:HB2   | 1:b1:369:ASP:HB2   | 1.93                     | 0.50              |
| 1:g1:385:LEU:N     | 1:g1:428:ASP:OD2   | 2.36                     | 0.50              |
| 2:A2:121:ILE:HG23  | 2:A2:125:GLU:HG2   | 1.94                     | 0.50              |
| 2:A2:224:MET:HE3   | 2:B2:187:PHE:CD2   | 2.46                     | 0.50              |
| 2:E2:47:PHE:HZ     | 3:F2:71:LEU:HD13   | 1.74                     | 0.50              |
| 7:X2:4:LEU:HD23    | 7:X2:6:ILE:HG22    | 1.92                     | 0.50              |
| 9:l2:245:LYS:NZ    | 9:r2:260:LEU:O     | 2.44                     | 0.50              |
| 9:m2:40:VAL:HG13   | 9:m2:75:VAL:HG23   | 1.93                     | 0.50              |
| 9:p2:115:THR:HB    | 9:p2:191:LEU:HD23  | 1.93                     | 0.50              |
| 9:p2:163:GLY:HA3   | 9:l2:111:THR:HG21  | 1.92                     | 0.50              |
| 9:s2:254:LEU:O     | 9:s2:258:THR:HG23  | 2.12                     | 0.50              |
| 9:v2:153:ARG:HH21  | 9:22:189:GLU:CD    | 2.20                     | 0.50              |
| 9:w2:233:MET:HE1   | 9:22:245:LYS:HG2   | 1.92                     | 0.50              |
| 9:y2:16:GLN:HE22   | 9:42:2:ILE:HG23    | 1.76                     | 0.50              |
| 9:z2:136:VAL:HG11  | 9:z2:173:LEU:HD11  | 1.93                     | 0.50              |
| 10:F3:112:TYR:CE1  | 10:F3:113:LEU:HG   | 2.46                     | 0.50              |
| 10:I3:70:ARG:NH2   | 11:h3:72:THR:OG1   | 2.38                     | 0.50              |
| 10:J3:80:ILE:HD13  | 10:J3:195:VAL:CG1  | 2.39                     | 0.50              |
| 10:N3:51:ILE:CG1   | 11:p3:175:LEU:HD11 | 2.41                     | 0.50              |
| 10:Y3:170:ALA:HB3  | 10:Z3:206:GLU:HG3  | 1.92                     | 0.50              |
| 11:a3:251:ALA:HB1  | 11:a3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:d3:28:VAL:HB    | 11:d3:31:VAL:HG23  | 1.93                     | 0.50              |
| 11:g3:98:ARG:HA    | 11:g3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:g3:193:ASP:HB3  | 11:g3:196:MET:HB2  | 1.91                     | 0.50              |
| 11:i3:28:VAL:HB    | 11:i3:31:VAL:HG23  | 1.94                     | 0.50              |
| 11:j3:28:VAL:HB    | 11:j3:31:VAL:HG23  | 1.93                     | 0.50              |
| 11:j3:94:PRO:HB2   | 11:k3:219:ARG:NH2  | 2.27                     | 0.50              |
| 11:k3:275:VAL:HG21 | 11:k3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:p3:79:MET:HE2   | 11:q3:57:PHE:CD2   | 2.46                     | 0.50              |
| 11:q3:208:ARG:HH21 | 11:q3:238:ASP:HB2  | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:q3:251:ALA:HB1  | 11:q3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:v3:79:MET:HE2   | 11:w3:57:PHE:CD2   | 2.46                     | 0.50              |
| 11:x3:28:VAL:HB    | 11:x3:31:VAL:HG23  | 1.94                     | 0.50              |
| 11:x3:142:LEU:HD23 | 11:z3:350:GLN:NE2  | 2.25                     | 0.50              |
| 11:y3:254:VAL:CG2  | 11:z3:355:ALA:HB2  | 2.42                     | 0.50              |
| 11:z3:42:VAL:CG1   | 11:z3:119:GLY:HA3  | 2.41                     | 0.50              |
| 1:A1:389:VAL:HB    | 1:A1:432:VAL:HG22  | 1.94                     | 0.50              |
| 1:B1:126:PHE:HA    | 1:B1:129:GLN:HE22  | 1.77                     | 0.50              |
| 1:C1:129:GLN:OE1   | 1:C1:129:GLN:N     | 2.39                     | 0.50              |
| 1:K1:142:ARG:O     | 1:K1:146:THR:HG23  | 2.11                     | 0.50              |
| 1:N1:125:GLN:O     | 1:N1:128:GLU:HG3   | 2.11                     | 0.50              |
| 1:Q1:161:LYS:HD3   | 1:Q1:162:PRO:C     | 2.37                     | 0.50              |
| 1:U1:142:ARG:HG3   | 1:W1:154:ARG:NH1   | 2.27                     | 0.50              |
| 1:V1:393:TYR:CE2   | 1:V1:436:PRO:HD3   | 2.46                     | 0.50              |
| 1:W1:164:LEU:CD1   | 2:E2:143:ARG:C     | 2.76                     | 0.50              |
| 1:e1:271:ASP:OD1   | 1:e1:381:ASP:N     | 2.43                     | 0.50              |
| 8:b2:51:LEU:O      | 8:b2:53:THR:HG23   | 2.11                     | 0.50              |
| 9:g2:237:GLN:NE2   | 9:l2:252:GLN:OE1   | 2.44                     | 0.50              |
| 9:m2:36:ARG:NH1    | 9:m2:38:ARG:HB2    | 2.26                     | 0.50              |
| 9:o2:227:ALA:HA    | 9:y2:257:LEU:HD21  | 1.93                     | 0.50              |
| 9:p2:185:GLU:HB3   | 9:u2:52:PRO:HG2    | 1.92                     | 0.50              |
| 9:t2:6:TRP:O       | 9:t2:10:THR:HG23   | 2.12                     | 0.50              |
| 9:t2:230:LEU:HD11  | 9:y2:242:ILE:HG23  | 1.94                     | 0.50              |
| 9:32:179:MET:O     | 9:32:179:MET:HE3   | 2.11                     | 0.50              |
| 10:X3:112:TYR:CE1  | 10:X3:113:LEU:HG   | 2.46                     | 0.50              |
| 11:b3:42:VAL:CG1   | 11:b3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:c3:28:VAL:HB    | 11:c3:31:VAL:HG23  | 1.93                     | 0.50              |
| 11:c3:105:VAL:HG11 | 11:c3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:d3:275:VAL:HG21 | 11:d3:338:LEU:CD2  | 2.40                     | 0.50              |
| 11:h3:251:ALA:HB1  | 11:h3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:h3:275:VAL:HG21 | 11:h3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:i3:216:LEU:HD11 | 11:i3:222:GLN:HB2  | 1.92                     | 0.50              |
| 11:l3:208:ARG:HH21 | 11:l3:238:ASP:HB2  | 1.76                     | 0.50              |
| 11:m3:96:PHE:O     | 11:n3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:m3:172:GLU:OE1  | 11:m3:172:GLU:HA   | 2.09                     | 0.50              |
| 11:n3:98:ARG:HA    | 11:n3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:p3:251:ALA:HB1  | 11:p3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:w3:280:LEU:HD11 | 11:w3:340:ALA:HB2  | 1.92                     | 0.50              |
| 1:H1:125:GLN:OE1   | 4:H2:3:PRO:C       | 2.55                     | 0.50              |
| 1:K1:167:ARG:NE    | 2:A2:244:TYR:O     | 2.43                     | 0.50              |
| 1:K1:393:TYR:CE2   | 1:K1:436:PRO:HD3   | 2.46                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a1:176:VAL:O     | 1:a1:212:LEU:HA    | 2.12                     | 0.50              |
| 1:b1:257:VAL:O     | 1:b1:261:ASN:ND2   | 2.45                     | 0.50              |
| 1:d1:404:LEU:HB2   | 1:d1:434:ASN:ND2   | 2.27                     | 0.50              |
| 2:B2:185:ILE:HG23  | 4:H2:84:LEU:HD21   | 1.93                     | 0.50              |
| 2:E2:62:THR:HB     | 2:E2:101:MET:CE    | 2.40                     | 0.50              |
| 3:F2:193:LEU:HD13  | 3:F2:228:LEU:HD11  | 1.92                     | 0.50              |
| 8:c2:62:PRO:HB3    | 9:h2:62:LEU:HG     | 1.93                     | 0.50              |
| 8:c2:217:MET:SD    | 9:h2:245:LYS:HG2   | 2.51                     | 0.50              |
| 8:d2:27:ALA:C      | 9:i2:72:VAL:HG11   | 2.36                     | 0.50              |
| 8:f2:27:ALA:C      | 9:k2:72:VAL:HG11   | 2.37                     | 0.50              |
| 9:h2:26:LEU:HD21   | 9:m2:242:ILE:HG22  | 1.94                     | 0.50              |
| 9:k2:176:THR:OG1   | 9:k2:203:GLU:OE1   | 2.29                     | 0.50              |
| 9:n2:238:ARG:O     | 9:n2:242:ILE:HG12  | 2.12                     | 0.50              |
| 9:p2:150:THR:HA    | 9:p2:216:GLN:HE22  | 1.77                     | 0.50              |
| 9:q2:44:LEU:HB2    | 9:q2:70:THR:O      | 2.12                     | 0.50              |
| 9:x2:86:LEU:HD11   | 9:x2:98:LYS:HD3    | 1.93                     | 0.50              |
| 9:22:237:GLN:NE2   | 12:A4:53:LEU:HD11  | 2.15                     | 0.50              |
| 10:A3:112:TYR:CE1  | 10:A3:113:LEU:HG   | 2.46                     | 0.50              |
| 10:H3:51:ILE:CG1   | 11:j3:175:LEU:HD11 | 2.41                     | 0.50              |
| 10:R3:166:GLU:OE2  | 10:R3:168:GLN:NE2  | 2.27                     | 0.50              |
| 10:Y3:72:ARG:N     | 10:Y3:76:ASP:OD2   | 2.25                     | 0.50              |
| 11:a3:98:ARG:HA    | 11:a3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:b3:96:PHE:O     | 11:c3:219:ARG:HD2  | 2.12                     | 0.50              |
| 11:b3:105:VAL:HG11 | 11:b3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:b3:251:ALA:HB1  | 11:b3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:b3:280:LEU:CD1  | 11:b3:340:ALA:HB2  | 2.41                     | 0.50              |
| 11:c3:96:PHE:O     | 11:d3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:c3:251:ALA:HB1  | 11:c3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:d3:42:VAL:CG1   | 11:d3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:d3:105:VAL:HG11 | 11:d3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:e3:282:VAL:HG23 | 11:e3:317:GLY:O    | 2.12                     | 0.50              |
| 11:f3:42:VAL:CG1   | 11:f3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:g3:251:ALA:HB1  | 11:g3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:h3:96:PHE:O     | 11:i3:219:ARG:HD2  | 2.12                     | 0.50              |
| 11:l3:101:GLN:NE2  | 11:m3:219:ARG:HD3  | 2.25                     | 0.50              |
| 11:o3:251:ALA:HB1  | 11:o3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:p3:105:VAL:HG11 | 11:p3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:p3:208:ARG:HH21 | 11:p3:238:ASP:HB2  | 1.76                     | 0.50              |
| 11:r3:96:PHE:O     | 11:s3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:r3:251:ALA:HB1  | 11:r3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:s3:280:LEU:CD1  | 11:s3:340:ALA:HB2  | 2.41                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:s3:282:VAL:HG23 | 11:s3:317:GLY:O    | 2.12                     | 0.50              |
| 11:t3:89:VAL:HG11  | 11:t3:121:LEU:CD2  | 2.40                     | 0.50              |
| 11:v3:28:VAL:HB    | 11:v3:31:VAL:HG23  | 1.93                     | 0.50              |
| 11:w3:275:VAL:HG21 | 11:w3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:x3:94:PRO:HB2   | 11:y3:219:ARG:NH2  | 2.27                     | 0.50              |
| 11:y3:282:VAL:HG23 | 11:y3:317:GLY:O    | 2.12                     | 0.50              |
| 1:C1:125:GLN:HB3   | 4:H2:75:ASP:OD2    | 2.12                     | 0.50              |
| 1:D1:234:GLN:OE1   | 1:D1:234:GLN:N     | 2.38                     | 0.50              |
| 1:H1:165:PHE:CD2   | 2:B2:162:PRO:HA    | 2.47                     | 0.50              |
| 1:L1:256:ILE:HG21  | 1:L1:412:ILE:HD11  | 1.92                     | 0.50              |
| 1:L1:407:ASP:HA    | 1:L1:410:LYS:HE3   | 1.94                     | 0.50              |
| 1:M1:276:GLU:OE2   | 1:M1:374:HIS:NE2   | 2.38                     | 0.50              |
| 1:N1:277:GLN:HB3   | 1:N1:375:THR:HB    | 1.93                     | 0.50              |
| 1:Q1:393:TYR:HB3   | 1:Q1:402:LEU:N     | 2.27                     | 0.50              |
| 1:Y1:203:ALA:HA    | 1:a1:158:ALA:HB1   | 1.92                     | 0.50              |
| 3:F2:201:LEU:HD11  | 3:F2:213:ILE:HD12  | 1.93                     | 0.50              |
| 5:K2:67:ALA:HB3    | 5:K2:70:ASP:HB2    | 1.92                     | 0.50              |
| 7:X2:29:ALA:HA     | 8:c2:230:GLN:HE22  | 1.76                     | 0.50              |
| 7:X2:43:ARG:HB3    | 7:X2:69:GLU:CD     | 2.36                     | 0.50              |
| 8:c2:70:GLN:OE1    | 9:o2:3:SER:HB2     | 2.12                     | 0.50              |
| 9:j2:26:LEU:HD21   | 9:n2:242:ILE:HG22  | 1.93                     | 0.50              |
| 9:l2:227:ALA:HA    | 9:w2:257:LEU:HD21  | 1.93                     | 0.50              |
| 9:p2:36:ARG:NH1    | 9:p2:38:ARG:HB2    | 2.27                     | 0.50              |
| 10:E3:112:TYR:CE1  | 10:E3:113:LEU:HG   | 2.46                     | 0.50              |
| 11:a3:105:VAL:HG11 | 11:a3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:a3:350:GLN:NE2  | 11:y3:142:LEU:HD23 | 2.26                     | 0.50              |
| 11:f3:275:VAL:HG21 | 11:f3:338:LEU:CD2  | 2.40                     | 0.50              |
| 11:f3:282:VAL:HG23 | 11:f3:317:GLY:O    | 2.12                     | 0.50              |
| 11:g3:216:LEU:HD11 | 11:g3:222:GLN:HB2  | 1.92                     | 0.50              |
| 11:g3:282:VAL:HG23 | 11:g3:317:GLY:O    | 2.12                     | 0.50              |
| 11:h3:101:GLN:NE2  | 11:i3:219:ARG:HD3  | 2.25                     | 0.50              |
| 11:h3:275:VAL:HG21 | 11:h3:338:LEU:CD2  | 2.40                     | 0.50              |
| 11:h3:282:VAL:HG23 | 11:h3:317:GLY:O    | 2.12                     | 0.50              |
| 11:i3:280:LEU:CD1  | 11:i3:340:ALA:HB2  | 2.41                     | 0.50              |
| 11:j3:282:VAL:HG23 | 11:j3:317:GLY:O    | 2.12                     | 0.50              |
| 11:k3:28:VAL:HB    | 11:k3:31:VAL:HG23  | 1.93                     | 0.50              |
| 11:k3:251:ALA:HB1  | 11:k3:360:ALA:HB2  | 1.94                     | 0.50              |
| 11:k3:280:LEU:CD1  | 11:k3:340:ALA:HB2  | 2.41                     | 0.50              |
| 11:l3:98:ARG:HA    | 11:l3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:l3:254:VAL:CG2  | 11:m3:355:ALA:HB2  | 2.42                     | 0.50              |
| 11:l3:282:VAL:HG23 | 11:l3:317:GLY:O    | 2.12                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:m3:42:VAL:CG1   | 11:m3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:o3:245:ASN:OD1  | 11:o3:245:ASN:N    | 2.33                     | 0.50              |
| 11:q3:46:ASP:HA    | 11:r3:161:ASN:ND2  | 2.21                     | 0.50              |
| 11:q3:105:VAL:HG11 | 11:q3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:u3:42:VAL:CG1   | 11:u3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:w3:98:ARG:HA    | 11:w3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:x3:275:VAL:HG21 | 11:x3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:y3:275:VAL:HG21 | 11:y3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:z3:282:VAL:HG23 | 11:z3:317:GLY:O    | 2.12                     | 0.50              |
| 12:B4:227:GLU:HA   | 12:B4:229:ARG:HH12 | 1.76                     | 0.50              |
| 1:B1:154:ARG:HH12  | 1:h1:142:ARG:C     | 2.19                     | 0.50              |
| 1:B1:165:PHE:HE2   | 2:C2:161:GLY:O     | 1.41                     | 0.50              |
| 1:H1:137:GLU:HB2   | 1:H1:155:VAL:HG13  | 1.94                     | 0.50              |
| 1:U1:165:PHE:HZ    | 2:E2:244:TYR:CE2   | 2.29                     | 0.50              |
| 1:X1:256:ILE:HG22  | 1:X1:257:VAL:HG13  | 1.93                     | 0.50              |
| 1:a1:149:PRO:HA    | 1:a1:181:GLU:HG2   | 1.92                     | 0.50              |
| 2:B2:43:GLN:C      | 2:B2:45:LEU:H      | 2.20                     | 0.50              |
| 2:C2:100:ILE:O     | 2:C2:103:PRO:HD2   | 2.12                     | 0.50              |
| 7:a2:23:VAL:HG21   | 7:a2:47:VAL:HG13   | 1.94                     | 0.50              |
| 9:i2:190:ASN:N     | 9:o2:42:GLU:OE2    | 2.44                     | 0.50              |
| 9:w2:196:GLN:HE22  | 9:22:61:THR:HG23   | 1.77                     | 0.50              |
| 9:12:240:TYR:CE2   | 12:E4:49:PRO:HA    | 2.46                     | 0.50              |
| 10:B3:157:ALA:HB1  | 10:Z3:41:PRO:HA    | 1.94                     | 0.50              |
| 10:G3:51:ILE:CG1   | 11:i3:175:LEU:HD11 | 2.41                     | 0.50              |
| 11:d3:94:PRO:HB2   | 11:e3:219:ARG:NH2  | 2.27                     | 0.50              |
| 11:d3:282:VAL:HG23 | 11:d3:317:GLY:O    | 2.12                     | 0.50              |
| 11:f3:208:ARG:HH21 | 11:f3:238:ASP:HB2  | 1.76                     | 0.50              |
| 11:i3:98:ARG:HA    | 11:i3:174:GLU:OE2  | 2.11                     | 0.50              |
| 11:k3:42:VAL:CG1   | 11:k3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:k3:208:ARG:HH21 | 11:k3:238:ASP:HB2  | 1.76                     | 0.50              |
| 11:n3:282:VAL:HG23 | 11:n3:317:GLY:O    | 2.12                     | 0.50              |
| 11:o3:105:VAL:HG11 | 11:o3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:r3:282:VAL:HG23 | 11:r3:317:GLY:O    | 2.12                     | 0.50              |
| 11:s3:105:VAL:HG11 | 11:s3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:t3:96:PHE:O     | 11:u3:219:ARG:HD2  | 2.12                     | 0.50              |
| 11:u3:96:PHE:O     | 11:v3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:z3:105:VAL:HG11 | 11:z3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:z3:251:ALA:HB1  | 11:z3:360:ALA:HB2  | 1.93                     | 0.50              |
| 1:C1:291:ALA:HB1   | 1:C1:366:TYR:HE1   | 1.76                     | 0.50              |
| 1:I1:174:ALA:O     | 1:I1:210:VAL:HA    | 2.12                     | 0.50              |
| 1:J1:377:MET:HA    | 1:J1:377:MET:HE3   | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:K1:161:LYS:HG2   | 1:K1:162:PRO:HD2   | 1.93                     | 0.50              |
| 1:R1:248:ARG:NH1   | 1:S1:267:THR:HG22  | 2.27                     | 0.50              |
| 1:T1:262:VAL:HG23  | 1:T1:391:VAL:HG12  | 1.94                     | 0.50              |
| 1:V1:267:THR:OG1   | 1:V1:386:SER:HB2   | 2.12                     | 0.50              |
| 1:f1:170:LYS:HD2   | 1:f1:171:SER:O     | 2.12                     | 0.50              |
| 2:C2:42:VAL:HG11   | 5:N2:42:LEU:HB3    | 1.93                     | 0.50              |
| 2:C2:56:ALA:O      | 2:C2:60:MET:HE2    | 2.12                     | 0.50              |
| 2:E2:205:MET:HE3   | 4:J2:51:PHE:CD2    | 2.43                     | 0.50              |
| 6:T2:93:PRO:HB3    | 8:e2:48:GLY:HA3    | 1.94                     | 0.50              |
| 8:b2:81:ALA:HB3    | 8:b2:202:MET:HB3   | 1.94                     | 0.50              |
| 9:i2:152:GLY:HA3   | 9:y2:56:SER:O      | 2.11                     | 0.50              |
| 9:p2:95:VAL:O      | 9:p2:118:GLY:HA3   | 2.12                     | 0.50              |
| 9:t2:254:LEU:O     | 9:t2:258:THR:HG23  | 2.12                     | 0.50              |
| 9:v2:56:SER:OG     | 9:v2:60:THR:OG1    | 2.27                     | 0.50              |
| 9:w2:235:GLN:HG3   | 9:32:1:MET:HG3     | 1.94                     | 0.50              |
| 9:32:240:TYR:CZ    | 12:B4:49:PRO:HA    | 2.47                     | 0.50              |
| 10:M3:51:ILE:CG1   | 11:o3:175:LEU:HD11 | 2.42                     | 0.50              |
| 10:Q3:54:SER:HB2   | 11:r3:173:ARG:HH12 | 1.77                     | 0.50              |
| 11:b3:254:VAL:CG2  | 11:c3:355:ALA:HB2  | 2.42                     | 0.50              |
| 11:g3:96:PHE:O     | 11:h3:219:ARG:HD2  | 2.11                     | 0.50              |
| 11:i3:282:VAL:HG23 | 11:i3:317:GLY:O    | 2.12                     | 0.50              |
| 11:j3:275:VAL:HG21 | 11:j3:338:LEU:HD21 | 1.92                     | 0.50              |
| 11:k3:245:ASN:OD1  | 11:k3:245:ASN:N    | 2.33                     | 0.50              |
| 11:k3:282:VAL:HG23 | 11:k3:317:GLY:O    | 2.12                     | 0.50              |
| 11:m3:282:VAL:HG23 | 11:m3:317:GLY:O    | 2.12                     | 0.50              |
| 11:r3:42:VAL:CG1   | 11:r3:119:GLY:HA3  | 2.41                     | 0.50              |
| 11:r3:105:VAL:HG11 | 11:r3:169:ALA:HB2  | 1.94                     | 0.50              |
| 11:s3:251:ALA:HB1  | 11:s3:360:ALA:HB2  | 1.93                     | 0.50              |
| 11:t3:282:VAL:HG23 | 11:t3:317:GLY:O    | 2.12                     | 0.50              |
| 11:w3:42:VAL:CG1   | 11:w3:119:GLY:HA3  | 2.41                     | 0.50              |
| 12:B4:136:VAL:HG11 | 12:B4:156:LEU:HD12 | 1.93                     | 0.50              |
| 12:B4:149:ARG:HD2  | 12:B4:170:THR:HA   | 1.94                     | 0.50              |
| 1:B1:161:LYS:HZ3   | 1:B1:163:SER:HA    | 1.77                     | 0.50              |
| 1:B1:195:VAL:HG13  | 1:B1:210:VAL:CG2   | 2.42                     | 0.50              |
| 1:E1:143:THR:HG21  | 1:G1:156:HIS:NE2   | 2.26                     | 0.50              |
| 1:E1:393:TYR:CE2   | 1:E1:436:PRO:HD3   | 2.47                     | 0.50              |
| 1:P1:422:PHE:HE2   | 1:P1:424:ASP:HB3   | 1.76                     | 0.50              |
| 1:Q1:151:LYS:NZ    | 1:Q1:182:PRO:HD3   | 2.27                     | 0.50              |
| 1:T1:233:ALA:HA    | 1:T1:236:LYS:HD3   | 1.92                     | 0.50              |
| 1:W1:420:MET:HE1   | 1:W1:430:LEU:HB2   | 1.93                     | 0.50              |
| 1:d1:356:ARG:NH2   | 1:d1:358:THR:OG1   | 2.45                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:f1:233:ALA:HA    | 1:f1:236:LYS:HE2  | 1.94                     | 0.50              |
| 1:h1:192:SER:O     | 1:h1:196:HIS:ND1  | 2.39                     | 0.50              |
| 2:C2:221:PHE:O     | 2:C2:224:MET:HB3  | 2.12                     | 0.50              |
| 5:P2:66:ILE:HD12   | 5:P2:66:ILE:H     | 1.77                     | 0.50              |
| 9:h2:28:ASN:HD21   | 9:m2:43:ASP:HB3   | 1.75                     | 0.50              |
| 9:j2:44:LEU:HB2    | 9:j2:70:THR:O     | 2.12                     | 0.50              |
| 9:x2:248:SER:O     | 9:x2:252:GLN:HG2  | 2.12                     | 0.50              |
| 9:12:237:GLN:NE2   | 12:E4:53:LEU:C    | 2.70                     | 0.50              |
| 9:42:7:ILE:O       | 9:42:10:THR:OG1   | 2.30                     | 0.50              |
| 9:42:115:THR:HB    | 9:42:191:LEU:HD23 | 1.93                     | 0.50              |
| 10:L3:112:TYR:CE1  | 10:L3:113:LEU:HG  | 2.46                     | 0.50              |
| 10:P3:101:LYS:HZ3  | 10:P3:101:LYS:HB2 | 1.76                     | 0.50              |
| 10:V3:112:TYR:CE1  | 10:V3:113:LEU:HG  | 2.46                     | 0.50              |
| 11:c3:282:VAL:HG23 | 11:c3:317:GLY:O   | 2.12                     | 0.50              |
| 11:e3:105:VAL:HG11 | 11:e3:169:ALA:HB2 | 1.94                     | 0.50              |
| 11:f3:79:MET:HE2   | 11:g3:57:PHE:CD2  | 2.47                     | 0.50              |
| 11:g3:42:VAL:CG1   | 11:g3:119:GLY:HA3 | 2.41                     | 0.50              |
| 11:n3:105:VAL:HG11 | 11:n3:169:ALA:HB2 | 1.94                     | 0.50              |
| 11:n3:196:MET:HA   | 11:n3:196:MET:CE  | 2.34                     | 0.50              |
| 11:o3:254:VAL:CG2  | 11:p3:355:ALA:HB2 | 2.42                     | 0.50              |
| 11:t3:105:VAL:HG11 | 11:t3:169:ALA:HB2 | 1.94                     | 0.50              |
| 11:u3:28:VAL:HB    | 11:u3:31:VAL:HG23 | 1.93                     | 0.50              |
| 11:u3:141:ILE:HD13 | 11:u3:165:ILE:CD1 | 2.37                     | 0.50              |
| 1:E1:373:ARG:HH21  | 1:F1:275:LYS:HE3  | 1.77                     | 0.49              |
| 1:F1:407:ASP:OD1   | 1:F1:408:GLN:N    | 2.44                     | 0.49              |
| 1:G1:167:ARG:HH12  | 2:B2:245:SER:HB3  | 1.77                     | 0.49              |
| 1:H1:147:LEU:O     | 1:H1:149:PRO:HD2  | 2.12                     | 0.49              |
| 1:O1:180:LEU:H     | 1:O1:215:GLN:CD   | 2.20                     | 0.49              |
| 1:U1:161:LYS:HD3   | 1:U1:162:PRO:C    | 2.37                     | 0.49              |
| 1:W1:404:LEU:HD13  | 1:W1:434:ASN:HD21 | 1.77                     | 0.49              |
| 1:X1:140:LEU:O     | 1:X1:143:THR:OG1  | 2.27                     | 0.49              |
| 1:d1:426:ARG:NE    | 1:d1:428:ASP:OD1  | 2.38                     | 0.49              |
| 1:g1:213:VAL:HG22  | 1:g1:219:LEU:HD23 | 1.93                     | 0.49              |
| 2:B2:242:SER:HB3   | 4:H2:85:PRO:HB3   | 1.94                     | 0.49              |
| 2:C2:99:PHE:CE1    | 2:D2:154:ALA:HB2  | 2.46                     | 0.49              |
| 2:C2:138:MET:O     | 2:C2:142:THR:HG23 | 2.10                     | 0.49              |
| 3:F2:109:SER:O     | 3:F2:112:THR:OG1  | 2.30                     | 0.49              |
| 6:R2:106:ARG:NH1   | 8:c2:245:ASN:OD1  | 2.45                     | 0.49              |
| 6:T2:128:LYS:O     | 6:T2:132:ASN:ND2  | 2.39                     | 0.49              |
| 9:q2:89:THR:HG23   | 9:q2:91:ASN:H     | 1.77                     | 0.49              |
| 9:r2:195:THR:HG23  | 9:r2:197:SER:H    | 1.76                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:s2:120:PHE:O     | 9:s2:121:GLN:NE2   | 2.39                     | 0.49              |
| 9:z2:136:VAL:O     | 9:z2:137:GLN:NE2   | 2.45                     | 0.49              |
| 10:Z3:82:LEU:HA    | 10:Z3:197:SER:CB   | 2.39                     | 0.49              |
| 11:a3:282:VAL:HG23 | 11:a3:317:GLY:O    | 2.12                     | 0.49              |
| 11:g3:208:ARG:HH21 | 11:g3:238:ASP:HB2  | 1.76                     | 0.49              |
| 11:i3:42:VAL:CG1   | 11:i3:119:GLY:HA3  | 2.41                     | 0.49              |
| 11:j3:254:VAL:CG2  | 11:k3:355:ALA:HB2  | 2.41                     | 0.49              |
| 11:l3:28:VAL:HB    | 11:l3:31:VAL:HG23  | 1.93                     | 0.49              |
| 11:o3:282:VAL:HG23 | 11:o3:317:GLY:O    | 2.12                     | 0.49              |
| 11:p3:42:VAL:CG1   | 11:p3:119:GLY:HA3  | 2.41                     | 0.49              |
| 11:t3:28:VAL:HB    | 11:t3:31:VAL:HG23  | 1.93                     | 0.49              |
| 11:t3:254:VAL:CG2  | 11:u3:355:ALA:HB2  | 2.42                     | 0.49              |
| 11:v3:94:PRO:HB2   | 11:w3:219:ARG:NH2  | 2.27                     | 0.49              |
| 11:x3:282:VAL:HG23 | 11:x3:317:GLY:O    | 2.12                     | 0.49              |
| 12:E4:124:PRO:HG2  | 12:E4:200:PHE:HB2  | 1.94                     | 0.49              |
| 12:E4:128:GLU:HB3  | 12:E4:196:GLN:HB3  | 1.94                     | 0.49              |
| 12:E4:138:ALA:HB1  | 12:E4:182:ILE:HD11 | 1.93                     | 0.49              |
| 1:C1:144:ILE:HG22  | 1:C1:150:VAL:HG11  | 1.92                     | 0.49              |
| 1:J1:417:ARG:O     | 1:J1:422:PHE:HB2   | 2.11                     | 0.49              |
| 1:K1:157:LEU:HD21  | 1:K1:202:VAL:HG21  | 1.94                     | 0.49              |
| 1:N1:133:GLN:O     | 1:N1:136:LEU:N     | 2.43                     | 0.49              |
| 1:X1:407:ASP:OD1   | 1:X1:408:GLN:N     | 2.43                     | 0.49              |
| 1:c1:139:GLU:OE2   | 1:d1:134:ARG:NH2   | 2.45                     | 0.49              |
| 1:c1:200:SER:HB3   | 1:d1:175:SER:HB3   | 1.93                     | 0.49              |
| 1:c1:236:LYS:H     | 1:c1:236:LYS:HD2   | 1.77                     | 0.49              |
| 1:f1:302:GLU:HB3   | 1:f1:358:THR:HG23  | 1.95                     | 0.49              |
| 1:g1:257:VAL:O     | 1:g1:261:ASN:ND2   | 2.30                     | 0.49              |
| 1:h1:199:SER:OG    | 1:h1:205:LEU:O     | 2.24                     | 0.49              |
| 2:A2:52:THR:HG1    | 5:O2:91:LYS:HZ3    | 1.53                     | 0.49              |
| 9:j2:97:ILE:HD12   | 9:j2:116:ARG:HD2   | 1.93                     | 0.49              |
| 9:k2:44:LEU:HB2    | 9:k2:70:THR:O      | 2.12                     | 0.49              |
| 9:o2:14:ALA:HB2    | 9:o2:72:VAL:HG13   | 1.94                     | 0.49              |
| 9:r2:44:LEU:HD12   | 9:r2:71:GLY:HA3    | 1.95                     | 0.49              |
| 9:z2:120:PHE:O     | 9:z2:121:GLN:NE2   | 2.41                     | 0.49              |
| 9:22:257:LEU:O     | 9:22:260:LEU:HB3   | 2.12                     | 0.49              |
| 9:42:195:THR:HG1   | 9:42:198:SER:HG    | 1.60                     | 0.49              |
| 10:C3:112:TYR:CE1  | 10:C3:113:LEU:HG   | 2.46                     | 0.49              |
| 10:F3:51:ILE:CG1   | 11:h3:175:LEU:HD11 | 2.42                     | 0.49              |
| 10:L3:51:ILE:CG1   | 11:n3:175:LEU:HD11 | 2.42                     | 0.49              |
| 10:O3:54:SER:HB2   | 11:p3:173:ARG:HH12 | 1.77                     | 0.49              |
| 11:c3:254:VAL:CG2  | 11:d3:355:ALA:HB2  | 2.42                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:d3:79:MET:HE2   | 11:e3:57:PHE:CD2  | 2.46                     | 0.49              |
| 11:d3:98:ARG:HA    | 11:d3:174:GLU:OE2 | 2.11                     | 0.49              |
| 11:m3:28:VAL:HB    | 11:m3:31:VAL:HG23 | 1.93                     | 0.49              |
| 11:n3:254:VAL:CG2  | 11:o3:355:ALA:HB2 | 2.42                     | 0.49              |
| 11:p3:101:GLN:NE2  | 11:q3:219:ARG:HD3 | 2.26                     | 0.49              |
| 11:q3:89:VAL:HG11  | 11:q3:121:LEU:CD2 | 2.40                     | 0.49              |
| 11:s3:89:VAL:HG11  | 11:s3:121:LEU:CD2 | 2.40                     | 0.49              |
| 11:y3:251:ALA:HB1  | 11:y3:360:ALA:HB2 | 1.93                     | 0.49              |
| 11:y3:328:LEU:HD21 | 11:z3:273:CYS:HA  | 1.94                     | 0.49              |
| 1:A1:231:ASN:OD1   | 1:A1:232:ASP:N    | 2.45                     | 0.49              |
| 1:C1:161:LYS:HA    | 1:C1:161:LYS:HE2  | 1.93                     | 0.49              |
| 1:E1:191:ILE:HD13  | 1:E1:220:LEU:HB3  | 1.94                     | 0.49              |
| 1:K1:137:GLU:HB2   | 1:K1:155:VAL:HG13 | 1.94                     | 0.49              |
| 1:M1:375:THR:HG23  | 1:N1:275:LYS:HZ2  | 1.77                     | 0.49              |
| 1:N1:125:GLN:HG3   | 3:F2:238:PRO:HD3  | 1.88                     | 0.49              |
| 1:N1:166:VAL:HG21  | 2:A2:162:PRO:HD3  | 1.91                     | 0.49              |
| 1:N1:179:THR:HA    | 1:N1:215:GLN:HB3  | 1.94                     | 0.49              |
| 1:N1:244:ARG:CZ    | 1:O1:235:LEU:HB3  | 2.42                     | 0.49              |
| 1:O1:304:VAL:HG22  | 1:O1:356:ARG:HG2  | 1.94                     | 0.49              |
| 1:d1:166:VAL:HA    | 2:D2:161:GLY:HA2  | 1.94                     | 0.49              |
| 1:d1:407:ASP:HA    | 1:d1:410:LYS:HG3  | 1.94                     | 0.49              |
| 1:g1:234:GLN:HB3   | 1:g1:272:PHE:CE2  | 2.47                     | 0.49              |
| 6:U2:130:MET:O     | 6:U2:134:LEU:HD23 | 2.12                     | 0.49              |
| 7:W2:90:TYR:CE2    | 9:h2:45:LEU:HD22  | 2.46                     | 0.49              |
| 7:X2:113:GLN:OE1   | 8:c2:243:ARG:NH1  | 2.45                     | 0.49              |
| 8:e2:133:SER:HB2   | 8:e2:135:ILE:HG12 | 1.94                     | 0.49              |
| 9:i2:98:LYS:O      | 9:i2:212:GLY:CA   | 2.47                     | 0.49              |
| 9:o2:86:LEU:HD11   | 9:y2:45:LEU:HG    | 1.94                     | 0.49              |
| 9:v2:138:PRO:HD3   | 9:v2:174:ASN:OD1  | 2.12                     | 0.49              |
| 9:w2:238:ARG:HE    | 9:32:255:GLN:HE22 | 1.60                     | 0.49              |
| 9:x2:12:LEU:HD22   | 9:x2:243:ASN:HB3  | 1.93                     | 0.49              |
| 9:32:72:VAL:O      | 9:32:72:VAL:HG12  | 2.11                     | 0.49              |
| 9:42:143:PRO:HD3   | 9:42:170:VAL:HG21 | 1.94                     | 0.49              |
| 10:T3:70:ARG:NH2   | 11:s3:72:THR:OG1  | 2.39                     | 0.49              |
| 10:X3:219:MET:HE2  | 10:Z3:132:PHE:CB  | 2.43                     | 0.49              |
| 11:e3:42:VAL:CG1   | 11:e3:119:GLY:HA3 | 2.41                     | 0.49              |
| 11:f3:105:VAL:HG11 | 11:f3:169:ALA:HB2 | 1.94                     | 0.49              |
| 11:h3:208:ARG:HH21 | 11:h3:238:ASP:HB2 | 1.76                     | 0.49              |
| 11:l3:103:ILE:HG13 | 11:l3:169:ALA:HB3 | 1.95                     | 0.49              |
| 11:m3:105:VAL:HG11 | 11:m3:169:ALA:HB2 | 1.94                     | 0.49              |
| 11:n3:103:ILE:HG13 | 11:n3:169:ALA:HB3 | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:o3:103:ILE:HG13 | 11:o3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:p3:96:PHE:O     | 11:q3:219:ARG:HD2  | 2.11                     | 0.49              |
| 11:r3:79:MET:HE2   | 11:s3:57:PHE:CD2   | 2.47                     | 0.49              |
| 11:r3:254:VAL:CG2  | 11:s3:355:ALA:HB2  | 2.42                     | 0.49              |
| 11:t3:196:MET:HA   | 11:t3:196:MET:CE   | 2.34                     | 0.49              |
| 11:u3:282:VAL:HG23 | 11:u3:317:GLY:O    | 2.12                     | 0.49              |
| 11:v3:251:ALA:HB1  | 11:v3:360:ALA:HB2  | 1.94                     | 0.49              |
| 11:y3:105:VAL:HG11 | 11:y3:169:ALA:HB2  | 1.94                     | 0.49              |
| 1:B1:246:GLN:NE2   | 1:B1:264:ALA:O     | 2.45                     | 0.49              |
| 1:M1:252:ILE:HG22  | 1:M1:253:LEU:HD12  | 1.94                     | 0.49              |
| 1:T1:165:PHE:CD1   | 3:F2:166:SER:HB2   | 2.45                     | 0.49              |
| 1:W1:242:GLU:OE2   | 1:W1:268:ALA:N     | 2.39                     | 0.49              |
| 1:f1:164:LEU:HD21  | 2:D2:149:LEU:HA    | 1.93                     | 0.49              |
| 1:f1:275:LYS:HB3   | 1:f1:377:MET:HE2   | 1.94                     | 0.49              |
| 1:h1:407:ASP:HA    | 1:h1:410:LYS:HG2   | 1.95                     | 0.49              |
| 2:C2:166:PRO:HG2   | 2:C2:169:ILE:HG12  | 1.94                     | 0.49              |
| 4:J2:46:GLU:HG2    | 4:J2:47:MET:N      | 2.25                     | 0.49              |
| 6:Q2:117:GLN:CD    | 7:V2:128:LYS:HZ3   | 2.20                     | 0.49              |
| 8:d2:62:PRO:O      | 9:i2:63:PRO:HG2    | 2.12                     | 0.49              |
| 9:h2:152:GLY:HA3   | 9:x2:56:SER:O      | 2.13                     | 0.49              |
| 9:i2:190:ASN:ND2   | 9:o2:42:GLU:OE1    | 2.46                     | 0.49              |
| 9:u2:254:LEU:O     | 9:u2:258:THR:HG23  | 2.12                     | 0.49              |
| 9:22:2:ILE:HG22    | 9:22:4:SER:H       | 1.78                     | 0.49              |
| 10:A3:41:PRO:HA    | 10:C3:157:ALA:HB1  | 1.95                     | 0.49              |
| 10:I3:30:LEU:HD23  | 10:I3:30:LEU:H     | 1.78                     | 0.49              |
| 10:J3:30:LEU:HD23  | 10:J3:30:LEU:H     | 1.78                     | 0.49              |
| 10:T3:51:ILE:CG1   | 11:v3:175:LEU:HD11 | 2.41                     | 0.49              |
| 11:b3:282:VAL:HG23 | 11:b3:317:GLY:O    | 2.12                     | 0.49              |
| 11:i3:275:VAL:HG21 | 11:i3:338:LEU:HD21 | 1.92                     | 0.49              |
| 11:j3:208:ARG:HH21 | 11:j3:238:ASP:HB2  | 1.76                     | 0.49              |
| 11:k3:103:ILE:HG13 | 11:k3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:m3:103:ILE:HG13 | 11:m3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:p3:94:PRO:HB2   | 11:q3:219:ARG:NH2  | 2.27                     | 0.49              |
| 11:p3:282:VAL:HG23 | 11:p3:317:GLY:O    | 2.12                     | 0.49              |
| 11:q3:103:ILE:HG13 | 11:q3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:r3:89:VAL:HG11  | 11:r3:121:LEU:CD2  | 2.40                     | 0.49              |
| 11:t3:79:MET:HE2   | 11:u3:57:PHE:CD2   | 2.48                     | 0.49              |
| 11:u3:251:ALA:HB1  | 11:u3:360:ALA:HB2  | 1.94                     | 0.49              |
| 11:w3:251:ALA:HB1  | 11:w3:360:ALA:HB2  | 1.94                     | 0.49              |
| 11:y3:42:VAL:CG1   | 11:y3:119:GLY:HA3  | 2.41                     | 0.49              |
| 12:C4:148:VAL:O    | 12:C4:170:THR:N    | 2.44                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:E4:101:VAL:HG12 | 12:E4:231:ILE:HG23 | 1.94                     | 0.49              |
| 1:C1:250:GLU:O     | 1:C1:254:SER:OG    | 2.27                     | 0.49              |
| 1:F1:413:GLU:CD    | 1:F1:417:ARG:HH12  | 2.18                     | 0.49              |
| 1:G1:239:ASN:HA    | 1:G1:242:GLU:HG2   | 1.95                     | 0.49              |
| 1:I1:216:SER:O     | 1:I1:218:HIS:ND1   | 2.43                     | 0.49              |
| 1:N1:143:THR:HA    | 1:O1:154:ARG:HD3   | 1.94                     | 0.49              |
| 1:Q1:369:ASP:OD1   | 1:R1:282:TYR:N     | 2.44                     | 0.49              |
| 1:Y1:187:ASP:O     | 1:Y1:191:ILE:HG12  | 2.12                     | 0.49              |
| 1:a1:283:SER:HB2   | 1:a1:369:ASP:HB2   | 1.94                     | 0.49              |
| 1:e1:373:ARG:NH2   | 1:f1:377:MET:HE3   | 2.27                     | 0.49              |
| 1:f1:143:THR:HG23  | 1:g1:154:ARG:NE    | 2.27                     | 0.49              |
| 2:A2:128:ASP:OD1   | 2:A2:129:LYS:N     | 2.45                     | 0.49              |
| 2:A2:187:PHE:HA    | 2:A2:190:PHE:HD2   | 1.78                     | 0.49              |
| 2:B2:167:MET:HE3   | 2:B2:171:LEU:HD21  | 1.94                     | 0.49              |
| 4:H2:24:LEU:HD22   | 4:H2:58:VAL:HG13   | 1.94                     | 0.49              |
| 6:Q2:35:THR:HG23   | 6:Q2:38:TYR:HB2    | 1.94                     | 0.49              |
| 6:T2:40:ALA:HB2    | 6:T2:100:VAL:HG22  | 1.95                     | 0.49              |
| 6:T2:92:GLN:CD     | 7:Z2:19:LYS:HG2    | 2.37                     | 0.49              |
| 7:W2:76:LEU:H      | 9:h2:47:GLN:NE2    | 2.09                     | 0.49              |
| 8:b2:27:ALA:O      | 9:g2:72:VAL:HG11   | 2.12                     | 0.49              |
| 8:c2:134:GLU:HB2   | 8:c2:146:LEU:O     | 2.11                     | 0.49              |
| 8:e2:42:ARG:NH1    | 9:j2:64:SER:OG     | 2.34                     | 0.49              |
| 9:i2:37:GLN:OE1    | 9:i2:79:ARG:NH2    | 2.45                     | 0.49              |
| 9:z2:116:ARG:NE    | 9:z2:220:GLU:OE1   | 2.46                     | 0.49              |
| 9:22:7:ILE:HG23    | 9:22:71:GLY:H      | 1.76                     | 0.49              |
| 10:A3:70:ARG:NH2   | 11:z3:72:THR:OG1   | 2.41                     | 0.49              |
| 10:B3:132:PHE:CB   | 10:Z3:219:MET:HE2  | 2.43                     | 0.49              |
| 10:S3:54:SER:HB2   | 11:t3:173:ARG:HH12 | 1.78                     | 0.49              |
| 11:h3:254:VAL:CG2  | 11:i3:355:ALA:HB2  | 2.42                     | 0.49              |
| 11:i3:254:VAL:CG2  | 11:j3:355:ALA:HB2  | 2.42                     | 0.49              |
| 11:j3:101:GLN:NE2  | 11:k3:219:ARG:HD3  | 2.26                     | 0.49              |
| 11:j3:103:ILE:HG13 | 11:j3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:n3:96:PHE:O     | 11:o3:219:ARG:HD2  | 2.12                     | 0.49              |
| 11:p3:103:ILE:HG13 | 11:p3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:p3:120:THR:HG23 | 11:p3:139:GLY:O    | 2.13                     | 0.49              |
| 11:q3:282:VAL:HG23 | 11:q3:317:GLY:O    | 2.12                     | 0.49              |
| 11:r3:103:ILE:HG13 | 11:r3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:s3:96:PHE:O     | 11:t3:219:ARG:HD2  | 2.11                     | 0.49              |
| 11:s3:103:ILE:HG13 | 11:s3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:t3:251:ALA:HB1  | 11:t3:360:ALA:HB2  | 1.94                     | 0.49              |
| 11:v3:101:GLN:NE2  | 11:w3:219:ARG:HD3  | 2.26                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:x3:105:VAL:HG11 | 11:x3:169:ALA:HB2  | 1.94                     | 0.49              |
| 11:x3:251:ALA:HB1  | 11:x3:360:ALA:HB2  | 1.94                     | 0.49              |
| 12:C4:149:ARG:HG2  | 12:C4:165:TRP:HE1  | 1.77                     | 0.49              |
| 12:E4:169:GLN:HE21 | 12:E4:173:THR:HG1  | 1.56                     | 0.49              |
| 1:B1:191:ILE:HG23  | 1:B1:212:LEU:HD12  | 1.95                     | 0.49              |
| 1:C1:143:THR:HG22  | 1:E1:154:ARG:HD3   | 1.94                     | 0.49              |
| 1:C1:195:VAL:HG13  | 1:C1:210:VAL:HB    | 1.95                     | 0.49              |
| 1:H1:160:PRO:HD3   | 1:H1:172:PRO:HA    | 1.94                     | 0.49              |
| 1:K1:180:LEU:N     | 1:K1:215:GLN:OE1   | 2.37                     | 0.49              |
| 1:L1:298:LEU:HG    | 1:L1:362:GLU:OE2   | 2.12                     | 0.49              |
| 1:T1:147:LEU:HD23  | 1:T1:150:VAL:HG21  | 1.94                     | 0.49              |
| 1:T1:191:ILE:HD12  | 1:T1:220:LEU:HD13  | 1.95                     | 0.49              |
| 1:U1:161:LYS:HG2   | 1:U1:162:PRO:HD2   | 1.95                     | 0.49              |
| 1:W1:378:ASN:HB3   | 1:W1:381:ASP:OD2   | 2.12                     | 0.49              |
| 1:b1:277:GLN:HB3   | 1:b1:375:THR:HB    | 1.94                     | 0.49              |
| 1:d1:421:GLY:O     | 1:d1:426:ARG:NH2   | 2.45                     | 0.49              |
| 1:h1:287:ASP:HB3   | 1:h1:290:LYS:HE2   | 1.94                     | 0.49              |
| 2:A2:220:PRO:HB2   | 2:B2:187:PHE:CE1   | 2.48                     | 0.49              |
| 6:Q2:34:ASP:OD1    | 6:Q2:34:ASP:N      | 2.44                     | 0.49              |
| 7:V2:36:GLY:N      | 7:V2:40:GLN:O      | 2.45                     | 0.49              |
| 7:X2:90:TYR:CE2    | 9:i2:45:LEU:HD22   | 2.47                     | 0.49              |
| 8:b2:133:SER:OG    | 8:b2:134:GLU:N     | 2.45                     | 0.49              |
| 8:f2:122:GLY:HA2   | 8:f2:162:LYS:HB3   | 1.95                     | 0.49              |
| 9:j2:19:MET:HG2    | 9:n2:253:MET:HE1   | 1.94                     | 0.49              |
| 9:j2:152:GLY:HA3   | 9:z2:56:SER:O      | 2.12                     | 0.49              |
| 9:n2:168:VAL:CA    | 11:x3:78:ASN:ND2   | 2.45                     | 0.49              |
| 10:A3:82:LEU:HD13  | 10:A3:144:PHE:CE1  | 2.48                     | 0.49              |
| 10:B3:51:ILE:CG1   | 11:d3:175:LEU:HD11 | 2.41                     | 0.49              |
| 10:G3:30:LEU:HD23  | 10:G3:30:LEU:H     | 1.78                     | 0.49              |
| 10:I3:54:SER:HB2   | 11:j3:173:ARG:HH12 | 1.77                     | 0.49              |
| 10:K3:30:LEU:HD23  | 10:K3:30:LEU:H     | 1.78                     | 0.49              |
| 10:U3:54:SER:HB2   | 11:v3:173:ARG:HH12 | 1.77                     | 0.49              |
| 10:Z3:82:LEU:HD13  | 10:Z3:144:PHE:CE1  | 2.48                     | 0.49              |
| 11:l3:120:THR:HG23 | 11:l3:139:GLY:O    | 2.13                     | 0.49              |
| 11:n3:28:VAL:HB    | 11:n3:31:VAL:HG23  | 1.93                     | 0.49              |
| 11:s3:28:VAL:HB    | 11:s3:31:VAL:HG23  | 1.94                     | 0.49              |
| 11:s3:120:THR:HG23 | 11:s3:139:GLY:O    | 2.13                     | 0.49              |
| 11:t3:103:ILE:HG13 | 11:t3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:u3:105:VAL:HG11 | 11:u3:169:ALA:HB2  | 1.94                     | 0.49              |
| 11:w3:282:VAL:HG23 | 11:w3:317:GLY:O    | 2.12                     | 0.49              |
| 1:C1:389:VAL:HB    | 1:C1:432:VAL:HG13  | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:424:ASP:OD1   | 1:C1:425:LYS:N     | 2.46                     | 0.49              |
| 1:D1:295:SER:OG    | 6:U2:72:HIS:C      | 2.54                     | 0.49              |
| 1:G1:165:PHE:CZ    | 2:B2:143:ARG:NH1   | 2.80                     | 0.49              |
| 1:N1:212:LEU:HB2   | 1:N1:220:LEU:HB2   | 1.93                     | 0.49              |
| 1:U1:365:ASN:HD21  | 6:R2:65:LEU:HA     | 1.77                     | 0.49              |
| 1:c1:143:THR:HG22  | 1:d1:154:ARG:HD3   | 1.95                     | 0.49              |
| 1:d1:160:PRO:HD3   | 1:d1:172:PRO:HA    | 1.95                     | 0.49              |
| 2:A2:121:ILE:HG12  | 2:A2:125:GLU:HG3   | 1.94                     | 0.49              |
| 2:B2:189:ILE:HD11  | 4:H2:84:LEU:HD22   | 1.95                     | 0.49              |
| 2:C2:92:LEU:CD2    | 2:C2:236:MET:HE2   | 2.37                     | 0.49              |
| 4:H2:33:LEU:O      | 4:H2:37:ILE:HG12   | 2.12                     | 0.49              |
| 7:Z2:102:MET:CE    | 8:e2:232:LYS:HD3   | 2.43                     | 0.49              |
| 8:e2:14:GLN:HG3    | 8:e2:58:THR:HA     | 1.95                     | 0.49              |
| 8:e2:42:ARG:HD2    | 9:j2:64:SER:CB     | 2.42                     | 0.49              |
| 8:e2:122:GLY:HA2   | 8:e2:162:LYS:HB3   | 1.93                     | 0.49              |
| 9:o2:146:ALA:HB1   | 9:o2:159:VAL:HB    | 1.95                     | 0.49              |
| 9:x2:238:ARG:O     | 9:x2:241:GLU:HB2   | 2.12                     | 0.49              |
| 9:z2:238:ARG:O     | 9:z2:242:ILE:HG12  | 2.12                     | 0.49              |
| 10:D3:30:LEU:HD23  | 10:D3:30:LEU:H     | 1.78                     | 0.49              |
| 10:F3:30:LEU:H     | 10:F3:30:LEU:HD23  | 1.78                     | 0.49              |
| 10:S3:51:ILE:CG1   | 11:u3:175:LEU:HD11 | 2.42                     | 0.49              |
| 11:a3:20:GLU:O     | 11:a3:244:VAL:HG12 | 2.13                     | 0.49              |
| 11:a3:42:VAL:CG1   | 11:a3:119:GLY:HA3  | 2.41                     | 0.49              |
| 11:c3:42:VAL:CG1   | 11:c3:119:GLY:HA3  | 2.41                     | 0.49              |
| 11:d3:101:GLN:NE2  | 11:e3:188:GLN:HB3  | 2.28                     | 0.49              |
| 11:g3:105:VAL:HG11 | 11:g3:169:ALA:HB2  | 1.94                     | 0.49              |
| 11:i3:103:ILE:HG13 | 11:i3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:m3:120:THR:HG23 | 11:m3:139:GLY:O    | 2.13                     | 0.49              |
| 12:B4:30:ALA:HA    | 12:B4:33:GLN:HB3   | 1.95                     | 0.49              |
| 12:C4:102:MET:HB2  | 12:C4:229:ARG:HB2  | 1.95                     | 0.49              |
| 1:E1:134:ARG:O     | 1:E1:137:GLU:HB3   | 2.13                     | 0.49              |
| 1:K1:373:ARG:NH1   | 1:L1:277:GLN:OE1   | 2.46                     | 0.49              |
| 1:L1:142:ARG:HB3   | 1:N1:154:ARG:HH22  | 1.78                     | 0.49              |
| 1:P1:279:GLU:OE2   | 1:P1:281:HIS:HB2   | 2.13                     | 0.49              |
| 1:S1:295:SER:HG    | 6:R2:71:HIS:C      | 1.98                     | 0.49              |
| 1:U1:269:GLN:HB2   | 1:U1:383:GLU:HG2   | 1.94                     | 0.49              |
| 1:b1:245:ILE:HG21  | 1:b1:266:VAL:HG11  | 1.93                     | 0.49              |
| 2:C2:230:ASP:O     | 2:C2:234:LEU:HD23  | 2.12                     | 0.49              |
| 2:E2:56:ALA:O      | 2:E2:60:MET:HG2    | 2.13                     | 0.49              |
| 3:F2:73:LEU:O      | 3:F2:76:GLN:HB3    | 2.12                     | 0.49              |
| 3:F2:119:HIS:CE1   | 3:F2:121:ASN:HB2   | 2.47                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:g2:123:ASP:OD1   | 9:g2:127:GLN:N     | 2.45                     | 0.49              |
| 10:A3:82:LEU:HA    | 10:A3:197:SER:CB   | 2.38                     | 0.49              |
| 10:C3:82:LEU:O     | 10:C3:197:SER:OG   | 2.21                     | 0.49              |
| 10:H3:30:LEU:HD23  | 10:H3:30:LEU:H     | 1.78                     | 0.49              |
| 10:R3:51:ILE:CG1   | 11:t3:175:LEU:HD11 | 2.42                     | 0.49              |
| 10:T3:54:SER:HB2   | 11:u3:173:ARG:HH12 | 1.78                     | 0.49              |
| 10:U3:82:LEU:HD13  | 10:U3:144:PHE:CE1  | 2.48                     | 0.49              |
| 10:Y3:82:LEU:HD13  | 10:Y3:144:PHE:CE1  | 2.48                     | 0.49              |
| 11:b3:20:GLU:O     | 11:b3:244:VAL:HG12 | 2.13                     | 0.49              |
| 11:e3:277:GLN:HB3  | 11:e3:280:LEU:HD12 | 1.95                     | 0.49              |
| 11:h3:103:ILE:HG13 | 11:h3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:j3:79:MET:HE2   | 11:k3:57:PHE:CD2   | 2.46                     | 0.49              |
| 11:o3:28:VAL:HB    | 11:o3:31:VAL:HG23  | 1.93                     | 0.49              |
| 11:o3:120:THR:HG23 | 11:o3:139:GLY:O    | 2.13                     | 0.49              |
| 11:z3:20:GLU:O     | 11:z3:244:VAL:HG12 | 2.13                     | 0.49              |
| 1:G1:393:TYR:CE2   | 1:G1:436:PRO:HD3   | 2.48                     | 0.49              |
| 1:J1:387:VAL:HB    | 1:J1:420:MET:HE3   | 1.95                     | 0.49              |
| 1:T1:165:PHE:HZ    | 3:F2:170:MET:CG    | 2.25                     | 0.49              |
| 1:b1:239:ASN:O     | 1:b1:242:GLU:HG2   | 2.13                     | 0.49              |
| 1:c1:420:MET:HE3   | 1:c1:422:PHE:CD1   | 2.48                     | 0.49              |
| 2:D2:90:LEU:HD13   | 5:L2:100:MET:HA    | 1.94                     | 0.49              |
| 3:F2:51:THR:O      | 3:F2:55:ALA:N      | 2.45                     | 0.49              |
| 6:T2:103:ASP:OD1   | 7:Z2:112:TYR:OH    | 2.31                     | 0.49              |
| 8:b2:27:ALA:C      | 9:g2:72:VAL:HG11   | 2.37                     | 0.49              |
| 8:d2:115:ILE:HG22  | 8:d2:116:GLN:OE1   | 2.13                     | 0.49              |
| 8:d2:184:GLU:OE2   | 9:i2:55:GLN:HB2    | 2.13                     | 0.49              |
| 8:e2:138:ALA:HB3   | 8:e2:141:GLY:H     | 1.77                     | 0.49              |
| 9:g2:36:ARG:HH11   | 9:g2:80:LEU:HD12   | 1.77                     | 0.49              |
| 9:x2:118:GLY:HA2   | 9:x2:120:PHE:CE1   | 2.48                     | 0.49              |
| 10:B3:82:LEU:HD13  | 10:B3:144:PHE:CE1  | 2.48                     | 0.49              |
| 10:C3:30:LEU:H     | 10:C3:30:LEU:HD23  | 1.78                     | 0.49              |
| 10:E3:30:LEU:HD23  | 10:E3:30:LEU:H     | 1.78                     | 0.49              |
| 10:F3:82:LEU:HD13  | 10:F3:144:PHE:CE1  | 2.48                     | 0.49              |
| 10:K3:54:SER:HB2   | 11:l3:173:ARG:HH12 | 1.77                     | 0.49              |
| 10:T3:82:LEU:HD13  | 10:T3:144:PHE:CE1  | 2.48                     | 0.49              |
| 10:V3:82:LEU:HD13  | 10:V3:144:PHE:CE1  | 2.48                     | 0.49              |
| 11:a3:120:THR:HG23 | 11:a3:139:GLY:O    | 2.13                     | 0.49              |
| 11:h3:105:VAL:HG11 | 11:h3:169:ALA:HB2  | 1.94                     | 0.49              |
| 11:i3:208:ARG:HH21 | 11:i3:238:ASP:HB2  | 1.76                     | 0.49              |
| 11:l3:94:PRO:HB2   | 11:m3:219:ARG:NH2  | 2.28                     | 0.49              |
| 11:p3:28:VAL:HB    | 11:p3:31:VAL:HG23  | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:q3:28:VAL:HB    | 11:q3:31:VAL:HG23  | 1.93                     | 0.49              |
| 11:q3:79:MET:HE2   | 11:r3:57:PHE:CD2   | 2.48                     | 0.49              |
| 11:u3:79:MET:HE2   | 11:v3:57:PHE:CD2   | 2.48                     | 0.49              |
| 11:u3:103:ILE:HG13 | 11:u3:169:ALA:HB3  | 1.95                     | 0.49              |
| 11:v3:327:ASN:OD1  | 11:v3:330:SER:HB2  | 2.13                     | 0.49              |
| 11:y3:20:GLU:O     | 11:y3:244:VAL:HG12 | 2.13                     | 0.49              |
| 1:B1:182:PRO:O     | 1:B1:184:ARG:NH1   | 2.46                     | 0.49              |
| 1:B1:414:ASP:HB3   | 1:C1:431:ASN:ND2   | 2.27                     | 0.49              |
| 1:G1:164:LEU:CG    | 2:B2:144:GLU:OE1   | 2.58                     | 0.49              |
| 1:G1:187:ASP:O     | 1:G1:191:ILE:HG12  | 2.13                     | 0.49              |
| 1:L1:282:TYR:OH    | 1:L1:370:ARG:HD3   | 2.12                     | 0.49              |
| 1:O1:144:ILE:HG22  | 1:O1:150:VAL:HG11  | 1.94                     | 0.49              |
| 1:R1:203:ALA:HB1   | 1:T1:160:PRO:HG3   | 1.94                     | 0.49              |
| 1:V1:281:HIS:CE1   | 1:V1:282:TYR:O     | 2.65                     | 0.49              |
| 1:b1:252:ILE:HB    | 1:c1:265:GLN:HG3   | 1.95                     | 0.49              |
| 1:h1:125:GLN:NE2   | 4:I2:5:SER:HG      | 2.05                     | 0.49              |
| 1:h1:256:ILE:HG21  | 1:h1:412:ILE:HD11  | 1.95                     | 0.49              |
| 2:E2:40:LEU:HA     | 3:F2:66:PHE:HZ     | 1.74                     | 0.49              |
| 3:F2:7:GLU:HA      | 3:F2:10:LEU:HB2    | 1.95                     | 0.49              |
| 8:c2:116:GLN:NE2   | 9:h2:42:GLU:OE2    | 2.23                     | 0.49              |
| 8:d2:228:GLU:HB2   | 9:i2:256:LYS:HG2   | 1.95                     | 0.49              |
| 9:o2:254:LEU:O     | 9:o2:258:THR:HG23  | 2.12                     | 0.49              |
| 9:r2:26:LEU:HD11   | 9:w2:242:ILE:HG21  | 1.94                     | 0.49              |
| 9:r2:124:GLN:NE2   | 9:w2:197:SER:HA    | 2.28                     | 0.49              |
| 10:E3:82:LEU:HD13  | 10:E3:144:PHE:CE1  | 2.48                     | 0.49              |
| 10:H3:82:LEU:HA    | 10:H3:197:SER:CB   | 2.39                     | 0.49              |
| 10:J3:78:LEU:HD12  | 10:J3:193:ASN:O    | 2.13                     | 0.49              |
| 10:P3:78:LEU:HD12  | 10:P3:193:ASN:O    | 2.13                     | 0.49              |
| 10:Q3:78:LEU:HD12  | 10:Q3:193:ASN:O    | 2.13                     | 0.49              |
| 10:S3:124:MET:HE3  | 10:S3:124:MET:HB3  | 1.77                     | 0.49              |
| 11:d3:277:GLN:HB3  | 11:d3:280:LEU:HD12 | 1.95                     | 0.49              |
| 11:f3:94:PRO:HB2   | 11:g3:219:ARG:NH2  | 2.27                     | 0.49              |
| 11:h3:20:GLU:O     | 11:h3:244:VAL:HG12 | 2.13                     | 0.49              |
| 11:i3:120:THR:HG23 | 11:i3:139:GLY:O    | 2.13                     | 0.49              |
| 11:j3:101:GLN:NE2  | 11:k3:188:GLN:HB3  | 2.28                     | 0.49              |
| 11:j3:120:THR:HG23 | 11:j3:139:GLY:O    | 2.13                     | 0.49              |
| 11:k3:94:PRO:HB2   | 11:l3:219:ARG:NH2  | 2.28                     | 0.49              |
| 11:k3:120:THR:HG23 | 11:k3:139:GLY:O    | 2.13                     | 0.49              |
| 11:l3:105:VAL:HG11 | 11:l3:169:ALA:HB2  | 1.94                     | 0.49              |
| 11:p3:252:LYS:HB2  | 11:p3:252:LYS:HE3  | 1.52                     | 0.49              |
| 11:r3:28:VAL:HB    | 11:r3:31:VAL:HG23  | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:s3:338:LEU:O    | 11:s3:338:LEU:HG   | 2.13                     | 0.49              |
| 11:v3:141:ILE:HD13 | 11:v3:165:ILE:CD1  | 2.37                     | 0.49              |
| 11:w3:327:ASN:OD1  | 11:w3:330:SER:HB2  | 2.13                     | 0.49              |
| 12:C4:160:VAL:HG11 | 12:C4:229:ARG:HB3  | 1.95                     | 0.49              |
| 12:C4:215:LEU:N    | 12:C4:223:THR:O    | 2.32                     | 0.49              |
| 12:E4:102:MET:HB3  | 12:E4:230:GLN:HB3  | 1.94                     | 0.49              |
| 1:A1:276:GLU:HB3   | 1:h1:374:HIS:HB3   | 1.95                     | 0.48              |
| 1:B1:187:ASP:O     | 1:B1:191:ILE:HG12  | 2.12                     | 0.48              |
| 1:C1:404:LEU:H     | 1:C1:434:ASN:ND2   | 2.10                     | 0.48              |
| 1:L1:143:THR:HG21  | 1:N1:156:HIS:NE2   | 2.28                     | 0.48              |
| 1:L1:151:LYS:NZ    | 1:L1:179:THR:HG22  | 2.28                     | 0.48              |
| 1:L1:409:MET:CE    | 1:L1:434:ASN:HB2   | 2.43                     | 0.48              |
| 1:Q1:244:ARG:HH11  | 1:R1:239:ASN:HB2   | 1.78                     | 0.48              |
| 1:S1:368:VAL:HG22  | 1:S1:369:ASP:O     | 2.13                     | 0.48              |
| 1:T1:141:ALA:O     | 1:T1:144:ILE:HG22  | 2.13                     | 0.48              |
| 1:W1:410:LYS:HD2   | 1:W1:410:LYS:C     | 2.38                     | 0.48              |
| 1:Z1:252:ILE:O     | 1:Z1:255:PRO:HD2   | 2.14                     | 0.48              |
| 1:c1:125:GLN:NE2   | 4:J2:6:VAL:H       | 2.10                     | 0.48              |
| 1:f1:189:GLY:O     | 1:f1:192:SER:OG    | 2.25                     | 0.48              |
| 2:C2:60:MET:HG3    | 2:C2:65:THR:CG2    | 2.43                     | 0.48              |
| 6:Q2:95:LEU:CD1    | 8:b2:56:LEU:HD11   | 2.42                     | 0.48              |
| 7:W2:30:ASN:HB2    | 7:W2:42:TYR:CE2    | 2.48                     | 0.48              |
| 8:e2:165:LYS:O     | 8:e2:189:ARG:NH2   | 2.44                     | 0.48              |
| 8:e2:182:THR:C     | 8:e2:184:GLU:H     | 2.20                     | 0.48              |
| 9:k2:11:GLY:HA2    | 9:k2:72:VAL:HG21   | 1.94                     | 0.48              |
| 9:r2:205:THR:CG2   | 11:m3:80:GLN:OE1   | 2.61                     | 0.48              |
| 9:x2:89:THR:OG1    | 9:x2:91:ASN:OD1    | 2.27                     | 0.48              |
| 10:E3:54:SER:HB2   | 11:f3:173:ARG:HH12 | 1.77                     | 0.48              |
| 10:F3:58:ILE:HG13  | 10:F3:59:ASN:N     | 2.28                     | 0.48              |
| 10:G3:78:LEU:HD12  | 10:G3:193:ASN:O    | 2.13                     | 0.48              |
| 10:H3:58:ILE:HG13  | 10:H3:59:ASN:N     | 2.28                     | 0.48              |
| 10:I3:58:ILE:HG13  | 10:I3:59:ASN:N     | 2.28                     | 0.48              |
| 10:M3:78:LEU:HD12  | 10:M3:193:ASN:O    | 2.13                     | 0.48              |
| 10:O3:78:LEU:HD12  | 10:O3:193:ASN:O    | 2.13                     | 0.48              |
| 10:P3:82:LEU:HD13  | 10:P3:144:PHE:CE1  | 2.48                     | 0.48              |
| 11:b3:94:PRO:HB2   | 11:c3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:b3:120:THR:HG23 | 11:b3:139:GLY:O    | 2.13                     | 0.48              |
| 11:c3:20:GLU:O     | 11:c3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:f3:277:GLN:HB3  | 11:f3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:g3:20:GLU:O     | 11:g3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:h3:79:MET:HE2   | 11:i3:57:PHE:CD2   | 2.48                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:h3:94:PRO:HB2   | 11:i3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:l3:277:GLN:HB3  | 11:l3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:t3:120:THR:HG23 | 11:t3:139:GLY:O    | 2.13                     | 0.48              |
| 11:v3:105:VAL:HG11 | 11:v3:169:ALA:HB2  | 1.94                     | 0.48              |
| 11:w3:254:VAL:CG2  | 11:x3:355:ALA:HB2  | 2.43                     | 0.48              |
| 11:z3:120:THR:HG23 | 11:z3:139:GLY:O    | 2.13                     | 0.48              |
| 1:E1:167:ARG:O     | 2:B2:140:ARG:NH2   | 2.45                     | 0.48              |
| 1:G1:267:THR:HB    | 1:G1:386:SER:HB2   | 1.95                     | 0.48              |
| 1:H1:195:VAL:HG13  | 1:H1:210:VAL:HG21  | 1.94                     | 0.48              |
| 1:P1:293:LEU:O     | 1:Q1:366:TYR:HD2   | 1.95                     | 0.48              |
| 1:T1:424:ASP:OD1   | 1:T1:425:LYS:N     | 2.47                     | 0.48              |
| 1:U1:373:ARG:HG2   | 1:V1:277:GLN:OE1   | 2.13                     | 0.48              |
| 1:U1:419:ALA:O     | 1:V1:267:THR:HG21  | 2.11                     | 0.48              |
| 1:Z1:266:VAL:HG22  | 1:Z1:387:VAL:HG22  | 1.94                     | 0.48              |
| 1:a1:389:VAL:O     | 1:a1:432:VAL:HA    | 2.12                     | 0.48              |
| 1:b1:404:LEU:H     | 1:b1:434:ASN:ND2   | 2.11                     | 0.48              |
| 1:d1:187:ASP:O     | 1:d1:191:ILE:HG12  | 2.13                     | 0.48              |
| 1:f1:199:SER:OG    | 1:f1:205:LEU:O     | 2.19                     | 0.48              |
| 1:g1:394:LYS:HG3   | 1:g1:402:LEU:HB2   | 1.94                     | 0.48              |
| 2:A2:143:ARG:H     | 2:A2:177:SER:HB2   | 1.77                     | 0.48              |
| 2:D2:42:VAL:HG11   | 5:M2:42:LEU:HB3    | 1.96                     | 0.48              |
| 2:E2:40:LEU:HD13   | 3:F2:66:PHE:CZ     | 2.47                     | 0.48              |
| 5:M2:32:VAL:HG13   | 5:M2:33:SER:N      | 2.27                     | 0.48              |
| 7:Y2:78:TYR:CZ     | 7:Y2:80:PRO:HG3    | 2.48                     | 0.48              |
| 8:b2:182:THR:C     | 8:b2:184:GLU:H     | 2.22                     | 0.48              |
| 8:b2:218:THR:OG1   | 9:h2:9:LYS:HG3     | 2.12                     | 0.48              |
| 8:e2:91:GLN:O      | 8:e2:118:HIS:HB2   | 2.13                     | 0.48              |
| 9:h2:173:LEU:HD22  | 9:h2:214:LEU:HD21  | 1.94                     | 0.48              |
| 9:k2:46:TYR:HA     | 9:k2:69:GLY:HA2    | 1.95                     | 0.48              |
| 9:o2:2:ILE:HG13    | 9:o2:3:SER:N       | 2.21                     | 0.48              |
| 9:p2:238:ARG:HD3   | 9:p2:238:ARG:HA    | 1.65                     | 0.48              |
| 9:v2:230:LEU:HD21  | 9:l2:242:ILE:HG13  | 1.95                     | 0.48              |
| 10:B3:30:LEU:HD23  | 10:B3:30:LEU:H     | 1.78                     | 0.48              |
| 10:B3:72:ARG:N     | 10:B3:76:ASP:OD2   | 2.25                     | 0.48              |
| 10:G3:58:ILE:HG13  | 10:G3:59:ASN:N     | 2.28                     | 0.48              |
| 10:H3:54:SER:HB2   | 11:i3:173:ARG:HH12 | 1.78                     | 0.48              |
| 10:H3:78:LEU:HD12  | 10:H3:193:ASN:O    | 2.13                     | 0.48              |
| 10:I3:78:LEU:HD12  | 10:I3:193:ASN:O    | 2.13                     | 0.48              |
| 10:J3:58:ILE:HG13  | 10:J3:59:ASN:N     | 2.28                     | 0.48              |
| 10:J3:159:GLY:O    | 10:J3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:L3:30:LEU:HD23  | 10:L3:30:LEU:H     | 1.78                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L3:58:ILE:HG13  | 10:L3:59:ASN:N     | 2.28                     | 0.48              |
| 10:N3:54:SER:HB2   | 11:o3:173:ARG:HH12 | 1.78                     | 0.48              |
| 10:O3:82:LEU:O     | 10:O3:197:SER:OG   | 2.21                     | 0.48              |
| 11:g3:103:ILE:HG13 | 11:g3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:h3:105:VAL:CG1  | 11:h3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:i3:20:GLU:O     | 11:i3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:m3:338:LEU:O    | 11:m3:338:LEU:HG   | 2.13                     | 0.48              |
| 11:n3:338:LEU:HG   | 11:n3:338:LEU:O    | 2.13                     | 0.48              |
| 11:q3:254:VAL:CG2  | 11:r3:355:ALA:HB2  | 2.43                     | 0.48              |
| 11:t3:327:ASN:OD1  | 11:t3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:t3:338:LEU:HG   | 11:t3:338:LEU:O    | 2.13                     | 0.48              |
| 11:u3:327:ASN:OD1  | 11:u3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:v3:282:VAL:HG23 | 11:v3:317:GLY:O    | 2.12                     | 0.48              |
| 11:y3:164:ARG:HD2  | 11:z3:365:ILE:CG2  | 2.43                     | 0.48              |
| 1:H1:200:SER:HB3   | 1:I1:175:SER:HB3   | 1.95                     | 0.48              |
| 1:I1:193:ALA:HB1   | 1:K1:213:VAL:HG13  | 1.94                     | 0.48              |
| 1:L1:142:ARG:HA    | 1:L1:145:GLU:OE1   | 2.12                     | 0.48              |
| 1:L1:244:ARG:NH1   | 1:M1:235:LEU:O     | 2.46                     | 0.48              |
| 1:Q1:374:HIS:HB3   | 1:R1:276:GLU:HB3   | 1.95                     | 0.48              |
| 1:W1:188:GLU:HA    | 1:W1:191:ILE:HB    | 1.94                     | 0.48              |
| 1:Y1:182:PRO:O     | 1:Y1:184:ARG:NH1   | 2.46                     | 0.48              |
| 1:c1:137:GLU:OE2   | 1:c1:155:VAL:HG22  | 2.13                     | 0.48              |
| 1:g1:270:LEU:HD23  | 1:g1:382:ILE:HA    | 1.96                     | 0.48              |
| 1:h1:133:GLN:O     | 1:h1:137:GLU:HG2   | 2.14                     | 0.48              |
| 1:h1:266:VAL:HG22  | 1:h1:387:VAL:HG22  | 1.94                     | 0.48              |
| 2:A2:116:PHE:CD1   | 2:A2:122:SER:HA    | 2.48                     | 0.48              |
| 3:F2:32:ILE:HG21   | 3:F2:138:LEU:HD21  | 1.95                     | 0.48              |
| 5:N2:76:GLN:HB3    | 6:T2:127:LEU:HD13  | 1.94                     | 0.48              |
| 8:d2:196:ASP:O     | 8:d2:198:SER:N     | 2.43                     | 0.48              |
| 9:k2:175:LEU:HG    | 9:k2:206:PRO:HG3   | 1.94                     | 0.48              |
| 9:n2:230:LEU:HD21  | 9:t2:242:ILE:HG23  | 1.96                     | 0.48              |
| 9:r2:98:LYS:HG2    | 9:r2:213:LEU:HD12  | 1.93                     | 0.48              |
| 9:u2:89:THR:HG23   | 9:u2:91:ASN:H      | 1.79                     | 0.48              |
| 9:v2:56:SER:OG     | 9:v2:57:SER:N      | 2.46                     | 0.48              |
| 10:D3:82:LEU:HD13  | 10:D3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:E3:58:ILE:HG13  | 10:E3:59:ASN:N     | 2.28                     | 0.48              |
| 10:G3:54:SER:HB2   | 11:h3:173:ARG:HH12 | 1.78                     | 0.48              |
| 10:G3:82:LEU:HD13  | 10:G3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:I3:159:GLY:O    | 10:I3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:K3:58:ILE:HG13  | 10:K3:59:ASN:N     | 2.28                     | 0.48              |
| 10:K3:159:GLY:O    | 10:K3:186:PRO:HG3  | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L3:159:GLY:O    | 10:L3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:M3:58:ILE:HG13  | 10:M3:59:ASN:N     | 2.28                     | 0.48              |
| 10:M3:159:GLY:O    | 10:M3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:O3:40:ILE:H     | 10:O3:40:ILE:HG12  | 1.48                     | 0.48              |
| 10:R3:54:SER:HB2   | 11:s3:173:ARG:HH12 | 1.79                     | 0.48              |
| 10:S3:82:LEU:HD13  | 10:S3:144:PHE:CE1  | 2.48                     | 0.48              |
| 11:a3:252:LYS:HB2  | 11:a3:252:LYS:HE3  | 1.52                     | 0.48              |
| 11:c3:105:VAL:CG1  | 11:c3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:c3:277:GLN:HB3  | 11:c3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:d3:105:VAL:CG1  | 11:d3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:e3:105:VAL:CG1  | 11:e3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:e3:254:VAL:CG2  | 11:f3:355:ALA:HB2  | 2.43                     | 0.48              |
| 11:f3:101:GLN:NE2  | 11:g3:219:ARG:HD3  | 2.26                     | 0.48              |
| 11:f3:105:VAL:CG1  | 11:f3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:h3:120:THR:HG23 | 11:h3:139:GLY:O    | 2.13                     | 0.48              |
| 11:i3:94:PRO:HB2   | 11:j3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:m3:20:GLU:O     | 11:m3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:r3:338:LEU:HG   | 11:r3:338:LEU:O    | 2.13                     | 0.48              |
| 11:t3:20:GLU:O     | 11:t3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:u3:254:VAL:CG2  | 11:v3:355:ALA:HB2  | 2.43                     | 0.48              |
| 11:w3:79:MET:HE2   | 11:x3:57:PHE:CD2   | 2.48                     | 0.48              |
| 11:w3:105:VAL:HG11 | 11:w3:169:ALA:HB2  | 1.94                     | 0.48              |
| 11:x3:277:GLN:HB3  | 11:x3:280:LEU:HD12 | 1.95                     | 0.48              |
| 12:E4:217:LEU:HB2  | 12:E4:220:TYR:HB2  | 1.95                     | 0.48              |
| 1:A1:405:THR:HG22  | 1:A1:408:GLN:HB2   | 1.94                     | 0.48              |
| 1:G1:407:ASP:OD1   | 1:G1:408:GLN:N     | 2.47                     | 0.48              |
| 1:H1:264:ALA:HB2   | 1:H1:389:VAL:HG22  | 1.96                     | 0.48              |
| 1:K1:205:LEU:HD11  | 1:K1:209:ASN:HB2   | 1.95                     | 0.48              |
| 1:O1:405:THR:OG1   | 1:O1:407:ASP:OD1   | 2.20                     | 0.48              |
| 1:P1:299:ASN:ND2   | 1:P1:361:ASN:HD22  | 2.11                     | 0.48              |
| 1:Q1:160:PRO:HG2   | 1:Q1:170:LYS:O     | 2.12                     | 0.48              |
| 1:U1:245:ILE:HG21  | 1:U1:266:VAL:HG11  | 1.95                     | 0.48              |
| 1:X1:166:VAL:O     | 1:X1:169:GLN:NE2   | 2.46                     | 0.48              |
| 1:a1:423:SER:HB3   | 1:a1:426:ARG:HB2   | 1.96                     | 0.48              |
| 1:h1:164:LEU:CD1   | 2:C2:143:ARG:NE    | 2.58                     | 0.48              |
| 2:E2:104:VAL:HG23  | 2:E2:133:PRO:HB2   | 1.95                     | 0.48              |
| 4:H2:59:PHE:HD1    | 4:I2:14:MET:HE2    | 1.76                     | 0.48              |
| 7:W2:43:ARG:HB3    | 7:W2:69:GLU:OE2    | 2.14                     | 0.48              |
| 8:c2:27:ALA:O      | 9:h2:72:VAL:HG11   | 2.14                     | 0.48              |
| 8:d2:152:PRO:HB2   | 9:n2:195:THR:HG22  | 1.94                     | 0.48              |
| 9:m2:239:ALA:HB2   | 9:s2:1:MET:HE3     | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:m2:248:SER:O     | 9:m2:252:GLN:HG3   | 2.13                     | 0.48              |
| 9:p2:16:GLN:NE2    | 9:u2:2:ILE:HD12    | 2.28                     | 0.48              |
| 9:42:42:GLU:OE1    | 9:42:73:ARG:HB3    | 2.14                     | 0.48              |
| 9:42:130:THR:HG22  | 9:42:134:PHE:HB2   | 1.93                     | 0.48              |
| 10:A3:30:LEU:HD23  | 10:A3:30:LEU:H     | 1.78                     | 0.48              |
| 10:D3:58:ILE:HG13  | 10:D3:59:ASN:N     | 2.28                     | 0.48              |
| 10:L3:78:LEU:HD12  | 10:L3:193:ASN:O    | 2.13                     | 0.48              |
| 10:L3:82:LEU:HD13  | 10:L3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:N3:58:ILE:HG13  | 10:N3:59:ASN:N     | 2.28                     | 0.48              |
| 10:N3:78:LEU:HD12  | 10:N3:193:ASN:O    | 2.13                     | 0.48              |
| 10:N3:159:GLY:O    | 10:N3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:O3:58:ILE:HG13  | 10:O3:59:ASN:N     | 2.28                     | 0.48              |
| 10:R3:78:LEU:HD12  | 10:R3:193:ASN:O    | 2.13                     | 0.48              |
| 11:c3:94:PRO:HB2   | 11:d3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:c3:120:THR:HG23 | 11:c3:139:GLY:O    | 2.13                     | 0.48              |
| 11:f3:103:ILE:HG13 | 11:f3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:g3:277:GLN:HB3  | 11:g3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:k3:105:VAL:CG1  | 11:k3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:k3:277:GLN:HB3  | 11:k3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:m3:277:GLN:HB3  | 11:m3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:q3:120:THR:HG23 | 11:q3:139:GLY:O    | 2.13                     | 0.48              |
| 11:r3:20:GLU:O     | 11:r3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:r3:120:THR:HG23 | 11:r3:139:GLY:O    | 2.13                     | 0.48              |
| 11:s3:20:GLU:O     | 11:s3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:u3:20:GLU:O     | 11:u3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:v3:103:ILE:HG13 | 11:v3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:x3:327:ASN:OD1  | 11:x3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:y3:256:ASN:O    | 11:y3:257:SER:OG   | 2.30                     | 0.48              |
| 1:B1:187:ASP:OD1   | 1:B1:190:GLN:HG3   | 2.13                     | 0.48              |
| 1:J1:389:VAL:HB    | 1:J1:432:VAL:HG22  | 1.95                     | 0.48              |
| 1:O1:244:ARG:NE    | 1:P1:239:ASN:HD21  | 2.10                     | 0.48              |
| 1:P1:240:ASP:O     | 1:P1:244:ARG:HG3   | 2.14                     | 0.48              |
| 1:P1:374:HIS:HB3   | 1:Q1:276:GLU:HB3   | 1.94                     | 0.48              |
| 1:Q1:187:ASP:OD1   | 1:Q1:190:GLN:HG3   | 2.13                     | 0.48              |
| 1:Q1:275:LYS:CB    | 1:Q1:377:MET:HB2   | 2.43                     | 0.48              |
| 1:R1:138:GLY:O     | 1:R1:142:ARG:HG2   | 2.13                     | 0.48              |
| 1:T1:392:ASN:OD1   | 1:T1:436:PRO:HA    | 2.14                     | 0.48              |
| 1:U1:143:THR:HG21  | 1:W1:156:HIS:CD2   | 2.48                     | 0.48              |
| 1:Y1:407:ASP:HA    | 1:Y1:410:LYS:HG3   | 1.94                     | 0.48              |
| 1:c1:283:SER:OG    | 1:c1:369:ASP:HB2   | 2.14                     | 0.48              |
| 1:h1:125:GLN:HB2   | 4:I2:8:MET:HB2     | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:h1:164:LEU:HD11  | 2:C2:143:ARG:HE    | 1.74                     | 0.48              |
| 3:F2:149:LEU:O     | 3:F2:153:THR:HG23  | 2.12                     | 0.48              |
| 4:G2:2:THR:HG23    | 4:G2:5:SER:H       | 1.79                     | 0.48              |
| 6:S2:70:SER:C      | 6:S2:72:HIS:H      | 2.22                     | 0.48              |
| 8:c2:182:THR:C     | 8:c2:184:GLU:H     | 2.21                     | 0.48              |
| 9:i2:230:LEU:HD12  | 9:t2:257:LEU:HG    | 1.95                     | 0.48              |
| 9:o2:2:ILE:HB      | 9:o2:254:LEU:HD11  | 1.95                     | 0.48              |
| 9:q2:7:ILE:O       | 9:q2:10:THR:OG1    | 2.27                     | 0.48              |
| 9:s2:72:VAL:O      | 9:s2:72:VAL:HG12   | 2.14                     | 0.48              |
| 9:u2:72:VAL:O      | 9:u2:72:VAL:HG12   | 2.14                     | 0.48              |
| 9:u2:231:VAL:HG11  | 9:12:9:LYS:HG2     | 1.96                     | 0.48              |
| 9:w2:36:ARG:HH21   | 9:w2:80:LEU:HD13   | 1.77                     | 0.48              |
| 9:w2:48:THR:HG21   | 9:w2:51:GLN:NE2    | 2.27                     | 0.48              |
| 9:12:105:VAL:CG1   | 9:12:134:PHE:HB3   | 2.44                     | 0.48              |
| 10:F3:78:LEU:HD12  | 10:F3:193:ASN:O    | 2.14                     | 0.48              |
| 10:H3:159:GLY:O    | 10:H3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:P3:54:SER:HB2   | 11:q3:173:ARG:HH12 | 1.79                     | 0.48              |
| 10:P3:58:ILE:HG13  | 10:P3:59:ASN:N     | 2.28                     | 0.48              |
| 10:R3:41:PRO:HA    | 10:T3:157:ALA:HB1  | 1.95                     | 0.48              |
| 10:W3:54:SER:HB2   | 11:x3:173:ARG:HH12 | 1.77                     | 0.48              |
| 10:W3:82:LEU:HD13  | 10:W3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:X3:82:LEU:HD13  | 10:X3:144:PHE:CE1  | 2.48                     | 0.48              |
| 11:b3:105:VAL:CG1  | 11:b3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:e3:79:MET:HE2   | 11:f3:57:PHE:CD2   | 2.48                     | 0.48              |
| 11:e3:94:PRO:HB2   | 11:f3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:i3:105:VAL:HG11 | 11:i3:169:ALA:HB2  | 1.94                     | 0.48              |
| 11:k3:20:GLU:O     | 11:k3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:k3:105:VAL:HG11 | 11:k3:169:ALA:HB2  | 1.94                     | 0.48              |
| 11:n3:20:GLU:O     | 11:n3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:o3:20:GLU:O     | 11:o3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:o3:79:MET:HE2   | 11:p3:57:PHE:CD2   | 2.48                     | 0.48              |
| 11:p3:20:GLU:O     | 11:p3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:q3:20:GLU:O     | 11:q3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:q3:327:ASN:OD1  | 11:q3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:s3:79:MET:HE2   | 11:t3:57:PHE:CD2   | 2.49                     | 0.48              |
| 11:v3:20:GLU:O     | 11:v3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:w3:94:PRO:HB2   | 11:x3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:x3:20:GLU:O     | 11:x3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:x3:103:ILE:HG13 | 11:x3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:y3:277:GLN:HB3  | 11:y3:280:LEU:HD12 | 1.95                     | 0.48              |
| 1:B1:417:ARG:HG3   | 1:B1:422:PHE:CB    | 2.43                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C1:165:PHE:CZ    | 2:C2:145:ALA:HA    | 2.49                     | 0.48              |
| 1:E1:424:ASP:OD1   | 1:E1:425:LYS:N     | 2.46                     | 0.48              |
| 1:I1:275:LYS:HB2   | 1:I1:377:MET:HB2   | 1.96                     | 0.48              |
| 1:Q1:410:LYS:HD2   | 1:Q1:411:GLN:N     | 2.29                     | 0.48              |
| 1:S1:248:ARG:NH1   | 1:T1:267:THR:OG1   | 2.46                     | 0.48              |
| 1:T1:203:ALA:HB3   | 1:U1:160:PRO:HG3   | 1.95                     | 0.48              |
| 1:X1:167:ARG:NH2   | 2:E2:158:PRO:O     | 2.46                     | 0.48              |
| 1:a1:203:ALA:HA    | 1:c1:158:ALA:HB1   | 1.95                     | 0.48              |
| 1:d1:410:LYS:HD2   | 1:d1:411:GLN:N     | 2.28                     | 0.48              |
| 3:F2:244:PHE:O     | 3:F2:247:ILE:HG22  | 2.14                     | 0.48              |
| 7:X2:29:ALA:HB1    | 8:c2:11:ALA:HB2    | 1.95                     | 0.48              |
| 8:b2:140:ASP:O     | 8:b2:160:ARG:NH1   | 2.45                     | 0.48              |
| 8:b2:189:ARG:HE    | 8:b2:193:LEU:HD23  | 1.78                     | 0.48              |
| 8:c2:27:ALA:C      | 9:h2:72:VAL:HG11   | 2.39                     | 0.48              |
| 9:i2:95:VAL:O      | 9:i2:118:GLY:HA3   | 2.13                     | 0.48              |
| 9:l2:99:GLY:O      | 9:l2:116:ARG:NH2   | 2.47                     | 0.48              |
| 9:q2:248:SER:O     | 9:q2:252:GLN:HG2   | 2.13                     | 0.48              |
| 9:w2:241:GLU:OE1   | 9:22:256:LYS:HD2   | 2.13                     | 0.48              |
| 9:z2:89:THR:HG23   | 9:z2:91:ASN:H      | 1.77                     | 0.48              |
| 9:12:237:GLN:HE22  | 12:E4:53:LEU:C     | 2.19                     | 0.48              |
| 9:32:120:PHE:HB3   | 9:32:128:LEU:HD22  | 1.94                     | 0.48              |
| 10:A3:219:MET:HE2  | 10:C3:132:PHE:CB   | 2.44                     | 0.48              |
| 10:B3:219:MET:HE2  | 10:D3:132:PHE:CB   | 2.44                     | 0.48              |
| 10:C3:54:SER:HB2   | 11:d3:173:ARG:HH12 | 1.77                     | 0.48              |
| 10:C3:58:ILE:HG13  | 10:C3:59:ASN:N     | 2.28                     | 0.48              |
| 10:I3:82:LEU:HD13  | 10:I3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:K3:82:LEU:HD13  | 10:K3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:M3:54:SER:HB2   | 11:n3:173:ARG:HH12 | 1.78                     | 0.48              |
| 10:M3:82:LEU:HD13  | 10:M3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:M3:101:LYS:HZ3  | 10:M3:101:LYS:HB2  | 1.78                     | 0.48              |
| 10:N3:82:LEU:HD13  | 10:N3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:O3:159:GLY:O    | 10:O3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:Q3:58:ILE:HG13  | 10:Q3:59:ASN:N     | 2.28                     | 0.48              |
| 10:Q3:82:LEU:HD13  | 10:Q3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:U3:159:GLY:O    | 10:U3:186:PRO:HG3  | 2.14                     | 0.48              |
| 11:f3:20:GLU:O     | 11:f3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:f3:327:ASN:OD1  | 11:f3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:h3:277:GLN:HB3  | 11:h3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:j3:20:GLU:O     | 11:j3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:j3:105:VAL:HG11 | 11:j3:169:ALA:HB2  | 1.94                     | 0.48              |
| 11:j3:105:VAL:CG1  | 11:j3:169:ALA:HB2  | 2.44                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:j3:327:ASN:OD1  | 11:j3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:k3:254:VAL:CG2  | 11:l3:355:ALA:HB2  | 2.43                     | 0.48              |
| 11:l3:20:GLU:O     | 11:l3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:l3:93:TYR:OH    | 11:l3:173:ARG:O    | 2.25                     | 0.48              |
| 11:n3:94:PRO:HB2   | 11:o3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:r3:94:PRO:HB2   | 11:s3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:w3:103:ILE:HG13 | 11:w3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:y3:120:THR:HG23 | 11:y3:139:GLY:O    | 2.13                     | 0.48              |
| 12:A4:108:ILE:HD12 | 12:A4:182:ILE:HG21 | 1.94                     | 0.48              |
| 1:F1:392:ASN:OD1   | 1:F1:393:TYR:N     | 2.46                     | 0.48              |
| 1:J1:370:ARG:HG2   | 1:J1:371:THR:N     | 2.29                     | 0.48              |
| 1:L1:165:PHE:CD1   | 2:A2:143:ARG:HA    | 2.49                     | 0.48              |
| 1:T1:281:HIS:HB3   | 1:T1:371:THR:HB    | 1.96                     | 0.48              |
| 1:W1:154:ARG:HG3   | 1:W1:177:THR:HG23  | 1.96                     | 0.48              |
| 1:X1:275:LYS:HB2   | 1:X1:377:MET:HB2   | 1.96                     | 0.48              |
| 1:d1:139:GLU:HB3   | 1:f1:156:HIS:HE1   | 1.79                     | 0.48              |
| 2:D2:45:LEU:O      | 2:D2:49:THR:HG23   | 2.13                     | 0.48              |
| 3:F2:7:GLU:HB2     | 5:K2:74:ASP:OD2    | 2.13                     | 0.48              |
| 7:a2:74:GLU:HA     | 7:a2:95:ASN:HB3    | 1.95                     | 0.48              |
| 8:d2:173:ARG:HB3   | 9:i2:67:GLN:HE22   | 1.78                     | 0.48              |
| 9:m2:46:TYR:HA     | 9:m2:69:GLY:HA2    | 1.95                     | 0.48              |
| 9:n2:36:ARG:HH21   | 9:n2:80:LEU:HB2    | 1.78                     | 0.48              |
| 9:t2:26:LEU:HD23   | 9:y2:246:ALA:HB2   | 1.94                     | 0.48              |
| 9:u2:202:ASN:ND2   | 11:a3:78:ASN:HD21  | 1.99                     | 0.48              |
| 10:B3:82:LEU:HA    | 10:B3:197:SER:CB   | 2.38                     | 0.48              |
| 10:C3:82:LEU:HD13  | 10:C3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:D3:219:MET:HE2  | 10:F3:132:PHE:CB   | 2.44                     | 0.48              |
| 10:E3:78:LEU:HD12  | 10:E3:193:ASN:O    | 2.13                     | 0.48              |
| 10:G3:159:GLY:O    | 10:G3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:O3:82:LEU:HD13  | 10:O3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:S3:219:MET:HE2  | 10:U3:132:PHE:CB   | 2.43                     | 0.48              |
| 10:V3:159:GLY:O    | 10:V3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:V3:219:MET:HE2  | 10:X3:132:PHE:CB   | 2.44                     | 0.48              |
| 10:W3:159:GLY:O    | 10:W3:186:PRO:HG3  | 2.13                     | 0.48              |
| 11:a3:105:VAL:CG1  | 11:a3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:b3:277:GLN:HB3  | 11:b3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:c3:338:LEU:HG   | 11:c3:338:LEU:O    | 2.13                     | 0.48              |
| 11:d3:120:THR:HG23 | 11:d3:139:GLY:O    | 2.13                     | 0.48              |
| 11:g3:105:VAL:CG1  | 11:g3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:i3:327:ASN:OD1  | 11:i3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:k3:96:PHE:O     | 11:l3:219:ARG:HD2  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:k3:101:GLN:NE2 | 11:l3:188:GLN:HB3  | 2.29                     | 0.48              |
| 11:m3:105:VAL:CG1 | 11:m3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:n3:327:ASN:OD1 | 11:n3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:o3:338:LEU:HG  | 11:o3:338:LEU:O    | 2.13                     | 0.48              |
| 11:q3:338:LEU:HG  | 11:q3:338:LEU:O    | 2.13                     | 0.48              |
| 11:r3:83:ASN:ND2  | 11:s3:109:SER:OG   | 2.45                     | 0.48              |
| 11:r3:327:ASN:OD1 | 11:r3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:v3:83:ASN:ND2  | 11:w3:109:SER:OG   | 2.45                     | 0.48              |
| 11:w3:21:ARG:O    | 11:w3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:w3:277:GLN:HB3 | 11:w3:280:LEU:HD12 | 1.96                     | 0.48              |
| 11:y3:46:ASP:OD1  | 11:z3:161:ASN:N    | 2.47                     | 0.48              |
| 11:y3:327:ASN:OD1 | 11:y3:330:SER:HB2  | 2.13                     | 0.48              |
| 1:A1:267:THR:HG22 | 1:h1:248:ARG:HD2   | 1.94                     | 0.48              |
| 1:B1:194:VAL:HG13 | 1:B1:212:LEU:HD11  | 1.96                     | 0.48              |
| 1:B1:408:GLN:O    | 1:B1:412:ILE:HG12  | 2.14                     | 0.48              |
| 1:G1:165:PHE:CE2  | 4:H2:88:ILE:CG2    | 2.93                     | 0.48              |
| 1:H1:143:THR:HG22 | 1:I1:154:ARG:CD    | 2.43                     | 0.48              |
| 1:M1:365:ASN:ND2  | 6:Q2:72:HIS:O      | 2.45                     | 0.48              |
| 1:N1:374:HIS:HB3  | 1:O1:276:GLU:HB2   | 1.95                     | 0.48              |
| 1:N1:415:LEU:HD11 | 1:O1:433:VAL:HG21  | 1.95                     | 0.48              |
| 1:Q1:244:ARG:HG2  | 1:Q1:247:ARG:HH22  | 1.77                     | 0.48              |
| 1:R1:187:ASP:O    | 1:R1:191:ILE:HG12  | 2.14                     | 0.48              |
| 1:W1:375:THR:HG23 | 1:X1:275:LYS:HZ1   | 1.78                     | 0.48              |
| 1:Y1:392:ASN:OD1  | 1:Y1:393:TYR:N     | 2.44                     | 0.48              |
| 1:Z1:301:SER:OG   | 1:Z1:303:GLN:NE2   | 2.46                     | 0.48              |
| 1:c1:231:ASN:OD1  | 1:c1:232:ASP:N     | 2.42                     | 0.48              |
| 1:d1:244:ARG:HH21 | 1:e1:239:ASN:HD21  | 1.60                     | 0.48              |
| 2:B2:39:SER:C     | 2:B2:41:SER:N      | 2.72                     | 0.48              |
| 2:B2:53:PHE:HD2   | 2:B2:57:ILE:HD12   | 1.78                     | 0.48              |
| 2:E2:115:PRO:CB   | 2:E2:121:ILE:HD12  | 2.44                     | 0.48              |
| 4:G2:43:GLN:H     | 4:G2:43:GLN:CD     | 2.21                     | 0.48              |
| 6:U2:18:LEU:HD21  | 6:U2:48:GLU:HB2    | 1.96                     | 0.48              |
| 8:c2:76:ARG:HG2   | 8:c2:77:PRO:HD2    | 1.95                     | 0.48              |
| 8:d2:134:GLU:HB3  | 8:d2:146:LEU:O     | 2.13                     | 0.48              |
| 8:e2:142:THR:HG21 | 9:u2:58:GLU:HG3    | 1.95                     | 0.48              |
| 9:j2:86:LEU:HD11  | 9:u2:45:LEU:HG     | 1.96                     | 0.48              |
| 9:m2:7:ILE:O      | 9:m2:10:THR:OG1    | 2.28                     | 0.48              |
| 9:t2:105:VAL:HG11 | 9:t2:134:PHE:HB3   | 1.96                     | 0.48              |
| 9:v2:105:VAL:CG1  | 9:v2:134:PHE:HB3   | 2.44                     | 0.48              |
| 9:v2:254:LEU:O    | 9:v2:258:THR:HG23  | 2.13                     | 0.48              |
| 9:12:106:MET:HE2  | 9:12:135:GLN:HB3   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:32:238:ARG:CG    | 12:B4:55:ASN:HD21  | 2.26                     | 0.48              |
| 9:42:102:PHE:HB3   | 9:42:114:TYR:HB3   | 1.96                     | 0.48              |
| 10:C3:219:MET:HE2  | 10:E3:132:PHE:CB   | 2.44                     | 0.48              |
| 10:F3:54:SER:HB2   | 11:g3:173:ARG:HH12 | 1.78                     | 0.48              |
| 10:P3:159:GLY:O    | 10:P3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:S3:41:PRO:HA    | 10:U3:157:ALA:HB1  | 1.96                     | 0.48              |
| 10:S3:78:LEU:HD12  | 10:S3:193:ASN:O    | 2.13                     | 0.48              |
| 10:V3:51:ILE:CG1   | 11:x3:175:LEU:HD11 | 2.39                     | 0.48              |
| 10:Y3:124:MET:HE3  | 10:Y3:124:MET:HB3  | 1.77                     | 0.48              |
| 10:Z3:30:LEU:HD23  | 10:Z3:30:LEU:H     | 1.78                     | 0.48              |
| 11:b3:101:GLN:NE2  | 11:c3:188:GLN:HB3  | 2.29                     | 0.48              |
| 11:d3:20:GLU:O     | 11:d3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:g3:327:ASN:OD1  | 11:g3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:j3:277:GLN:HB3  | 11:j3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:l3:21:ARG:O     | 11:l3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:l3:338:LEU:HG   | 11:l3:338:LEU:O    | 2.13                     | 0.48              |
| 11:n3:120:THR:HG23 | 11:n3:139:GLY:O    | 2.13                     | 0.48              |
| 11:q3:96:PHE:O     | 11:r3:219:ARG:HD2  | 2.13                     | 0.48              |
| 11:r3:50:ASP:OD1   | 11:r3:113:ALA:N    | 2.47                     | 0.48              |
| 11:u3:120:THR:HG23 | 11:u3:139:GLY:O    | 2.13                     | 0.48              |
| 11:u3:338:LEU:O    | 11:u3:338:LEU:HG   | 2.13                     | 0.48              |
| 11:v3:120:THR:HG23 | 11:v3:139:GLY:O    | 2.13                     | 0.48              |
| 11:w3:20:GLU:O     | 11:w3:244:VAL:HG12 | 2.13                     | 0.48              |
| 11:w3:120:THR:HG23 | 11:w3:139:GLY:O    | 2.13                     | 0.48              |
| 11:x3:21:ARG:O     | 11:x3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:y3:21:ARG:O     | 11:y3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:y3:50:ASP:OD1   | 11:y3:113:ALA:N    | 2.47                     | 0.48              |
| 11:y3:103:ILE:HG13 | 11:y3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:z3:103:ILE:HG13 | 11:z3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:z3:105:VAL:CG1  | 11:z3:169:ALA:HB2  | 2.44                     | 0.48              |
| 12:C4:100:GLY:HA3  | 12:C4:200:PHE:CE1  | 2.49                     | 0.48              |
| 1:E1:365:ASN:C     | 6:U2:72:HIS:NE2    | 2.72                     | 0.48              |
| 1:H1:189:GLY:O     | 1:H1:192:SER:OG    | 2.25                     | 0.48              |
| 1:I1:283:SER:HB2   | 1:I1:369:ASP:HB2   | 1.96                     | 0.48              |
| 1:J1:267:THR:HB    | 1:J1:386:SER:HB2   | 1.95                     | 0.48              |
| 1:L1:245:ILE:HG21  | 1:L1:266:VAL:HG11  | 1.96                     | 0.48              |
| 1:O1:139:GLU:O     | 1:O1:143:THR:HG23  | 2.14                     | 0.48              |
| 1:X1:234:GLN:HB2   | 1:X1:272:PHE:CE2   | 2.49                     | 0.48              |
| 1:Y1:298:LEU:HD13  | 1:Y1:362:GLU:HB3   | 1.95                     | 0.48              |
| 1:Z1:245:ILE:O     | 1:Z1:249:ILE:HG12  | 2.14                     | 0.48              |
| 1:g1:266:VAL:HG22  | 1:g1:387:VAL:HG22  | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A2:135:ARG:CG    | 2:A2:167:MET:HE1   | 2.44                     | 0.48              |
| 2:E2:42:VAL:HG22   | 5:L2:42:LEU:HD12   | 1.96                     | 0.48              |
| 2:E2:65:THR:O      | 2:E2:69:ILE:HG12   | 2.13                     | 0.48              |
| 4:H2:46:GLU:OE2    | 4:H2:49:LEU:HG     | 2.14                     | 0.48              |
| 7:a2:64:VAL:O      | 7:a2:64:VAL:HG22   | 2.14                     | 0.48              |
| 9:h2:7:ILE:O       | 9:h2:10:THR:OG1    | 2.24                     | 0.48              |
| 9:n2:49:ILE:HD12   | 9:n2:66:LEU:HD11   | 1.96                     | 0.48              |
| 9:n2:168:VAL:HG21  | 11:x3:80:GLN:OE1   | 2.14                     | 0.48              |
| 9:s2:98:LYS:NZ     | 9:y2:187:ILE:O     | 2.39                     | 0.48              |
| 9:u2:26:LEU:HD13   | 9:u2:229:GLU:HB3   | 1.96                     | 0.48              |
| 9:u2:208:LEU:HD22  | 9:12:109:ASP:OD1   | 2.14                     | 0.48              |
| 9:u2:257:LEU:O     | 9:u2:260:LEU:HB3   | 2.14                     | 0.48              |
| 9:v2:174:ASN:HA    | 9:v2:206:PRO:HD3   | 1.96                     | 0.48              |
| 10:H3:82:LEU:HD13  | 10:H3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:J3:82:LEU:HD13  | 10:J3:144:PHE:CE1  | 2.48                     | 0.48              |
| 10:L3:54:SER:HB2   | 11:m3:173:ARG:HH12 | 1.78                     | 0.48              |
| 10:M3:219:MET:HE2  | 10:O3:132:PHE:CB   | 2.43                     | 0.48              |
| 10:R3:58:ILE:HG13  | 10:R3:59:ASN:N     | 2.28                     | 0.48              |
| 10:S3:159:GLY:O    | 10:S3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:T3:159:GLY:O    | 10:T3:186:PRO:HG3  | 2.14                     | 0.48              |
| 11:b3:338:LEU:HG   | 11:b3:338:LEU:O    | 2.13                     | 0.48              |
| 11:c3:103:ILE:HG13 | 11:c3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:e3:101:GLN:NE2  | 11:f3:188:GLN:HB3  | 2.29                     | 0.48              |
| 11:e3:103:ILE:HG13 | 11:e3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:e3:338:LEU:O    | 11:e3:338:LEU:HG   | 2.13                     | 0.48              |
| 11:g3:50:ASP:OD1   | 11:g3:113:ALA:N    | 2.47                     | 0.48              |
| 11:g3:79:MET:HE2   | 11:h3:57:PHE:CD2   | 2.49                     | 0.48              |
| 11:h3:50:ASP:OD1   | 11:h3:113:ALA:N    | 2.47                     | 0.48              |
| 11:k3:21:ARG:O     | 11:k3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:m3:254:VAL:CG2  | 11:n3:355:ALA:HB2  | 2.44                     | 0.48              |
| 11:n3:50:ASP:OD1   | 11:n3:113:ALA:N    | 2.47                     | 0.48              |
| 11:n3:277:GLN:HB3  | 11:n3:280:LEU:HD12 | 1.95                     | 0.48              |
| 11:o3:327:ASN:OD1  | 11:o3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:q3:50:ASP:OD1   | 11:q3:113:ALA:N    | 2.47                     | 0.48              |
| 11:q3:94:PRO:HB2   | 11:r3:219:ARG:NH2  | 2.28                     | 0.48              |
| 11:s3:21:ARG:O     | 11:s3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:t3:105:VAL:CG1  | 11:t3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:v3:21:ARG:O     | 11:v3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:v3:50:ASP:OD1   | 11:v3:113:ALA:N    | 2.47                     | 0.48              |
| 11:v3:101:GLN:NE2  | 11:w3:188:GLN:HB3  | 2.28                     | 0.48              |
| 11:z3:21:ARG:O     | 11:z3:25:LEU:HD22  | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:D4:134:ASP:HA   | 12:D4:155:GLU:HA   | 1.96                     | 0.48              |
| 1:C1:164:LEU:CD2   | 2:C2:149:LEU:HA    | 2.43                     | 0.48              |
| 1:E1:178:VAL:HG12  | 1:E1:180:LEU:HD22  | 1.96                     | 0.48              |
| 1:E1:197:LEU:HD12  | 1:G1:175:SER:HB2   | 1.96                     | 0.48              |
| 1:F1:393:TYR:CE2   | 1:F1:436:PRO:HD3   | 2.48                     | 0.48              |
| 1:G1:191:ILE:HD11  | 1:G1:220:LEU:HD13  | 1.96                     | 0.48              |
| 1:I1:151:LYS:NZ    | 1:I1:182:PRO:HD3   | 2.29                     | 0.48              |
| 1:N1:275:LYS:CB    | 1:N1:377:MET:HB2   | 2.44                     | 0.48              |
| 1:R1:203:ALA:HB2   | 1:T1:158:ALA:HB1   | 1.95                     | 0.48              |
| 1:T1:250:GLU:O     | 1:T1:254:SER:OG    | 2.25                     | 0.48              |
| 1:Y1:393:TYR:CE2   | 1:Y1:436:PRO:HD3   | 2.49                     | 0.48              |
| 1:Z1:294:ARG:CG    | 6:S2:68:THR:HB     | 2.43                     | 0.48              |
| 1:a1:423:SER:HB3   | 1:a1:426:ARG:HE    | 1.79                     | 0.48              |
| 1:c1:391:VAL:HG21  | 1:c1:409:MET:HE1   | 1.95                     | 0.48              |
| 2:D2:128:ASP:O     | 2:D2:132:GLN:HG2   | 2.14                     | 0.48              |
| 5:K2:99:VAL:O      | 5:K2:102:MET:HG2   | 2.14                     | 0.48              |
| 5:N2:69:ASN:OD1    | 5:N2:70:ASP:N      | 2.47                     | 0.48              |
| 6:U2:76:GLN:HG2    | 6:U2:77:ALA:H      | 1.79                     | 0.48              |
| 7:Y2:29:ALA:HB1    | 8:d2:11:ALA:HB2    | 1.96                     | 0.48              |
| 8:b2:62:PRO:HB3    | 9:g2:62:LEU:HG     | 1.96                     | 0.48              |
| 8:b2:66:MET:HG3    | 8:b2:168:GLY:H     | 1.78                     | 0.48              |
| 9:s2:95:VAL:O      | 9:s2:118:GLY:HA3   | 2.14                     | 0.48              |
| 9:u2:105:VAL:CG1   | 9:u2:134:PHE:HB3   | 2.43                     | 0.48              |
| 9:y2:195:THR:HG23  | 9:y2:197:SER:H     | 1.78                     | 0.48              |
| 9:z2:237:GLN:HG2   | 12:D4:53:LEU:HD12  | 1.91                     | 0.48              |
| 9:32:52:PRO:HA     | 9:32:65:GLY:H      | 1.79                     | 0.48              |
| 10:F3:159:GLY:O    | 10:F3:186:PRO:HG3  | 2.14                     | 0.48              |
| 10:T3:219:MET:HE2  | 10:V3:132:PHE:CB   | 2.44                     | 0.48              |
| 10:X3:54:SER:HB2   | 11:y3:173:ARG:HH12 | 1.77                     | 0.48              |
| 10:Y3:171:ILE:O    | 10:Z3:207:TYR:O    | 2.31                     | 0.48              |
| 10:Z3:54:SER:HB2   | 11:a3:173:ARG:HH12 | 1.77                     | 0.48              |
| 11:a3:103:ILE:HG13 | 11:a3:169:ALA:HB3  | 1.95                     | 0.48              |
| 11:h3:338:LEU:O    | 11:h3:338:LEU:HG   | 2.13                     | 0.48              |
| 11:i3:79:MET:HE2   | 11:j3:57:PHE:CD2   | 2.48                     | 0.48              |
| 11:l3:79:MET:HE2   | 11:m3:57:PHE:CD2   | 2.47                     | 0.48              |
| 11:m3:21:ARG:O     | 11:m3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:p3:327:ASN:OD1  | 11:p3:330:SER:HB2  | 2.13                     | 0.48              |
| 11:r3:21:ARG:O     | 11:r3:25:LEU:HD22  | 2.14                     | 0.48              |
| 11:s3:105:VAL:CG1  | 11:s3:169:ALA:HB2  | 2.44                     | 0.48              |
| 11:s3:327:ASN:OD1  | 11:s3:330:SER:HB2  | 2.14                     | 0.48              |
| 11:u3:50:ASP:OD1   | 11:u3:113:ALA:N    | 2.47                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:w3:96:PHE:O     | 11:x3:219:ARG:HD2  | 2.13                     | 0.48              |
| 11:x3:80:GLN:HB3   | 11:y3:54:GLN:HB3   | 1.96                     | 0.48              |
| 11:x3:120:THR:HG23 | 11:x3:139:GLY:O    | 2.13                     | 0.48              |
| 11:y3:96:PHE:O     | 11:z3:219:ARG:HD2  | 2.13                     | 0.48              |
| 11:z3:50:ASP:OD1   | 11:z3:113:ALA:N    | 2.47                     | 0.48              |
| 11:z3:277:GLN:HB3  | 11:z3:280:LEU:HD12 | 1.95                     | 0.48              |
| 12:A4:149:ARG:NH1  | 12:A4:168:LYS:O    | 2.37                     | 0.48              |
| 12:E4:224:THR:OG1  | 12:E4:226:ASP:OD1  | 2.24                     | 0.48              |
| 1:I1:282:TYR:CZ    | 1:I1:370:ARG:HD3   | 2.49                     | 0.47              |
| 1:K1:372:ILE:O     | 1:L1:277:GLN:HA    | 2.14                     | 0.47              |
| 1:L1:179:THR:HG23  | 1:L1:215:GLN:HB3   | 1.96                     | 0.47              |
| 1:L1:373:ARG:HH21  | 1:M1:275:LYS:HD2   | 1.79                     | 0.47              |
| 1:Q1:178:VAL:HG12  | 1:Q1:213:VAL:O     | 2.13                     | 0.47              |
| 1:Q1:412:ILE:O     | 1:Q1:416:THR:HG23  | 2.14                     | 0.47              |
| 1:T1:417:ARG:HG3   | 1:T1:422:PHE:HB3   | 1.96                     | 0.47              |
| 1:Y1:180:LEU:H     | 1:Y1:215:GLN:CD    | 2.22                     | 0.47              |
| 1:Z1:404:LEU:H     | 1:Z1:434:ASN:ND2   | 2.12                     | 0.47              |
| 2:D2:109:TYR:HE2   | 2:D2:114:GLN:HE22  | 1.62                     | 0.47              |
| 6:R2:100:VAL:HG13  | 6:R2:105:GLU:HG3   | 1.96                     | 0.47              |
| 6:U2:68:THR:HG22   | 6:U2:69:SER:N      | 2.23                     | 0.47              |
| 7:Y2:32:ASP:HB2    | 9:j2:1:MET:N       | 2.28                     | 0.47              |
| 8:b2:228:GLU:HG3   | 9:h2:258:THR:HB    | 1.96                     | 0.47              |
| 8:c2:101:ARG:NH2   | 8:c2:207:GLU:OE2   | 2.45                     | 0.47              |
| 9:g2:98:LYS:O      | 9:g2:212:GLY:CA    | 2.62                     | 0.47              |
| 9:k2:152:GLY:HA3   | 9:12:56:SER:O      | 2.14                     | 0.47              |
| 9:r2:190:ASN:OD1   | 9:w2:42:GLU:HA     | 2.13                     | 0.47              |
| 9:z2:114:TYR:CE1   | 9:z2:178:PHE:HZ    | 2.31                     | 0.47              |
| 9:12:77:THR:O      | 9:12:77:THR:OG1    | 2.32                     | 0.47              |
| 9:12:173:LEU:HD23  | 9:12:214:LEU:HD21  | 1.96                     | 0.47              |
| 10:E3:219:MET:HE2  | 10:G3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:G3:219:MET:HE2  | 10:I3:132:PHE:CB   | 2.43                     | 0.47              |
| 10:J3:54:SER:HB2   | 11:k3:173:ARG:HH12 | 1.79                     | 0.47              |
| 10:N3:124:MET:HE3  | 10:N3:124:MET:HB3  | 1.77                     | 0.47              |
| 10:S3:58:ILE:HG13  | 10:S3:59:ASN:N     | 2.28                     | 0.47              |
| 10:X3:159:GLY:O    | 10:X3:186:PRO:HG3  | 2.14                     | 0.47              |
| 10:Y3:30:LEU:HD23  | 10:Y3:30:LEU:H     | 1.78                     | 0.47              |
| 10:Z3:58:ILE:HG13  | 10:Z3:59:ASN:N     | 2.28                     | 0.47              |
| 11:a3:21:ARG:O     | 11:a3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:a3:254:VAL:CG2  | 11:b3:355:ALA:HB2  | 2.44                     | 0.47              |
| 11:a3:355:ALA:HB2  | 11:z3:254:VAL:CG2  | 2.44                     | 0.47              |
| 11:b3:252:LYS:HB2  | 11:b3:252:LYS:HE3  | 1.52                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:e3:21:ARG:O    | 11:e3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:f3:338:LEU:HG  | 11:f3:338:LEU:O    | 2.13                     | 0.47              |
| 11:g3:42:VAL:HA   | 11:g3:120:THR:O    | 2.14                     | 0.47              |
| 11:g3:338:LEU:HG  | 11:g3:338:LEU:O    | 2.13                     | 0.47              |
| 11:i3:21:ARG:O    | 11:i3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:j3:21:ARG:O    | 11:j3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:l3:89:VAL:HG21 | 11:l3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:m3:89:VAL:HG21 | 11:m3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:m3:327:ASN:OD1 | 11:m3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:n3:79:MET:HE2  | 11:o3:57:PHE:CD2   | 2.47                     | 0.47              |
| 11:r3:42:VAL:HA   | 11:r3:120:THR:O    | 2.14                     | 0.47              |
| 11:s3:42:VAL:HA   | 11:s3:120:THR:O    | 2.14                     | 0.47              |
| 11:t3:42:VAL:HA   | 11:t3:120:THR:O    | 2.14                     | 0.47              |
| 11:t3:101:GLN:NE2 | 11:u3:188:GLN:HB3  | 2.29                     | 0.47              |
| 11:u3:21:ARG:O    | 11:u3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:u3:94:PRO:HB2  | 11:v3:219:ARG:NH2  | 2.28                     | 0.47              |
| 11:w3:105:VAL:CG1 | 11:w3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:y3:105:VAL:CG1 | 11:y3:169:ALA:HB2  | 2.44                     | 0.47              |
| 1:B1:252:ILE:HD11 | 1:C1:265:GLN:HB2   | 1.95                     | 0.47              |
| 1:E1:413:GLU:OE2  | 1:E1:432:VAL:HB    | 2.14                     | 0.47              |
| 1:G1:140:LEU:HA   | 1:G1:143:THR:OG1   | 2.15                     | 0.47              |
| 1:I1:139:GLU:O    | 1:I1:143:THR:HG23  | 2.14                     | 0.47              |
| 1:I1:393:TYR:HB3  | 1:I1:402:LEU:N     | 2.29                     | 0.47              |
| 1:M1:279:GLU:OE2  | 1:M1:281:HIS:N     | 2.46                     | 0.47              |
| 1:O1:244:ARG:NH1  | 1:P1:235:LEU:O     | 2.47                     | 0.47              |
| 1:W1:378:ASN:HD22 | 1:W1:381:ASP:CG    | 2.20                     | 0.47              |
| 1:Y1:266:VAL:HG22 | 1:Y1:387:VAL:HG22  | 1.95                     | 0.47              |
| 1:Y1:295:SER:HB3  | 6:S2:72:HIS:HA     | 1.95                     | 0.47              |
| 2:C2:150:PHE:CZ   | 2:C2:172:PRO:HB2   | 2.48                     | 0.47              |
| 2:E2:63:SER:C     | 2:E2:65:THR:H      | 2.23                     | 0.47              |
| 4:J2:39:GLN:O     | 4:J2:43:GLN:HA     | 2.14                     | 0.47              |
| 5:L2:38:LEU:O     | 5:L2:42:LEU:HD23   | 2.14                     | 0.47              |
| 5:O2:76:GLN:HB3   | 6:U2:127:LEU:HD13  | 1.95                     | 0.47              |
| 6:Q2:32:ASN:OD1   | 7:V2:62:VAL:HB     | 2.13                     | 0.47              |
| 7:X2:75:LYS:HA    | 9:i2:47:GLN:OE1    | 2.14                     | 0.47              |
| 9:i2:162:GLN:HE21 | 9:i2:162:GLN:HB2   | 1.44                     | 0.47              |
| 9:q2:28:ASN:OD1   | 9:v2:72:VAL:HG22   | 2.13                     | 0.47              |
| 9:y2:175:LEU:HG   | 9:y2:206:PRO:HG3   | 1.95                     | 0.47              |
| 9:12:72:VAL:O     | 9:12:72:VAL:HG12   | 2.14                     | 0.47              |
| 10:A3:51:ILE:CG1  | 11:c3:175:LEU:HD11 | 2.43                     | 0.47              |
| 10:A3:54:SER:HB2  | 11:b3:173:ARG:HH12 | 1.78                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:E3:159:GLY:O    | 10:E3:186:PRO:HG3  | 2.13                     | 0.47              |
| 10:F3:72:ARG:N     | 10:F3:76:ASP:OD2   | 2.25                     | 0.47              |
| 10:F3:110:PRO:O    | 10:F3:114:GLN:HG2  | 2.14                     | 0.47              |
| 10:I3:101:LYS:HB2  | 10:I3:101:LYS:HZ3  | 1.79                     | 0.47              |
| 10:I3:110:PRO:O    | 10:I3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:L3:219:MET:HE2  | 10:N3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:M3:30:LEU:HD23  | 10:M3:30:LEU:H     | 1.78                     | 0.47              |
| 10:Q3:30:LEU:HD23  | 10:Q3:30:LEU:H     | 1.78                     | 0.47              |
| 10:Q3:159:GLY:O    | 10:Q3:186:PRO:HG3  | 2.14                     | 0.47              |
| 10:R3:82:LEU:HD13  | 10:R3:144:PHE:CE1  | 2.48                     | 0.47              |
| 10:S3:30:LEU:HD23  | 10:S3:30:LEU:H     | 1.78                     | 0.47              |
| 10:T3:78:LEU:HD12  | 10:T3:193:ASN:O    | 2.13                     | 0.47              |
| 10:V3:30:LEU:H     | 10:V3:30:LEU:HD23  | 1.78                     | 0.47              |
| 10:W3:30:LEU:HD23  | 10:W3:30:LEU:H     | 1.78                     | 0.47              |
| 10:X3:78:LEU:HD12  | 10:X3:193:ASN:O    | 2.13                     | 0.47              |
| 10:Y3:58:ILE:HG13  | 10:Y3:59:ASN:N     | 2.28                     | 0.47              |
| 11:a3:89:VAL:HG21  | 11:a3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:a3:327:ASN:OD1  | 11:a3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:b3:50:ASP:OD1   | 11:b3:113:ALA:N    | 2.47                     | 0.47              |
| 11:b3:103:ILE:HG13 | 11:b3:169:ALA:HB3  | 1.95                     | 0.47              |
| 11:d3:103:ILE:HG13 | 11:d3:169:ALA:HB3  | 1.95                     | 0.47              |
| 11:d3:327:ASN:OD1  | 11:d3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:d3:338:LEU:HG   | 11:d3:338:LEU:O    | 2.13                     | 0.47              |
| 11:e3:20:GLU:O     | 11:e3:244:VAL:HG12 | 2.13                     | 0.47              |
| 11:e3:96:PHE:O     | 11:f3:219:ARG:HD2  | 2.13                     | 0.47              |
| 11:f3:21:ARG:O     | 11:f3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:g3:21:ARG:O     | 11:g3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:h3:21:ARG:O     | 11:h3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:i3:105:VAL:CG1  | 11:i3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:m3:93:TYR:OH    | 11:m3:173:ARG:O    | 2.25                     | 0.47              |
| 11:n3:21:ARG:O     | 11:n3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:n3:105:VAL:CG1  | 11:n3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:o3:105:VAL:CG1  | 11:o3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:p3:101:GLN:NE2  | 11:q3:188:GLN:HB3  | 2.28                     | 0.47              |
| 11:q3:42:VAL:HA    | 11:q3:120:THR:O    | 2.14                     | 0.47              |
| 11:r3:277:GLN:HB3  | 11:r3:280:LEU:HD12 | 1.95                     | 0.47              |
| 11:v3:89:VAL:HG21  | 11:v3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:v3:277:GLN:HB3  | 11:v3:280:LEU:HD12 | 1.95                     | 0.47              |
| 11:x3:46:ASP:HA    | 11:y3:161:ASN:ND2  | 2.25                     | 0.47              |
| 11:x3:105:VAL:CG1  | 11:x3:169:ALA:HB2  | 2.43                     | 0.47              |
| 12:A4:65:ILE:HD11  | 12:E4:62:LEU:HD11  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:D4:122:THR:OG1 | 12:D4:165:TRP:O    | 2.30                     | 0.47              |
| 1:E1:180:LEU:HD23 | 1:E1:214:ASP:HB2   | 1.96                     | 0.47              |
| 1:E1:206:PRO:HG2  | 1:E1:209:ASN:OD1   | 2.14                     | 0.47              |
| 1:I1:200:SER:HG   | 1:K1:173:SER:HG    | 1.59                     | 0.47              |
| 1:L1:143:THR:HG22 | 1:N1:154:ARG:CD    | 2.45                     | 0.47              |
| 1:O1:182:PRO:O    | 1:O1:184:ARG:NH1   | 2.47                     | 0.47              |
| 1:Q1:167:ARG:CG   | 3:F2:156:THR:CG2   | 2.84                     | 0.47              |
| 1:X1:190:GLN:CD   | 1:Y1:217:GLY:HA3   | 2.39                     | 0.47              |
| 1:h1:165:PHE:CE1  | 1:h1:166:VAL:HG23  | 2.50                     | 0.47              |
| 1:h1:244:ARG:NH2  | 1:h1:248:ARG:HH22  | 2.12                     | 0.47              |
| 8:d2:14:GLN:HG3   | 8:d2:58:THR:HA     | 1.97                     | 0.47              |
| 8:d2:174:SER:OG   | 8:d2:178:LEU:O     | 2.25                     | 0.47              |
| 8:f2:131:GLU:HG2  | 9:k2:179:MET:HG3   | 1.96                     | 0.47              |
| 9:g2:174:ASN:HA   | 9:g2:206:PRO:HD3   | 1.97                     | 0.47              |
| 9:j2:26:LEU:HD11  | 9:n2:242:ILE:HG21  | 1.95                     | 0.47              |
| 9:k2:145:ASN:HD22 | 9:p2:209:ASN:C     | 2.22                     | 0.47              |
| 9:l2:98:LYS:HD3   | 9:l2:215:TYR:CZ    | 2.50                     | 0.47              |
| 9:t2:42:GLU:CB    | 9:t2:75:VAL:HB     | 2.44                     | 0.47              |
| 9:y2:142:ILE:HG21 | 9:y2:149:ILE:HD11  | 1.96                     | 0.47              |
| 9:z2:105:VAL:HG11 | 9:z2:134:PHE:HB3   | 1.95                     | 0.47              |
| 9:22:56:SER:OG    | 9:22:57:SER:N      | 2.47                     | 0.47              |
| 10:A3:58:ILE:HG13 | 10:A3:59:ASN:N     | 2.28                     | 0.47              |
| 10:J3:219:MET:HE2 | 10:L3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:P3:30:LEU:HD23 | 10:P3:30:LEU:H     | 1.78                     | 0.47              |
| 10:T3:110:PRO:O   | 10:T3:114:GLN:HG2  | 2.14                     | 0.47              |
| 10:U3:219:MET:HE2 | 10:W3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:Y3:78:LEU:HD12 | 10:Y3:193:ASN:O    | 2.13                     | 0.47              |
| 11:b3:79:MET:HE2  | 11:c3:57:PHE:CD2   | 2.48                     | 0.47              |
| 11:c3:21:ARG:O    | 11:c3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:c3:327:ASN:OD1 | 11:c3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:e3:327:ASN:OD1 | 11:e3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:f3:42:VAL:HA   | 11:f3:120:THR:O    | 2.14                     | 0.47              |
| 11:i3:50:ASP:OD1  | 11:i3:113:ALA:N    | 2.47                     | 0.47              |
| 11:i3:338:LEU:HG  | 11:i3:338:LEU:O    | 2.13                     | 0.47              |
| 11:k3:42:VAL:HA   | 11:k3:120:THR:O    | 2.14                     | 0.47              |
| 11:l3:101:GLN:NE2 | 11:m3:188:GLN:HB3  | 2.30                     | 0.47              |
| 11:l3:105:VAL:CG1 | 11:l3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:n3:101:GLN:NE2 | 11:o3:188:GLN:HB3  | 2.29                     | 0.47              |
| 11:o3:50:ASP:OD1  | 11:o3:113:ALA:N    | 2.47                     | 0.47              |
| 11:p3:105:VAL:CG1 | 11:p3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:q3:277:GLN:HB3 | 11:q3:280:LEU:HD12 | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:r3:101:GLN:NE2 | 11:s3:188:GLN:HB3 | 2.29                     | 0.47              |
| 11:t3:21:ARG:O    | 11:t3:25:LEU:HD22 | 2.14                     | 0.47              |
| 11:t3:94:PRO:HB2  | 11:u3:219:ARG:NH2 | 2.28                     | 0.47              |
| 11:u3:42:VAL:HA   | 11:u3:120:THR:O   | 2.14                     | 0.47              |
| 11:x3:338:LEU:O   | 11:x3:338:LEU:HG  | 2.13                     | 0.47              |
| 12:D4:47:GLN:O    | 12:D4:51:ASN:N    | 2.47                     | 0.47              |
| 1:B1:165:PHE:CD2  | 2:C2:161:GLY:C    | 2.91                     | 0.47              |
| 1:E1:151:LYS:HZ1  | 1:E1:181:GLU:HA   | 1.79                     | 0.47              |
| 1:K1:257:VAL:C    | 1:K1:261:ASN:HD22 | 2.23                     | 0.47              |
| 1:O1:167:ARG:CD   | 2:A2:152:ARG:O    | 2.62                     | 0.47              |
| 1:X1:241:VAL:HG22 | 1:Y1:235:LEU:HD21 | 1.96                     | 0.47              |
| 1:Y1:231:ASN:OD1  | 1:Y1:232:ASP:N    | 2.47                     | 0.47              |
| 1:Z1:408:GLN:O    | 1:Z1:412:ILE:HG12 | 2.14                     | 0.47              |
| 1:a1:254:SER:HB2  | 1:a1:255:PRO:HD3  | 1.96                     | 0.47              |
| 1:d1:165:PHE:HE1  | 2:D2:147:LEU:HB2  | 1.79                     | 0.47              |
| 1:f1:137:GLU:HB2  | 1:f1:155:VAL:HG13 | 1.96                     | 0.47              |
| 1:g1:389:VAL:HB   | 1:g1:432:VAL:HG13 | 1.97                     | 0.47              |
| 1:h1:263:HIS:HB2  | 1:h1:390:VAL:HG22 | 1.97                     | 0.47              |
| 1:h1:387:VAL:HB   | 1:h1:420:MET:SD   | 2.54                     | 0.47              |
| 2:B2:63:SER:C     | 2:B2:65:THR:H     | 2.21                     | 0.47              |
| 2:D2:138:MET:HE3  | 2:D2:170:LEU:HG   | 1.96                     | 0.47              |
| 6:S2:65:LEU:HB2   | 6:S2:74:PRO:HA    | 1.96                     | 0.47              |
| 8:c2:60:SER:HB2   | 9:h2:64:SER:HB2   | 1.94                     | 0.47              |
| 8:c2:80:VAL:O     | 8:c2:103:GLY:HA3  | 2.13                     | 0.47              |
| 8:f2:115:ILE:O    | 8:f2:116:GLN:C    | 2.58                     | 0.47              |
| 9:g2:241:GLU:HG2  | 9:l2:256:LYS:HE3  | 1.96                     | 0.47              |
| 9:h2:77:THR:HG23  | 9:h2:77:THR:O     | 2.14                     | 0.47              |
| 9:i2:18:ASN:HB2   | 9:i2:41:PHE:HZ    | 1.80                     | 0.47              |
| 9:p2:226:VAL:O    | 9:p2:230:LEU:HD23 | 2.15                     | 0.47              |
| 9:v2:194:GLU:OE2  | 9:v2:201:PRO:HD3  | 2.14                     | 0.47              |
| 9:x2:241:GLU:OE1  | 9:32:256:LYS:HD2  | 2.14                     | 0.47              |
| 9:12:101:GLY:O    | 9:12:116:ARG:NH2  | 2.47                     | 0.47              |
| 10:B3:40:ILE:H    | 10:B3:40:ILE:HG12 | 1.48                     | 0.47              |
| 10:B3:78:LEU:HD12 | 10:B3:193:ASN:O   | 2.13                     | 0.47              |
| 10:G3:41:PRO:HA   | 10:I3:157:ALA:HB1 | 1.96                     | 0.47              |
| 10:I3:82:LEU:HA   | 10:I3:197:SER:CB  | 2.39                     | 0.47              |
| 10:K3:78:LEU:HD12 | 10:K3:193:ASN:O   | 2.14                     | 0.47              |
| 10:N3:40:ILE:H    | 10:N3:40:ILE:HG12 | 1.48                     | 0.47              |
| 10:R3:30:LEU:HD23 | 10:R3:30:LEU:H    | 1.78                     | 0.47              |
| 10:T3:30:LEU:HD23 | 10:T3:30:LEU:H    | 1.78                     | 0.47              |
| 10:T3:58:ILE:HG13 | 10:T3:59:ASN:N    | 2.28                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:V3:54:SER:HB2   | 11:w3:173:ARG:HH12 | 1.79                     | 0.47              |
| 10:V3:110:PRO:O    | 10:V3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:X3:30:LEU:HD23  | 10:X3:30:LEU:H     | 1.78                     | 0.47              |
| 10:X3:58:ILE:HG13  | 10:X3:59:ASN:N     | 2.28                     | 0.47              |
| 10:Y3:159:GLY:O    | 10:Y3:186:PRO:HG3  | 2.13                     | 0.47              |
| 10:Z3:78:LEU:HD12  | 10:Z3:193:ASN:O    | 2.13                     | 0.47              |
| 11:a3:338:LEU:HG   | 11:a3:338:LEU:O    | 2.13                     | 0.47              |
| 11:b3:21:ARG:O     | 11:b3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:c3:50:ASP:OD1   | 11:c3:113:ALA:N    | 2.47                     | 0.47              |
| 11:e3:120:THR:HG23 | 11:e3:139:GLY:O    | 2.13                     | 0.47              |
| 11:f3:50:ASP:OD1   | 11:f3:113:ALA:N    | 2.47                     | 0.47              |
| 11:g3:89:VAL:HG21  | 11:g3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:h3:89:VAL:HG21  | 11:h3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:l3:327:ASN:OD1  | 11:l3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:o3:21:ARG:O     | 11:o3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:p3:42:VAL:HA    | 11:p3:120:THR:O    | 2.15                     | 0.47              |
| 11:p3:83:ASN:ND2   | 11:q3:109:SER:OG   | 2.45                     | 0.47              |
| 11:q3:21:ARG:O     | 11:q3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:s3:277:GLN:HB3  | 11:s3:280:LEU:HD12 | 1.95                     | 0.47              |
| 11:u3:89:VAL:HG21  | 11:u3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:x3:50:ASP:OD1   | 11:x3:113:ALA:N    | 2.47                     | 0.47              |
| 11:y3:101:GLN:NE2  | 11:z3:219:ARG:HD3  | 2.28                     | 0.47              |
| 11:z3:89:VAL:HG21  | 11:z3:124:THR:OG1  | 2.14                     | 0.47              |
| 12:C4:54:GLN:HB2   | 12:C4:57:GLU:HG2   | 1.95                     | 0.47              |
| 1:D1:297:GLN:OE1   | 1:E1:363:THR:HG22  | 2.14                     | 0.47              |
| 1:F1:267:THR:OG1   | 1:F1:386:SER:HB2   | 2.14                     | 0.47              |
| 1:I1:174:ALA:HB3   | 1:I1:210:VAL:HG22  | 1.95                     | 0.47              |
| 1:M1:293:LEU:HD21  | 1:M1:296:ARG:NH2   | 2.29                     | 0.47              |
| 1:U1:420:MET:HE3   | 1:U1:422:PHE:HB2   | 1.95                     | 0.47              |
| 1:V1:389:VAL:O     | 1:V1:432:VAL:HA    | 2.14                     | 0.47              |
| 1:W1:404:LEU:H     | 1:W1:434:ASN:ND2   | 2.12                     | 0.47              |
| 1:X1:206:PRO:HG2   | 1:X1:209:ASN:OD1   | 2.14                     | 0.47              |
| 1:X1:254:SER:HB2   | 1:X1:255:PRO:HD3   | 1.96                     | 0.47              |
| 1:c1:140:LEU:O     | 1:c1:144:ILE:HG12  | 2.15                     | 0.47              |
| 1:f1:165:PHE:HD1   | 2:D2:148:ALA:HB1   | 1.77                     | 0.47              |
| 2:B2:89:LEU:HB2    | 5:N2:104:VAL:HG21  | 1.95                     | 0.47              |
| 2:B2:142:THR:HG22  | 2:B2:174:TYR:HA    | 1.95                     | 0.47              |
| 2:E2:166:PRO:HG2   | 2:E2:169:ILE:HG12  | 1.97                     | 0.47              |
| 3:F2:6:SER:HA      | 5:K2:75:MET:CE     | 2.45                     | 0.47              |
| 3:F2:219:PRO:O     | 3:F2:223:THR:HG23  | 2.14                     | 0.47              |
| 6:R2:37:GLY:N      | 6:R2:96:ASP:O      | 2.48                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:S2:92:GLN:HE21   | 7:Y2:19:LYS:HA     | 1.78                     | 0.47              |
| 7:V2:6:ILE:CG2     | 7:V2:122:VAL:HG11  | 2.44                     | 0.47              |
| 7:X2:36:GLY:O      | 8:c2:42:ARG:NH2    | 2.45                     | 0.47              |
| 7:Z2:32:ASP:OD2    | 9:k2:1:MET:N       | 2.35                     | 0.47              |
| 8:b2:217:MET:HE3   | 8:b2:217:MET:HB3   | 1.78                     | 0.47              |
| 8:c2:170:GLU:OE1   | 8:c2:189:ARG:NH1   | 2.48                     | 0.47              |
| 8:f2:87:TRP:NE1    | 8:f2:166:ALA:O     | 2.39                     | 0.47              |
| 8:f2:226:ARG:O     | 8:f2:230:GLN:HG2   | 2.14                     | 0.47              |
| 9:h2:106:MET:HB2   | 9:h2:137:GLN:HG3   | 1.97                     | 0.47              |
| 9:l2:164:GLN:CG    | 11:j3:80:GLN:NE2   | 2.59                     | 0.47              |
| 9:s2:55:GLN:HG2    | 9:s2:57:SER:O      | 2.14                     | 0.47              |
| 9:x2:231:VAL:HG11  | 9:42:9:LYS:HG3     | 1.97                     | 0.47              |
| 9:22:136:VAL:O     | 9:22:137:GLN:NE2   | 2.46                     | 0.47              |
| 9:42:44:LEU:HD21   | 9:42:73:ARG:HB2    | 1.97                     | 0.47              |
| 10:B3:41:PRO:HA    | 10:D3:157:ALA:HB1  | 1.97                     | 0.47              |
| 10:B3:58:ILE:HG13  | 10:B3:59:ASN:N     | 2.28                     | 0.47              |
| 10:C3:78:LEU:HD12  | 10:C3:193:ASN:O    | 2.13                     | 0.47              |
| 10:D3:78:LEU:HD12  | 10:D3:193:ASN:O    | 2.14                     | 0.47              |
| 10:J3:101:LYS:HZ3  | 10:J3:101:LYS:HB2  | 1.79                     | 0.47              |
| 10:N3:30:LEU:H     | 10:N3:30:LEU:HD23  | 1.78                     | 0.47              |
| 10:N3:82:LEU:HA    | 10:N3:197:SER:CB   | 2.39                     | 0.47              |
| 10:O3:219:MET:HE2  | 10:Q3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:R3:159:GLY:O    | 10:R3:186:PRO:HG3  | 2.14                     | 0.47              |
| 10:U3:30:LEU:HD23  | 10:U3:30:LEU:H     | 1.78                     | 0.47              |
| 10:W3:58:ILE:HG13  | 10:W3:59:ASN:N     | 2.28                     | 0.47              |
| 10:W3:78:LEU:HD12  | 10:W3:193:ASN:O    | 2.13                     | 0.47              |
| 10:X3:110:PRO:O    | 10:X3:114:GLN:HG2  | 2.15                     | 0.47              |
| 11:a3:277:GLN:HB3  | 11:a3:280:LEU:HD12 | 1.95                     | 0.47              |
| 11:b3:89:VAL:HG21  | 11:b3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:d3:21:ARG:O     | 11:d3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:g3:120:THR:HG23 | 11:g3:139:GLY:O    | 2.13                     | 0.47              |
| 11:h3:327:ASN:OD1  | 11:h3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:i3:277:GLN:HB3  | 11:i3:280:LEU:HD12 | 1.95                     | 0.47              |
| 11:k3:50:ASP:OD1   | 11:k3:113:ALA:N    | 2.47                     | 0.47              |
| 11:o3:42:VAL:HA    | 11:o3:120:THR:O    | 2.14                     | 0.47              |
| 11:p3:338:LEU:O    | 11:p3:338:LEU:HG   | 2.13                     | 0.47              |
| 11:s3:50:ASP:OD1   | 11:s3:113:ALA:N    | 2.47                     | 0.47              |
| 11:v3:42:VAL:HA    | 11:v3:120:THR:O    | 2.14                     | 0.47              |
| 11:w3:89:VAL:HG21  | 11:w3:124:THR:OG1  | 2.15                     | 0.47              |
| 11:w3:101:GLN:NE2  | 11:x3:188:GLN:HB3  | 2.29                     | 0.47              |
| 11:z3:327:ASN:OD1  | 11:z3:330:SER:HB2  | 2.13                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:z3:338:LEU:HG  | 11:z3:338:LEU:O    | 2.13                     | 0.47              |
| 12:C4:169:GLN:HB3 | 12:C4:175:VAL:HG12 | 1.96                     | 0.47              |
| 12:E4:92:GLN:O    | 12:E4:95:THR:OG1   | 2.33                     | 0.47              |
| 12:E4:100:GLY:HA2 | 12:E4:202:LEU:HA   | 1.96                     | 0.47              |
| 1:I1:143:THR:HG22 | 1:K1:154:ARG:CD    | 2.45                     | 0.47              |
| 1:M1:375:THR:HG23 | 1:N1:275:LYS:NZ    | 2.29                     | 0.47              |
| 1:O1:161:LYS:HZ2  | 1:O1:163:SER:HA    | 1.80                     | 0.47              |
| 1:Q1:193:ALA:HA   | 1:R1:219:LEU:HG    | 1.96                     | 0.47              |
| 1:R1:302:GLU:HA   | 1:R1:357:SER:O     | 2.15                     | 0.47              |
| 1:U1:126:PHE:O    | 1:U1:129:GLN:HG2   | 2.15                     | 0.47              |
| 1:V1:275:LYS:CB   | 1:V1:377:MET:HE2   | 2.45                     | 0.47              |
| 1:W1:404:LEU:HD23 | 1:W1:408:GLN:HG2   | 1.96                     | 0.47              |
| 2:B2:96:LEU:CG    | 2:B2:236:MET:HE3   | 2.39                     | 0.47              |
| 2:D2:184:GLN:HA   | 2:D2:187:PHE:CD2   | 2.50                     | 0.47              |
| 3:F2:22:ARG:NH2   | 3:F2:158:PRO:O     | 2.48                     | 0.47              |
| 5:K2:69:ASN:OD1   | 5:K2:69:ASN:N      | 2.47                     | 0.47              |
| 8:e2:76:ARG:O     | 8:e2:204:GLY:HA2   | 2.15                     | 0.47              |
| 8:f2:62:PRO:HB3   | 9:k2:62:LEU:HG     | 1.97                     | 0.47              |
| 9:i2:118:GLY:O    | 9:i2:120:PHE:N     | 2.47                     | 0.47              |
| 9:i2:175:LEU:HG   | 9:i2:206:PRO:HG3   | 1.96                     | 0.47              |
| 9:j2:98:LYS:HB3   | 9:j2:213:LEU:HB2   | 1.95                     | 0.47              |
| 9:u2:175:LEU:HD11 | 9:u2:214:LEU:HD11  | 1.97                     | 0.47              |
| 9:w2:35:LYS:NZ    | 9:w2:82:SER:O      | 2.38                     | 0.47              |
| 9:w2:213:LEU:HD21 | 9:32:108:PRO:HG2   | 1.96                     | 0.47              |
| 9:x2:10:THR:OG1   | 9:x2:71:GLY:HA2    | 2.15                     | 0.47              |
| 10:B3:54:SER:HB2  | 11:c3:173:ARG:HH12 | 1.78                     | 0.47              |
| 10:D3:110:PRO:O   | 10:D3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:N3:219:MET:HE2 | 10:P3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:O3:30:LEU:HD23 | 10:O3:30:LEU:H     | 1.78                     | 0.47              |
| 10:P3:110:PRO:O   | 10:P3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:Q3:41:PRO:HA   | 10:S3:157:ALA:HB1  | 1.96                     | 0.47              |
| 10:R3:110:PRO:O   | 10:R3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:S3:110:PRO:O   | 10:S3:114:GLN:HG2  | 2.14                     | 0.47              |
| 10:V3:78:LEU:HD12 | 10:V3:193:ASN:O    | 2.13                     | 0.47              |
| 11:b3:42:VAL:HA   | 11:b3:120:THR:O    | 2.14                     | 0.47              |
| 11:b3:327:ASN:OD1 | 11:b3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:j3:42:VAL:HA   | 11:j3:120:THR:O    | 2.14                     | 0.47              |
| 11:l3:42:VAL:HA   | 11:l3:120:THR:O    | 2.14                     | 0.47              |
| 11:m3:50:ASP:OD1  | 11:m3:113:ALA:N    | 2.47                     | 0.47              |
| 11:o3:94:PRO:HB2  | 11:p3:219:ARG:NH2  | 2.28                     | 0.47              |
| 11:q3:83:ASN:ND2  | 11:r3:109:SER:OG   | 2.46                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:q3:105:VAL:CG1 | 11:q3:169:ALA:HB2 | 2.44                     | 0.47              |
| 11:v3:105:VAL:CG1 | 11:v3:169:ALA:HB2 | 2.44                     | 0.47              |
| 11:w3:50:ASP:OD1  | 11:w3:113:ALA:N   | 2.47                     | 0.47              |
| 11:y3:338:LEU:HG  | 11:y3:338:LEU:O   | 2.13                     | 0.47              |
| 12:C4:77:THR:HG23 | 12:D4:85:ILE:HD11 | 1.96                     | 0.47              |
| 12:D4:100:GLY:HA3 | 12:D4:200:PHE:CZ  | 2.49                     | 0.47              |
| 1:A1:268:ALA:HB2  | 1:A1:385:LEU:HD23 | 1.97                     | 0.47              |
| 1:B1:409:MET:HE2  | 1:B1:434:ASN:HB2  | 1.96                     | 0.47              |
| 1:D1:378:ASN:ND2  | 1:D1:381:ASP:OD1  | 2.38                     | 0.47              |
| 1:E1:382:ILE:H    | 1:E1:382:ILE:HD12 | 1.80                     | 0.47              |
| 1:H1:134:ARG:HA   | 1:H1:137:GLU:OE2  | 2.15                     | 0.47              |
| 1:H1:150:VAL:HG22 | 1:H1:178:VAL:HG21 | 1.96                     | 0.47              |
| 1:I1:145:GLU:HG2  | 1:I1:152:SER:HA   | 1.96                     | 0.47              |
| 1:K1:128:GLU:HG2  | 1:K1:129:GLN:N    | 2.28                     | 0.47              |
| 1:N1:298:LEU:HD12 | 1:N1:361:ASN:O    | 2.15                     | 0.47              |
| 1:O1:128:GLU:HG2  | 1:O1:129:GLN:N    | 2.30                     | 0.47              |
| 1:T1:197:LEU:HD11 | 1:U1:154:ARG:HH21 | 1.79                     | 0.47              |
| 1:W1:164:LEU:HD11 | 2:E2:143:ARG:HA   | 0.49                     | 0.47              |
| 1:a1:190:GLN:NE2  | 1:c1:216:SER:O    | 2.48                     | 0.47              |
| 1:b1:412:ILE:O    | 1:b1:416:THR:HG23 | 2.15                     | 0.47              |
| 1:d1:409:MET:CE   | 1:d1:434:ASN:HB2  | 2.45                     | 0.47              |
| 1:e1:393:TYR:CE2  | 1:e1:436:PRO:HD3  | 2.50                     | 0.47              |
| 1:f1:199:SER:HA   | 1:f1:205:LEU:HD23 | 1.97                     | 0.47              |
| 2:A2:100:ILE:HG21 | 2:A2:243:PHE:HD2  | 1.80                     | 0.47              |
| 2:A2:116:PHE:HD1  | 2:A2:122:SER:HA   | 1.78                     | 0.47              |
| 2:B2:224:MET:HE2  | 2:B2:224:MET:HB3  | 1.77                     | 0.47              |
| 2:D2:211:MET:HE2  | 2:E2:211:MET:O    | 2.15                     | 0.47              |
| 2:E2:96:LEU:HB2   | 2:E2:236:MET:HE1  | 1.97                     | 0.47              |
| 3:F2:140:PHE:HZ   | 3:F2:241:GLU:OE2  | 1.98                     | 0.47              |
| 4:I2:52:ILE:H     | 4:I2:52:ILE:HD12  | 1.80                     | 0.47              |
| 5:O2:86:ILE:HD11  | 6:T2:133:VAL:HG22 | 1.96                     | 0.47              |
| 6:Q2:78:VAL:CG1   | 7:V2:57:GLN:CG    | 2.91                     | 0.47              |
| 6:U2:92:GLN:OE1   | 8:f2:54:ARG:NH2   | 2.48                     | 0.47              |
| 8:b2:133:SER:HB2  | 8:b2:135:ILE:HG12 | 1.96                     | 0.47              |
| 8:b2:138:ALA:HB1  | 9:r2:56:SER:C     | 2.39                     | 0.47              |
| 9:i2:21:VAL:HG21  | 9:i2:39:ALA:HB2   | 1.97                     | 0.47              |
| 9:i2:94:ASP:OD1   | 9:i2:95:VAL:N     | 2.48                     | 0.47              |
| 9:j2:1:MET:HE1    | 9:j2:9:LYS:HD2    | 1.97                     | 0.47              |
| 9:k2:122:VAL:O    | 9:p2:180:ASN:ND2  | 2.48                     | 0.47              |
| 9:l2:167:PRO:CD   | 9:w2:196:GLN:HG2  | 2.44                     | 0.47              |
| 9:n2:254:LEU:O    | 9:n2:258:THR:HG23 | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:p2:2:ILE:HG13    | 9:p2:3:SER:H       | 1.80                     | 0.47              |
| 9:p2:172:GLN:NE2   | 11:d3:54:GLN:NE2   | 2.61                     | 0.47              |
| 9:s2:26:LEU:HD23   | 9:x2:246:ALA:HB2   | 1.96                     | 0.47              |
| 9:y2:91:ASN:O      | 9:y2:217:GLY:HA2   | 2.14                     | 0.47              |
| 9:12:51:GLN:HG3    | 9:12:53:GLY:H      | 1.80                     | 0.47              |
| 9:12:121:GLN:N     | 9:12:129:VAL:O     | 2.39                     | 0.47              |
| 10:A3:78:LEU:HD12  | 10:A3:193:ASN:O    | 2.13                     | 0.47              |
| 10:A3:232:MET:HG3  | 10:Z3:223:GLN:HB2  | 1.97                     | 0.47              |
| 10:C3:110:PRO:O    | 10:C3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:D3:54:SER:HB2   | 11:e3:173:ARG:HH12 | 1.78                     | 0.47              |
| 10:D3:159:GLY:O    | 10:D3:186:PRO:HG3  | 2.14                     | 0.47              |
| 10:F3:41:PRO:HA    | 10:H3:157:ALA:HB1  | 1.96                     | 0.47              |
| 10:H3:223:GLN:HB2  | 10:I3:232:MET:HG3  | 1.97                     | 0.47              |
| 10:K3:110:PRO:O    | 10:K3:114:GLN:HG2  | 2.14                     | 0.47              |
| 10:K3:219:MET:HE2  | 10:M3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:L3:110:PRO:O    | 10:L3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:N3:110:PRO:O    | 10:N3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:R3:82:LEU:O     | 10:R3:197:SER:OG   | 2.21                     | 0.47              |
| 10:R3:219:MET:HE2  | 10:T3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:R3:223:GLN:HB2  | 10:S3:232:MET:HG3  | 1.97                     | 0.47              |
| 10:T3:41:PRO:HA    | 10:V3:157:ALA:HB1  | 1.97                     | 0.47              |
| 10:T3:223:GLN:HB2  | 10:U3:232:MET:HG3  | 1.97                     | 0.47              |
| 10:W3:41:PRO:HA    | 10:Y3:157:ALA:HB1  | 1.97                     | 0.47              |
| 10:X3:41:PRO:HA    | 10:Z3:157:ALA:HB1  | 1.97                     | 0.47              |
| 10:Y3:168:GLN:HG3  | 10:Z3:204:ARG:NE   | 2.29                     | 0.47              |
| 11:c3:42:VAL:HA    | 11:c3:120:THR:O    | 2.15                     | 0.47              |
| 11:c3:79:MET:HE2   | 11:d3:57:PHE:CD2   | 2.48                     | 0.47              |
| 11:c3:117:ARG:NH1  | 11:c3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:e3:50:ASP:OD1   | 11:e3:113:ALA:N    | 2.47                     | 0.47              |
| 11:e3:117:ARG:NH1  | 11:e3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:f3:89:VAL:HG21  | 11:f3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:f3:120:THR:HG23 | 11:f3:139:GLY:O    | 2.13                     | 0.47              |
| 11:h3:42:VAL:HA    | 11:h3:120:THR:O    | 2.14                     | 0.47              |
| 11:i3:89:VAL:HG21  | 11:i3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:j3:341:THR:OG1  | 11:j3:343:MET:HE2  | 2.15                     | 0.47              |
| 11:k3:89:VAL:HG21  | 11:k3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:k3:123:MET:CE   | 11:k3:136:LEU:HD22 | 2.38                     | 0.47              |
| 11:k3:277:GLN:HG3  | 11:k3:278:GLY:N    | 2.30                     | 0.47              |
| 11:k3:327:ASN:OD1  | 11:k3:330:SER:HB2  | 2.13                     | 0.47              |
| 11:k3:338:LEU:HG   | 11:k3:338:LEU:O    | 2.13                     | 0.47              |
| 11:l3:50:ASP:OD1   | 11:l3:113:ALA:N    | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:l3:123:MET:CE   | 11:l3:136:LEU:HD22 | 2.38                     | 0.47              |
| 11:m3:277:GLN:HG3  | 11:m3:278:GLY:N    | 2.30                     | 0.47              |
| 11:n3:89:VAL:HG21  | 11:n3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:o3:89:VAL:HG21  | 11:o3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:p3:21:ARG:O     | 11:p3:25:LEU:HD22  | 2.14                     | 0.47              |
| 11:p3:50:ASP:OD1   | 11:p3:113:ALA:N    | 2.47                     | 0.47              |
| 11:p3:89:VAL:HG21  | 11:p3:124:THR:OG1  | 2.15                     | 0.47              |
| 11:q3:89:VAL:HG21  | 11:q3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:q3:141:ILE:HD13 | 11:q3:165:ILE:CD1  | 2.38                     | 0.47              |
| 11:r3:89:VAL:HG21  | 11:r3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:r3:105:VAL:CG1  | 11:r3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:t3:50:ASP:OD1   | 11:t3:113:ALA:N    | 2.47                     | 0.47              |
| 11:t3:256:ASN:O    | 11:t3:257:SER:OG   | 2.30                     | 0.47              |
| 11:t3:341:THR:OG1  | 11:t3:343:MET:HE2  | 2.15                     | 0.47              |
| 11:v3:117:ARG:NH1  | 11:v3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:v3:338:LEU:HG   | 11:v3:338:LEU:O    | 2.13                     | 0.47              |
| 11:w3:196:MET:HA   | 11:w3:196:MET:CE   | 2.34                     | 0.47              |
| 11:w3:338:LEU:HG   | 11:w3:338:LEU:O    | 2.13                     | 0.47              |
| 11:w3:341:THR:OG1  | 11:w3:343:MET:HE2  | 2.15                     | 0.47              |
| 12:A4:215:LEU:H    | 12:A4:223:THR:H    | 1.63                     | 0.47              |
| 12:E4:72:GLU:OE1   | 12:E4:73:LYS:HD2   | 2.14                     | 0.47              |
| 1:E1:261:ASN:HB3   | 1:E1:392:ASN:HB3   | 1.96                     | 0.47              |
| 1:I1:408:GLN:O     | 1:I1:412:ILE:HG12  | 2.15                     | 0.47              |
| 1:J1:238:ALA:O     | 1:J1:242:GLU:HG2   | 2.14                     | 0.47              |
| 1:K1:162:PRO:O     | 4:G2:86:TYR:CZ     | 2.67                     | 0.47              |
| 1:M1:234:GLN:HB2   | 1:M1:272:PHE:CE2   | 2.50                     | 0.47              |
| 1:O1:144:ILE:HG22  | 1:O1:150:VAL:HG21  | 1.97                     | 0.47              |
| 1:T1:172:PRO:HG2   | 1:T1:204:GLY:O     | 2.15                     | 0.47              |
| 1:T1:284:PRO:O     | 1:T1:290:LYS:NZ    | 2.32                     | 0.47              |
| 1:W1:164:LEU:HD11  | 2:E2:143:ARG:CG    | 2.43                     | 0.47              |
| 1:Z1:277:GLN:HB3   | 1:Z1:375:THR:HB    | 1.96                     | 0.47              |
| 1:c1:389:VAL:HB    | 1:c1:432:VAL:HG22  | 1.95                     | 0.47              |
| 1:e1:420:MET:SD    | 1:e1:422:PHE:HB2   | 2.55                     | 0.47              |
| 2:E2:84:PRO:HB2    | 2:E2:87:GLN:HB2    | 1.97                     | 0.47              |
| 2:E2:91:GLY:HA3    | 3:F2:86:PHE:CE1    | 2.50                     | 0.47              |
| 5:P2:38:LEU:O      | 5:P2:42:LEU:HG     | 2.15                     | 0.47              |
| 7:a2:30:ASN:ND2    | 8:f2:57:VAL:HG22   | 2.30                     | 0.47              |
| 8:c2:167:GLU:OE1   | 8:c2:167:GLU:N     | 2.47                     | 0.47              |
| 8:e2:170:GLU:O     | 8:e2:181:LEU:HD13  | 2.15                     | 0.47              |
| 8:e2:228:GLU:HG3   | 9:k2:258:THR:HG21  | 1.97                     | 0.47              |
| 9:p2:27:ALA:C      | 9:u2:72:VAL:HG21   | 2.40                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:u2:153:ARG:HH22 | 9:12:108:PRO:HD3   | 1.80                     | 0.47              |
| 9:u2:238:ARG:HA   | 9:u2:238:ARG:HD3   | 1.69                     | 0.47              |
| 9:12:257:LEU:O    | 9:12:260:LEU:HB3   | 2.14                     | 0.47              |
| 10:C3:82:LEU:HA   | 10:C3:197:SER:CB   | 2.39                     | 0.47              |
| 10:E3:223:GLN:HB2 | 10:F3:232:MET:HG3  | 1.97                     | 0.47              |
| 10:F3:219:MET:HE2 | 10:H3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:G3:110:PRO:O   | 10:G3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:I3:219:MET:HE2 | 10:K3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:O3:82:LEU:HA   | 10:O3:197:SER:CB   | 2.39                     | 0.47              |
| 10:Q3:110:PRO:O   | 10:Q3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:U3:41:PRO:HA   | 10:W3:157:ALA:HB1  | 1.97                     | 0.47              |
| 10:V3:41:PRO:HA   | 10:X3:157:ALA:HB1  | 1.97                     | 0.47              |
| 10:V3:58:ILE:HG13 | 10:V3:59:ASN:N     | 2.28                     | 0.47              |
| 11:a3:50:ASP:OD1  | 11:a3:113:ALA:N    | 2.47                     | 0.47              |
| 11:b3:277:GLN:HG3 | 11:b3:278:GLY:N    | 2.30                     | 0.47              |
| 11:d3:50:ASP:OD1  | 11:d3:113:ALA:N    | 2.47                     | 0.47              |
| 11:d3:277:GLN:HG3 | 11:d3:278:GLY:N    | 2.30                     | 0.47              |
| 11:f3:101:GLN:NE2 | 11:g3:188:GLN:HB3  | 2.30                     | 0.47              |
| 11:f3:277:GLN:HG3 | 11:f3:278:GLY:N    | 2.30                     | 0.47              |
| 11:g3:341:THR:OG1 | 11:g3:343:MET:HE2  | 2.15                     | 0.47              |
| 11:h3:101:GLN:NE2 | 11:i3:188:GLN:HB3  | 2.29                     | 0.47              |
| 11:j3:89:VAL:HG21 | 11:j3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:j3:338:LEU:HG  | 11:j3:338:LEU:O    | 2.13                     | 0.47              |
| 11:n3:42:VAL:HA   | 11:n3:120:THR:O    | 2.14                     | 0.47              |
| 11:p3:123:MET:CE  | 11:p3:136:LEU:HD22 | 2.38                     | 0.47              |
| 11:s3:117:ARG:NH1 | 11:s3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:s3:254:VAL:CG2 | 11:t3:355:ALA:HB2  | 2.44                     | 0.47              |
| 11:t3:89:VAL:HG21 | 11:t3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:t3:277:GLN:HB3 | 11:t3:280:LEU:HD12 | 1.95                     | 0.47              |
| 11:u3:105:VAL:CG1 | 11:u3:169:ALA:HB2  | 2.44                     | 0.47              |
| 11:w3:42:VAL:HA   | 11:w3:120:THR:O    | 2.14                     | 0.47              |
| 12:B4:215:LEU:N   | 12:B4:223:THR:O    | 2.35                     | 0.47              |
| 12:E4:137:THR:OG1 | 12:E4:185:THR:OG1  | 2.32                     | 0.47              |
| 1:E1:166:VAL:HG22 | 1:E1:168:GLU:HG3   | 1.96                     | 0.47              |
| 1:H1:133:GLN:O    | 1:H1:136:LEU:N     | 2.48                     | 0.47              |
| 1:N1:280:GLU:HG2  | 1:N1:282:TYR:HE2   | 1.80                     | 0.47              |
| 1:O1:152:SER:OG   | 1:O1:179:THR:OG1   | 2.30                     | 0.47              |
| 1:O1:197:LEU:CD2  | 1:Q1:213:VAL:HG21  | 2.45                     | 0.47              |
| 1:U1:302:GLU:HA   | 1:U1:357:SER:O     | 2.15                     | 0.47              |
| 1:W1:142:ARG:HG3  | 1:X1:154:ARG:HH12  | 1.80                     | 0.47              |
| 1:W1:374:HIS:HB3  | 1:X1:276:GLU:HB3   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:X1:244:ARG:NH2  | 1:Y1:235:LEU:HB3   | 2.30                     | 0.47              |
| 1:Y1:298:LEU:HD11 | 1:Y1:300:ILE:HD11  | 1.95                     | 0.47              |
| 1:d1:287:ASP:HB3  | 1:d1:290:LYS:HE3   | 1.97                     | 0.47              |
| 1:e1:413:GLU:O    | 1:e1:416:THR:OG1   | 2.27                     | 0.47              |
| 2:D2:119:GLN:OE1  | 2:D2:120:LYS:NZ    | 2.35                     | 0.47              |
| 3:F2:65:LEU:O     | 3:F2:68:ILE:HG13   | 2.15                     | 0.47              |
| 5:M2:59:PHE:CD2   | 6:R2:118:MET:HE2   | 2.50                     | 0.47              |
| 7:a2:83:PRO:O     | 7:a2:84:LEU:HB2    | 2.15                     | 0.47              |
| 8:d2:91:GLN:O     | 8:d2:118:HIS:HB2   | 2.14                     | 0.47              |
| 9:i2:44:LEU:HB2   | 9:i2:70:THR:O      | 2.14                     | 0.47              |
| 9:n2:169:GLN:N    | 11:x3:78:ASN:ND2   | 2.52                     | 0.47              |
| 9:42:158:SER:HA   | 9:42:170:VAL:HG12  | 1.97                     | 0.47              |
| 10:A3:110:PRO:O   | 10:A3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:A3:132:PHE:CB  | 10:Y3:219:MET:HE2  | 2.45                     | 0.47              |
| 10:B3:159:GLY:O   | 10:B3:186:PRO:HG3  | 2.14                     | 0.47              |
| 10:C3:41:PRO:HA   | 10:E3:157:ALA:HB1  | 1.97                     | 0.47              |
| 10:Q3:223:GLN:HB2 | 10:R3:232:MET:HG3  | 1.97                     | 0.47              |
| 10:U3:110:PRO:O   | 10:U3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:Z3:110:PRO:O   | 10:Z3:114:GLN:HG2  | 2.15                     | 0.47              |
| 11:a3:277:GLN:HG3 | 11:a3:278:GLY:N    | 2.30                     | 0.47              |
| 11:c3:89:VAL:HG21 | 11:c3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:c3:252:LYS:HB2 | 11:c3:252:LYS:HE3  | 1.52                     | 0.47              |
| 11:e3:42:VAL:HA   | 11:e3:120:THR:O    | 2.14                     | 0.47              |
| 11:e3:252:LYS:HB2 | 11:e3:252:LYS:HE3  | 1.52                     | 0.47              |
| 11:g3:254:VAL:CG2 | 11:h3:355:ALA:HB2  | 2.44                     | 0.47              |
| 11:i3:277:GLN:HG3 | 11:i3:278:GLY:N    | 2.30                     | 0.47              |
| 11:j3:50:ASP:OD1  | 11:j3:113:ALA:N    | 2.47                     | 0.47              |
| 11:j3:123:MET:CE  | 11:j3:136:LEU:HD22 | 2.38                     | 0.47              |
| 11:n3:341:THR:OG1 | 11:n3:343:MET:HE2  | 2.15                     | 0.47              |
| 11:o3:123:MET:CE  | 11:o3:136:LEU:HD22 | 2.38                     | 0.47              |
| 11:p3:277:GLN:HB3 | 11:p3:280:LEU:HD12 | 1.95                     | 0.47              |
| 11:q3:101:GLN:NE2 | 11:r3:188:GLN:HB3  | 2.29                     | 0.47              |
| 11:q3:117:ARG:NH1 | 11:q3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:q3:341:THR:OG1 | 11:q3:343:MET:HE2  | 2.15                     | 0.47              |
| 11:s3:89:VAL:HG21 | 11:s3:124:THR:OG1  | 2.14                     | 0.47              |
| 11:x3:79:MET:HE2  | 11:y3:57:PHE:CD2   | 2.50                     | 0.47              |
| 11:x3:117:ARG:NH1 | 11:x3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:y3:89:VAL:HG21 | 11:y3:124:THR:OG1  | 2.14                     | 0.47              |
| 1:B1:165:PHE:CD2  | 2:C2:162:PRO:CA    | 2.79                     | 0.47              |
| 1:C1:165:PHE:C    | 2:C2:152:ARG:HE    | 2.21                     | 0.47              |
| 1:E1:165:PHE:CZ   | 2:C2:153:LEU:HB3   | 2.49                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:E1:244:ARG:HD2  | 1:F1:235:LEU:HD12  | 1.97                     | 0.47              |
| 1:G1:187:ASP:OD1  | 1:G1:187:ASP:N     | 2.35                     | 0.47              |
| 1:K1:167:ARG:CZ   | 2:A2:244:TYR:CA    | 2.69                     | 0.47              |
| 1:L1:139:GLU:OE2  | 1:N1:154:ARG:NH1   | 2.43                     | 0.47              |
| 1:L1:374:HIS:HB3  | 1:M1:276:GLU:HB3   | 1.96                     | 0.47              |
| 1:M1:363:THR:CG2  | 6:Q2:73:ILE:CG1    | 2.90                     | 0.47              |
| 1:T1:192:SER:HB2  | 1:T1:196:HIS:CE1   | 2.50                     | 0.47              |
| 1:U1:393:TYR:CE2  | 1:U1:436:PRO:HD3   | 2.49                     | 0.47              |
| 1:V1:240:ASP:OD1  | 1:W1:235:LEU:HD13  | 2.15                     | 0.47              |
| 1:a1:140:LEU:O    | 1:a1:143:THR:OG1   | 2.26                     | 0.47              |
| 1:d1:155:VAL:HG22 | 1:d1:156:HIS:N     | 2.30                     | 0.47              |
| 1:d1:167:ARG:H    | 2:D2:160:GLN:C     | 2.22                     | 0.47              |
| 1:d1:408:GLN:HA   | 1:d1:411:GLN:NE2   | 2.30                     | 0.47              |
| 1:g1:423:SER:OG   | 1:g1:425:LYS:HE2   | 2.15                     | 0.47              |
| 2:B2:100:ILE:HG21 | 2:B2:243:PHE:HD2   | 1.80                     | 0.47              |
| 2:B2:207:LEU:HD22 | 2:B2:209:MET:HG2   | 1.97                     | 0.47              |
| 2:C2:195:ILE:HD11 | 4:I2:13:ALA:HB1    | 1.97                     | 0.47              |
| 6:Q2:78:VAL:CG1   | 7:V2:57:GLN:HG2    | 2.45                     | 0.47              |
| 7:X2:28:LEU:HD11  | 8:c2:229:MET:HE2   | 1.96                     | 0.47              |
| 9:j2:25:ASN:ND2   | 9:j2:37:GLN:H      | 2.13                     | 0.47              |
| 9:p2:44:LEU:CD2   | 9:p2:73:ARG:HB2    | 2.44                     | 0.47              |
| 9:u2:180:ASN:HB3  | 9:u2:198:SER:HA    | 1.97                     | 0.47              |
| 10:C3:159:GLY:O   | 10:C3:186:PRO:HG3  | 2.14                     | 0.47              |
| 10:H3:110:PRO:O   | 10:H3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:J3:110:PRO:O   | 10:J3:114:GLN:HG2  | 2.14                     | 0.47              |
| 10:O3:110:PRO:O   | 10:O3:114:GLN:HG2  | 2.14                     | 0.47              |
| 10:Q3:219:MET:HE2 | 10:S3:132:PHE:CB   | 2.44                     | 0.47              |
| 10:U3:58:ILE:HG13 | 10:U3:59:ASN:N     | 2.28                     | 0.47              |
| 10:U3:78:LEU:HD12 | 10:U3:193:ASN:O    | 2.13                     | 0.47              |
| 10:W3:110:PRO:O   | 10:W3:114:GLN:HG2  | 2.15                     | 0.47              |
| 10:Y3:110:PRO:O   | 10:Y3:114:GLN:HG2  | 2.15                     | 0.47              |
| 11:a3:42:VAL:HA   | 11:a3:120:THR:O    | 2.14                     | 0.47              |
| 11:b3:341:THR:OG1 | 11:b3:343:MET:HE2  | 2.15                     | 0.47              |
| 11:k3:79:MET:HE2  | 11:l3:57:PHE:CD2   | 2.48                     | 0.47              |
| 11:l3:117:ARG:NH1 | 11:l3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:m3:94:PRO:HB2  | 11:n3:219:ARG:NH2  | 2.29                     | 0.47              |
| 11:m3:117:ARG:NH1 | 11:m3:145:GLY:HA2  | 2.30                     | 0.47              |
| 11:m3:123:MET:CE  | 11:m3:136:LEU:HD22 | 2.38                     | 0.47              |
| 11:n3:123:MET:CE  | 11:n3:136:LEU:HD22 | 2.38                     | 0.47              |
| 11:r3:341:THR:OG1 | 11:r3:343:MET:HE2  | 2.15                     | 0.47              |
| 11:s3:94:PRO:HB2  | 11:t3:219:ARG:NH2  | 2.30                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:s3:277:GLN:HG3 | 11:s3:278:GLY:N   | 2.30                     | 0.47              |
| 11:v3:341:THR:OG1 | 11:v3:343:MET:HE2 | 2.15                     | 0.47              |
| 11:x3:89:VAL:HG21 | 11:x3:124:THR:OG1 | 2.14                     | 0.47              |
| 11:y3:277:GLN:HG3 | 11:y3:278:GLY:N   | 2.30                     | 0.47              |
| 12:D4:137:THR:OG1 | 12:D4:185:THR:OG1 | 2.31                     | 0.47              |
| 1:C1:139:GLU:O    | 1:C1:143:THR:HG23 | 2.14                     | 0.46              |
| 1:C1:165:PHE:CZ   | 2:C2:145:ALA:CA   | 2.98                     | 0.46              |
| 1:D1:254:SER:HB2  | 1:D1:255:PRO:HD3  | 1.97                     | 0.46              |
| 1:F1:245:ILE:O    | 1:F1:249:ILE:HG12 | 2.15                     | 0.46              |
| 1:I1:416:THR:O    | 1:I1:420:MET:HG3  | 2.14                     | 0.46              |
| 1:L1:157:LEU:HA   | 1:L1:174:ALA:HA   | 1.97                     | 0.46              |
| 1:O1:237:PHE:HE1  | 1:P1:232:ASP:HA   | 1.79                     | 0.46              |
| 1:T1:236:LYS:H    | 1:T1:236:LYS:HD2  | 1.80                     | 0.46              |
| 1:U1:173:SER:OG   | 1:U1:174:ALA:N    | 2.46                     | 0.46              |
| 1:Y1:250:GLU:O    | 1:Y1:254:SER:OG   | 2.32                     | 0.46              |
| 1:c1:151:LYS:HD3  | 1:c1:182:PRO:HD3  | 1.96                     | 0.46              |
| 1:d1:296:ARG:NH1  | 1:d1:364:SER:OG   | 2.48                     | 0.46              |
| 1:f1:151:LYS:HZ2  | 1:f1:179:THR:HG22 | 1.79                     | 0.46              |
| 2:E2:96:LEU:HD21  | 2:E2:236:MET:HE3  | 1.92                     | 0.46              |
| 4:I2:59:PHE:CE1   | 4:J2:18:LEU:HG    | 2.50                     | 0.46              |
| 6:S2:106:ARG:HE   | 8:d2:248:LEU:CD1  | 2.29                     | 0.46              |
| 6:T2:51:LYS:NZ    | 6:T2:55:ARG:HE    | 2.13                     | 0.46              |
| 8:b2:115:ILE:O    | 8:b2:116:GLN:C    | 2.57                     | 0.46              |
| 8:f2:221:ILE:O    | 8:f2:225:ARG:HG2  | 2.15                     | 0.46              |
| 9:n2:129:VAL:HG21 | 9:y2:63:PRO:HG3   | 1.97                     | 0.46              |
| 9:u2:115:THR:HB   | 9:u2:191:LEU:HD23 | 1.97                     | 0.46              |
| 10:A3:159:GLY:O   | 10:A3:186:PRO:HG3 | 2.14                     | 0.46              |
| 10:B3:223:GLN:HB2 | 10:C3:232:MET:HG3 | 1.97                     | 0.46              |
| 10:G3:223:GLN:HB2 | 10:H3:232:MET:HG3 | 1.98                     | 0.46              |
| 10:P3:82:LEU:HA   | 10:P3:197:SER:CB  | 2.39                     | 0.46              |
| 10:U3:82:LEU:O    | 10:U3:197:SER:OG  | 2.20                     | 0.46              |
| 10:W3:223:GLN:HB2 | 10:X3:232:MET:HG3 | 1.97                     | 0.46              |
| 10:X3:74:ILE:CD1  | 10:X3:154:GLN:HA  | 2.46                     | 0.46              |
| 10:Z3:74:ILE:CD1  | 10:Z3:154:GLN:HA  | 2.46                     | 0.46              |
| 10:Z3:159:GLY:O   | 10:Z3:186:PRO:HG3 | 2.14                     | 0.46              |
| 11:a3:117:ARG:NH1 | 11:a3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:f3:284:VAL:CG2 | 11:f3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:g3:117:ARG:NH1 | 11:g3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:h3:284:VAL:CG2 | 11:h3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:j3:252:LYS:HB2 | 11:j3:252:LYS:HE3 | 1.52                     | 0.46              |
| 11:m3:341:THR:OG1 | 11:m3:343:MET:HE2 | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:n3:277:GLN:HG3  | 11:n3:278:GLY:N    | 2.30                     | 0.46              |
| 11:o3:117:ARG:NH1  | 11:o3:145:GLY:HA2  | 2.30                     | 0.46              |
| 11:o3:277:GLN:HB3  | 11:o3:280:LEU:HD12 | 1.96                     | 0.46              |
| 11:q3:123:MET:CE   | 11:q3:136:LEU:HD22 | 2.38                     | 0.46              |
| 11:q3:204:ILE:HG21 | 11:q3:213:ALA:HB2  | 1.97                     | 0.46              |
| 11:t3:117:ARG:NH1  | 11:t3:145:GLY:HA2  | 2.30                     | 0.46              |
| 11:t3:277:GLN:HG3  | 11:t3:278:GLY:N    | 2.30                     | 0.46              |
| 11:y3:341:THR:OG1  | 11:y3:343:MET:HE2  | 2.15                     | 0.46              |
| 12:A4:201:ALA:HB3  | 12:A4:217:LEU:HD13 | 1.97                     | 0.46              |
| 12:C4:136:VAL:HG21 | 12:C4:156:LEU:HD12 | 1.97                     | 0.46              |
| 1:H1:245:ILE:HG21  | 1:H1:266:VAL:HG11  | 1.98                     | 0.46              |
| 1:I1:257:VAL:O     | 1:I1:261:ASN:ND2   | 2.39                     | 0.46              |
| 1:I1:416:THR:HG23  | 1:I1:430:LEU:HD21  | 1.97                     | 0.46              |
| 1:L1:423:SER:HB2   | 1:M1:384:ARG:NH1   | 2.30                     | 0.46              |
| 1:M1:360:ARG:HG2   | 1:M1:362:GLU:OE2   | 2.15                     | 0.46              |
| 1:R1:172:PRO:HG2   | 1:R1:205:LEU:HD13  | 1.96                     | 0.46              |
| 1:W1:166:VAL:O     | 2:E2:144:GLU:OE2   | 2.34                     | 0.46              |
| 1:W1:293:LEU:HD11  | 1:W1:296:ARG:HH21  | 1.80                     | 0.46              |
| 1:Z1:231:ASN:O     | 1:Z1:234:GLN:NE2   | 2.48                     | 0.46              |
| 2:A2:128:ASP:O     | 2:A2:132:GLN:HG2   | 2.16                     | 0.46              |
| 2:B2:178:GLU:OE2   | 2:B2:243:PHE:HE1   | 1.98                     | 0.46              |
| 2:D2:181:THR:HG23  | 4:J2:88:ILE:HG21   | 1.97                     | 0.46              |
| 2:E2:220:PRO:O     | 2:E2:224:MET:HG2   | 2.15                     | 0.46              |
| 2:E2:220:PRO:HG3   | 3:F2:105:GLN:HE22  | 1.80                     | 0.46              |
| 5:P2:48:ARG:HH21   | 5:P2:77:LYS:HE3    | 1.80                     | 0.46              |
| 6:S2:90:PRO:O      | 8:d2:50:SER:OG     | 2.33                     | 0.46              |
| 9:g2:105:VAL:CG1   | 9:g2:134:PHE:HB3   | 2.46                     | 0.46              |
| 9:i2:231:VAL:HG21  | 9:n2:9:LYS:HG3     | 1.96                     | 0.46              |
| 9:j2:46:TYR:HA     | 9:j2:69:GLY:HA2    | 1.97                     | 0.46              |
| 9:p2:44:LEU:HD21   | 9:p2:73:ARG:HB2    | 1.97                     | 0.46              |
| 9:s2:94:ASP:HA     | 9:s2:118:GLY:O     | 2.16                     | 0.46              |
| 9:w2:230:LEU:HD21  | 9:22:242:ILE:HG23  | 1.97                     | 0.46              |
| 9:42:40:VAL:HG23   | 9:42:75:VAL:HG23   | 1.98                     | 0.46              |
| 10:D3:41:PRO:HA    | 10:F3:157:ALA:HB1  | 1.97                     | 0.46              |
| 10:D3:223:GLN:HB2  | 10:E3:232:MET:HG3  | 1.98                     | 0.46              |
| 10:H3:219:MET:HE2  | 10:J3:132:PHE:CB   | 2.44                     | 0.46              |
| 10:M3:41:PRO:HA    | 10:O3:157:ALA:HB1  | 1.96                     | 0.46              |
| 10:P3:219:MET:HE2  | 10:R3:132:PHE:CB   | 2.44                     | 0.46              |
| 10:T3:74:ILE:CD1   | 10:T3:154:GLN:HA   | 2.45                     | 0.46              |
| 10:V3:74:ILE:CD1   | 10:V3:154:GLN:HA   | 2.46                     | 0.46              |
| 11:a3:361:LYS:O    | 11:a3:361:LYS:HG3  | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:b3:361:LYS:HG3  | 11:b3:361:LYS:O    | 2.15                     | 0.46              |
| 11:c3:101:GLN:NE2  | 11:d3:188:GLN:HB3  | 2.31                     | 0.46              |
| 11:d3:341:THR:OG1  | 11:d3:343:MET:HE2  | 2.15                     | 0.46              |
| 11:e3:341:THR:OG1  | 11:e3:343:MET:HE2  | 2.15                     | 0.46              |
| 11:g3:94:PRO:HB2   | 11:h3:219:ARG:NH2  | 2.30                     | 0.46              |
| 11:i3:117:ARG:NH1  | 11:i3:145:GLY:HA2  | 2.30                     | 0.46              |
| 11:k3:117:ARG:NH1  | 11:k3:145:GLY:HA2  | 2.30                     | 0.46              |
| 11:m3:42:VAL:HA    | 11:m3:120:THR:O    | 2.14                     | 0.46              |
| 11:m3:79:MET:HE2   | 11:n3:57:PHE:CD2   | 2.49                     | 0.46              |
| 11:n3:117:ARG:NH1  | 11:n3:145:GLY:HA2  | 2.30                     | 0.46              |
| 11:p3:204:ILE:HG21 | 11:p3:213:ALA:HB2  | 1.97                     | 0.46              |
| 11:r3:204:ILE:HG21 | 11:r3:213:ALA:HB2  | 1.98                     | 0.46              |
| 11:s3:341:THR:OG1  | 11:s3:343:MET:HE2  | 2.15                     | 0.46              |
| 11:u3:277:GLN:HB3  | 11:u3:280:LEU:HD12 | 1.95                     | 0.46              |
| 11:w3:83:ASN:ND2   | 11:x3:109:SER:OG   | 2.46                     | 0.46              |
| 11:x3:42:VAL:HA    | 11:x3:120:THR:O    | 2.14                     | 0.46              |
| 11:z3:341:THR:OG1  | 11:z3:343:MET:HE2  | 2.15                     | 0.46              |
| 1:F1:415:LEU:HD23  | 1:F1:415:LEU:HA    | 1.78                     | 0.46              |
| 1:K1:140:LEU:O     | 1:K1:143:THR:OG1   | 2.30                     | 0.46              |
| 1:M1:366:TYR:N     | 6:Q2:72:HIS:CE1    | 2.51                     | 0.46              |
| 1:N1:167:ARG:HD2   | 2:A2:160:GLN:HG2   | 1.66                     | 0.46              |
| 1:O1:193:ALA:HA    | 1:Q1:219:LEU:HD21  | 1.96                     | 0.46              |
| 1:P1:422:PHE:CE2   | 1:P1:424:ASP:HB3   | 2.50                     | 0.46              |
| 1:Q1:181:GLU:HB3   | 1:Q1:184:ARG:NH2   | 2.31                     | 0.46              |
| 1:S1:276:GLU:HG2   | 1:S1:374:HIS:HE1   | 1.79                     | 0.46              |
| 1:U1:408:GLN:O     | 1:U1:411:GLN:HG2   | 2.14                     | 0.46              |
| 1:c1:297:GLN:NE2   | 6:S2:55:ARG:NH2    | 2.64                     | 0.46              |
| 1:e1:417:ARG:HG3   | 1:e1:422:PHE:HB3   | 1.98                     | 0.46              |
| 5:P2:84:MET:CE     | 7:V2:130:LEU:HD11  | 2.45                     | 0.46              |
| 7:Y2:75:LYS:HA     | 9:j2:47:GLN:NE2    | 2.30                     | 0.46              |
| 8:b2:9:MET:HE3     | 8:b2:9:MET:HB3     | 1.76                     | 0.46              |
| 8:b2:42:ARG:HD2    | 9:g2:64:SER:CB     | 2.45                     | 0.46              |
| 8:d2:182:THR:C     | 8:d2:184:GLU:H     | 2.22                     | 0.46              |
| 8:e2:2:ASP:O       | 8:e2:5:ILE:HG22    | 2.16                     | 0.46              |
| 9:j2:233:MET:HE1   | 9:n2:245:LYS:HG3   | 1.96                     | 0.46              |
| 9:l2:117:ASP:OD1   | 9:l2:118:GLY:N     | 2.46                     | 0.46              |
| 9:22:138:PRO:O     | 9:22:140:ILE:HG12  | 2.15                     | 0.46              |
| 9:32:102:PHE:CB    | 9:32:114:TYR:HB3   | 2.44                     | 0.46              |
| 10:L3:74:ILE:CD1   | 10:L3:154:GLN:HA   | 2.45                     | 0.46              |
| 10:M3:40:ILE:H     | 10:M3:40:ILE:HG12  | 1.48                     | 0.46              |
| 10:S3:74:ILE:CD1   | 10:S3:154:GLN:HA   | 2.45                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:U3:74:ILE:CD1   | 10:U3:154:GLN:HA  | 2.46                     | 0.46              |
| 11:a3:249:GLN:O    | 11:z3:23:ARG:NH1  | 2.49                     | 0.46              |
| 11:b3:284:VAL:CG2  | 11:b3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:c3:277:GLN:HG3  | 11:c3:278:GLY:N   | 2.30                     | 0.46              |
| 11:d3:42:VAL:HA    | 11:d3:120:THR:O   | 2.14                     | 0.46              |
| 11:d3:284:VAL:CG2  | 11:d3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:h3:277:GLN:HG3  | 11:h3:278:GLY:N   | 2.30                     | 0.46              |
| 11:h3:341:THR:OG1  | 11:h3:343:MET:HE2 | 2.15                     | 0.46              |
| 11:i3:101:GLN:NE2  | 11:j3:188:GLN:HB3 | 2.31                     | 0.46              |
| 11:j3:254:VAL:HG13 | 11:j3:365:ILE:CG1 | 2.46                     | 0.46              |
| 11:j3:284:VAL:CG2  | 11:j3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:p3:277:GLN:HG3  | 11:p3:278:GLY:N   | 2.30                     | 0.46              |
| 11:p3:341:THR:OG1  | 11:p3:343:MET:HE2 | 2.15                     | 0.46              |
| 11:u3:117:ARG:NH1  | 11:u3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:y3:117:ARG:NH1  | 11:y3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:z3:117:ARG:NH1  | 11:z3:145:GLY:HA2 | 2.30                     | 0.46              |
| 1:F1:253:LEU:CD1   | 1:F1:412:ILE:HG23 | 2.46                     | 0.46              |
| 1:L1:164:LEU:HD23  | 1:L1:164:LEU:H    | 1.80                     | 0.46              |
| 1:L1:244:ARG:HH11  | 1:M1:235:LEU:HB3  | 1.79                     | 0.46              |
| 1:M1:287:ASP:OD2   | 1:M1:289:SER:HB3  | 2.16                     | 0.46              |
| 1:M1:402:LEU:HD23  | 1:M1:403:PRO:O    | 2.16                     | 0.46              |
| 1:N1:245:ILE:O     | 1:N1:249:ILE:HG12 | 2.15                     | 0.46              |
| 1:Q1:393:TYR:CE2   | 1:Q1:436:PRO:HD3  | 2.50                     | 0.46              |
| 1:T1:414:ASP:HB3   | 1:U1:431:ASN:ND2  | 2.30                     | 0.46              |
| 1:U1:393:TYR:HB3   | 1:U1:402:LEU:N    | 2.31                     | 0.46              |
| 1:Y1:180:LEU:HB2   | 1:Y1:215:GLN:HE22 | 1.80                     | 0.46              |
| 1:Z1:411:GLN:O     | 1:Z1:415:LEU:HD23 | 2.16                     | 0.46              |
| 1:a1:237:PHE:HE2   | 1:b1:232:ASP:HA   | 1.80                     | 0.46              |
| 1:c1:125:GLN:HB2   | 4:J2:5:SER:HA     | 1.66                     | 0.46              |
| 1:h1:246:GLN:HB2   | 1:h1:266:VAL:HG23 | 1.96                     | 0.46              |
| 2:B2:66:ARG:NE     | 2:B2:178:GLU:OE2  | 2.49                     | 0.46              |
| 4:G2:52:ILE:H      | 4:G2:52:ILE:HD12  | 1.80                     | 0.46              |
| 6:Q2:26:LEU:HD12   | 6:Q2:112:ASN:HD22 | 1.80                     | 0.46              |
| 8:c2:216:ALA:O     | 8:c2:220:MET:HG3  | 2.16                     | 0.46              |
| 8:e2:171:VAL:CG1   | 8:e2:179:PHE:HB3  | 2.46                     | 0.46              |
| 9:h2:88:GLN:NE2    | 9:h2:90:ASN:OD1   | 2.49                     | 0.46              |
| 9:p2:145:ASN:HB3   | 9:p2:162:GLN:NE2  | 2.31                     | 0.46              |
| 9:s2:154:ASP:OD1   | 9:s2:156:VAL:HG22 | 2.15                     | 0.46              |
| 9:t2:189:GLU:HB2   | 9:t2:191:LEU:HD12 | 1.98                     | 0.46              |
| 9:v2:226:VAL:HG13  | 9:12:242:ILE:HD12 | 1.97                     | 0.46              |
| 9:y2:175:LEU:HD21  | 9:y2:214:LEU:HD11 | 1.98                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:z2:91:ASN:O      | 9:z2:217:GLY:HA2  | 2.16                     | 0.46              |
| 9:32:234:ILE:HG22  | 12:B4:55:ASN:HD22 | 1.79                     | 0.46              |
| 10:A3:223:GLN:HB2  | 10:B3:232:MET:HG3 | 1.97                     | 0.46              |
| 10:B3:74:ILE:CD1   | 10:B3:154:GLN:HA  | 2.45                     | 0.46              |
| 10:M3:223:GLN:HB2  | 10:N3:232:MET:HG3 | 1.97                     | 0.46              |
| 10:N3:74:ILE:CD1   | 10:N3:154:GLN:HA  | 2.46                     | 0.46              |
| 10:N3:223:GLN:HB2  | 10:O3:232:MET:HG3 | 1.97                     | 0.46              |
| 10:Q3:82:LEU:HA    | 10:Q3:197:SER:CB  | 2.38                     | 0.46              |
| 10:V3:223:GLN:HB2  | 10:W3:232:MET:HG3 | 1.98                     | 0.46              |
| 10:W3:74:ILE:CD1   | 10:W3:154:GLN:HA  | 2.46                     | 0.46              |
| 11:a3:284:VAL:CG2  | 11:a3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:h3:254:VAL:HG13 | 11:h3:365:ILE:CG1 | 2.46                     | 0.46              |
| 11:j3:117:ARG:NH1  | 11:j3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:k3:341:THR:OG1  | 11:k3:343:MET:HE2 | 2.15                     | 0.46              |
| 11:o3:341:THR:OG1  | 11:o3:343:MET:HE2 | 2.15                     | 0.46              |
| 11:p3:114:LYS:HD2  | 11:p3:114:LYS:HA  | 1.77                     | 0.46              |
| 11:q3:252:LYS:HB2  | 11:q3:252:LYS:HE3 | 1.52                     | 0.46              |
| 11:s3:204:ILE:HG21 | 11:s3:213:ALA:HB2 | 1.98                     | 0.46              |
| 11:t3:361:LYS:HG3  | 11:t3:361:LYS:O   | 2.15                     | 0.46              |
| 11:u3:277:GLN:HG3  | 11:u3:278:GLY:N   | 2.30                     | 0.46              |
| 11:z3:361:LYS:O    | 11:z3:361:LYS:HG3 | 2.15                     | 0.46              |
| 12:C4:86:ASP:O     | 12:C4:89:GLN:HG3  | 2.14                     | 0.46              |
| 1:B1:166:VAL:HA    | 2:C2:161:GLY:CA   | 2.43                     | 0.46              |
| 1:B1:407:ASP:O     | 1:B1:410:LYS:HG3  | 2.16                     | 0.46              |
| 1:E1:162:PRO:HA    | 1:E1:169:GLN:HG3  | 1.98                     | 0.46              |
| 1:F1:279:GLU:H     | 1:F1:373:ARG:HB2  | 1.81                     | 0.46              |
| 1:N1:359:GLN:OE1   | 7:V2:55:PRO:HG3   | 2.15                     | 0.46              |
| 1:U1:164:LEU:HD12  | 1:U1:164:LEU:HA   | 1.68                     | 0.46              |
| 1:U1:193:ALA:HA    | 1:W1:219:LEU:HD21 | 1.97                     | 0.46              |
| 1:U1:415:LEU:HD21  | 1:V1:433:VAL:HG22 | 1.97                     | 0.46              |
| 1:X1:203:ALA:C     | 1:Y1:170:LYS:HZ3  | 2.23                     | 0.46              |
| 1:Y1:404:LEU:HD23  | 1:Y1:408:GLN:HG2  | 1.97                     | 0.46              |
| 1:b1:298:LEU:HD13  | 1:b1:362:GLU:HB3  | 1.97                     | 0.46              |
| 1:e1:283:SER:HB2   | 1:e1:369:ASP:HB2  | 1.97                     | 0.46              |
| 1:g1:360:ARG:NH1   | 1:g1:362:GLU:OE1  | 2.47                     | 0.46              |
| 5:P2:80:VAL:HG11   | 7:V2:126:MET:CE   | 2.46                     | 0.46              |
| 9:r2:1:MET:HE2     | 9:r2:1:MET:HA     | 1.97                     | 0.46              |
| 9:u2:151:ILE:N     | 9:u2:216:GLN:OE1  | 2.28                     | 0.46              |
| 9:u2:225:ASN:HB3   | 9:u2:228:GLU:HB3  | 1.96                     | 0.46              |
| 9:v2:248:SER:O     | 9:v2:252:GLN:HG2  | 2.16                     | 0.46              |
| 9:x2:43:ASP:OD2    | 9:x2:43:ASP:N     | 2.47                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:22:123:ASP:OD1   | 9:22:126:GLY:N     | 2.48                     | 0.46              |
| 9:42:250:THR:O     | 9:42:253:MET:HB2   | 2.16                     | 0.46              |
| 10:A3:40:ILE:H     | 10:A3:40:ILE:HG12  | 1.48                     | 0.46              |
| 10:I3:124:MET:HE3  | 10:I3:124:MET:HB3  | 1.77                     | 0.46              |
| 10:K3:74:ILE:CD1   | 10:K3:154:GLN:HA   | 2.46                     | 0.46              |
| 10:K3:223:GLN:HB2  | 10:L3:232:MET:HG3  | 1.97                     | 0.46              |
| 10:M3:74:ILE:CD1   | 10:M3:154:GLN:HA   | 2.46                     | 0.46              |
| 10:P3:41:PRO:HA    | 10:R3:157:ALA:HB1  | 1.97                     | 0.46              |
| 10:Q3:124:MET:HE3  | 10:Q3:124:MET:HB3  | 1.77                     | 0.46              |
| 10:S3:223:GLN:HB2  | 10:T3:232:MET:HG3  | 1.98                     | 0.46              |
| 10:W3:51:ILE:CG1   | 11:y3:175:LEU:HD11 | 2.41                     | 0.46              |
| 11:g3:277:GLN:HG3  | 11:g3:278:GLY:N    | 2.30                     | 0.46              |
| 11:i3:42:VAL:HA    | 11:i3:120:THR:O    | 2.14                     | 0.46              |
| 11:i3:123:MET:CE   | 11:i3:136:LEU:HD22 | 2.38                     | 0.46              |
| 11:o3:204:ILE:HG21 | 11:o3:213:ALA:HB2  | 1.98                     | 0.46              |
| 11:p3:254:VAL:HG13 | 11:p3:365:ILE:CG1  | 2.46                     | 0.46              |
| 11:s3:361:LYS:HG3  | 11:s3:361:LYS:O    | 2.15                     | 0.46              |
| 11:u3:93:TYR:OH    | 11:u3:173:ARG:O    | 2.25                     | 0.46              |
| 11:v3:217:ASP:OD1  | 11:v3:219:ARG:N    | 2.37                     | 0.46              |
| 11:x3:254:VAL:HG13 | 11:x3:365:ILE:CG1  | 2.46                     | 0.46              |
| 11:y3:42:VAL:HA    | 11:y3:120:THR:O    | 2.14                     | 0.46              |
| 12:D4:102:MET:N    | 12:D4:230:GLN:O    | 2.44                     | 0.46              |
| 1:B1:181:GLU:CD    | 1:B1:184:ARG:HH21  | 2.22                     | 0.46              |
| 1:B1:190:GLN:HG2   | 1:C1:217:GLY:HA3   | 1.97                     | 0.46              |
| 1:Q1:173:SER:OG    | 1:Q1:174:ALA:N     | 2.48                     | 0.46              |
| 1:R1:389:VAL:HB    | 1:R1:432:VAL:HG13  | 1.97                     | 0.46              |
| 1:U1:276:GLU:OE2   | 1:U1:374:HIS:NE2   | 2.42                     | 0.46              |
| 1:X1:404:LEU:HB2   | 1:X1:434:ASN:ND2   | 2.30                     | 0.46              |
| 1:Z1:267:THR:OG1   | 1:Z1:386:SER:HB2   | 2.15                     | 0.46              |
| 1:a1:373:ARG:HH21  | 1:b1:275:LYS:HE2   | 1.80                     | 0.46              |
| 1:c1:362:GLU:N     | 1:c1:362:GLU:OE2   | 2.49                     | 0.46              |
| 1:e1:244:ARG:NH2   | 1:f1:235:LEU:HB3   | 2.30                     | 0.46              |
| 1:f1:214:ASP:HB2   | 1:f1:220:LEU:HD11  | 1.97                     | 0.46              |
| 1:g1:404:LEU:H     | 1:g1:434:ASN:HD21  | 1.63                     | 0.46              |
| 2:A2:39:SER:C      | 2:A2:41:SER:N      | 2.69                     | 0.46              |
| 2:A2:187:PHE:O     | 2:A2:191:ILE:HG12  | 2.16                     | 0.46              |
| 2:C2:43:GLN:HG2    | 2:C2:123:MET:SD    | 2.56                     | 0.46              |
| 2:C2:125:GLU:O     | 2:C2:129:LYS:HG2   | 2.16                     | 0.46              |
| 2:E2:101:MET:HE3   | 2:E2:104:VAL:HG11  | 1.97                     | 0.46              |
| 4:I2:56:VAL:O      | 4:I2:60:ILE:HG12   | 2.16                     | 0.46              |
| 4:J2:50:SER:O      | 4:J2:54:LYS:HG3    | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:S2:35:THR:HG23   | 6:S2:38:TYR:HB2    | 1.97                     | 0.46              |
| 8:e2:139:ALA:O     | 8:e2:201:ILE:N     | 2.42                     | 0.46              |
| 8:e2:147:ASN:HB2   | 8:e2:150:ASP:OD2   | 2.15                     | 0.46              |
| 9:q2:241:GLU:HG3   | 9:v2:256:LYS:HG2   | 1.97                     | 0.46              |
| 9:s2:185:GLU:OE1   | 9:x2:51:GLN:NE2    | 2.49                     | 0.46              |
| 9:u2:20:ASP:OD2    | 9:z2:3:SER:OG      | 2.28                     | 0.46              |
| 9:u2:238:ARG:NH2   | 9:12:255:GLN:HE22  | 2.13                     | 0.46              |
| 9:y2:127:GLN:HG3   | 9:y2:141:THR:HG22  | 1.97                     | 0.46              |
| 10:D3:82:LEU:HD12  | 10:D3:146:GLY:HA3  | 1.98                     | 0.46              |
| 10:E3:71:PRO:HD2   | 10:E3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:E3:110:PRO:O    | 10:E3:114:GLN:HG2  | 2.15                     | 0.46              |
| 10:I3:71:PRO:HD2   | 10:I3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:J3:74:ILE:CD1   | 10:J3:154:GLN:HA   | 2.45                     | 0.46              |
| 10:J3:223:GLN:HB2  | 10:K3:232:MET:HG3  | 1.98                     | 0.46              |
| 10:P3:74:ILE:CD1   | 10:P3:154:GLN:HA   | 2.46                     | 0.46              |
| 10:R3:74:ILE:CD1   | 10:R3:154:GLN:HA   | 2.46                     | 0.46              |
| 10:U3:82:LEU:HD12  | 10:U3:146:GLY:HA3  | 1.98                     | 0.46              |
| 10:Y3:71:PRO:HD3   | 10:Y3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:Y3:74:ILE:CD1   | 10:Y3:154:GLN:HA   | 2.45                     | 0.46              |
| 11:c3:254:VAL:HG13 | 11:c3:365:ILE:CG1  | 2.46                     | 0.46              |
| 11:c3:341:THR:OG1  | 11:c3:343:MET:HE2  | 2.15                     | 0.46              |
| 11:c3:361:LYS:HG3  | 11:c3:361:LYS:O    | 2.15                     | 0.46              |
| 11:e3:89:VAL:HG21  | 11:e3:124:THR:OG1  | 2.15                     | 0.46              |
| 11:e3:114:LYS:HD2  | 11:e3:114:LYS:HA   | 1.77                     | 0.46              |
| 11:i3:341:THR:OG1  | 11:i3:343:MET:HE2  | 2.15                     | 0.46              |
| 11:i3:361:LYS:O    | 11:i3:361:LYS:HG3  | 2.15                     | 0.46              |
| 11:l3:277:GLN:HG3  | 11:l3:278:GLY:N    | 2.30                     | 0.46              |
| 11:m3:284:VAL:CG2  | 11:m3:316:GLY:HA2  | 2.46                     | 0.46              |
| 11:n3:204:ILE:HG21 | 11:n3:213:ALA:HB2  | 1.97                     | 0.46              |
| 11:o3:277:GLN:HG3  | 11:o3:278:GLY:N    | 2.30                     | 0.46              |
| 11:r3:123:MET:CE   | 11:r3:136:LEU:HD22 | 2.38                     | 0.46              |
| 11:r3:361:LYS:O    | 11:r3:361:LYS:HG3  | 2.15                     | 0.46              |
| 11:u3:341:THR:OG1  | 11:u3:343:MET:HE2  | 2.15                     | 0.46              |
| 11:u3:361:LYS:O    | 11:u3:361:LYS:HG3  | 2.15                     | 0.46              |
| 11:v3:196:MET:HA   | 11:v3:196:MET:CE   | 2.34                     | 0.46              |
| 11:y3:361:LYS:HG3  | 11:y3:361:LYS:O    | 2.15                     | 0.46              |
| 11:z3:284:VAL:CG2  | 11:z3:316:GLY:HA2  | 2.46                     | 0.46              |
| 1:G1:250:GLU:O     | 1:G1:254:SER:OG    | 2.20                     | 0.46              |
| 1:N1:375:THR:HG23  | 1:O1:275:LYS:NZ    | 2.31                     | 0.46              |
| 1:Q1:161:LYS:HE2   | 3:F2:249:ASN:HD22  | 1.68                     | 0.46              |
| 1:U1:149:PRO:HA    | 1:U1:181:GLU:HB2   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:X1:143:THR:HG21 | 1:Y1:156:HIS:NE2   | 2.30                     | 0.46              |
| 1:a1:304:VAL:HB   | 1:b1:356:ARG:H     | 1.81                     | 0.46              |
| 1:c1:168:GLU:OE1  | 1:c1:170:LYS:HB2   | 2.16                     | 0.46              |
| 1:c1:190:GLN:CD   | 1:d1:217:GLY:HA3   | 2.41                     | 0.46              |
| 1:f1:385:LEU:HD12 | 1:f1:426:ARG:NH2   | 2.31                     | 0.46              |
| 2:C2:101:MET:HE1  | 2:C2:137:PHE:CE2   | 2.51                     | 0.46              |
| 2:D2:52:THR:O     | 2:D2:55:PRO:HD2    | 2.16                     | 0.46              |
| 3:F2:20:LEU:HD13  | 3:F2:48:ILE:HA     | 1.98                     | 0.46              |
| 4:G2:67:PRO:HD3   | 4:H2:7:MET:HE2     | 1.97                     | 0.46              |
| 6:S2:102:MET:HG3  | 6:S2:106:ARG:HD3   | 1.98                     | 0.46              |
| 7:Z2:112:TYR:HE2  | 8:e2:244:ALA:HB2   | 1.80                     | 0.46              |
| 8:b2:86:GLY:O     | 8:b2:101:ARG:HD3   | 2.14                     | 0.46              |
| 8:b2:131:GLU:OE2  | 8:b2:131:GLU:N     | 2.47                     | 0.46              |
| 8:b2:173:ARG:HB3  | 9:g2:67:GLN:NE2    | 2.30                     | 0.46              |
| 9:l2:7:ILE:O      | 9:l2:10:THR:OG1    | 2.26                     | 0.46              |
| 9:l2:105:VAL:CG1  | 9:l2:134:PHE:HB3   | 2.45                     | 0.46              |
| 9:v2:257:LEU:O    | 9:v2:260:LEU:HB3   | 2.15                     | 0.46              |
| 9:42:7:ILE:HG23   | 9:42:71:GLY:H      | 1.81                     | 0.46              |
| 9:42:226:VAL:O    | 9:42:230:LEU:HD23  | 2.16                     | 0.46              |
| 10:B3:110:PRO:O   | 10:B3:114:GLN:HG2  | 2.14                     | 0.46              |
| 10:E3:41:PRO:HA   | 10:G3:157:ALA:HB1  | 1.97                     | 0.46              |
| 10:E3:50:SER:HB3  | 11:f3:99:GLN:HE21  | 1.81                     | 0.46              |
| 10:E3:71:PRO:HD3  | 10:E3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:F3:71:PRO:HD2  | 10:F3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:G3:71:PRO:HD2  | 10:G3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:H3:71:PRO:HD2  | 10:H3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:H3:71:PRO:HD3  | 10:H3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:J3:71:PRO:HD2  | 10:J3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:J3:82:LEU:HA   | 10:J3:197:SER:CB   | 2.39                     | 0.46              |
| 10:M3:110:PRO:O   | 10:M3:114:GLN:HG2  | 2.14                     | 0.46              |
| 10:P3:71:PRO:HD3  | 10:P3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:Q3:71:PRO:HD3  | 10:Q3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:Q3:74:ILE:CD1  | 10:Q3:154:GLN:HA   | 2.45                     | 0.46              |
| 10:T3:82:LEU:HD12 | 10:T3:146:GLY:HA3  | 1.98                     | 0.46              |
| 10:X3:71:PRO:HD3  | 10:X3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:Y3:223:GLN:HB2 | 10:Z3:232:MET:HG3  | 1.97                     | 0.46              |
| 10:Z3:71:PRO:HD3  | 10:Z3:193:ASN:OD1  | 2.16                     | 0.46              |
| 11:a3:94:PRO:HB2  | 11:b3:219:ARG:NH2  | 2.30                     | 0.46              |
| 11:h3:361:LYS:O   | 11:h3:361:LYS:HG3  | 2.15                     | 0.46              |
| 11:i3:252:LYS:HB2 | 11:i3:252:LYS:HE3  | 1.52                     | 0.46              |
| 11:j3:361:LYS:HG3 | 11:j3:361:LYS:O    | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:k3:361:LYS:HG3  | 11:k3:361:LYS:O    | 2.15                     | 0.46              |
| 11:l3:361:LYS:HG3  | 11:l3:361:LYS:O    | 2.15                     | 0.46              |
| 11:m3:204:ILE:HG21 | 11:m3:213:ALA:HB2  | 1.97                     | 0.46              |
| 11:r3:277:GLN:HG3  | 11:r3:278:GLY:N    | 2.30                     | 0.46              |
| 11:t3:204:ILE:HG21 | 11:t3:213:ALA:HB2  | 1.98                     | 0.46              |
| 12:E4:142:ASP:OD2  | 12:E4:146:ARG:NE   | 2.48                     | 0.46              |
| 12:E4:169:GLN:NE2  | 12:E4:173:THR:OG1  | 2.32                     | 0.46              |
| 1:B1:156:HIS:CE1   | 1:h1:140:LEU:HD22  | 2.51                     | 0.46              |
| 1:I1:192:SER:O     | 1:I1:196:HIS:ND1   | 2.49                     | 0.46              |
| 1:M1:365:ASN:OD1   | 6:Q2:72:HIS:C      | 2.58                     | 0.46              |
| 1:N1:212:LEU:CB    | 1:N1:220:LEU:HB2   | 2.46                     | 0.46              |
| 1:O1:195:VAL:HG13  | 1:O1:210:VAL:HB    | 1.96                     | 0.46              |
| 1:P1:421:GLY:O     | 1:P1:426:ARG:NH2   | 2.49                     | 0.46              |
| 1:T1:173:SER:OG    | 1:T1:174:ALA:N     | 2.48                     | 0.46              |
| 1:c1:236:LYS:HD2   | 1:c1:236:LYS:N     | 2.30                     | 0.46              |
| 2:A2:149:LEU:HD22  | 3:F2:144:LEU:HB3   | 1.98                     | 0.46              |
| 2:D2:75:ARG:NH2    | 2:D2:85:PRO:HB3    | 2.31                     | 0.46              |
| 2:D2:119:GLN:O     | 2:D2:120:LYS:HG2   | 2.15                     | 0.46              |
| 3:F2:68:ILE:HD12   | 3:F2:68:ILE:H      | 1.80                     | 0.46              |
| 3:F2:242:HIS:O     | 3:F2:246:GLU:HG3   | 2.16                     | 0.46              |
| 4:J2:36:SER:HA     | 4:J2:39:GLN:HB2    | 1.97                     | 0.46              |
| 6:R2:65:LEU:HD12   | 6:R2:75:ALA:H      | 1.81                     | 0.46              |
| 7:V2:6:ILE:HG21    | 7:V2:122:VAL:HG11  | 1.97                     | 0.46              |
| 7:a2:127:LEU:HD11  | 8:f2:250:MET:HE3   | 1.98                     | 0.46              |
| 8:c2:122:GLY:HA2   | 8:c2:162:LYS:HB3   | 1.98                     | 0.46              |
| 8:d2:139:ALA:O     | 8:d2:201:ILE:N     | 2.46                     | 0.46              |
| 8:e2:136:THR:OG1   | 8:e2:144:SER:OG    | 2.33                     | 0.46              |
| 9:j2:9:LYS:HE3     | 9:j2:9:LYS:HB3     | 1.71                     | 0.46              |
| 9:n2:170:VAL:HG23  | 11:x3:80:GLN:NE2   | 2.30                     | 0.46              |
| 9:p2:42:GLU:HB2    | 9:p2:75:VAL:HB     | 1.97                     | 0.46              |
| 9:t2:129:VAL:HG21  | 9:42:63:PRO:HG3    | 1.97                     | 0.46              |
| 9:w2:79:ARG:O      | 9:w2:182:THR:HG22  | 2.15                     | 0.46              |
| 9:w2:238:ARG:NH2   | 9:32:255:GLN:OE1   | 2.49                     | 0.46              |
| 10:A3:124:MET:HE3  | 10:A3:124:MET:HB3  | 1.77                     | 0.46              |
| 10:C3:71:PRO:HD2   | 10:C3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:C3:82:LEU:HD12  | 10:C3:146:GLY:HA3  | 1.98                     | 0.46              |
| 10:H3:41:PRO:HA    | 10:J3:157:ALA:HB1  | 1.97                     | 0.46              |
| 10:Y3:222:LEU:HB2  | 10:Z3:231:PRO:HB3  | 1.98                     | 0.46              |
| 11:b3:117:ARG:NH1  | 11:b3:145:GLY:HA2  | 2.30                     | 0.46              |
| 11:d3:89:VAL:HG21  | 11:d3:124:THR:OG1  | 2.14                     | 0.46              |
| 11:d3:252:LYS:HB2  | 11:d3:252:LYS:HE3  | 1.52                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:g3:284:VAL:CG2  | 11:g3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:h3:117:ARG:NH1  | 11:h3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:j3:277:GLN:HG3  | 11:j3:278:GLY:N   | 2.30                     | 0.46              |
| 11:k3:204:ILE:HG21 | 11:k3:213:ALA:HB2 | 1.97                     | 0.46              |
| 11:l3:204:ILE:HG21 | 11:l3:213:ALA:HB2 | 1.97                     | 0.46              |
| 11:l3:254:VAL:HG13 | 11:l3:365:ILE:CG1 | 2.46                     | 0.46              |
| 11:l3:284:VAL:CG2  | 11:l3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:l3:341:THR:OG1  | 11:l3:343:MET:HE2 | 2.15                     | 0.46              |
| 11:m3:254:VAL:HG13 | 11:m3:365:ILE:CG1 | 2.46                     | 0.46              |
| 11:m3:361:LYS:O    | 11:m3:361:LYS:HG3 | 2.15                     | 0.46              |
| 11:p3:117:ARG:NH1  | 11:p3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:q3:93:TYR:OH    | 11:q3:173:ARG:O   | 2.25                     | 0.46              |
| 11:r3:117:ARG:NH1  | 11:r3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:u3:101:GLN:NE2  | 11:v3:188:GLN:HB3 | 2.31                     | 0.46              |
| 11:v3:277:GLN:HG3  | 11:v3:278:GLY:N   | 2.30                     | 0.46              |
| 11:v3:361:LYS:HG3  | 11:v3:361:LYS:O   | 2.15                     | 0.46              |
| 11:w3:277:GLN:HG3  | 11:w3:278:GLY:N   | 2.30                     | 0.46              |
| 11:x3:284:VAL:CG2  | 11:x3:316:GLY:HA2 | 2.46                     | 0.46              |
| 11:z3:42:VAL:HA    | 11:z3:120:THR:O   | 2.14                     | 0.46              |
| 11:z3:277:GLN:HG3  | 11:z3:278:GLY:N   | 2.30                     | 0.46              |
| 12:B4:208:LYS:NZ   | 12:C4:225:LEU:O   | 2.40                     | 0.46              |
| 12:C4:156:LEU:HD21 | 12:C4:163:PHE:HZ  | 1.81                     | 0.46              |
| 1:E1:140:LEU:HD23  | 1:E1:140:LEU:HA   | 1.82                     | 0.46              |
| 1:H1:187:ASP:OD1   | 1:H1:187:ASP:N    | 2.49                     | 0.46              |
| 1:H1:191:ILE:HG23  | 1:H1:212:LEU:HD12 | 1.97                     | 0.46              |
| 1:K1:193:ALA:HA    | 1:L1:219:LEU:HG   | 1.98                     | 0.46              |
| 1:K1:249:ILE:HD13  | 1:K1:419:ALA:HB3  | 1.98                     | 0.46              |
| 1:N1:190:GLN:NE2   | 1:O1:216:SER:O    | 2.46                     | 0.46              |
| 1:R1:186:LEU:HD11  | 1:R1:190:GLN:OE1  | 2.16                     | 0.46              |
| 1:S1:279:GLU:OE1   | 1:S1:281:HIS:HB2  | 2.16                     | 0.46              |
| 1:S1:382:ILE:HG21  | 1:S1:385:LEU:HG   | 1.98                     | 0.46              |
| 1:U1:197:LEU:HD12  | 1:W1:175:SER:HB2  | 1.97                     | 0.46              |
| 1:e1:237:PHE:HE1   | 1:f1:232:ASP:HA   | 1.80                     | 0.46              |
| 1:f1:416:THR:O     | 1:f1:420:MET:HG2  | 2.15                     | 0.46              |
| 2:B2:87:GLN:HB3    | 2:C2:60:MET:HE3   | 1.98                     | 0.46              |
| 3:F2:131:MET:HA    | 3:F2:134:MET:HB2  | 1.97                     | 0.46              |
| 7:a2:125:MET:HA    | 7:a2:128:LYS:HE3  | 1.98                     | 0.46              |
| 8:b2:70:GLN:CD     | 9:m2:3:SER:HB2    | 2.40                     | 0.46              |
| 8:e2:152:PRO:HB3   | 9:u2:51:GLN:NE2   | 2.30                     | 0.46              |
| 9:j2:175:LEU:HG    | 9:j2:206:PRO:HG3  | 1.98                     | 0.46              |
| 9:n2:175:LEU:HG    | 9:n2:206:PRO:HG3  | 1.96                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:p2:170:VAL:C     | 11:c3:53:THR:HG21  | 2.39                     | 0.46              |
| 9:u2:238:ARG:O     | 9:u2:242:ILE:HG12  | 2.16                     | 0.46              |
| 9:v2:26:LEU:HD23   | 9:v2:26:LEU:HA     | 1.61                     | 0.46              |
| 9:x2:106:MET:HB2   | 9:x2:137:GLN:HE21  | 1.80                     | 0.46              |
| 9:y2:35:LYS:NZ     | 9:y2:82:SER:O      | 2.37                     | 0.46              |
| 10:A3:71:PRO:HD3   | 10:A3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:D3:71:PRO:HD2   | 10:D3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:D3:74:ILE:CD1   | 10:D3:154:GLN:HA   | 2.45                     | 0.46              |
| 10:I3:71:PRO:HD3   | 10:I3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:K3:71:PRO:HD2   | 10:K3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:L3:41:PRO:HA    | 10:N3:157:ALA:HB1  | 1.96                     | 0.46              |
| 10:O3:74:ILE:CD1   | 10:O3:154:GLN:HA   | 2.46                     | 0.46              |
| 10:U3:223:GLN:HB2  | 10:V3:232:MET:HG3  | 1.98                     | 0.46              |
| 10:W3:71:PRO:HD3   | 10:W3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:Z3:40:ILE:H     | 10:Z3:40:ILE:HG12  | 1.48                     | 0.46              |
| 11:a3:79:MET:HE2   | 11:b3:57:PHE:CD2   | 2.50                     | 0.46              |
| 11:e3:277:GLN:HG3  | 11:e3:278:GLY:N    | 2.30                     | 0.46              |
| 11:f3:254:VAL:HG13 | 11:f3:365:ILE:CG1  | 2.46                     | 0.46              |
| 11:g3:101:GLN:NE2  | 11:h3:188:GLN:HB3  | 2.31                     | 0.46              |
| 11:j3:328:LEU:HD21 | 11:k3:273:CYS:HA   | 1.98                     | 0.46              |
| 11:q3:361:LYS:HG3  | 11:q3:361:LYS:O    | 2.15                     | 0.46              |
| 11:s3:254:VAL:HG13 | 11:s3:365:ILE:CG1  | 2.46                     | 0.46              |
| 11:t3:254:VAL:HG13 | 11:t3:365:ILE:CG1  | 2.46                     | 0.46              |
| 11:u3:204:ILE:HG21 | 11:u3:213:ALA:HB2  | 1.98                     | 0.46              |
| 11:v3:204:ILE:HG21 | 11:v3:213:ALA:HB2  | 1.97                     | 0.46              |
| 11:w3:117:ARG:NH1  | 11:w3:145:GLY:HA2  | 2.30                     | 0.46              |
| 11:x3:101:GLN:NE2  | 11:y3:188:GLN:HB3  | 2.29                     | 0.46              |
| 11:x3:361:LYS:HG3  | 11:x3:361:LYS:O    | 2.15                     | 0.46              |
| 11:y3:284:VAL:CG2  | 11:y3:316:GLY:HA2  | 2.46                     | 0.46              |
| 12:A4:86:ASP:OD1   | 12:A4:213:ASN:ND2  | 2.48                     | 0.46              |
| 12:B4:94:THR:HG22  | 12:C4:231:ILE:HG21 | 1.97                     | 0.46              |
| 12:B4:215:LEU:HD11 | 12:B4:225:LEU:HG   | 1.97                     | 0.46              |
| 1:A1:393:TYR:CE2   | 1:A1:436:PRO:HD3   | 2.51                     | 0.46              |
| 1:B1:372:ILE:O     | 1:C1:277:GLN:HA    | 2.16                     | 0.46              |
| 1:F1:247:ARG:NH1   | 1:F1:247:ARG:HB2   | 2.31                     | 0.46              |
| 1:F1:279:GLU:OE2   | 1:F1:281:HIS:N     | 2.38                     | 0.46              |
| 1:G1:202:VAL:HB    | 1:G1:205:LEU:HD22  | 1.97                     | 0.46              |
| 1:H1:174:ALA:O     | 1:H1:210:VAL:HA    | 2.15                     | 0.46              |
| 1:H1:413:GLU:OE1   | 1:H1:417:ARG:NH1   | 2.49                     | 0.46              |
| 1:J1:256:ILE:HD12  | 1:K1:435:SER:OG    | 2.16                     | 0.46              |
| 1:K1:167:ARG:HD2   | 2:A2:245:SER:C     | 2.39                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L1:151:LYS:HZ1   | 1:L1:179:THR:HG22  | 1.79                     | 0.46              |
| 1:L1:244:ARG:HH22  | 1:M1:239:ASN:CB    | 2.20                     | 0.46              |
| 1:M1:411:GLN:O     | 1:M1:415:LEU:HD23  | 2.16                     | 0.46              |
| 1:P1:258:GLY:HA3   | 1:P1:261:ASN:HD22  | 1.81                     | 0.46              |
| 1:W1:382:ILE:HD13  | 1:W1:385:LEU:HD21  | 1.98                     | 0.46              |
| 1:Y1:262:VAL:HG23  | 1:Y1:391:VAL:HG12  | 1.98                     | 0.46              |
| 1:g1:186:LEU:HD12  | 1:g1:186:LEU:HA    | 1.78                     | 0.46              |
| 1:g1:212:LEU:HD23  | 1:g1:220:LEU:HD12  | 1.97                     | 0.46              |
| 1:h1:257:VAL:HG23  | 1:h1:261:ASN:HB2   | 1.98                     | 0.46              |
| 2:A2:220:PRO:HB2   | 2:B2:187:PHE:CD1   | 2.51                     | 0.46              |
| 2:B2:195:ILE:O     | 2:B2:199:VAL:HG12  | 2.16                     | 0.46              |
| 2:C2:64:PHE:HB2    | 2:C2:97:THR:HG21   | 1.98                     | 0.46              |
| 2:D2:227:VAL:HG13  | 2:D2:228:LEU:HD22  | 1.98                     | 0.46              |
| 5:N2:58:LYS:HG2    | 5:N2:66:ILE:HD13   | 1.98                     | 0.46              |
| 6:R2:16:LEU:HD13   | 6:R2:123:LEU:HD12  | 1.98                     | 0.46              |
| 6:R2:70:SER:OG     | 6:R2:71:HIS:N      | 2.49                     | 0.46              |
| 7:V2:131:THR:HA    | 7:V2:134:GLN:NE2   | 2.30                     | 0.46              |
| 7:X2:42:TYR:HB3    | 7:X2:94:PRO:HG3    | 1.98                     | 0.46              |
| 7:a2:72:ALA:HB3    | 7:a2:95:ASN:ND2    | 2.31                     | 0.46              |
| 8:d2:22:THR:O      | 8:d2:26:LEU:N      | 2.48                     | 0.46              |
| 8:e2:225:ARG:NE    | 8:e2:228:GLU:OE2   | 2.26                     | 0.46              |
| 8:f2:73:TYR:CD1    | 9:q2:73:ARG:HG3    | 2.50                     | 0.46              |
| 9:h2:9:LYS:HD3     | 9:h2:12:LEU:HD12   | 1.97                     | 0.46              |
| 9:n2:28:ASN:OD1    | 9:t2:72:VAL:HG22   | 2.16                     | 0.46              |
| 9:22:184:LEU:HB3   | 9:22:192:TYR:HB3   | 1.98                     | 0.46              |
| 9:32:184:LEU:HB3   | 9:32:192:TYR:HB3   | 1.98                     | 0.46              |
| 10:B3:71:PRO:HD2   | 10:B3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:B3:82:LEU:HD12  | 10:B3:146:GLY:HA3  | 1.98                     | 0.46              |
| 10:C3:223:GLN:HB2  | 10:D3:232:MET:HG3  | 1.98                     | 0.46              |
| 10:D3:71:PRO:HD3   | 10:D3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:H3:74:ILE:CD1   | 10:H3:154:GLN:HA   | 2.46                     | 0.46              |
| 10:L3:71:PRO:HD2   | 10:L3:189:ILE:HD13 | 1.98                     | 0.46              |
| 10:L3:71:PRO:HD3   | 10:L3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:M3:71:PRO:HD3   | 10:M3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:O3:41:PRO:HA    | 10:Q3:157:ALA:HB1  | 1.97                     | 0.46              |
| 10:P3:223:GLN:HB2  | 10:Q3:232:MET:HG3  | 1.98                     | 0.46              |
| 10:R3:82:LEU:HA    | 10:R3:197:SER:CB   | 2.39                     | 0.46              |
| 10:T3:71:PRO:HD3   | 10:T3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:V3:71:PRO:HD3   | 10:V3:193:ASN:OD1  | 2.16                     | 0.46              |
| 10:V3:82:LEU:HD12  | 10:V3:146:GLY:HA3  | 1.98                     | 0.46              |
| 11:a3:254:VAL:HG13 | 11:a3:365:ILE:CG1  | 2.46                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:a3:341:THR:OG1  | 11:a3:343:MET:HE2 | 2.15                     | 0.46              |
| 11:c3:340:ALA:HB1  | 11:c3:344:ASP:HB2 | 1.98                     | 0.46              |
| 11:d3:328:LEU:HD21 | 11:e3:273:CYS:HA  | 1.98                     | 0.46              |
| 11:d3:361:LYS:O    | 11:d3:361:LYS:HG3 | 2.15                     | 0.46              |
| 11:f3:117:ARG:NH1  | 11:f3:145:GLY:HA2 | 2.30                     | 0.46              |
| 11:f3:256:ASN:O    | 11:f3:257:SER:OG  | 2.30                     | 0.46              |
| 11:f3:341:THR:OG1  | 11:f3:343:MET:HE2 | 2.15                     | 0.46              |
| 11:g3:252:LYS:HE3  | 11:g3:252:LYS:HB2 | 1.52                     | 0.46              |
| 11:m3:101:GLN:NE2  | 11:n3:188:GLN:HB3 | 2.31                     | 0.46              |
| 11:o3:254:VAL:HG13 | 11:o3:365:ILE:CG1 | 2.46                     | 0.46              |
| 11:p3:328:LEU:HD21 | 11:q3:273:CYS:HA  | 1.98                     | 0.46              |
| 11:q3:254:VAL:HG13 | 11:q3:365:ILE:CG1 | 2.46                     | 0.46              |
| 11:r3:245:ASN:OD1  | 11:r3:245:ASN:N   | 2.32                     | 0.46              |
| 11:v3:328:LEU:HD21 | 11:w3:273:CYS:HA  | 1.98                     | 0.46              |
| 11:v3:340:ALA:HB1  | 11:v3:344:ASP:HB2 | 1.98                     | 0.46              |
| 11:w3:204:ILE:HG21 | 11:w3:213:ALA:HB2 | 1.97                     | 0.46              |
| 11:x3:340:ALA:HB1  | 11:x3:344:ASP:HB2 | 1.98                     | 0.46              |
| 11:x3:341:THR:OG1  | 11:x3:343:MET:HE2 | 2.15                     | 0.46              |
| 12:B4:102:MET:HA   | 12:B4:199:GLN:O   | 2.16                     | 0.46              |
| 12:D4:91:LEU:HD21  | 12:E4:91:LEU:HB3  | 1.98                     | 0.46              |
| 1:B1:393:TYR:HB3   | 1:B1:402:LEU:N    | 2.31                     | 0.45              |
| 1:C1:180:LEU:H     | 1:C1:215:GLN:CD   | 2.23                     | 0.45              |
| 1:F1:294:ARG:HD2   | 1:F1:294:ARG:HA   | 1.81                     | 0.45              |
| 1:I1:138:GLY:O     | 1:I1:142:ARG:HG2  | 2.16                     | 0.45              |
| 1:J1:423:SER:OG    | 1:J1:425:LYS:HG2  | 2.16                     | 0.45              |
| 1:L1:165:PHE:HD1   | 2:A2:143:ARG:HA   | 1.80                     | 0.45              |
| 1:L1:166:VAL:O     | 1:L1:166:VAL:HG12 | 2.16                     | 0.45              |
| 1:O1:141:ALA:O     | 1:O1:145:GLU:HG2  | 2.16                     | 0.45              |
| 1:O1:245:ILE:O     | 1:O1:249:ILE:HG12 | 2.16                     | 0.45              |
| 1:R1:160:PRO:HG3   | 1:R1:169:GLN:HG3  | 1.98                     | 0.45              |
| 1:S1:294:ARG:CG    | 6:R2:71:HIS:O     | 2.59                     | 0.45              |
| 1:U1:363:THR:HG21  | 6:R2:65:LEU:HD21  | 1.91                     | 0.45              |
| 1:Z1:295:SER:CB    | 6:S2:66:THR:H     | 2.29                     | 0.45              |
| 1:f1:143:THR:HG21  | 1:g1:156:HIS:NE2  | 2.31                     | 0.45              |
| 1:h1:165:PHE:O     | 1:h1:167:ARG:NH1  | 2.49                     | 0.45              |
| 2:A2:61:MET:SD     | 2:A2:171:LEU:HD11 | 2.56                     | 0.45              |
| 2:A2:143:ARG:HB2   | 2:A2:146:ASP:OD2  | 2.16                     | 0.45              |
| 4:I2:24:LEU:HD21   | 4:I2:62:ILE:HG13  | 1.98                     | 0.45              |
| 7:X2:77:VAL:O      | 7:X2:90:TYR:HA    | 2.15                     | 0.45              |
| 7:Y2:35:THR:OG1    | 7:Y2:39:GLY:HA2   | 2.16                     | 0.45              |
| 8:c2:202:MET:HE1   | 9:i2:189:GLU:HG3  | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:h2:167:PRO:HG3   | 9:x2:54:ALA:H      | 1.81                     | 0.45              |
| 9:m2:121:GLN:NE2   | 9:w2:63:PRO:HG2    | 2.31                     | 0.45              |
| 9:s2:86:LEU:HB3    | 9:s2:218:TYR:HD2   | 1.81                     | 0.45              |
| 9:t2:189:GLU:HA    | 9:y2:42:GLU:HG2    | 1.98                     | 0.45              |
| 9:u2:185:GLU:HB2   | 9:z2:52:PRO:HG2    | 1.98                     | 0.45              |
| 9:w2:105:VAL:CG1   | 9:w2:134:PHE:HB3   | 2.46                     | 0.45              |
| 9:w2:235:GLN:HB2   | 9:32:5:LEU:HD21    | 1.96                     | 0.45              |
| 9:12:56:SER:OG     | 9:12:57:SER:N      | 2.48                     | 0.45              |
| 9:32:238:ARG:HH22  | 12:B4:56:ASN:H     | 1.41                     | 0.45              |
| 9:42:10:THR:OG1    | 9:42:71:GLY:HA2    | 2.16                     | 0.45              |
| 10:A3:71:PRO:HD2   | 10:A3:189:ILE:HD13 | 1.98                     | 0.45              |
| 10:B3:71:PRO:HD3   | 10:B3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:D3:82:LEU:HA    | 10:D3:197:SER:CB   | 2.39                     | 0.45              |
| 10:E3:82:LEU:HD12  | 10:E3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:F3:74:ILE:CD1   | 10:F3:154:GLN:HA   | 2.46                     | 0.45              |
| 10:I3:41:PRO:HA    | 10:K3:157:ALA:HB1  | 1.97                     | 0.45              |
| 10:I3:74:ILE:CD1   | 10:I3:154:GLN:HA   | 2.46                     | 0.45              |
| 10:K3:82:LEU:HD12  | 10:K3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:L3:223:GLN:HB2  | 10:M3:232:MET:HG3  | 1.98                     | 0.45              |
| 10:N3:41:PRO:HA    | 10:P3:157:ALA:HB1  | 1.97                     | 0.45              |
| 10:S3:82:LEU:HD12  | 10:S3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:W3:219:MET:HE2  | 10:Y3:132:PHE:CB   | 2.46                     | 0.45              |
| 11:c3:284:VAL:CG2  | 11:c3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:d3:117:ARG:NH1  | 11:d3:145:GLY:HA2  | 2.30                     | 0.45              |
| 11:g3:361:LYS:O    | 11:g3:361:LYS:HG3  | 2.15                     | 0.45              |
| 11:n3:83:ASN:ND2   | 11:o3:109:SER:OG   | 2.47                     | 0.45              |
| 11:n3:361:LYS:O    | 11:n3:361:LYS:HG3  | 2.15                     | 0.45              |
| 11:r3:328:LEU:HD21 | 11:s3:273:CYS:HA   | 1.98                     | 0.45              |
| 12:C4:133:ALA:HA   | 12:C4:188:ASN:HB3  | 1.98                     | 0.45              |
| 1:B1:151:LYS:HD3   | 1:B1:151:LYS:N     | 2.31                     | 0.45              |
| 1:C1:246:GLN:HE22  | 1:C1:250:GLU:CD    | 2.24                     | 0.45              |
| 1:I1:181:GLU:HB3   | 1:I1:184:ARG:NH2   | 2.32                     | 0.45              |
| 1:J1:253:LEU:O     | 1:J1:257:VAL:HG22  | 2.16                     | 0.45              |
| 1:N1:303:GLN:OE1   | 1:N1:303:GLN:N     | 2.48                     | 0.45              |
| 1:P1:419:ALA:O     | 1:Q1:267:THR:OG1   | 2.28                     | 0.45              |
| 1:U1:385:LEU:N     | 1:U1:428:ASP:OD2   | 2.20                     | 0.45              |
| 1:c1:394:LYS:HE3   | 1:c1:402:LEU:HD13  | 1.96                     | 0.45              |
| 1:f1:212:LEU:HG    | 1:f1:220:LEU:HD13  | 1.98                     | 0.45              |
| 1:g1:302:GLU:HA    | 1:g1:357:SER:O     | 2.16                     | 0.45              |
| 2:A2:98:PHE:HE2    | 2:B2:168:ARG:HD2   | 1.80                     | 0.45              |
| 2:A2:121:ILE:HG12  | 2:A2:125:GLU:CG    | 2.46                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:P2:76:GLN:CG     | 7:V2:123:LYS:HD3   | 2.47                     | 0.45              |
| 6:S2:118:MET:HE3   | 6:S2:118:MET:HB3   | 1.88                     | 0.45              |
| 7:W2:78:TYR:CZ     | 7:W2:80:PRO:HG3    | 2.51                     | 0.45              |
| 7:Y2:34:VAL:HG22   | 7:Y2:93:MET:HE1    | 1.98                     | 0.45              |
| 8:e2:60:SER:HB2    | 9:j2:64:SER:HB2    | 1.97                     | 0.45              |
| 9:g2:205:THR:HG23  | 9:g2:208:LEU:HB2   | 1.98                     | 0.45              |
| 9:m2:147:LEU:HD21  | 9:m2:162:GLN:HG3   | 1.98                     | 0.45              |
| 9:p2:26:LEU:HD23   | 9:p2:26:LEU:HA     | 1.80                     | 0.45              |
| 9:y2:238:ARG:O     | 9:y2:242:ILE:HG13  | 2.16                     | 0.45              |
| 9:12:194:GLU:CD    | 9:12:201:PRO:HD3   | 2.42                     | 0.45              |
| 9:42:237:GLN:CG    | 12:C4:58:LEU:HD22  | 2.39                     | 0.45              |
| 10:A3:82:LEU:HD12  | 10:A3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:L3:82:LEU:HD12  | 10:L3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:M3:71:PRO:HD2   | 10:M3:189:ILE:HD13 | 1.98                     | 0.45              |
| 10:N3:71:PRO:HD3   | 10:N3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:O3:71:PRO:HD3   | 10:O3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:O3:223:GLN:HB2  | 10:P3:232:MET:HG3  | 1.98                     | 0.45              |
| 11:a3:123:MET:HE1  | 11:a3:136:LEU:HB3  | 1.99                     | 0.45              |
| 11:a3:204:ILE:HG21 | 11:a3:213:ALA:HB2  | 1.98                     | 0.45              |
| 11:b3:204:ILE:HG21 | 11:b3:213:ALA:HB2  | 1.97                     | 0.45              |
| 11:d3:254:VAL:HG13 | 11:d3:365:ILE:CG1  | 2.46                     | 0.45              |
| 11:e3:284:VAL:CG2  | 11:e3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:e3:340:ALA:HB1  | 11:e3:344:ASP:HB2  | 1.99                     | 0.45              |
| 11:f3:23:ARG:NH1   | 11:g3:249:GLN:O    | 2.50                     | 0.45              |
| 11:h3:123:MET:CE   | 11:h3:136:LEU:HD22 | 2.38                     | 0.45              |
| 11:k3:284:VAL:CG2  | 11:k3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:k3:319:LEU:HD12 | 11:k3:319:LEU:HA   | 1.82                     | 0.45              |
| 11:l3:319:LEU:HD12 | 11:l3:319:LEU:HA   | 1.82                     | 0.45              |
| 11:o3:101:GLN:NE2  | 11:p3:188:GLN:HB3  | 2.31                     | 0.45              |
| 11:t3:340:ALA:HB1  | 11:t3:344:ASP:HB2  | 1.98                     | 0.45              |
| 11:u3:254:VAL:HG13 | 11:u3:365:ILE:CG1  | 2.46                     | 0.45              |
| 11:v3:252:LYS:HB2  | 11:v3:252:LYS:HE3  | 1.52                     | 0.45              |
| 11:z3:254:VAL:HG13 | 11:z3:365:ILE:CG1  | 2.46                     | 0.45              |
| 12:A4:132:PRO:HB3  | 12:A4:157:ARG:HA   | 1.98                     | 0.45              |
| 1:B1:424:ASP:OD2   | 1:B1:425:LYS:HG3   | 2.16                     | 0.45              |
| 1:E1:287:ASP:OD1   | 1:E1:289:SER:N     | 2.43                     | 0.45              |
| 1:G1:245:ILE:O     | 1:G1:249:ILE:HG12  | 2.16                     | 0.45              |
| 1:H1:164:LEU:HD21  | 2:B2:148:ALA:CA    | 2.47                     | 0.45              |
| 1:L1:377:MET:HA    | 1:M1:273:ALA:HB1   | 1.98                     | 0.45              |
| 1:N1:419:ALA:O     | 1:O1:267:THR:OG1   | 2.31                     | 0.45              |
| 1:O1:157:LEU:HD22  | 1:O1:202:VAL:HG21  | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:P1:231:ASN:O     | 1:P1:234:GLN:HG3   | 2.16                     | 0.45              |
| 1:T1:149:PRO:HA    | 1:T1:181:GLU:HG2   | 1.97                     | 0.45              |
| 1:e1:405:THR:HG23  | 1:e1:408:GLN:H     | 1.81                     | 0.45              |
| 2:A2:75:ARG:NH2    | 5:O2:104:VAL:O     | 2.49                     | 0.45              |
| 2:B2:100:ILE:HG21  | 2:B2:243:PHE:CD2   | 2.51                     | 0.45              |
| 3:F2:9:TRP:CD1     | 5:P2:34:PHE:CE1    | 3.04                     | 0.45              |
| 4:G2:42:THR:C      | 4:G2:44:ILE:H      | 2.25                     | 0.45              |
| 7:W2:116:ILE:HG21  | 8:b2:244:ALA:HA    | 1.99                     | 0.45              |
| 9:g2:38:ARG:NH2    | 9:g2:78:GLU:OE1    | 2.25                     | 0.45              |
| 9:g2:175:LEU:HG    | 9:g2:206:PRO:HG3   | 1.98                     | 0.45              |
| 9:l2:144:ALA:HA    | 9:q2:179:MET:SD    | 2.56                     | 0.45              |
| 9:m2:121:GLN:HE21  | 9:w2:63:PRO:HG2    | 1.82                     | 0.45              |
| 9:r2:125:ASN:HB3   | 11:l3:54:GLN:HE22  | 1.77                     | 0.45              |
| 9:t2:42:GLU:HB2    | 9:t2:75:VAL:HB     | 1.98                     | 0.45              |
| 9:u2:185:GLU:HG3   | 9:z2:67:GLN:OE1    | 2.15                     | 0.45              |
| 9:w2:72:VAL:O      | 9:w2:72:VAL:HG12   | 2.15                     | 0.45              |
| 10:C3:71:PRO:HD3   | 10:C3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:F3:71:PRO:HD3   | 10:F3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:F3:82:LEU:HD12  | 10:F3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:F3:223:GLN:HB2  | 10:G3:232:MET:HG3  | 1.98                     | 0.45              |
| 10:G3:74:ILE:CD1   | 10:G3:154:GLN:HA   | 2.45                     | 0.45              |
| 10:J3:82:LEU:HD12  | 10:J3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:K3:71:PRO:HD3   | 10:K3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:Z3:71:PRO:HD2   | 10:Z3:189:ILE:HD13 | 1.98                     | 0.45              |
| 11:a3:340:ALA:HB1  | 11:a3:344:ASP:HB2  | 1.99                     | 0.45              |
| 11:e3:254:VAL:HG13 | 11:e3:365:ILE:CG1  | 2.46                     | 0.45              |
| 11:f3:361:LYS:HG3  | 11:f3:361:LYS:O    | 2.15                     | 0.45              |
| 11:i3:284:VAL:CG2  | 11:i3:316:GLY:HA2  | 2.45                     | 0.45              |
| 11:j3:204:ILE:HG21 | 11:j3:213:ALA:HB2  | 1.98                     | 0.45              |
| 11:o3:361:LYS:O    | 11:o3:361:LYS:HG3  | 2.15                     | 0.45              |
| 11:q3:284:VAL:CG2  | 11:q3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:v3:123:MET:HE1  | 11:v3:136:LEU:HB3  | 1.99                     | 0.45              |
| 11:w3:361:LYS:O    | 11:w3:361:LYS:HG3  | 2.15                     | 0.45              |
| 11:x3:204:ILE:HG21 | 11:x3:213:ALA:HB2  | 1.97                     | 0.45              |
| 12:A4:102:MET:HE1  | 12:A4:232:ILE:HG12 | 1.98                     | 0.45              |
| 12:A4:104:PRO:HA   | 12:A4:198:LEU:HD23 | 1.98                     | 0.45              |
| 12:A4:127:VAL:HG12 | 12:A4:163:PHE:HE2  | 1.81                     | 0.45              |
| 12:C4:156:LEU:HD22 | 12:C4:161:HIS:CG   | 2.51                     | 0.45              |
| 1:A1:267:THR:HG22  | 1:h1:248:ARG:NH1   | 2.20                     | 0.45              |
| 1:D1:267:THR:HB    | 1:D1:386:SER:HB2   | 1.99                     | 0.45              |
| 1:H1:404:LEU:HD23  | 1:H1:408:GLN:HG2   | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:J1:246:GLN:HG2   | 1:J1:264:ALA:HB3   | 1.98                     | 0.45              |
| 1:N1:411:GLN:O     | 1:N1:415:LEU:HG    | 2.16                     | 0.45              |
| 1:Q1:243:SER:O     | 1:Q1:247:ARG:HG3   | 2.16                     | 0.45              |
| 1:c1:142:ARG:HB2   | 1:d1:154:ARG:HH12  | 1.81                     | 0.45              |
| 1:d1:199:SER:HB2   | 1:d1:207:PRO:HA    | 1.98                     | 0.45              |
| 1:h1:252:ILE:O     | 1:h1:255:PRO:HD2   | 2.16                     | 0.45              |
| 2:A2:75:ARG:NH2    | 2:A2:85:PRO:HB3    | 2.32                     | 0.45              |
| 2:C2:189:ILE:O     | 2:C2:192:PRO:HD2   | 2.16                     | 0.45              |
| 2:C2:230:ASP:OD2   | 2:C2:233:GLN:HB2   | 2.17                     | 0.45              |
| 5:M2:32:VAL:HG13   | 5:M2:33:SER:H      | 1.80                     | 0.45              |
| 7:X2:4:LEU:HB3     | 7:X2:7:PHE:HB2     | 1.98                     | 0.45              |
| 7:Z2:64:VAL:HG22   | 7:Z2:64:VAL:O      | 2.17                     | 0.45              |
| 8:c2:42:ARG:HH11   | 9:h2:64:SER:CB     | 2.28                     | 0.45              |
| 8:e2:222:ALA:HB1   | 9:k2:1:MET:HB3     | 1.98                     | 0.45              |
| 9:i2:98:LYS:CB     | 9:t2:45:LEU:HD21   | 2.45                     | 0.45              |
| 9:s2:128:LEU:HD12  | 9:s2:140:ILE:HD12  | 1.99                     | 0.45              |
| 9:x2:189:GLU:HA    | 9:32:42:GLU:HG2    | 1.98                     | 0.45              |
| 9:z2:86:LEU:HB3    | 9:z2:218:TYR:HD2   | 1.82                     | 0.45              |
| 9:12:50:ARG:HG3    | 9:12:66:LEU:HB3    | 1.99                     | 0.45              |
| 9:12:104:GLN:HG3   | 9:12:112:SER:OG    | 2.15                     | 0.45              |
| 9:42:51:GLN:HG3    | 9:42:53:GLY:H      | 1.81                     | 0.45              |
| 10:E3:74:ILE:CD1   | 10:E3:154:GLN:HA   | 2.46                     | 0.45              |
| 10:I3:223:GLN:HB2  | 10:J3:232:MET:HG3  | 1.98                     | 0.45              |
| 10:J3:41:PRO:HA    | 10:L3:157:ALA:HB1  | 1.97                     | 0.45              |
| 10:J3:71:PRO:HD3   | 10:J3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:L3:40:ILE:H     | 10:L3:40:ILE:HG12  | 1.48                     | 0.45              |
| 10:R3:71:PRO:HD3   | 10:R3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:S3:71:PRO:HD3   | 10:S3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:V3:124:MET:HE3  | 10:V3:124:MET:HB3  | 1.76                     | 0.45              |
| 11:h3:340:ALA:HB1  | 11:h3:344:ASP:HB2  | 1.98                     | 0.45              |
| 11:n3:284:VAL:CG2  | 11:n3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:r3:141:ILE:HD13 | 11:r3:165:ILE:CD1  | 2.38                     | 0.45              |
| 11:s3:123:MET:CE   | 11:s3:136:LEU:HD22 | 2.38                     | 0.45              |
| 11:s3:252:LYS:HB2  | 11:s3:252:LYS:HE3  | 1.52                     | 0.45              |
| 11:s3:284:VAL:CG2  | 11:s3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:u3:123:MET:HE1  | 11:u3:136:LEU:HB3  | 1.98                     | 0.45              |
| 11:u3:217:ASP:OD1  | 11:u3:219:ARG:N    | 2.37                     | 0.45              |
| 11:z3:123:MET:HE1  | 11:z3:136:LEU:HB3  | 1.99                     | 0.45              |
| 11:z3:204:ILE:HG21 | 11:z3:213:ALA:HB2  | 1.98                     | 0.45              |
| 12:A4:206:VAL:O    | 12:B4:230:GLN:HA   | 2.16                     | 0.45              |
| 12:D4:135:LYS:O    | 12:D4:135:LYS:HD3  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:E1:191:ILE:HD11 | 1:E1:220:LEU:HD22  | 1.98                     | 0.45              |
| 1:H1:417:ARG:HA   | 1:H1:420:MET:HE3   | 1.99                     | 0.45              |
| 1:K1:187:ASP:OD2  | 1:K1:190:GLN:HG3   | 2.17                     | 0.45              |
| 1:L1:150:VAL:HG13 | 1:L1:178:VAL:HG23  | 1.97                     | 0.45              |
| 1:M1:295:SER:OG   | 6:Q2:66:THR:HG23   | 2.16                     | 0.45              |
| 1:O1:293:LEU:HD23 | 1:O1:293:LEU:HA    | 1.70                     | 0.45              |
| 1:P1:404:LEU:H    | 1:P1:434:ASN:HD21  | 1.63                     | 0.45              |
| 1:Q1:394:LYS:CG   | 1:Q1:402:LEU:HB2   | 2.47                     | 0.45              |
| 1:T1:245:ILE:HG23 | 1:T1:266:VAL:HG21  | 1.97                     | 0.45              |
| 1:T1:409:MET:HE1  | 1:T1:434:ASN:HB2   | 1.97                     | 0.45              |
| 1:X1:252:ILE:O    | 1:X1:255:PRO:HD2   | 2.16                     | 0.45              |
| 1:X1:299:ASN:HB2  | 1:X1:361:ASN:HB2   | 1.97                     | 0.45              |
| 1:g1:147:LEU:HD12 | 1:g1:149:PRO:HD2   | 1.98                     | 0.45              |
| 2:C2:117:SER:O    | 2:C2:117:SER:OG    | 2.29                     | 0.45              |
| 2:C2:119:GLN:HE22 | 2:C2:120:LYS:NZ    | 2.13                     | 0.45              |
| 2:D2:163:GLU:CD   | 2:D2:163:GLU:H     | 2.24                     | 0.45              |
| 2:E2:91:GLY:HA3   | 3:F2:86:PHE:CZ     | 2.52                     | 0.45              |
| 5:K2:68:LEU:HD11  | 5:P2:84:MET:CE     | 2.47                     | 0.45              |
| 6:S2:22:ARG:HB3   | 6:S2:112:ASN:HD21  | 1.80                     | 0.45              |
| 7:W2:83:PRO:O     | 7:W2:84:LEU:HB2    | 2.16                     | 0.45              |
| 7:Z2:32:ASP:OD2   | 8:e2:226:ARG:NH1   | 2.49                     | 0.45              |
| 8:c2:2:ASP:O      | 8:c2:5:ILE:HG22    | 2.17                     | 0.45              |
| 8:f2:35:ARG:HD3   | 8:f2:35:ARG:HA     | 1.77                     | 0.45              |
| 9:k2:18:ASN:HB2   | 9:k2:41:PHE:HZ     | 1.79                     | 0.45              |
| 9:l2:189:GLU:HA   | 9:q2:42:GLU:OE2    | 2.16                     | 0.45              |
| 9:n2:163:GLY:HA2  | 9:z2:111:THR:HG21  | 1.98                     | 0.45              |
| 9:o2:156:VAL:HG23 | 9:o2:156:VAL:O     | 2.17                     | 0.45              |
| 9:p2:98:LYS:HD2   | 9:p2:213:LEU:HG    | 1.98                     | 0.45              |
| 9:q2:235:GLN:HG2  | 9:w2:5:LEU:HD23    | 1.99                     | 0.45              |
| 9:y2:72:VAL:O     | 9:y2:72:VAL:HG12   | 2.15                     | 0.45              |
| 9:12:29:VAL:O     | 9:12:30:SER:OG     | 2.29                     | 0.45              |
| 10:C3:50:SER:HB3  | 11:d3:99:GLN:HE21  | 1.82                     | 0.45              |
| 10:K3:90:LYS:CE   | 10:K3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:N3:71:PRO:HD2  | 10:N3:189:ILE:HD13 | 1.98                     | 0.45              |
| 10:R3:101:LYS:HB2 | 10:R3:101:LYS:NZ   | 2.32                     | 0.45              |
| 10:U3:50:SER:HB3  | 11:v3:99:GLN:HE21  | 1.82                     | 0.45              |
| 10:W3:50:SER:HB3  | 11:x3:99:GLN:HE21  | 1.81                     | 0.45              |
| 10:W3:82:LEU:HD12 | 10:W3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:Y3:54:SER:HB2  | 11:z3:173:ARG:HH12 | 1.80                     | 0.45              |
| 11:a3:23:ARG:NH1  | 11:b3:249:GLN:O    | 2.50                     | 0.45              |
| 11:b3:123:MET:HE1 | 11:b3:136:LEU:HB3  | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:g3:204:ILE:HG21 | 11:g3:213:ALA:HB2  | 1.98                     | 0.45              |
| 11:h3:204:ILE:HG21 | 11:h3:213:ALA:HB2  | 1.97                     | 0.45              |
| 11:i3:141:ILE:HD13 | 11:i3:165:ILE:CD1  | 2.38                     | 0.45              |
| 11:j3:319:LEU:HD12 | 11:j3:319:LEU:HA   | 1.82                     | 0.45              |
| 11:o3:284:VAL:CG2  | 11:o3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:t3:284:VAL:CG2  | 11:t3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:v3:284:VAL:CG2  | 11:v3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:w3:123:MET:HE1  | 11:w3:136:LEU:HB3  | 1.99                     | 0.45              |
| 11:y3:254:VAL:HG13 | 11:y3:365:ILE:CG1  | 2.46                     | 0.45              |
| 11:z3:340:ALA:HB1  | 11:z3:344:ASP:HB2  | 1.98                     | 0.45              |
| 12:A4:169:GLN:HB3  | 12:A4:175:VAL:HG12 | 1.99                     | 0.45              |
| 1:A1:377:MET:HA    | 1:A1:377:MET:HE3   | 1.98                     | 0.45              |
| 1:B1:150:VAL:HG22  | 1:B1:178:VAL:HG21  | 1.99                     | 0.45              |
| 1:C1:166:VAL:H     | 2:C2:152:ARG:CZ    | 2.25                     | 0.45              |
| 1:C1:404:LEU:HD13  | 1:C1:434:ASN:HD21  | 1.81                     | 0.45              |
| 1:F1:253:LEU:HD11  | 1:F1:412:ILE:HG23  | 1.97                     | 0.45              |
| 1:H1:143:THR:HG22  | 1:I1:154:ARG:NE    | 2.32                     | 0.45              |
| 1:H1:191:ILE:HD11  | 1:H1:220:LEU:HD13  | 1.99                     | 0.45              |
| 1:I1:280:GLU:HG3   | 1:I1:372:ILE:CD1   | 2.47                     | 0.45              |
| 1:L1:244:ARG:HA    | 1:L1:247:ARG:NH1   | 2.31                     | 0.45              |
| 1:P1:269:GLN:O     | 1:P1:382:ILE:HD12  | 2.16                     | 0.45              |
| 1:R1:294:ARG:NE    | 1:R1:367:GLU:OE1   | 2.47                     | 0.45              |
| 1:U1:187:ASP:O     | 1:U1:191:ILE:N     | 2.46                     | 0.45              |
| 1:X1:218:HIS:O     | 1:X1:220:LEU:N     | 2.49                     | 0.45              |
| 1:Y1:435:SER:HB2   | 1:Y1:436:PRO:HD2   | 1.99                     | 0.45              |
| 1:g1:246:GLN:O     | 1:g1:250:GLU:HG2   | 2.16                     | 0.45              |
| 2:C2:66:ARG:NE     | 2:C2:178:GLU:OE2   | 2.48                     | 0.45              |
| 2:C2:207:LEU:HD21  | 4:I2:58:VAL:HG11   | 1.99                     | 0.45              |
| 2:C2:211:MET:O     | 3:F2:114:VAL:HG21  | 2.17                     | 0.45              |
| 6:Q2:92:GLN:O      | 8:b2:54:ARG:NH1    | 2.50                     | 0.45              |
| 8:e2:49:LEU:HA     | 8:e2:49:LEU:HD23   | 1.84                     | 0.45              |
| 9:j2:254:LEU:O     | 9:j2:258:THR:HG23  | 2.17                     | 0.45              |
| 9:k2:185:GLU:HB2   | 9:k2:195:THR:CG2   | 2.46                     | 0.45              |
| 9:q2:27:ALA:C      | 9:v2:72:VAL:HG21   | 2.42                     | 0.45              |
| 9:r2:38:ARG:NH2    | 9:r2:40:VAL:HG22   | 2.32                     | 0.45              |
| 9:y2:2:ILE:HD13    | 9:y2:2:ILE:HA      | 1.84                     | 0.45              |
| 9:y2:122:VAL:HG21  | 9:42:179:MET:HE3   | 1.98                     | 0.45              |
| 9:32:23:ALA:CB     | 12:B4:45:LYS:HG3   | 2.45                     | 0.45              |
| 9:42:238:ARG:NE    | 12:C4:55:ASN:CB    | 2.57                     | 0.45              |
| 10:A3:74:ILE:CD1   | 10:A3:154:GLN:HA   | 2.46                     | 0.45              |
| 10:C3:74:ILE:CD1   | 10:C3:154:GLN:HA   | 2.45                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:F3:101:LYS:HB2  | 10:F3:101:LYS:NZ   | 2.32                     | 0.45              |
| 10:G3:71:PRO:HD3   | 10:G3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:I3:90:LYS:CE    | 10:I3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:M3:82:LEU:HD12  | 10:M3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:M3:90:LYS:CE    | 10:M3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:Q3:50:SER:HB3   | 11:r3:99:GLN:HE21  | 1.81                     | 0.45              |
| 10:S3:82:LEU:HA    | 10:S3:197:SER:CB   | 2.39                     | 0.45              |
| 10:U3:71:PRO:HD3   | 10:U3:193:ASN:OD1  | 2.16                     | 0.45              |
| 10:Y3:37:ALA:HB1   | 10:Z3:74:ILE:CG2   | 2.47                     | 0.45              |
| 10:Y3:71:PRO:HD2   | 10:Y3:189:ILE:HD13 | 1.98                     | 0.45              |
| 10:Y3:74:ILE:HD13  | 10:Y3:154:GLN:HA   | 1.99                     | 0.45              |
| 11:f3:252:LYS:HB2  | 11:f3:252:LYS:HE3  | 1.52                     | 0.45              |
| 11:h3:252:LYS:HB2  | 11:h3:252:LYS:HE3  | 1.52                     | 0.45              |
| 11:i3:204:ILE:HG21 | 11:i3:213:ALA:HB2  | 1.98                     | 0.45              |
| 11:j3:141:ILE:HD13 | 11:j3:165:ILE:CD1  | 2.38                     | 0.45              |
| 11:m3:319:LEU:HD12 | 11:m3:319:LEU:HA   | 1.82                     | 0.45              |
| 11:n3:328:LEU:HD21 | 11:o3:273:CYS:HA   | 1.99                     | 0.45              |
| 11:p3:361:LYS:HG3  | 11:p3:361:LYS:O    | 2.15                     | 0.45              |
| 11:s3:340:ALA:HB1  | 11:s3:344:ASP:HB2  | 1.99                     | 0.45              |
| 11:x3:277:GLN:HG3  | 11:x3:278:GLY:N    | 2.30                     | 0.45              |
| 11:z3:114:LYS:HA   | 11:z3:114:LYS:HD2  | 1.77                     | 0.45              |
| 1:C1:125:GLN:O     | 1:C1:128:GLU:HG2   | 2.16                     | 0.45              |
| 1:D1:295:SER:CB    | 6:U2:71:HIS:O      | 2.64                     | 0.45              |
| 1:E1:160:PRO:HG2   | 1:E1:170:LYS:O     | 2.17                     | 0.45              |
| 1:G1:199:SER:OG    | 1:G1:205:LEU:O     | 2.31                     | 0.45              |
| 1:L1:418:GLU:HB3   | 1:M1:388:ALA:HB2   | 1.99                     | 0.45              |
| 1:O1:143:THR:HG22  | 1:Q1:154:ARG:HD3   | 1.99                     | 0.45              |
| 1:S1:407:ASP:HA    | 1:S1:410:LYS:HG2   | 1.99                     | 0.45              |
| 1:W1:186:LEU:HD12  | 1:W1:186:LEU:HA    | 1.81                     | 0.45              |
| 1:W1:420:MET:HG3   | 1:W1:422:PHE:N     | 2.31                     | 0.45              |
| 1:X1:142:ARG:HB2   | 1:Y1:154:ARG:HH22  | 1.81                     | 0.45              |
| 1:Y1:410:LYS:HD2   | 1:Y1:411:GLN:N     | 2.32                     | 0.45              |
| 1:c1:237:PHE:HE1   | 1:d1:232:ASP:HA    | 1.82                     | 0.45              |
| 1:h1:237:PHE:HA    | 1:h1:240:ASP:OD1   | 2.17                     | 0.45              |
| 2:A2:210:MET:HG2   | 2:B2:211:MET:HB3   | 1.99                     | 0.45              |
| 2:B2:235:LEU:HD12  | 2:B2:235:LEU:HA    | 1.68                     | 0.45              |
| 3:F2:39:PRO:HG2    | 3:F2:42:VAL:HG23   | 1.99                     | 0.45              |
| 5:N2:58:LYS:HG3    | 5:N2:63:GLU:HG3    | 1.98                     | 0.45              |
| 5:O2:92:LEU:HD23   | 5:O2:92:LEU:HA     | 1.78                     | 0.45              |
| 7:Y2:83:PRO:O      | 7:Y2:84:LEU:HB2    | 2.17                     | 0.45              |
| 7:Z2:75:LYS:HA     | 9:k2:47:GLN:CD     | 2.42                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:a2:131:THR:HA    | 7:a2:134:GLN:NE2   | 2.32                     | 0.45              |
| 8:d2:57:VAL:O      | 8:d2:57:VAL:HG12   | 2.16                     | 0.45              |
| 9:k2:185:GLU:HB3   | 9:k2:193:ILE:HG13  | 1.97                     | 0.45              |
| 9:l2:129:VAL:HG21  | 9:v2:63:PRO:HG3    | 1.99                     | 0.45              |
| 9:l2:238:ARG:HD3   | 9:l2:238:ARG:HA    | 1.67                     | 0.45              |
| 9:o2:255:GLN:O     | 9:o2:259:GLN:HG2   | 2.17                     | 0.45              |
| 9:r2:181:ASP:O     | 9:r2:184:LEU:HD23  | 2.17                     | 0.45              |
| 9:u2:118:GLY:O     | 9:u2:120:PHE:N     | 2.48                     | 0.45              |
| 9:22:233:MET:SD    | 12:A4:58:LEU:CD1   | 3.02                     | 0.45              |
| 9:32:238:ARG:CD    | 12:C4:46:ASN:O     | 2.65                     | 0.45              |
| 10:B3:74:ILE:HD13  | 10:B3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:C3:74:ILE:HD13  | 10:C3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:K3:41:PRO:HA    | 10:M3:157:ALA:HB1  | 1.97                     | 0.45              |
| 10:O3:71:PRO:HD2   | 10:O3:189:ILE:HD13 | 1.98                     | 0.45              |
| 10:O3:82:LEU:HD12  | 10:O3:146:GLY:HA3  | 1.98                     | 0.45              |
| 10:Q3:101:LYS:HB2  | 10:Q3:101:LYS:NZ   | 2.32                     | 0.45              |
| 10:R3:90:LYS:CE    | 10:R3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:T3:90:LYS:CE    | 10:T3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:X3:74:ILE:HD13  | 10:X3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:X3:82:LEU:O     | 10:X3:197:SER:OG   | 2.20                     | 0.45              |
| 10:Z3:74:ILE:HD13  | 10:Z3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:Z3:82:LEU:HD12  | 10:Z3:146:GLY:HA3  | 1.98                     | 0.45              |
| 11:c3:204:ILE:HG21 | 11:c3:213:ALA:HB2  | 1.98                     | 0.45              |
| 11:e3:361:LYS:HG3  | 11:e3:361:LYS:O    | 2.15                     | 0.45              |
| 11:f3:204:ILE:HG21 | 11:f3:213:ALA:HB2  | 1.98                     | 0.45              |
| 11:f3:217:ASP:OD1  | 11:f3:219:ARG:N    | 2.37                     | 0.45              |
| 11:f3:340:ALA:HB1  | 11:f3:344:ASP:HB2  | 1.99                     | 0.45              |
| 11:g3:340:ALA:HB1  | 11:g3:344:ASP:HB2  | 1.99                     | 0.45              |
| 11:i3:319:LEU:HD12 | 11:i3:319:LEU:HA   | 1.82                     | 0.45              |
| 11:j3:340:ALA:HB1  | 11:j3:344:ASP:HB2  | 1.98                     | 0.45              |
| 11:p3:284:VAL:CG2  | 11:p3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:q3:340:ALA:HB1  | 11:q3:344:ASP:HB2  | 1.98                     | 0.45              |
| 11:r3:340:ALA:HB1  | 11:r3:344:ASP:HB2  | 1.98                     | 0.45              |
| 11:t3:328:LEU:HD21 | 11:u3:273:CYS:HA   | 1.99                     | 0.45              |
| 11:u3:340:ALA:HB1  | 11:u3:344:ASP:HB2  | 1.98                     | 0.45              |
| 11:y3:204:ILE:HG21 | 11:y3:213:ALA:HB2  | 1.97                     | 0.45              |
| 11:z3:252:LYS:HB2  | 11:z3:252:LYS:HE3  | 1.52                     | 0.45              |
| 12:C4:176:PRO:O    | 12:C4:180:TYR:OH   | 2.24                     | 0.45              |
| 1:C1:254:SER:HB2   | 1:C1:255:PRO:HD3   | 1.99                     | 0.45              |
| 1:D1:409:MET:SD    | 1:D1:434:ASN:HB2   | 2.57                     | 0.45              |
| 1:H1:298:LEU:HD13  | 1:H1:362:GLU:HB3   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:K1:147:LEU:O     | 1:K1:149:PRO:HD2  | 2.16                     | 0.45              |
| 1:N1:268:ALA:HB1   | 1:N1:382:ILE:HD13 | 1.98                     | 0.45              |
| 1:O1:250:GLU:O     | 1:O1:254:SER:OG   | 2.27                     | 0.45              |
| 1:U1:368:VAL:HG22  | 1:U1:369:ASP:O    | 2.17                     | 0.45              |
| 2:E2:82:SER:HB3    | 3:F2:97:THR:HG23  | 1.98                     | 0.45              |
| 2:E2:137:PHE:CZ    | 2:E2:243:PHE:HE2  | 2.34                     | 0.45              |
| 3:F2:41:ARG:NH1    | 5:O2:98:GLU:OE1   | 2.49                     | 0.45              |
| 7:V2:76:LEU:HD23   | 7:V2:90:TYR:CG    | 2.52                     | 0.45              |
| 7:X2:23:VAL:HG21   | 7:X2:47:VAL:HG13  | 1.98                     | 0.45              |
| 7:Y2:75:LYS:HA     | 9:j2:47:GLN:HE22  | 1.81                     | 0.45              |
| 7:a2:72:ALA:C      | 7:a2:95:ASN:HD22  | 2.25                     | 0.45              |
| 8:b2:83:GLN:HG2    | 8:b2:84:GLN:N     | 2.32                     | 0.45              |
| 9:g2:184:LEU:HB3   | 9:g2:192:TYR:HB3  | 1.99                     | 0.45              |
| 9:k2:150:THR:HG21  | 9:12:54:ALA:HB1   | 1.99                     | 0.45              |
| 9:q2:167:PRO:HD3   | 9:22:196:GLN:HB2  | 1.99                     | 0.45              |
| 9:z2:127:GLN:HG3   | 9:z2:141:THR:HG22 | 1.98                     | 0.45              |
| 10:A3:74:ILE:HD13  | 10:A3:154:GLN:HA  | 1.99                     | 0.45              |
| 10:D3:90:LYS:CE    | 10:D3:138:ALA:HB3 | 2.47                     | 0.45              |
| 10:G3:74:ILE:HD13  | 10:G3:154:GLN:HA  | 1.99                     | 0.45              |
| 10:I3:50:SER:HB3   | 11:j3:99:GLN:HE21 | 1.82                     | 0.45              |
| 10:M3:149:THR:OG1  | 10:N3:198:THR:O   | 2.34                     | 0.45              |
| 10:P3:170:ALA:HB3  | 10:Q3:206:GLU:HG3 | 1.99                     | 0.45              |
| 10:Y3:101:LYS:HB2  | 10:Y3:101:LYS:NZ  | 2.32                     | 0.45              |
| 11:a3:57:PHE:CD2   | 11:z3:79:MET:HE2  | 2.50                     | 0.45              |
| 11:g3:31:VAL:HG12  | 11:g3:95:PRO:HG3  | 1.99                     | 0.45              |
| 11:h3:141:ILE:HD13 | 11:h3:165:ILE:CD1 | 2.38                     | 0.45              |
| 11:i3:57:PHE:CE1   | 11:i3:110:MET:HE2 | 2.52                     | 0.45              |
| 11:i3:254:VAL:HG13 | 11:i3:365:ILE:CG1 | 2.46                     | 0.45              |
| 11:i3:256:ASN:O    | 11:i3:257:SER:OG  | 2.30                     | 0.45              |
| 11:l3:359:ARG:HD2  | 11:l3:359:ARG:N   | 2.32                     | 0.45              |
| 11:m3:352:MET:O    | 11:m3:356:GLY:O   | 2.35                     | 0.45              |
| 11:n3:254:VAL:HG13 | 11:n3:365:ILE:CG1 | 2.46                     | 0.45              |
| 11:n3:359:ARG:N    | 11:n3:359:ARG:HD2 | 2.32                     | 0.45              |
| 11:s3:57:PHE:CE1   | 11:s3:110:MET:HE2 | 2.52                     | 0.45              |
| 11:v3:254:VAL:HG13 | 11:v3:365:ILE:CG1 | 2.46                     | 0.45              |
| 11:y3:340:ALA:HB1  | 11:y3:344:ASP:HB2 | 1.98                     | 0.45              |
| 12:A4:61:GLN:HB3   | 12:E4:62:LEU:HD23 | 1.97                     | 0.45              |
| 12:A4:196:GLN:NE2  | 12:A4:197:PRO:O   | 2.50                     | 0.45              |
| 1:A1:374:HIS:HB3   | 1:B1:276:GLU:HB3  | 1.99                     | 0.45              |
| 1:C1:166:VAL:HG13  | 1:C1:169:GLN:H    | 1.81                     | 0.45              |
| 1:C1:301:SER:HB3   | 1:C1:359:GLN:NE2  | 2.32                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E1:166:VAL:N     | 2:B2:244:TYR:CE2   | 2.62                     | 0.45              |
| 1:E1:246:GLN:O     | 1:E1:250:GLU:HG3   | 2.17                     | 0.45              |
| 1:E1:415:LEU:HD12  | 1:F1:431:ASN:ND2   | 2.32                     | 0.45              |
| 1:G1:287:ASP:HB3   | 1:G1:290:LYS:HG2   | 1.99                     | 0.45              |
| 1:I1:426:ARG:NE    | 1:I1:428:ASP:OD1   | 2.45                     | 0.45              |
| 1:M1:385:LEU:N     | 1:M1:428:ASP:OD2   | 2.43                     | 0.45              |
| 1:O1:299:ASN:HD22  | 1:O1:361:ASN:HD22  | 1.65                     | 0.45              |
| 1:P1:407:ASP:HA    | 1:P1:410:LYS:HG3   | 1.99                     | 0.45              |
| 1:S1:423:SER:HB3   | 1:S1:426:ARG:HB2   | 1.98                     | 0.45              |
| 1:T1:266:VAL:HG22  | 1:T1:387:VAL:HG22  | 1.98                     | 0.45              |
| 1:a1:385:LEU:HB2   | 1:a1:428:ASP:OD2   | 2.16                     | 0.45              |
| 1:d1:248:ARG:NH1   | 1:e1:267:THR:HG22  | 2.32                     | 0.45              |
| 1:e1:393:TYR:HB3   | 1:e1:402:LEU:N     | 2.32                     | 0.45              |
| 2:A2:210:MET:HE3   | 2:A2:210:MET:O     | 2.16                     | 0.45              |
| 3:F2:24:LEU:HB3    | 5:K2:89:ARG:HH21   | 1.81                     | 0.45              |
| 4:I2:39:GLN:O      | 4:I2:43:GLN:HA     | 2.17                     | 0.45              |
| 4:J2:21:ALA:HB1    | 4:J2:25:LEU:HD23   | 1.99                     | 0.45              |
| 7:a2:56:GLY:C      | 7:a2:58:ALA:H      | 2.23                     | 0.45              |
| 9:h2:9:LYS:HD3     | 9:h2:9:LYS:HA      | 1.71                     | 0.45              |
| 9:j2:25:ASN:HD21   | 9:j2:37:GLN:H      | 1.64                     | 0.45              |
| 9:t2:238:ARG:HD3   | 9:z2:254:LEU:HB3   | 1.99                     | 0.45              |
| 9:z2:56:SER:OG     | 9:z2:57:SER:N      | 2.49                     | 0.45              |
| 9:12:103:PHE:O     | 9:12:114:TYR:HA    | 2.17                     | 0.45              |
| 9:32:36:ARG:HH21   | 9:32:80:LEU:HD22   | 1.81                     | 0.45              |
| 9:42:151:ILE:HG12  | 9:42:157:VAL:HG23  | 1.97                     | 0.45              |
| 10:C3:90:LYS:CE    | 10:C3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:E3:90:LYS:CE    | 10:E3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:F3:74:ILE:HD13  | 10:F3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:H3:74:ILE:HD13  | 10:H3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:I3:74:ILE:HD13  | 10:I3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:O3:50:SER:HB3   | 11:p3:99:GLN:HE21  | 1.82                     | 0.45              |
| 10:O3:90:LYS:CE    | 10:O3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:P3:90:LYS:CE    | 10:P3:138:ALA:HB3  | 2.47                     | 0.45              |
| 10:W3:71:PRO:HD2   | 10:W3:189:ILE:HD13 | 1.98                     | 0.45              |
| 10:W3:74:ILE:HD13  | 10:W3:154:GLN:HA   | 1.99                     | 0.45              |
| 10:X3:50:SER:HB3   | 11:y3:99:GLN:HE21  | 1.82                     | 0.45              |
| 10:X3:71:PRO:HD2   | 10:X3:189:ILE:HD13 | 1.98                     | 0.45              |
| 11:a3:57:PHE:CE1   | 11:a3:110:MET:HE2  | 2.52                     | 0.45              |
| 11:b3:254:VAL:HG13 | 11:b3:365:ILE:CG1  | 2.46                     | 0.45              |
| 11:b3:328:LEU:HD21 | 11:c3:273:CYS:HA   | 1.99                     | 0.45              |
| 11:d3:340:ALA:HB1  | 11:d3:344:ASP:HB2  | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:e3:93:TYR:OH    | 11:e3:173:ARG:O    | 2.25                     | 0.45              |
| 11:g3:57:PHE:CE1   | 11:g3:110:MET:HE2  | 2.52                     | 0.45              |
| 11:h3:93:TYR:OH    | 11:h3:173:ARG:O    | 2.25                     | 0.45              |
| 11:i3:352:MET:O    | 11:i3:356:GLY:O    | 2.35                     | 0.45              |
| 11:j3:83:ASN:ND2   | 11:k3:109:SER:OG   | 2.45                     | 0.45              |
| 11:k3:254:VAL:HG13 | 11:k3:365:ILE:CG1  | 2.46                     | 0.45              |
| 11:k3:352:MET:O    | 11:k3:356:GLY:O    | 2.35                     | 0.45              |
| 11:m3:32:ARG:H     | 11:m3:95:PRO:HB3   | 1.82                     | 0.45              |
| 11:r3:284:VAL:CG2  | 11:r3:316:GLY:HA2  | 2.46                     | 0.45              |
| 11:s3:31:VAL:HG12  | 11:s3:95:PRO:HG3   | 1.99                     | 0.45              |
| 11:s3:359:ARG:N    | 11:s3:359:ARG:HD2  | 2.32                     | 0.45              |
| 11:u3:359:ARG:N    | 11:u3:359:ARG:HD2  | 2.32                     | 0.45              |
| 11:w3:328:LEU:HD21 | 11:x3:273:CYS:HA   | 1.99                     | 0.45              |
| 11:x3:32:ARG:H     | 11:x3:95:PRO:HB3   | 1.82                     | 0.45              |
| 11:y3:93:TYR:OH    | 11:y3:173:ARG:O    | 2.25                     | 0.45              |
| 11:y3:136:LEU:HD13 | 11:z3:129:VAL:HG11 | 1.99                     | 0.45              |
| 11:z3:217:ASP:OD1  | 11:z3:219:ARG:N    | 2.37                     | 0.45              |
| 1:H1:248:ARG:HD2   | 1:I1:267:THR:HG22  | 1.98                     | 0.45              |
| 1:R1:140:LEU:O     | 1:R1:144:ILE:HG12  | 2.16                     | 0.45              |
| 1:R1:186:LEU:HB3   | 1:R1:191:ILE:HD11  | 1.99                     | 0.45              |
| 1:R1:244:ARG:CZ    | 1:S1:235:LEU:HB3   | 2.46                     | 0.45              |
| 1:W1:250:GLU:O     | 1:W1:254:SER:OG    | 2.27                     | 0.45              |
| 1:X1:173:SER:HA    | 1:X1:209:ASN:HB3   | 1.97                     | 0.45              |
| 1:Z1:246:GLN:O     | 1:Z1:250:GLU:OE1   | 2.35                     | 0.45              |
| 1:f1:279:GLU:OE1   | 1:f1:281:HIS:HB2   | 2.17                     | 0.45              |
| 1:h1:133:GLN:NE2   | 1:h1:137:GLU:OE2   | 2.50                     | 0.45              |
| 2:A2:42:VAL:O      | 2:A2:45:LEU:HB2    | 2.16                     | 0.45              |
| 3:F2:204:LEU:HA    | 3:F2:207:MET:HE2   | 1.98                     | 0.45              |
| 5:O2:50:ALA:O      | 5:O2:54:VAL:HG23   | 2.17                     | 0.45              |
| 6:Q2:100:VAL:HG13  | 6:Q2:105:GLU:HG3   | 1.98                     | 0.45              |
| 6:S2:123:LEU:HD23  | 7:X2:132:LEU:HD21  | 1.98                     | 0.45              |
| 6:T2:118:MET:HA    | 7:Z2:130:LEU:HD11  | 1.99                     | 0.45              |
| 6:U2:102:MET:HE2   | 6:U2:102:MET:HA    | 1.97                     | 0.45              |
| 7:X2:28:LEU:HD11   | 8:c2:229:MET:CE    | 2.47                     | 0.45              |
| 7:a2:30:ASN:OD1    | 8:f2:55:THR:HG23   | 2.17                     | 0.45              |
| 8:c2:165:LYS:HB2   | 8:c2:196:ASP:OD1   | 2.17                     | 0.45              |
| 8:f2:76:ARG:O      | 8:f2:204:GLY:HA2   | 2.17                     | 0.45              |
| 9:h2:143:PRO:HD2   | 9:h2:159:VAL:HG11  | 1.99                     | 0.45              |
| 9:j2:150:THR:HG21  | 9:z2:54:ALA:HB1    | 1.99                     | 0.45              |
| 9:k2:129:VAL:HG21  | 9:u2:63:PRO:HG3    | 1.99                     | 0.45              |
| 9:k2:164:GLN:CG    | 11:e3:82:LYS:HZ3   | 2.30                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:n2:167:PRO:HD3   | 9:z2:196:GLN:HB3  | 1.99                     | 0.45              |
| 9:u2:36:ARG:HH12   | 9:u2:38:ARG:HB2   | 1.82                     | 0.45              |
| 9:w2:77:THR:HG23   | 9:22:66:LEU:HD13  | 1.99                     | 0.45              |
| 9:y2:239:ALA:HA    | 9:y2:242:ILE:HD12 | 1.98                     | 0.45              |
| 9:12:130:THR:O     | 9:12:134:PHE:HD2  | 2.00                     | 0.45              |
| 9:32:237:GLN:NE2   | 12:B4:52:PRO:HB2  | 2.31                     | 0.45              |
| 9:42:94:ASP:HA     | 9:42:119:SER:HA   | 1.97                     | 0.45              |
| 10:B3:50:SER:HB3   | 11:c3:99:GLN:HE21 | 1.82                     | 0.45              |
| 10:D3:74:ILE:HD13  | 10:D3:154:GLN:HA  | 1.99                     | 0.45              |
| 10:E3:74:ILE:HD13  | 10:E3:154:GLN:HA  | 1.99                     | 0.45              |
| 10:H3:50:SER:HB3   | 11:i3:99:GLN:HE21 | 1.82                     | 0.45              |
| 10:I3:101:LYS:HB2  | 10:I3:101:LYS:NZ  | 2.32                     | 0.45              |
| 10:J3:74:ILE:HD13  | 10:J3:154:GLN:HA  | 1.99                     | 0.45              |
| 10:K3:82:LEU:HA    | 10:K3:197:SER:CB  | 2.39                     | 0.45              |
| 10:N3:82:LEU:HD12  | 10:N3:146:GLY:HA3 | 1.98                     | 0.45              |
| 10:U3:101:LYS:HB2  | 10:U3:101:LYS:NZ  | 2.32                     | 0.45              |
| 10:V3:74:ILE:HD13  | 10:V3:154:GLN:HA  | 1.99                     | 0.45              |
| 11:a3:101:GLN:NE2  | 11:b3:188:GLN:HB3 | 2.32                     | 0.45              |
| 11:a3:219:ARG:NH2  | 11:z3:94:PRO:HB2  | 2.31                     | 0.45              |
| 11:e3:204:ILE:HG21 | 11:e3:213:ALA:HB2 | 1.97                     | 0.45              |
| 11:f3:31:VAL:HG12  | 11:f3:95:PRO:HG3  | 1.99                     | 0.45              |
| 11:g3:352:MET:O    | 11:g3:356:GLY:O   | 2.35                     | 0.45              |
| 11:k3:123:MET:HE1  | 11:k3:136:LEU:HB3 | 1.99                     | 0.45              |
| 11:k3:141:ILE:HD13 | 11:k3:165:ILE:CD1 | 2.38                     | 0.45              |
| 11:l3:57:PHE:CE1   | 11:l3:110:MET:HE2 | 2.52                     | 0.45              |
| 11:n3:32:ARG:H     | 11:n3:95:PRO:HB3  | 1.82                     | 0.45              |
| 11:n3:319:LEU:HD12 | 11:n3:319:LEU:HA  | 1.82                     | 0.45              |
| 11:o3:32:ARG:H     | 11:o3:95:PRO:HB3  | 1.82                     | 0.45              |
| 11:q3:277:GLN:HG3  | 11:q3:278:GLY:N   | 2.30                     | 0.45              |
| 11:q3:328:LEU:HD21 | 11:r3:273:CYS:HA  | 1.99                     | 0.45              |
| 11:r3:192:GLU:HB2  | 11:r3:219:ARG:HB2 | 1.99                     | 0.45              |
| 11:u3:284:VAL:CG2  | 11:u3:316:GLY:HA2 | 2.46                     | 0.45              |
| 11:w3:31:VAL:HG12  | 11:w3:95:PRO:HG3  | 1.99                     | 0.45              |
| 11:y3:32:ARG:H     | 11:y3:95:PRO:HB3  | 1.82                     | 0.45              |
| 11:z3:57:PHE:CE1   | 11:z3:110:MET:HE2 | 2.52                     | 0.45              |
| 1:A1:267:THR:CG2   | 1:h1:248:ARG:HD2  | 2.47                     | 0.44              |
| 1:B1:404:LEU:H     | 1:B1:434:ASN:ND2  | 2.16                     | 0.44              |
| 1:C1:404:LEU:HD23  | 1:C1:408:GLN:HG2  | 1.99                     | 0.44              |
| 1:G1:200:SER:HB3   | 1:H1:175:SER:HB3  | 1.98                     | 0.44              |
| 1:H1:192:SER:O     | 1:H1:196:HIS:ND1  | 2.41                     | 0.44              |
| 1:I1:179:THR:HA    | 1:I1:215:GLN:HB3  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:J1:248:ARG:NH1  | 1:K1:267:THR:OG1   | 2.49                     | 0.44              |
| 1:J1:261:ASN:HB3  | 1:J1:392:ASN:HB3   | 1.98                     | 0.44              |
| 1:O1:200:SER:OG   | 1:Q1:173:SER:OG    | 2.35                     | 0.44              |
| 1:P1:413:GLU:HG3  | 1:P1:417:ARG:HH12  | 1.82                     | 0.44              |
| 1:Q1:128:GLU:HG2  | 1:Q1:129:GLN:OE1   | 2.17                     | 0.44              |
| 1:Q1:160:PRO:O    | 1:Q1:161:LYS:HB2   | 2.17                     | 0.44              |
| 1:Q1:161:LYS:NZ   | 3:F2:249:ASN:HD21  | 1.87                     | 0.44              |
| 1:R1:145:GLU:HG2  | 1:R1:152:SER:HA    | 1.99                     | 0.44              |
| 1:T1:137:GLU:OE1  | 1:T1:155:VAL:HG13  | 2.17                     | 0.44              |
| 1:U1:389:VAL:HB   | 1:U1:432:VAL:HG22  | 1.99                     | 0.44              |
| 1:V1:245:ILE:HG21 | 1:V1:266:VAL:HG11  | 1.99                     | 0.44              |
| 1:Y1:157:LEU:HD23 | 1:Y1:157:LEU:HA    | 1.79                     | 0.44              |
| 1:c1:393:TYR:HB3  | 1:c1:402:LEU:N     | 2.33                     | 0.44              |
| 1:d1:142:ARG:O    | 1:d1:146:THR:HG23  | 2.16                     | 0.44              |
| 1:h1:252:ILE:HG22 | 1:h1:253:LEU:HD23  | 1.98                     | 0.44              |
| 2:A2:66:ARG:NE    | 2:A2:178:GLU:OE2   | 2.49                     | 0.44              |
| 2:B2:189:ILE:O    | 2:B2:192:PRO:HD2   | 2.17                     | 0.44              |
| 2:D2:63:SER:O     | 2:D2:64:PHE:HB3    | 2.17                     | 0.44              |
| 2:E2:204:LEU:O    | 2:E2:209:MET:HB2   | 2.16                     | 0.44              |
| 4:G2:12:GLU:HA    | 4:G2:15:LYS:HG2    | 1.97                     | 0.44              |
| 7:X2:113:GLN:HB2  | 8:c2:243:ARG:HH11  | 1.80                     | 0.44              |
| 8:d2:35:ARG:HD2   | 8:d2:101:ARG:HD3   | 1.99                     | 0.44              |
| 8:d2:117:GLY:O    | 8:d2:118:HIS:CG    | 2.70                     | 0.44              |
| 9:h2:11:GLY:HA2   | 9:h2:72:VAL:HG21   | 1.99                     | 0.44              |
| 9:h2:130:THR:O    | 9:h2:130:THR:HG23  | 2.17                     | 0.44              |
| 9:j2:123:ASP:OD1  | 9:j2:123:ASP:N     | 2.49                     | 0.44              |
| 9:m2:26:LEU:HA    | 9:m2:26:LEU:HD23   | 1.81                     | 0.44              |
| 9:o2:11:GLY:HA2   | 9:o2:72:VAL:HG11   | 1.99                     | 0.44              |
| 9:o2:175:LEU:HD13 | 9:o2:206:PRO:HG3   | 1.98                     | 0.44              |
| 9:w2:238:ARG:HE   | 9:32:255:GLN:NE2   | 2.15                     | 0.44              |
| 9:32:98:LYS:O     | 9:32:212:GLY:CA    | 2.65                     | 0.44              |
| 9:32:237:GLN:HE22 | 12:B4:52:PRO:CB    | 2.30                     | 0.44              |
| 10:D3:50:SER:HB3  | 11:e3:99:GLN:HE21  | 1.82                     | 0.44              |
| 10:D3:170:ALA:HB3 | 10:E3:206:GLU:HG3  | 1.99                     | 0.44              |
| 10:F3:90:LYS:CE   | 10:F3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:K3:50:SER:HB3  | 11:l3:99:GLN:HE21  | 1.81                     | 0.44              |
| 10:R3:71:PRO:HD2  | 10:R3:189:ILE:HD13 | 1.98                     | 0.44              |
| 10:S3:71:PRO:HD2  | 10:S3:189:ILE:HD13 | 1.98                     | 0.44              |
| 10:T3:71:PRO:HD2  | 10:T3:189:ILE:HD13 | 1.98                     | 0.44              |
| 10:T3:82:LEU:HA   | 10:T3:197:SER:CB   | 2.38                     | 0.44              |
| 10:V3:71:PRO:HD2  | 10:V3:189:ILE:HD13 | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:W3:90:LYS:CE    | 10:W3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:X3:82:LEU:HD12  | 10:X3:146:GLY:HA3  | 1.98                     | 0.44              |
| 10:X3:90:LYS:CE    | 10:X3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:X3:124:MET:HE3  | 10:X3:124:MET:HB3  | 1.77                     | 0.44              |
| 11:b3:57:PHE:CE1   | 11:b3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:b3:83:ASN:ND2   | 11:c3:109:SER:OG   | 2.47                     | 0.44              |
| 11:c3:123:MET:HE1  | 11:c3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:f3:352:MET:O    | 11:f3:356:GLY:O    | 2.35                     | 0.44              |
| 11:g3:254:VAL:HG13 | 11:g3:365:ILE:CG1  | 2.46                     | 0.44              |
| 11:h3:352:MET:O    | 11:h3:356:GLY:O    | 2.35                     | 0.44              |
| 11:i3:340:ALA:HB1  | 11:i3:344:ASP:HB2  | 1.99                     | 0.44              |
| 11:j3:352:MET:O    | 11:j3:356:GLY:O    | 2.35                     | 0.44              |
| 11:l3:32:ARG:H     | 11:l3:95:PRO:HB3   | 1.82                     | 0.44              |
| 11:l3:123:MET:HE1  | 11:l3:136:LEU:HB3  | 1.99                     | 0.44              |
| 11:l3:352:MET:O    | 11:l3:356:GLY:O    | 2.35                     | 0.44              |
| 11:n3:57:PHE:CE1   | 11:n3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:n3:123:MET:HE1  | 11:n3:136:LEU:HB3  | 1.99                     | 0.44              |
| 11:n3:352:MET:O    | 11:n3:356:GLY:O    | 2.35                     | 0.44              |
| 11:o3:352:MET:O    | 11:o3:356:GLY:O    | 2.35                     | 0.44              |
| 11:p3:57:PHE:CE1   | 11:p3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:p3:192:GLU:HB2  | 11:p3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:p3:340:ALA:HB1  | 11:p3:344:ASP:HB2  | 1.98                     | 0.44              |
| 11:p3:352:MET:O    | 11:p3:356:GLY:O    | 2.35                     | 0.44              |
| 11:q3:114:LYS:HD2  | 11:q3:114:LYS:HA   | 1.77                     | 0.44              |
| 11:q3:359:ARG:N    | 11:q3:359:ARG:HD2  | 2.32                     | 0.44              |
| 11:r3:31:VAL:HG12  | 11:r3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:r3:46:ASP:OD1   | 11:s3:160:LEU:HD12 | 2.17                     | 0.44              |
| 11:s3:83:ASN:ND2   | 11:t3:109:SER:OG   | 2.48                     | 0.44              |
| 11:t3:31:VAL:HG12  | 11:t3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:t3:123:MET:HE1  | 11:t3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:t3:192:GLU:HB2  | 11:t3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:u3:57:PHE:CE1   | 11:u3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:v3:31:VAL:HG12  | 11:v3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:w3:32:ARG:H     | 11:w3:95:PRO:HB3   | 1.83                     | 0.44              |
| 11:w3:254:VAL:HG13 | 11:w3:365:ILE:CG1  | 2.46                     | 0.44              |
| 11:w3:284:VAL:CG2  | 11:w3:316:GLY:HA2  | 2.46                     | 0.44              |
| 11:y3:123:MET:HE1  | 11:y3:136:LEU:HB3  | 1.99                     | 0.44              |
| 1:D1:387:VAL:HG21  | 1:D1:420:MET:HG3   | 1.99                     | 0.44              |
| 1:E1:126:PHE:HA    | 1:E1:129:GLN:NE2   | 2.32                     | 0.44              |
| 1:G1:180:LEU:HD13  | 1:G1:185:ALA:HA    | 1.98                     | 0.44              |
| 1:M1:235:LEU:HD23  | 1:M1:235:LEU:HA    | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S1:410:LYS:HA    | 1:S1:413:GLU:HG3   | 2.00                     | 0.44              |
| 1:T1:176:VAL:HG13  | 1:T1:212:LEU:HD13  | 1.99                     | 0.44              |
| 1:W1:302:GLU:HB3   | 1:W1:358:THR:HG23  | 1.99                     | 0.44              |
| 1:Y1:234:GLN:HG3   | 1:Y1:272:PHE:CZ    | 2.52                     | 0.44              |
| 1:Z1:244:ARG:NH2   | 1:a1:235:LEU:O     | 2.33                     | 0.44              |
| 1:d1:165:PHE:CZ    | 2:D2:144:GLU:HB3   | 2.19                     | 0.44              |
| 1:g1:157:LEU:HD12  | 1:g1:173:SER:O     | 2.16                     | 0.44              |
| 1:h1:242:GLU:HB3   | 1:h1:266:VAL:HB    | 1.98                     | 0.44              |
| 2:A2:79:GLY:HA3    | 2:A2:219:LEU:HD13  | 1.98                     | 0.44              |
| 2:A2:196:ILE:HD11  | 4:G2:73:LEU:HD21   | 1.99                     | 0.44              |
| 2:B2:121:ILE:HG12  | 2:B2:125:GLU:HG3   | 1.99                     | 0.44              |
| 7:V2:42:TYR:O      | 7:V2:94:PRO:HB3    | 2.18                     | 0.44              |
| 9:g2:19:MET:HG2    | 9:l2:253:MET:HE1   | 1.99                     | 0.44              |
| 9:h2:238:ARG:HD3   | 9:h2:238:ARG:HA    | 1.71                     | 0.44              |
| 9:j2:227:ALA:HA    | 9:u2:257:LEU:HD21  | 1.99                     | 0.44              |
| 9:o2:128:LEU:HD23  | 9:o2:136:VAL:HG21  | 1.99                     | 0.44              |
| 9:s2:56:SER:HB3    | 9:s2:62:LEU:HB2    | 1.98                     | 0.44              |
| 9:w2:154:ASP:OD1   | 9:w2:156:VAL:HG22  | 2.17                     | 0.44              |
| 9:12:129:VAL:HA    | 9:12:134:PHE:O     | 2.17                     | 0.44              |
| 10:A3:157:ALA:HB1  | 10:Y3:41:PRO:HA    | 1.99                     | 0.44              |
| 10:B3:90:LYS:CE    | 10:B3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:C3:124:MET:HE3  | 10:C3:124:MET:HB3  | 1.77                     | 0.44              |
| 10:E3:82:LEU:O     | 10:E3:197:SER:OG   | 2.20                     | 0.44              |
| 10:G3:82:LEU:HD12  | 10:G3:146:GLY:HA3  | 1.98                     | 0.44              |
| 10:M3:171:ILE:O    | 10:M3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:N3:90:LYS:CE    | 10:N3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:O3:171:ILE:O    | 10:O3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:P3:71:PRO:HD2   | 10:P3:189:ILE:HD13 | 1.98                     | 0.44              |
| 10:Q3:90:LYS:CE    | 10:Q3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:T3:170:ALA:HB3  | 10:U3:206:GLU:HG3  | 1.99                     | 0.44              |
| 10:V3:90:LYS:CE    | 10:V3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:V3:170:ALA:HB3  | 10:W3:206:GLU:HG3  | 1.99                     | 0.44              |
| 10:Y3:82:LEU:HD12  | 10:Y3:146:GLY:HA3  | 1.98                     | 0.44              |
| 11:c3:57:PHE:CE1   | 11:c3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:e3:34:ASN:HB2   | 11:e3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:f3:123:MET:HE1  | 11:f3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:h3:319:LEU:HD12 | 11:h3:319:LEU:HA   | 1.82                     | 0.44              |
| 11:h3:328:LEU:HD21 | 11:i3:273:CYS:HA   | 1.99                     | 0.44              |
| 11:i3:123:MET:HE1  | 11:i3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:j3:31:VAL:HG12  | 11:j3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:k3:31:VAL:HG12  | 11:k3:95:PRO:HG3   | 1.99                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:k3:57:PHE:CE1   | 11:k3:110:MET:HE2 | 2.52                     | 0.44              |
| 11:k3:328:LEU:HD21 | 11:l3:273:CYS:HA  | 1.99                     | 0.44              |
| 11:l3:328:LEU:HD21 | 11:m3:273:CYS:HA  | 2.00                     | 0.44              |
| 11:l3:340:ALA:HB1  | 11:l3:344:ASP:HB2 | 1.98                     | 0.44              |
| 11:o3:83:ASN:ND2   | 11:p3:109:SER:OG  | 2.47                     | 0.44              |
| 11:o3:340:ALA:HB1  | 11:o3:344:ASP:HB2 | 1.99                     | 0.44              |
| 11:q3:57:PHE:CE1   | 11:q3:110:MET:HE2 | 2.52                     | 0.44              |
| 11:u3:31:VAL:HG12  | 11:u3:95:PRO:HG3  | 1.99                     | 0.44              |
| 11:v3:32:ARG:H     | 11:v3:95:PRO:HB3  | 1.82                     | 0.44              |
| 11:x3:31:VAL:HG12  | 11:x3:95:PRO:HG3  | 1.99                     | 0.44              |
| 11:z3:32:ARG:H     | 11:z3:95:PRO:HB3  | 1.82                     | 0.44              |
| 12:D4:78:LEU:HA    | 12:D4:81:ILE:HG22 | 1.99                     | 0.44              |
| 1:B1:166:VAL:HG22  | 2:C2:162:PRO:HG3  | 1.99                     | 0.44              |
| 1:C1:165:PHE:CZ    | 2:C2:145:ALA:HB1  | 2.49                     | 0.44              |
| 1:F1:283:SER:HB2   | 1:F1:369:ASP:HB2  | 2.00                     | 0.44              |
| 1:L1:147:LEU:O     | 1:L1:149:PRO:HD2  | 2.18                     | 0.44              |
| 1:O1:159:MET:HE3   | 1:O1:159:MET:HB3  | 1.92                     | 0.44              |
| 1:P1:407:ASP:O     | 1:P1:410:LYS:HG3  | 2.17                     | 0.44              |
| 1:Q1:417:ARG:HG3   | 1:Q1:422:PHE:HB3  | 2.00                     | 0.44              |
| 1:W1:164:LEU:CA    | 2:E2:144:GLU:OE1  | 2.51                     | 0.44              |
| 1:a1:129:GLN:O     | 1:a1:133:GLN:HG2  | 2.17                     | 0.44              |
| 1:b1:256:ILE:HG22  | 1:b1:257:VAL:HG13 | 1.98                     | 0.44              |
| 1:h1:181:GLU:HB3   | 1:h1:184:ARG:NH2  | 2.29                     | 0.44              |
| 1:h1:416:THR:O     | 1:h1:420:MET:HG3  | 2.17                     | 0.44              |
| 2:A2:236:MET:HE2   | 2:B2:150:PHE:HZ   | 1.82                     | 0.44              |
| 2:B2:204:LEU:HD13  | 2:B2:212:VAL:HG13 | 1.98                     | 0.44              |
| 2:C2:137:PHE:HZ    | 2:C2:243:PHE:CE2  | 2.34                     | 0.44              |
| 2:C2:217:ILE:HG23  | 2:D2:194:LEU:HD11 | 2.00                     | 0.44              |
| 2:D2:140:ARG:NH1   | 2:D2:244:TYR:O    | 2.50                     | 0.44              |
| 2:E2:122:SER:O     | 2:E2:124:GLN:N    | 2.51                     | 0.44              |
| 3:F2:30:ALA:O      | 3:F2:34:SER:OG    | 2.20                     | 0.44              |
| 7:a2:42:TYR:HB3    | 7:a2:94:PRO:HG3   | 1.98                     | 0.44              |
| 8:b2:35:ARG:HD3    | 8:b2:35:ARG:HA    | 1.72                     | 0.44              |
| 8:f2:235:THR:HG23  | 9:k2:260:LEU:HD23 | 1.99                     | 0.44              |
| 9:h2:143:PRO:HG2   | 9:h2:159:VAL:HG21 | 1.98                     | 0.44              |
| 9:i2:146:ALA:HB1   | 9:i2:159:VAL:HB   | 1.99                     | 0.44              |
| 9:j2:98:LYS:HG3    | 9:u2:45:LEU:CD2   | 2.47                     | 0.44              |
| 9:j2:207:GLY:O     | 9:j2:208:LEU:HD23 | 2.17                     | 0.44              |
| 9:k2:113:ALA:CB    | 9:k2:191:LEU:HD23 | 2.45                     | 0.44              |
| 9:l2:44:LEU:HD13   | 9:l2:71:GLY:C     | 2.42                     | 0.44              |
| 9:o2:149:ILE:HG13  | 9:o2:159:VAL:HG12 | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:q2:86:LEU:HD11   | 9:22:45:LEU:HG     | 1.99                     | 0.44              |
| 9:s2:36:ARG:NH2    | 9:s2:80:LEU:HB2    | 2.33                     | 0.44              |
| 9:t2:145:ASN:OD1   | 9:t2:145:ASN:N     | 2.51                     | 0.44              |
| 9:u2:173:LEU:HD22  | 9:u2:214:LEU:HD21  | 1.99                     | 0.44              |
| 9:x2:233:MET:HB2   | 9:x2:233:MET:HE3   | 1.83                     | 0.44              |
| 9:32:104:GLN:HE21  | 9:32:112:SER:CB    | 2.30                     | 0.44              |
| 9:42:104:GLN:HG2   | 9:42:137:GLN:HB2   | 1.98                     | 0.44              |
| 10:G3:90:LYS:CE    | 10:G3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:G3:171:ILE:O    | 10:G3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:K3:40:ILE:H     | 10:K3:40:ILE:HG12  | 1.48                     | 0.44              |
| 10:K3:74:ILE:HD13  | 10:K3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:K3:171:ILE:O    | 10:K3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:L3:74:ILE:HD13  | 10:L3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:N3:50:SER:HB3   | 11:o3:99:GLN:HE21  | 1.82                     | 0.44              |
| 10:O3:74:ILE:HD13  | 10:O3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:O3:90:LYS:HE3   | 10:O3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:Q3:74:ILE:HD13  | 10:Q3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:Q3:170:ALA:HB3  | 10:R3:206:GLU:HG3  | 1.99                     | 0.44              |
| 10:Q3:171:ILE:O    | 10:Q3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:R3:170:ALA:HB3  | 10:S3:206:GLU:HG3  | 1.99                     | 0.44              |
| 10:S3:90:LYS:HE3   | 10:S3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:U3:90:LYS:CE    | 10:U3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:X3:223:GLN:HB2  | 10:Y3:232:MET:HG3  | 1.99                     | 0.44              |
| 11:a3:34:ASN:HB2   | 11:a3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:b3:73:VAL:HG11  | 11:b3:79:MET:HE1   | 2.00                     | 0.44              |
| 11:b3:340:ALA:HB1  | 11:b3:344:ASP:HB2  | 1.98                     | 0.44              |
| 11:c3:31:VAL:HG12  | 11:c3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:c3:34:ASN:HB2   | 11:c3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:d3:204:ILE:HG21 | 11:d3:213:ALA:HB2  | 1.97                     | 0.44              |
| 11:e3:31:VAL:HG12  | 11:e3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:e3:123:MET:HE1  | 11:e3:136:LEU:HB3  | 1.99                     | 0.44              |
| 11:f3:34:ASN:HB2   | 11:f3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:f3:114:LYS:HD2  | 11:f3:114:LYS:HA   | 1.77                     | 0.44              |
| 11:g3:123:MET:CE   | 11:g3:136:LEU:HD22 | 2.38                     | 0.44              |
| 11:h3:31:VAL:HG12  | 11:h3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:i3:359:ARG:HD2  | 11:i3:359:ARG:N    | 2.32                     | 0.44              |
| 11:j3:359:ARG:N    | 11:j3:359:ARG:HD2  | 2.32                     | 0.44              |
| 11:k3:32:ARG:H     | 11:k3:95:PRO:HB3   | 1.83                     | 0.44              |
| 11:l3:46:ASP:OD1   | 11:m3:160:LEU:HD12 | 2.18                     | 0.44              |
| 11:m3:123:MET:HE1  | 11:m3:136:LEU:HB3  | 1.99                     | 0.44              |
| 11:m3:340:ALA:HB1  | 11:m3:344:ASP:HB2  | 1.98                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:o3:31:VAL:HG12 | 11:o3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:o3:57:PHE:CE1  | 11:o3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:p3:32:ARG:H    | 11:p3:95:PRO:HB3   | 1.82                     | 0.44              |
| 11:p3:359:ARG:N   | 11:p3:359:ARG:HD2  | 2.32                     | 0.44              |
| 11:s3:101:GLN:NE2 | 11:t3:188:GLN:HB3  | 2.31                     | 0.44              |
| 11:s3:192:GLU:HB2 | 11:s3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:t3:123:MET:CE  | 11:t3:136:LEU:HD22 | 2.38                     | 0.44              |
| 11:u3:192:GLU:HB2 | 11:u3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:v3:114:LYS:HD2 | 11:v3:114:LYS:HA   | 1.77                     | 0.44              |
| 11:v3:192:GLU:HB2 | 11:v3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:v3:359:ARG:HD2 | 11:v3:359:ARG:N    | 2.32                     | 0.44              |
| 11:x3:123:MET:HE1 | 11:x3:136:LEU:HB3  | 1.99                     | 0.44              |
| 11:y3:252:LYS:HB2 | 11:y3:252:LYS:HE3  | 1.52                     | 0.44              |
| 1:C1:165:PHE:CE2  | 2:C2:145:ALA:HB1   | 2.52                     | 0.44              |
| 1:C1:252:ILE:O    | 1:C1:255:PRO:HD2   | 2.17                     | 0.44              |
| 1:H1:195:VAL:HG13 | 1:H1:210:VAL:CG2   | 2.47                     | 0.44              |
| 1:H1:394:LYS:HE2  | 1:H1:402:LEU:HD13  | 1.99                     | 0.44              |
| 1:J1:375:THR:HG23 | 1:K1:275:LYS:NZ    | 2.33                     | 0.44              |
| 1:L1:248:ARG:HH11 | 1:M1:267:THR:HG22  | 1.83                     | 0.44              |
| 1:M1:269:GLN:OE1  | 1:M1:384:ARG:NH1   | 2.49                     | 0.44              |
| 1:M1:270:LEU:HD13 | 1:M1:382:ILE:HA    | 1.99                     | 0.44              |
| 1:N1:166:VAL:HG21 | 2:A2:162:PRO:CG    | 2.47                     | 0.44              |
| 1:T1:161:LYS:HD2  | 1:T1:163:SER:HA    | 2.00                     | 0.44              |
| 1:U1:139:GLU:O    | 1:U1:142:ARG:HG2   | 2.18                     | 0.44              |
| 1:e1:418:GLU:HB3  | 1:f1:388:ALA:HB2   | 1.99                     | 0.44              |
| 1:f1:256:ILE:HD11 | 1:g1:390:VAL:HG11  | 2.00                     | 0.44              |
| 1:h1:132:TYR:CE2  | 1:h1:136:LEU:HD11  | 2.52                     | 0.44              |
| 2:A2:193:PHE:HB3  | 2:A2:222:LYS:NZ    | 2.33                     | 0.44              |
| 2:C2:90:LEU:HD23  | 2:C2:90:LEU:HA     | 1.87                     | 0.44              |
| 2:D2:38:TRP:HA    | 5:M2:46:SER:OG     | 2.17                     | 0.44              |
| 2:D2:234:LEU:CD2  | 4:J2:81:PHE:HB3    | 2.48                     | 0.44              |
| 7:W2:110:ARG:NH1  | 7:W2:113:GLN:OE1   | 2.49                     | 0.44              |
| 8:b2:171:VAL:HG13 | 8:b2:179:PHE:HB3   | 1.99                     | 0.44              |
| 8:c2:113:LEU:O    | 8:c2:120:VAL:HG12  | 2.17                     | 0.44              |
| 8:c2:228:GLU:HB2  | 9:h2:256:LYS:HE3   | 2.00                     | 0.44              |
| 8:d2:249:SER:OG   | 8:d2:250:MET:N     | 2.51                     | 0.44              |
| 8:f2:155:VAL:O    | 8:f2:155:VAL:HG12  | 2.17                     | 0.44              |
| 8:f2:165:LYS:HD2  | 8:f2:199:ILE:HD11  | 2.00                     | 0.44              |
| 9:h2:1:MET:HE1    | 9:h2:6:TRP:HB2     | 2.00                     | 0.44              |
| 9:i2:184:LEU:HB3  | 9:i2:192:TYR:HB3   | 1.98                     | 0.44              |
| 9:m2:98:LYS:HG2   | 9:x2:45:LEU:HG     | 1.97                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:r2:238:ARG:O     | 9:r2:242:ILE:HG12  | 2.17                     | 0.44              |
| 9:t2:72:VAL:O      | 9:t2:72:VAL:HG12   | 2.17                     | 0.44              |
| 9:t2:106:MET:CG    | 11:v3:54:GLN:HE21  | 2.25                     | 0.44              |
| 9:y2:8:ALA:O       | 9:y2:12:LEU:HD23   | 2.16                     | 0.44              |
| 9:y2:27:ALA:O      | 9:42:72:VAL:HG21   | 2.18                     | 0.44              |
| 9:y2:56:SER:OG     | 9:y2:57:SER:N      | 2.50                     | 0.44              |
| 9:z2:237:GLN:HG3   | 12:D4:55:ASN:ND2   | 2.30                     | 0.44              |
| 9:42:23:ALA:CA     | 12:C4:41:VAL:CG2   | 2.95                     | 0.44              |
| 10:E3:171:ILE:O    | 10:E3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:F3:50:SER:HB3   | 11:g3:99:GLN:HE21  | 1.82                     | 0.44              |
| 10:G3:50:SER:HB3   | 11:h3:99:GLN:HE21  | 1.82                     | 0.44              |
| 10:G3:124:MET:HE3  | 10:G3:124:MET:HB3  | 1.77                     | 0.44              |
| 10:I3:171:ILE:O    | 10:I3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:L3:90:LYS:CE    | 10:L3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:L3:124:MET:HE3  | 10:L3:124:MET:HB3  | 1.77                     | 0.44              |
| 10:M3:74:ILE:HD13  | 10:M3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:N3:74:ILE:HD13  | 10:N3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:P3:90:LYS:HE3   | 10:P3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:Q3:71:PRO:HD2   | 10:Q3:189:ILE:HD13 | 1.98                     | 0.44              |
| 10:U3:71:PRO:HD2   | 10:U3:189:ILE:HD13 | 1.98                     | 0.44              |
| 10:U3:74:ILE:HD13  | 10:U3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:Y3:90:LYS:CE    | 10:Y3:138:ALA:HB3  | 2.47                     | 0.44              |
| 11:a3:32:ARG:H     | 11:a3:95:PRO:HB3   | 1.82                     | 0.44              |
| 11:b3:34:ASN:HB2   | 11:b3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:d3:31:VAL:HG12  | 11:d3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:d3:34:ASN:HB2   | 11:d3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:f3:192:GLU:HB2  | 11:f3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:h3:34:ASN:HB2   | 11:h3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:i3:31:VAL:HG12  | 11:i3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:k3:114:LYS:HD2  | 11:k3:114:LYS:HA   | 1.77                     | 0.44              |
| 11:k3:340:ALA:HB1  | 11:k3:344:ASP:HB2  | 1.99                     | 0.44              |
| 11:n3:31:VAL:HG12  | 11:n3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:n3:340:ALA:HB1  | 11:n3:344:ASP:HB2  | 1.99                     | 0.44              |
| 11:q3:192:GLU:HB2  | 11:q3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:s3:23:ARG:NH1   | 11:t3:249:GLN:O    | 2.51                     | 0.44              |
| 11:x3:34:ASN:HB2   | 11:x3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:y3:31:VAL:HG12  | 11:y3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:y3:57:PHE:CE1   | 11:y3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:z3:34:ASN:HB2   | 11:z3:93:TYR:HB3   | 2.00                     | 0.44              |
| 12:B4:108:ILE:HG23 | 12:B4:123:THR:HG22 | 1.99                     | 0.44              |
| 12:B4:128:GLU:HA   | 12:B4:159:GLY:O    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:B4:206:VAL:HB  | 12:C4:231:ILE:HG22 | 1.99                     | 0.44              |
| 1:A1:405:THR:HG23 | 1:A1:408:GLN:H     | 1.82                     | 0.44              |
| 1:E1:151:LYS:HZ3  | 1:E1:181:GLU:HA    | 1.82                     | 0.44              |
| 1:G1:143:THR:HA   | 1:H1:154:ARG:NH1   | 2.30                     | 0.44              |
| 1:G1:147:LEU:O    | 1:G1:149:PRO:HD2   | 2.18                     | 0.44              |
| 1:K1:211:THR:HA   | 1:K1:221:THR:HG21  | 1.99                     | 0.44              |
| 1:K1:393:TYR:HB3  | 1:K1:402:LEU:N     | 2.33                     | 0.44              |
| 1:O1:191:ILE:HD13 | 1:O1:220:LEU:HB3   | 1.99                     | 0.44              |
| 1:R1:151:LYS:HZ1  | 1:R1:181:GLU:HA    | 1.83                     | 0.44              |
| 1:R1:258:GLY:HA3  | 1:R1:261:ASN:HD22  | 1.83                     | 0.44              |
| 1:T1:165:PHE:CE2  | 3:F2:167:ASN:CA    | 2.70                     | 0.44              |
| 1:U1:231:ASN:OD1  | 1:U1:232:ASP:N     | 2.51                     | 0.44              |
| 1:V1:280:GLU:O    | 1:V1:280:GLU:HG2   | 2.16                     | 0.44              |
| 1:V1:415:LEU:HD22 | 1:W1:431:ASN:ND2   | 2.32                     | 0.44              |
| 1:X1:165:PHE:HE1  | 2:E2:144:GLU:HB3   | 1.76                     | 0.44              |
| 1:Z1:415:LEU:HD22 | 1:a1:431:ASN:ND2   | 2.32                     | 0.44              |
| 1:d1:302:GLU:HA   | 1:d1:357:SER:O     | 2.17                     | 0.44              |
| 1:f1:216:SER:O    | 1:f1:216:SER:OG    | 2.36                     | 0.44              |
| 1:g1:205:LEU:HD11 | 1:g1:209:ASN:HB2   | 2.00                     | 0.44              |
| 1:h1:142:ARG:HA   | 1:h1:145:GLU:OE2   | 2.18                     | 0.44              |
| 2:A2:107:LYS:HD2  | 2:A2:133:PRO:HB3   | 1.98                     | 0.44              |
| 2:C2:115:PRO:HA   | 2:C2:119:GLN:HE21  | 1.83                     | 0.44              |
| 2:D2:80:THR:OG1   | 2:D2:82:SER:OG     | 2.36                     | 0.44              |
| 4:H2:50:SER:O     | 4:H2:54:LYS:HG3    | 2.18                     | 0.44              |
| 5:O2:68:LEU:HD13  | 6:T2:118:MET:SD    | 2.58                     | 0.44              |
| 9:j2:129:VAL:HG21 | 9:t2:63:PRO:HG3    | 1.99                     | 0.44              |
| 9:l2:36:ARG:NH1   | 9:l2:38:ARG:HB2    | 2.33                     | 0.44              |
| 9:t2:151:ILE:N    | 9:t2:216:GLN:OE1   | 2.36                     | 0.44              |
| 9:u2:162:GLN:HE21 | 9:z2:210:GLY:HA2   | 1.81                     | 0.44              |
| 9:y2:26:LEU:HD12  | 9:y2:26:LEU:HA     | 1.76                     | 0.44              |
| 9:y2:185:GLU:HB2  | 9:42:52:PRO:HG2    | 1.99                     | 0.44              |
| 9:22:120:PHE:CE2  | 9:22:173:LEU:HD21  | 2.51                     | 0.44              |
| 10:A3:101:LYS:HB2 | 10:A3:101:LYS:NZ   | 2.32                     | 0.44              |
| 10:B3:222:LEU:HB2 | 10:C3:231:PRO:HB3  | 2.00                     | 0.44              |
| 10:D3:82:LEU:O    | 10:D3:197:SER:OG   | 2.20                     | 0.44              |
| 10:J3:90:LYS:HE3  | 10:J3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:K3:90:LYS:HE3  | 10:K3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:L3:90:LYS:HE3  | 10:L3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:N3:90:LYS:HE3  | 10:N3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:P3:74:ILE:HD13 | 10:P3:154:GLN:HA   | 1.99                     | 0.44              |
| 10:R3:90:LYS:HE3  | 10:R3:138:ALA:HB3  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:S3:74:ILE:HD13  | 10:S3:154:GLN:HA  | 1.99                     | 0.44              |
| 10:S3:101:LYS:HB2  | 10:S3:101:LYS:NZ  | 2.32                     | 0.44              |
| 10:S3:171:ILE:O    | 10:S3:172:ASN:HB3 | 2.18                     | 0.44              |
| 10:T3:74:ILE:HD13  | 10:T3:154:GLN:HA  | 1.99                     | 0.44              |
| 10:T3:82:LEU:O     | 10:T3:197:SER:OG  | 2.20                     | 0.44              |
| 10:T3:90:LYS:HE3   | 10:T3:138:ALA:HB3 | 2.00                     | 0.44              |
| 10:T3:124:MET:HE3  | 10:T3:124:MET:HB3 | 1.77                     | 0.44              |
| 10:X3:101:LYS:HB2  | 10:X3:101:LYS:NZ  | 2.32                     | 0.44              |
| 10:X3:106:PHE:O    | 10:X3:107:ASP:HB2 | 2.18                     | 0.44              |
| 10:Z3:50:SER:HB3   | 11:a3:99:GLN:HE21 | 1.83                     | 0.44              |
| 11:a3:22:ILE:HA    | 11:a3:25:LEU:CD2  | 2.48                     | 0.44              |
| 11:a3:31:VAL:HG12  | 11:a3:95:PRO:HG3  | 1.99                     | 0.44              |
| 11:b3:31:VAL:HG12  | 11:b3:95:PRO:HG3  | 2.00                     | 0.44              |
| 11:c3:86:ALA:O     | 11:c3:110:MET:HB2 | 2.18                     | 0.44              |
| 11:g3:34:ASN:HB2   | 11:g3:93:TYR:HB3  | 2.00                     | 0.44              |
| 11:g3:123:MET:HE1  | 11:g3:136:LEU:HB3 | 1.99                     | 0.44              |
| 11:g3:141:ILE:HD13 | 11:g3:165:ILE:CD1 | 2.38                     | 0.44              |
| 11:g3:359:ARG:N    | 11:g3:359:ARG:HD2 | 2.32                     | 0.44              |
| 11:i3:34:ASN:HB2   | 11:i3:93:TYR:HB3  | 2.00                     | 0.44              |
| 11:j3:32:ARG:H     | 11:j3:95:PRO:HB3  | 1.82                     | 0.44              |
| 11:l3:31:VAL:HG12  | 11:l3:95:PRO:HG3  | 1.99                     | 0.44              |
| 11:p3:31:VAL:HG12  | 11:p3:95:PRO:HG3  | 1.99                     | 0.44              |
| 11:q3:32:ARG:H     | 11:q3:95:PRO:HB3  | 1.82                     | 0.44              |
| 11:q3:352:MET:O    | 11:q3:356:GLY:O   | 2.35                     | 0.44              |
| 11:r3:254:VAL:HG13 | 11:r3:365:ILE:CG1 | 2.46                     | 0.44              |
| 11:w3:192:GLU:HB2  | 11:w3:219:ARG:HB2 | 1.99                     | 0.44              |
| 11:x3:359:ARG:N    | 11:x3:359:ARG:HD2 | 2.32                     | 0.44              |
| 11:y3:34:ASN:HB2   | 11:y3:93:TYR:HB3  | 2.00                     | 0.44              |
| 1:B1:280:GLU:HG3   | 1:B1:372:ILE:CD1  | 2.48                     | 0.44              |
| 1:B1:393:TYR:CE2   | 1:B1:436:PRO:HD3  | 2.52                     | 0.44              |
| 1:C1:188:GLU:H     | 1:C1:188:GLU:CD   | 2.24                     | 0.44              |
| 1:F1:407:ASP:HA    | 1:F1:410:LYS:NZ   | 2.32                     | 0.44              |
| 1:H1:206:PRO:HG2   | 1:H1:209:ASN:OD1  | 2.17                     | 0.44              |
| 1:H1:283:SER:HB2   | 1:H1:369:ASP:HB2  | 1.99                     | 0.44              |
| 1:P1:275:LYS:HB2   | 1:P1:275:LYS:HE3  | 1.64                     | 0.44              |
| 1:R1:183:GLY:C     | 1:R1:184:ARG:HD3  | 2.43                     | 0.44              |
| 1:T1:167:ARG:NH1   | 2:E2:107:LYS:CA   | 2.81                     | 0.44              |
| 1:Y1:141:ALA:O     | 1:Y1:145:GLU:HG2  | 2.18                     | 0.44              |
| 1:c1:360:ARG:HG2   | 1:c1:362:GLU:OE2  | 2.17                     | 0.44              |
| 1:d1:151:LYS:NZ    | 1:d1:182:PRO:HD3  | 2.32                     | 0.44              |
| 1:f1:147:LEU:HB3   | 1:f1:150:VAL:HG21 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:f1:157:LEU:HB3  | 1:f1:159:MET:HE3  | 1.99                     | 0.44              |
| 2:E2:140:ARG:NH1  | 2:E2:244:TYR:HB2  | 2.32                     | 0.44              |
| 2:E2:232:TRP:CD1  | 3:F2:177:GLY:N    | 2.86                     | 0.44              |
| 4:G2:51:PHE:CE1   | 4:G2:55:ILE:HD11  | 2.52                     | 0.44              |
| 6:R2:42:ASP:OD1   | 6:R2:43:ILE:N     | 2.46                     | 0.44              |
| 7:X2:52:ASP:CG    | 7:X2:53:ALA:H     | 2.25                     | 0.44              |
| 7:a2:78:TYR:HB2   | 7:a2:90:TYR:HE1   | 1.81                     | 0.44              |
| 8:c2:73:TYR:CE1   | 9:o2:73:ARG:HG3   | 2.51                     | 0.44              |
| 8:c2:187:ALA:O    | 8:c2:188:GLU:HG2  | 2.17                     | 0.44              |
| 8:d2:71:LEU:HB3   | 8:d2:205:VAL:CG1  | 2.48                     | 0.44              |
| 8:f2:228:GLU:CG   | 9:k2:256:LYS:HG3  | 2.48                     | 0.44              |
| 9:g2:98:LYS:HG3   | 9:r2:45:LEU:CD2   | 2.48                     | 0.44              |
| 9:n2:72:VAL:O     | 9:n2:72:VAL:HG22  | 2.18                     | 0.44              |
| 9:t2:118:GLY:O    | 9:t2:120:PHE:N    | 2.51                     | 0.44              |
| 9:t2:189:GLU:HA   | 9:y2:42:GLU:CG    | 2.47                     | 0.44              |
| 9:w2:26:LEU:HD11  | 9:22:242:ILE:CG2  | 2.47                     | 0.44              |
| 9:z2:107:LEU:HD23 | 9:z2:109:ASP:H    | 1.83                     | 0.44              |
| 9:22:35:LYS:NZ    | 9:22:220:GLU:OE2  | 2.51                     | 0.44              |
| 9:32:234:ILE:HG23 | 12:B4:55:ASN:HB2  | 2.00                     | 0.44              |
| 10:A3:50:SER:HB3  | 11:b3:99:GLN:HE21 | 1.83                     | 0.44              |
| 10:A3:90:LYS:CE   | 10:A3:138:ALA:HB3 | 2.47                     | 0.44              |
| 10:D3:37:ALA:HB1  | 10:E3:74:ILE:CG2  | 2.48                     | 0.44              |
| 10:D3:106:PHE:O   | 10:D3:107:ASP:HB2 | 2.18                     | 0.44              |
| 10:E3:37:ALA:HB1  | 10:F3:74:ILE:CG2  | 2.48                     | 0.44              |
| 10:E3:82:LEU:HA   | 10:E3:197:SER:CB  | 2.39                     | 0.44              |
| 10:E3:106:PHE:O   | 10:E3:107:ASP:HB2 | 2.18                     | 0.44              |
| 10:E3:170:ALA:HB3 | 10:F3:206:GLU:HG3 | 1.99                     | 0.44              |
| 10:G3:170:ALA:HB3 | 10:H3:206:GLU:HG3 | 2.00                     | 0.44              |
| 10:H3:170:ALA:HB3 | 10:I3:206:GLU:HG3 | 1.99                     | 0.44              |
| 10:J3:170:ALA:HB3 | 10:K3:206:GLU:HG3 | 1.99                     | 0.44              |
| 10:L3:50:SER:HB3  | 11:m3:99:GLN:HE21 | 1.82                     | 0.44              |
| 10:M3:90:LYS:HE3  | 10:M3:138:ALA:HB3 | 2.00                     | 0.44              |
| 10:O3:37:ALA:HB1  | 10:P3:74:ILE:CG2  | 2.48                     | 0.44              |
| 10:Q3:37:ALA:HB1  | 10:R3:74:ILE:CG2  | 2.48                     | 0.44              |
| 10:R3:74:ILE:HD13 | 10:R3:154:GLN:HA  | 1.99                     | 0.44              |
| 10:S3:90:LYS:CE   | 10:S3:138:ALA:HB3 | 2.47                     | 0.44              |
| 10:U3:37:ALA:HB1  | 10:V3:74:ILE:CG2  | 2.47                     | 0.44              |
| 10:U3:90:LYS:HE3  | 10:U3:138:ALA:HB3 | 1.99                     | 0.44              |
| 10:V3:50:SER:HB3  | 11:w3:99:GLN:HE21 | 1.82                     | 0.44              |
| 10:V3:222:LEU:HB2 | 10:W3:231:PRO:HB3 | 2.00                     | 0.44              |
| 11:a3:86:ALA:O    | 11:a3:110:MET:HB2 | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a3:160:LEU:HD12 | 11:z3:46:ASP:OD1   | 2.16                     | 0.44              |
| 11:b3:86:ALA:O     | 11:b3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:c3:23:ARG:NH1   | 11:d3:249:GLN:O    | 2.51                     | 0.44              |
| 11:c3:185:ILE:O    | 11:c3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:c3:217:ASP:OD1  | 11:c3:219:ARG:N    | 2.37                     | 0.44              |
| 11:f3:46:ASP:OD1   | 11:g3:160:LEU:HD12 | 2.17                     | 0.44              |
| 11:g3:93:TYR:OH    | 11:g3:173:ARG:O    | 2.25                     | 0.44              |
| 11:j3:86:ALA:O     | 11:j3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:j3:123:MET:HE1  | 11:j3:136:LEU:HB3  | 1.99                     | 0.44              |
| 11:k3:359:ARG:N    | 11:k3:359:ARG:HD2  | 2.32                     | 0.44              |
| 11:l3:141:ILE:HD13 | 11:l3:165:ILE:CD1  | 2.37                     | 0.44              |
| 11:n3:185:ILE:O    | 11:n3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:o3:73:VAL:HG11  | 11:o3:79:MET:HE1   | 2.00                     | 0.44              |
| 11:o3:319:LEU:HD12 | 11:o3:319:LEU:HA   | 1.82                     | 0.44              |
| 11:q3:31:VAL:HG12  | 11:q3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:q3:123:MET:HE1  | 11:q3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:r3:22:ILE:HA    | 11:r3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:r3:57:PHE:CE1   | 11:r3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:r3:352:MET:O    | 11:r3:356:GLY:O    | 2.35                     | 0.44              |
| 11:u3:32:ARG:H     | 11:u3:95:PRO:HB3   | 1.82                     | 0.44              |
| 11:v3:86:ALA:O     | 11:v3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:w3:340:ALA:HB1  | 11:w3:344:ASP:HB2  | 1.98                     | 0.44              |
| 11:x3:66:LEU:HD21  | 11:y3:110:MET:HE1  | 2.00                     | 0.44              |
| 11:y3:185:ILE:O    | 11:y3:223:VAL:HG22 | 2.18                     | 0.44              |
| 12:B4:89:GLN:HG3   | 12:B4:225:LEU:HD22 | 1.99                     | 0.44              |
| 1:C1:426:ARG:HH21  | 1:C1:428:ASP:CG    | 2.26                     | 0.44              |
| 1:K1:404:LEU:HD23  | 1:K1:408:GLN:HG2   | 2.00                     | 0.44              |
| 1:O1:246:GLN:O     | 1:O1:250:GLU:HG2   | 2.18                     | 0.44              |
| 1:O1:413:GLU:CD    | 1:O1:417:ARG:HH12  | 2.25                     | 0.44              |
| 1:Q1:257:VAL:HG21  | 1:Q1:262:VAL:HB    | 2.00                     | 0.44              |
| 1:T1:188:GLU:O     | 1:T1:191:ILE:HB    | 2.18                     | 0.44              |
| 1:W1:370:ARG:NH1   | 1:W1:372:ILE:HD11  | 2.32                     | 0.44              |
| 1:Y1:165:PHE:CG    | 2:E2:152:ARG:NH2   | 2.85                     | 0.44              |
| 1:Y1:180:LEU:HD23  | 1:Y1:185:ALA:HA    | 1.99                     | 0.44              |
| 1:c1:204:GLY:O     | 1:d1:170:LYS:NZ    | 2.28                     | 0.44              |
| 3:F2:12:TRP:HD1    | 5:P2:34:PHE:CZ     | 2.33                     | 0.44              |
| 4:G2:46:GLU:HG2    | 4:G2:47:MET:N      | 2.25                     | 0.44              |
| 5:O2:71:VAL:HG12   | 5:O2:72:MET:HE2    | 2.00                     | 0.44              |
| 9:n2:26:LEU:HD11   | 9:t2:242:ILE:HG21  | 1.99                     | 0.44              |
| 9:n2:27:ALA:O      | 9:t2:72:VAL:HG21   | 2.17                     | 0.44              |
| 9:r2:44:LEU:HD21   | 9:r2:73:ARG:HB2    | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:r2:140:ILE:HD13  | 9:r2:157:VAL:HG11  | 2.00                     | 0.44              |
| 9:u2:26:LEU:HD11   | 9:z2:242:ILE:HG21  | 1.99                     | 0.44              |
| 9:32:151:ILE:HG12  | 9:32:157:VAL:HG23  | 2.00                     | 0.44              |
| 10:A3:198:THR:O    | 10:Z3:149:THR:OG1  | 2.32                     | 0.44              |
| 10:C3:106:PHE:O    | 10:C3:107:ASP:HB2  | 2.18                     | 0.44              |
| 10:G3:101:LYS:HB2  | 10:G3:101:LYS:NZ   | 2.32                     | 0.44              |
| 10:H3:90:LYS:CE    | 10:H3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:J3:222:LEU:HB2  | 10:K3:231:PRO:HB3  | 2.00                     | 0.44              |
| 10:P3:50:SER:HB3   | 11:q3:99:GLN:HE21  | 1.82                     | 0.44              |
| 10:Q3:90:LYS:HE3   | 10:Q3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:S3:170:ALA:HB3  | 10:T3:206:GLU:HG3  | 2.00                     | 0.44              |
| 10:T3:37:ALA:HB1   | 10:U3:74:ILE:CG2   | 2.48                     | 0.44              |
| 10:T3:101:LYS:HB2  | 10:T3:101:LYS:NZ   | 2.32                     | 0.44              |
| 10:W3:37:ALA:HB1   | 10:X3:74:ILE:CG2   | 2.48                     | 0.44              |
| 10:W3:106:PHE:O    | 10:W3:107:ASP:HB2  | 2.18                     | 0.44              |
| 10:W3:170:ALA:HB3  | 10:X3:206:GLU:HG3  | 1.99                     | 0.44              |
| 11:b3:22:ILE:HA    | 11:b3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:d3:57:PHE:CE1   | 11:d3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:d3:86:ALA:O     | 11:d3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:d3:352:MET:O    | 11:d3:356:GLY:O    | 2.35                     | 0.44              |
| 11:e3:57:PHE:CE1   | 11:e3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:e3:86:ALA:O     | 11:e3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:e3:328:LEU:HD21 | 11:f3:273:CYS:HA   | 1.99                     | 0.44              |
| 11:e3:352:MET:O    | 11:e3:356:GLY:O    | 2.35                     | 0.44              |
| 11:f3:57:PHE:CE1   | 11:f3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:f3:86:ALA:O     | 11:f3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:g3:185:ILE:O    | 11:g3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:g3:192:GLU:HB2  | 11:g3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:j3:57:PHE:CE1   | 11:j3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:k3:86:ALA:O     | 11:k3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:k3:185:ILE:O    | 11:k3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:m3:23:ARG:NH1   | 11:n3:249:GLN:O    | 2.51                     | 0.44              |
| 11:m3:31:VAL:HG12  | 11:m3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:m3:46:ASP:OD1   | 11:n3:160:LEU:HD12 | 2.18                     | 0.44              |
| 11:m3:57:PHE:CE1   | 11:m3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:m3:359:ARG:N    | 11:m3:359:ARG:HD2  | 2.32                     | 0.44              |
| 11:o3:123:MET:HE1  | 11:o3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:o3:359:ARG:N    | 11:o3:359:ARG:HD2  | 2.32                     | 0.44              |
| 11:p3:123:MET:HE1  | 11:p3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:q3:185:ILE:O    | 11:q3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:r3:32:ARG:H     | 11:r3:95:PRO:HB3   | 1.82                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:r3:123:MET:HE1 | 11:r3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:t3:185:ILE:O   | 11:t3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:t3:208:ARG:HG3 | 11:t3:235:PHE:CZ   | 2.53                     | 0.44              |
| 11:w3:34:ASN:HB2  | 11:w3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:w3:73:VAL:HG11 | 11:w3:79:MET:HE1   | 1.99                     | 0.44              |
| 11:w3:86:ALA:O    | 11:w3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:w3:359:ARG:N   | 11:w3:359:ARG:HD2  | 2.32                     | 0.44              |
| 11:x3:57:PHE:CE1  | 11:x3:110:MET:HE2  | 2.52                     | 0.44              |
| 11:x3:101:GLN:OE1 | 11:y3:219:ARG:HD3  | 2.17                     | 0.44              |
| 11:x3:192:GLU:HB2 | 11:x3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:x3:352:MET:O   | 11:x3:356:GLY:O    | 2.35                     | 0.44              |
| 11:y3:86:ALA:O    | 11:y3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:z3:22:ILE:HA   | 11:z3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:z3:31:VAL:HG12 | 11:z3:95:PRO:HG3   | 1.99                     | 0.44              |
| 11:z3:73:VAL:HG11 | 11:z3:79:MET:HE1   | 2.00                     | 0.44              |
| 11:z3:86:ALA:O    | 11:z3:110:MET:HB2  | 2.18                     | 0.44              |
| 12:B4:96:LEU:HD23 | 12:B4:96:LEU:H     | 1.81                     | 0.44              |
| 1:B1:385:LEU:N    | 1:B1:428:ASP:OD2   | 2.27                     | 0.44              |
| 1:I1:239:ASN:HA   | 1:I1:242:GLU:HG2   | 1.98                     | 0.44              |
| 1:I1:387:VAL:HB   | 1:I1:420:MET:SD    | 2.58                     | 0.44              |
| 1:K1:143:THR:HG22 | 1:L1:154:ARG:HD3   | 1.99                     | 0.44              |
| 1:K1:200:SER:HB3  | 1:L1:175:SER:HB3   | 2.00                     | 0.44              |
| 1:Q1:272:PHE:HA   | 1:Q1:379:VAL:HG13  | 2.00                     | 0.44              |
| 1:R1:145:GLU:HG3  | 1:R1:153:ALA:HB3   | 2.00                     | 0.44              |
| 1:U1:266:VAL:HG22 | 1:U1:387:VAL:HG22  | 1.98                     | 0.44              |
| 1:Z1:413:GLU:OE1  | 1:Z1:432:VAL:HB    | 2.17                     | 0.44              |
| 1:b1:369:ASP:OD1  | 1:c1:282:TYR:N     | 2.46                     | 0.44              |
| 1:c1:244:ARG:NH2  | 1:c1:248:ARG:HH22  | 2.15                     | 0.44              |
| 1:e1:297:GLN:OE1  | 1:f1:363:THR:OG1   | 2.27                     | 0.44              |
| 1:h1:416:THR:HG23 | 1:h1:430:LEU:HD21  | 1.98                     | 0.44              |
| 2:E2:43:GLN:HB3   | 3:F2:67:SER:OG     | 2.18                     | 0.44              |
| 2:E2:57:ILE:HG22  | 2:E2:58:LEU:HD22   | 2.00                     | 0.44              |
| 3:F2:66:PHE:HB3   | 6:Q2:4:ARG:HB2     | 2.00                     | 0.44              |
| 3:F2:195:LEU:HD23 | 3:F2:195:LEU:HA    | 1.82                     | 0.44              |
| 4:I2:59:PHE:CZ    | 4:J2:14:MET:HG2    | 2.51                     | 0.44              |
| 6:T2:100:VAL:HG13 | 6:T2:105:GLU:HG3   | 2.00                     | 0.44              |
| 6:U2:34:ASP:OD1   | 6:U2:34:ASP:N      | 2.50                     | 0.44              |
| 7:Z2:83:PRO:O     | 7:Z2:84:LEU:HB2    | 2.18                     | 0.44              |
| 8:f2:147:ASN:O    | 8:f2:149:GLY:N     | 2.51                     | 0.44              |
| 9:h2:9:LYS:HZ3    | 9:h2:12:LEU:HD13   | 1.83                     | 0.44              |
| 9:i2:98:LYS:HD2   | 9:i2:213:LEU:HD12  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:j2:226:VAL:O     | 9:j2:230:LEU:HD23  | 2.18                     | 0.44              |
| 9:k2:98:LYS:O      | 9:k2:212:GLY:CA    | 2.64                     | 0.44              |
| 9:l2:130:THR:HG22  | 9:l2:134:PHE:O     | 2.18                     | 0.44              |
| 9:x2:26:LEU:HD12   | 9:x2:26:LEU:HA     | 1.73                     | 0.44              |
| 9:y2:16:GLN:NE2    | 9:42:2:ILE:HG23    | 2.32                     | 0.44              |
| 9:y2:125:ASN:HB3   | 9:y2:127:GLN:HE22  | 1.82                     | 0.44              |
| 9:12:183:GLY:O     | 9:12:197:SER:OG    | 2.36                     | 0.44              |
| 9:32:89:THR:HG23   | 9:32:91:ASN:H      | 1.82                     | 0.44              |
| 10:B3:171:ILE:O    | 10:B3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:C3:171:ILE:O    | 10:C3:172:ASN:HB3  | 2.17                     | 0.44              |
| 10:E3:124:MET:HE3  | 10:E3:124:MET:HB3  | 1.76                     | 0.44              |
| 10:F3:106:PHE:O    | 10:F3:107:ASP:HB2  | 2.18                     | 0.44              |
| 10:F3:170:ALA:HB3  | 10:G3:206:GLU:HG3  | 2.00                     | 0.44              |
| 10:G3:106:PHE:O    | 10:G3:107:ASP:HB2  | 2.18                     | 0.44              |
| 10:H3:222:LEU:HB2  | 10:I3:231:PRO:HB3  | 2.00                     | 0.44              |
| 10:I3:90:LYS:HE3   | 10:I3:138:ALA:HB3  | 2.00                     | 0.44              |
| 10:J3:90:LYS:CE    | 10:J3:138:ALA:HB3  | 2.47                     | 0.44              |
| 10:M3:50:SER:HB3   | 11:n3:99:GLN:HE21  | 1.82                     | 0.44              |
| 10:W3:171:ILE:O    | 10:W3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:Y3:167:LYS:HD3  | 10:Z3:203:ALA:CB   | 2.46                     | 0.44              |
| 10:Y3:171:ILE:O    | 10:Y3:172:ASN:HB3  | 2.18                     | 0.44              |
| 10:Z3:51:ILE:CG1   | 11:b3:175:LEU:HD11 | 2.46                     | 0.44              |
| 10:Z3:135:LYS:HB2  | 10:Z3:135:LYS:HE2  | 1.76                     | 0.44              |
| 10:Z3:171:ILE:O    | 10:Z3:172:ASN:HB3  | 2.18                     | 0.44              |
| 11:c3:208:ARG:HG3  | 11:c3:235:PHE:CZ   | 2.53                     | 0.44              |
| 11:c3:319:LEU:HD12 | 11:c3:319:LEU:HA   | 1.82                     | 0.44              |
| 11:d3:73:VAL:HG11  | 11:d3:79:MET:HE1   | 2.00                     | 0.44              |
| 11:d3:123:MET:HE1  | 11:d3:136:LEU:HB3  | 1.99                     | 0.44              |
| 11:e3:73:VAL:HG11  | 11:e3:79:MET:HE1   | 2.00                     | 0.44              |
| 11:e3:192:GLU:HB2  | 11:e3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:f3:185:ILE:O    | 11:f3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:f3:208:ARG:HG3  | 11:f3:235:PHE:CZ   | 2.53                     | 0.44              |
| 11:g3:23:ARG:NH1   | 11:h3:249:GLN:O    | 2.51                     | 0.44              |
| 11:g3:319:LEU:HD12 | 11:g3:319:LEU:HA   | 1.82                     | 0.44              |
| 11:h3:123:MET:HE1  | 11:h3:136:LEU:HB3  | 1.98                     | 0.44              |
| 11:i3:23:ARG:NH1   | 11:j3:249:GLN:O    | 2.51                     | 0.44              |
| 11:i3:32:ARG:H     | 11:i3:95:PRO:HB3   | 1.82                     | 0.44              |
| 11:j3:34:ASN:HB2   | 11:j3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:j3:185:ILE:O    | 11:j3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:k3:93:TYR:OH    | 11:k3:173:ARG:O    | 2.25                     | 0.44              |
| 11:n3:192:GLU:HB2  | 11:n3:219:ARG:HB2  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:o3:192:GLU:HB2  | 11:o3:219:ARG:HB2  | 1.99                     | 0.44              |
| 11:p3:22:ILE:HA    | 11:p3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:p3:208:ARG:HG3  | 11:p3:235:PHE:CZ   | 2.53                     | 0.44              |
| 11:t3:359:ARG:HD2  | 11:t3:359:ARG:N    | 2.32                     | 0.44              |
| 11:u3:23:ARG:NH1   | 11:v3:249:GLN:O    | 2.51                     | 0.44              |
| 11:v3:185:ILE:O    | 11:v3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:w3:352:MET:O    | 11:w3:356:GLY:O    | 2.35                     | 0.44              |
| 11:x3:86:ALA:O     | 11:x3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:y3:22:ILE:HA    | 11:y3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:y3:73:VAL:HG11  | 11:y3:79:MET:HE1   | 2.00                     | 0.44              |
| 12:A4:215:LEU:HD22 | 12:A4:228:VAL:HG21 | 2.00                     | 0.44              |
| 12:C4:38:THR:HA    | 12:C4:41:VAL:HG12  | 1.99                     | 0.44              |
| 1:D1:420:MET:HE1   | 1:D1:428:ASP:HB3   | 1.99                     | 0.44              |
| 1:E1:297:GLN:HB3   | 1:E1:363:THR:OG1   | 2.18                     | 0.44              |
| 1:E1:419:ALA:O     | 1:F1:267:THR:HG21  | 2.18                     | 0.44              |
| 1:G1:203:ALA:HB1   | 1:H1:160:PRO:HA    | 2.00                     | 0.44              |
| 1:J1:393:TYR:CE2   | 1:J1:436:PRO:HD3   | 2.53                     | 0.44              |
| 1:L1:165:PHE:CD1   | 2:A2:142:THR:O     | 2.70                     | 0.44              |
| 1:N1:174:ALA:O     | 1:N1:210:VAL:HA    | 2.17                     | 0.44              |
| 1:N1:275:LYS:HA    | 1:N1:275:LYS:HE3   | 1.99                     | 0.44              |
| 1:P1:234:GLN:HB3   | 1:P1:272:PHE:CE2   | 2.53                     | 0.44              |
| 1:Q1:165:PHE:CE2   | 3:F2:145:TRP:HZ3   | 2.19                     | 0.44              |
| 1:U1:234:GLN:OE1   | 1:U1:234:GLN:N     | 2.48                     | 0.44              |
| 1:V1:303:GLN:HA    | 1:W1:357:SER:HA    | 1.99                     | 0.44              |
| 1:W1:164:LEU:CD1   | 2:E2:144:GLU:N     | 2.80                     | 0.44              |
| 1:W1:167:ARG:O     | 1:X1:165:PHE:HB3   | 2.18                     | 0.44              |
| 1:W1:257:VAL:HG23  | 1:W1:261:ASN:HB2   | 2.00                     | 0.44              |
| 1:X1:147:LEU:O     | 1:X1:149:PRO:HD2   | 2.17                     | 0.44              |
| 1:Z1:302:GLU:HA    | 1:Z1:357:SER:O     | 2.18                     | 0.44              |
| 1:f1:275:LYS:CB    | 1:f1:377:MET:HE2   | 2.48                     | 0.44              |
| 1:g1:167:ARG:HG3   | 2:C2:244:TYR:HD2   | 1.68                     | 0.44              |
| 2:A2:137:PHE:HZ    | 2:A2:243:PHE:CE2   | 2.35                     | 0.44              |
| 2:A2:217:ILE:H     | 2:A2:217:ILE:HD12  | 1.83                     | 0.44              |
| 2:C2:42:VAL:HA     | 2:C2:45:LEU:HB3    | 1.99                     | 0.44              |
| 2:D2:51:LEU:O      | 2:D2:54:LEU:HB3    | 2.18                     | 0.44              |
| 2:D2:128:ASP:OD1   | 2:D2:129:LYS:N     | 2.50                     | 0.44              |
| 2:E2:63:SER:HB3    | 2:E2:97:THR:OG1    | 2.18                     | 0.44              |
| 2:E2:150:PHE:CZ    | 2:E2:172:PRO:HB2   | 2.53                     | 0.44              |
| 3:F2:18:TRP:HE1    | 3:F2:62:ASP:HB2    | 1.82                     | 0.44              |
| 4:I2:47:MET:HE1    | 4:J2:54:LYS:NZ     | 2.32                     | 0.44              |
| 7:Z2:123:LYS:O     | 7:Z2:127:LEU:HD23  | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:e2:35:ARG:HH21   | 8:e2:210:ASN:ND2   | 2.16                     | 0.44              |
| 8:f2:46:VAL:O      | 8:f2:46:VAL:HG12   | 2.17                     | 0.44              |
| 9:m2:257:LEU:O     | 9:m2:260:LEU:HG    | 2.18                     | 0.44              |
| 9:o2:238:ARG:HA    | 9:o2:238:ARG:HD3   | 1.71                     | 0.44              |
| 9:p2:189:GLU:HA    | 9:u2:42:GLU:CG     | 2.47                     | 0.44              |
| 9:r2:127:GLN:OE1   | 9:r2:135:GLN:HG3   | 2.18                     | 0.44              |
| 9:x2:2:ILE:HG12    | 9:x2:254:LEU:HD11  | 1.99                     | 0.44              |
| 9:y2:36:ARG:HH21   | 9:y2:80:LEU:HD22   | 1.82                     | 0.44              |
| 10:B3:37:ALA:HB1   | 10:C3:74:ILE:CG2   | 2.48                     | 0.44              |
| 10:D3:101:LYS:NZ   | 10:D3:101:LYS:HB2  | 2.32                     | 0.44              |
| 10:H3:82:LEU:HD12  | 10:H3:146:GLY:HA3  | 1.98                     | 0.44              |
| 10:H3:101:LYS:HB2  | 10:H3:101:LYS:NZ   | 2.32                     | 0.44              |
| 10:H3:106:PHE:O    | 10:H3:107:ASP:HB2  | 2.18                     | 0.44              |
| 10:J3:101:LYS:HB2  | 10:J3:101:LYS:NZ   | 2.32                     | 0.44              |
| 10:K3:37:ALA:HB1   | 10:L3:74:ILE:CG2   | 2.48                     | 0.44              |
| 10:Y3:65:LEU:HD23  | 11:y3:68:GLN:HG2   | 2.00                     | 0.44              |
| 10:Y3:106:PHE:O    | 10:Y3:107:ASP:HB2  | 2.18                     | 0.44              |
| 10:Z3:90:LYS:CE    | 10:Z3:138:ALA:HB3  | 2.47                     | 0.44              |
| 11:a3:208:ARG:HG3  | 11:a3:235:PHE:CZ   | 2.53                     | 0.44              |
| 11:b3:185:ILE:O    | 11:b3:223:VAL:HG22 | 2.18                     | 0.44              |
| 11:c3:22:ILE:HA    | 11:c3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:c3:225:VAL:HG12 | 11:c3:235:PHE:CD1  | 2.53                     | 0.44              |
| 11:c3:352:MET:O    | 11:c3:356:GLY:O    | 2.35                     | 0.44              |
| 11:g3:86:ALA:O     | 11:g3:110:MET:HB2  | 2.18                     | 0.44              |
| 11:i3:22:ILE:HA    | 11:i3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:j3:22:ILE:HA    | 11:j3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:j3:225:VAL:HG12 | 11:j3:235:PHE:CD1  | 2.53                     | 0.44              |
| 11:k3:34:ASN:HB2   | 11:k3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:l3:23:ARG:NH1   | 11:m3:249:GLN:O    | 2.51                     | 0.44              |
| 11:l3:83:ASN:ND2   | 11:m3:109:SER:OG   | 2.46                     | 0.44              |
| 11:m3:208:ARG:HG3  | 11:m3:235:PHE:CZ   | 2.53                     | 0.44              |
| 11:m3:225:VAL:HG12 | 11:m3:235:PHE:CD1  | 2.53                     | 0.44              |
| 11:q3:22:ILE:HA    | 11:q3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:r3:23:ARG:NH1   | 11:s3:249:GLN:O    | 2.51                     | 0.44              |
| 11:t3:22:ILE:HA    | 11:t3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:t3:83:ASN:ND2   | 11:u3:109:SER:OG   | 2.47                     | 0.44              |
| 11:u3:319:LEU:HD12 | 11:u3:319:LEU:HA   | 1.82                     | 0.44              |
| 11:v3:34:ASN:HB2   | 11:v3:93:TYR:HB3   | 2.00                     | 0.44              |
| 11:v3:225:VAL:HG12 | 11:v3:235:PHE:CD1  | 2.53                     | 0.44              |
| 11:w3:22:ILE:HA    | 11:w3:25:LEU:CD2   | 2.48                     | 0.44              |
| 11:y3:352:MET:O    | 11:y3:356:GLY:O    | 2.35                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:z3:192:GLU:HB2 | 11:z3:219:ARG:HB2 | 1.99                     | 0.44              |
| 11:z3:359:ARG:N   | 11:z3:359:ARG:HD2 | 2.32                     | 0.44              |
| 12:B4:123:THR:OG1 | 12:B4:200:PHE:HB3 | 2.18                     | 0.44              |
| 1:E1:125:GLN:O    | 1:E1:128:GLU:HG3  | 2.18                     | 0.43              |
| 1:H1:140:LEU:HD23 | 1:H1:140:LEU:HA   | 1.83                     | 0.43              |
| 1:L1:139:GLU:HG3  | 1:N1:156:HIS:CE1  | 2.50                     | 0.43              |
| 1:L1:275:LYS:CB   | 1:L1:377:MET:HB2  | 2.47                     | 0.43              |
| 1:O1:407:ASP:O    | 1:O1:410:LYS:HG3  | 2.17                     | 0.43              |
| 1:Q1:161:LYS:HE3  | 3:F2:249:ASN:HD21 | 1.70                     | 0.43              |
| 1:T1:252:ILE:O    | 1:T1:255:PRO:HD2  | 2.17                     | 0.43              |
| 1:T1:409:MET:HE2  | 1:T1:409:MET:HB2  | 1.90                     | 0.43              |
| 1:X1:252:ILE:HD11 | 1:Y1:265:GLN:HB2  | 2.00                     | 0.43              |
| 1:X1:304:VAL:HG22 | 1:X1:356:ARG:HG2  | 1.99                     | 0.43              |
| 1:b1:411:GLN:O    | 1:b1:415:LEU:HD13 | 2.18                     | 0.43              |
| 2:A2:189:ILE:HD11 | 4:G2:84:LEU:HD22  | 2.00                     | 0.43              |
| 2:B2:42:VAL:HG11  | 5:O2:42:LEU:HB3   | 1.99                     | 0.43              |
| 2:B2:187:PHE:CZ   | 2:B2:191:ILE:HD11 | 2.53                     | 0.43              |
| 2:C2:142:THR:HG22 | 2:C2:174:TYR:HA   | 2.00                     | 0.43              |
| 2:D2:62:THR:O     | 2:D2:174:TYR:OH   | 2.21                     | 0.43              |
| 5:N2:84:MET:N     | 6:T2:134:LEU:HD21 | 2.33                     | 0.43              |
| 5:P2:61:LEU:HD21  | 6:U2:50:LYS:HZ3   | 1.83                     | 0.43              |
| 7:V2:42:TYR:CD1   | 7:a2:51:VAL:HG11  | 2.53                     | 0.43              |
| 7:Y2:32:ASP:HB2   | 9:j2:1:MET:H1     | 1.82                     | 0.43              |
| 8:e2:233:VAL:O    | 8:e2:237:VAL:HG23 | 2.18                     | 0.43              |
| 8:f2:147:ASN:HB2  | 8:f2:150:ASP:OD2  | 2.19                     | 0.43              |
| 9:g2:154:ASP:HA   | 9:g2:206:PRO:HB2  | 1.99                     | 0.43              |
| 9:m2:37:GLN:HG2   | 9:m2:77:THR:HB    | 2.00                     | 0.43              |
| 9:w2:86:LEU:HD11  | 9:w2:98:LYS:HD3   | 2.00                     | 0.43              |
| 9:x2:51:GLN:HG3   | 9:x2:53:GLY:H     | 1.83                     | 0.43              |
| 9:x2:137:GLN:OE1  | 9:x2:137:GLN:HA   | 2.18                     | 0.43              |
| 9:z2:77:THR:O     | 9:z2:77:THR:HG23  | 2.18                     | 0.43              |
| 9:22:194:GLU:CD   | 9:22:201:PRO:HD3  | 2.43                     | 0.43              |
| 10:B3:170:ALA:HB3 | 10:C3:206:GLU:HG3 | 2.00                     | 0.43              |
| 10:C3:37:ALA:HB1  | 10:D3:74:ILE:CG2  | 2.48                     | 0.43              |
| 10:D3:222:LEU:HB2 | 10:E3:231:PRO:HB3 | 2.00                     | 0.43              |
| 10:G3:37:ALA:HB1  | 10:H3:74:ILE:CG2  | 2.48                     | 0.43              |
| 10:H3:37:ALA:HB1  | 10:I3:74:ILE:CG2  | 2.48                     | 0.43              |
| 10:I3:106:PHE:O   | 10:I3:107:ASP:HB2 | 2.18                     | 0.43              |
| 10:J3:37:ALA:HB1  | 10:K3:74:ILE:CG2  | 2.48                     | 0.43              |
| 10:K3:101:LYS:HB2 | 10:K3:101:LYS:NZ  | 2.32                     | 0.43              |
| 10:R3:45:PRO:CG   | 10:S3:60:TYR:HD1  | 2.31                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:T3:222:LEU:HB2  | 10:U3:231:PRO:HB3  | 2.00                     | 0.43              |
| 10:U3:65:LEU:HD23  | 11:u3:68:GLN:HG2   | 2.00                     | 0.43              |
| 10:U3:82:LEU:HA    | 10:U3:197:SER:CB   | 2.39                     | 0.43              |
| 10:U3:171:ILE:O    | 10:U3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:V3:37:ALA:HB1   | 10:W3:74:ILE:CG2   | 2.48                     | 0.43              |
| 10:W3:101:LYS:NZ   | 10:W3:101:LYS:HB2  | 2.32                     | 0.43              |
| 11:a3:352:MET:O    | 11:a3:356:GLY:O    | 2.35                     | 0.43              |
| 11:b3:32:ARG:H     | 11:b3:95:PRO:HB3   | 1.83                     | 0.43              |
| 11:b3:319:LEU:HD12 | 11:b3:319:LEU:HA   | 1.82                     | 0.43              |
| 11:f3:328:LEU:HD21 | 11:g3:273:CYS:HA   | 2.00                     | 0.43              |
| 11:h3:22:ILE:HA    | 11:h3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:h3:192:GLU:HB2  | 11:h3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:h3:208:ARG:HG3  | 11:h3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:h3:245:ASN:OD1  | 11:h3:245:ASN:N    | 2.33                     | 0.43              |
| 11:j3:46:ASP:OD1   | 11:k3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:l3:208:ARG:HG3  | 11:l3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:o3:185:ILE:O    | 11:o3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:q3:208:ARG:HG3  | 11:q3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:r3:225:VAL:HG12 | 11:r3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:r3:252:LYS:HB2  | 11:r3:252:LYS:HE3  | 1.52                     | 0.43              |
| 11:r3:359:ARG:N    | 11:r3:359:ARG:HD2  | 2.32                     | 0.43              |
| 11:s3:22:ILE:HA    | 11:s3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:t3:32:ARG:H     | 11:t3:95:PRO:HB3   | 1.82                     | 0.43              |
| 11:t3:57:PHE:CE1   | 11:t3:110:MET:HE2  | 2.52                     | 0.43              |
| 11:u3:86:ALA:O     | 11:u3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:v3:57:PHE:CE1   | 11:v3:110:MET:HE2  | 2.52                     | 0.43              |
| 11:w3:185:ILE:O    | 11:w3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:x3:93:TYR:OH    | 11:x3:173:ARG:O    | 2.25                     | 0.43              |
| 11:x3:208:ARG:HG3  | 11:x3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:y3:319:LEU:HD12 | 11:y3:319:LEU:HA   | 1.82                     | 0.43              |
| 11:z3:225:VAL:HG12 | 11:z3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:z3:319:LEU:HD12 | 11:z3:319:LEU:HA   | 1.82                     | 0.43              |
| 1:A1:409:MET:HE2   | 1:A1:409:MET:HA    | 1.99                     | 0.43              |
| 1:F1:393:TYR:CE1   | 1:F1:403:PRO:HA    | 2.53                     | 0.43              |
| 1:G1:231:ASN:OD1   | 1:G1:232:ASP:N     | 2.45                     | 0.43              |
| 1:G1:420:MET:SD    | 1:G1:422:PHE:HD1   | 2.41                     | 0.43              |
| 1:H1:372:ILE:O     | 1:I1:277:GLN:HA    | 2.18                     | 0.43              |
| 1:M1:279:GLU:CD    | 1:M1:281:HIS:H     | 2.26                     | 0.43              |
| 1:R1:186:LEU:HD12  | 1:R1:186:LEU:HA    | 1.73                     | 0.43              |
| 1:U1:129:GLN:O     | 1:U1:133:GLN:HG2   | 2.18                     | 0.43              |
| 1:b1:407:ASP:O     | 1:b1:410:LYS:HG2   | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:c1:420:MET:HE3   | 1:c1:422:PHE:HB2   | 2.00                     | 0.43              |
| 1:h1:164:LEU:O     | 2:C2:144:GLU:N     | 2.50                     | 0.43              |
| 1:h1:252:ILE:HD13  | 1:h1:252:ILE:HA    | 1.90                     | 0.43              |
| 2:D2:45:LEU:HD13   | 6:R2:133:VAL:HG13  | 2.01                     | 0.43              |
| 6:U2:51:LYS:HB2    | 6:U2:51:LYS:HE3    | 1.53                     | 0.43              |
| 7:W2:37:PRO:HG3    | 8:b2:45:PRO:HD2    | 2.00                     | 0.43              |
| 9:h2:79:ARG:HD3    | 9:h2:79:ARG:HA     | 1.80                     | 0.43              |
| 9:j2:244:SER:OG    | 9:n2:260:LEU:HD23  | 2.18                     | 0.43              |
| 10:B3:106:PHE:O    | 10:B3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:H3:84:GLU:HG2   | 10:H3:197:SER:OG   | 2.19                     | 0.43              |
| 10:J3:106:PHE:O    | 10:J3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:K3:170:ALA:HB3  | 10:L3:206:GLU:HG3  | 1.99                     | 0.43              |
| 10:N3:37:ALA:HB1   | 10:O3:74:ILE:CG2   | 2.48                     | 0.43              |
| 10:N3:148:LEU:HD13 | 10:N3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:N3:170:ALA:HB3  | 10:O3:206:GLU:HG3  | 2.00                     | 0.43              |
| 10:N3:222:LEU:HB2  | 10:O3:231:PRO:HB3  | 2.00                     | 0.43              |
| 10:O3:170:ALA:HB3  | 10:P3:206:GLU:HG3  | 2.00                     | 0.43              |
| 10:Q3:84:GLU:HG2   | 10:Q3:197:SER:OG   | 2.19                     | 0.43              |
| 10:U3:170:ALA:HB3  | 10:V3:206:GLU:HG3  | 2.00                     | 0.43              |
| 10:V3:65:LEU:HD23  | 11:v3:68:GLN:HG2   | 2.00                     | 0.43              |
| 10:V3:106:PHE:O    | 10:V3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:V3:171:ILE:O    | 10:V3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:W3:222:LEU:HB2  | 10:X3:231:PRO:HB3  | 2.00                     | 0.43              |
| 10:X3:171:ILE:O    | 10:X3:172:ASN:HB3  | 2.18                     | 0.43              |
| 11:a3:185:ILE:O    | 11:a3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:c3:192:GLU:HB2  | 11:c3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:d3:32:ARG:H     | 11:d3:95:PRO:HB3   | 1.82                     | 0.43              |
| 11:d3:83:ASN:ND2   | 11:e3:109:SER:OG   | 2.45                     | 0.43              |
| 11:f3:123:MET:CE   | 11:f3:136:LEU:HD22 | 2.38                     | 0.43              |
| 11:f3:141:ILE:HD13 | 11:f3:165:ILE:CD1  | 2.37                     | 0.43              |
| 11:g3:73:VAL:HG11  | 11:g3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:h3:86:ALA:O     | 11:h3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:i3:86:ALA:O     | 11:i3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:k3:22:ILE:HA    | 11:k3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:m3:192:GLU:HB2  | 11:m3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:n3:73:VAL:HG11  | 11:n3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:o3:22:ILE:HA    | 11:o3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:o3:23:ARG:NH1   | 11:p3:249:GLN:O    | 2.51                     | 0.43              |
| 11:o3:328:LEU:HD21 | 11:p3:273:CYS:HA   | 2.00                     | 0.43              |
| 11:s3:32:ARG:H     | 11:s3:95:PRO:HB3   | 1.82                     | 0.43              |
| 11:s3:46:ASP:OD1   | 11:t3:160:LEU:HD12 | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:s3:208:ARG:HG3  | 11:s3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:s3:352:MET:O    | 11:s3:356:GLY:O    | 2.35                     | 0.43              |
| 11:t3:217:ASP:OD1  | 11:t3:219:ARG:N    | 2.37                     | 0.43              |
| 11:v3:22:ILE:HA    | 11:v3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:v3:352:MET:O    | 11:v3:356:GLY:O    | 2.35                     | 0.43              |
| 11:w3:57:PHE:CE1   | 11:w3:110:MET:HE2  | 2.52                     | 0.43              |
| 11:x3:252:LYS:HB2  | 11:x3:252:LYS:HE3  | 1.52                     | 0.43              |
| 11:y3:225:VAL:HG12 | 11:y3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:z3:185:ILE:O    | 11:z3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:z3:352:MET:O    | 11:z3:356:GLY:O    | 2.35                     | 0.43              |
| 12:A4:136:VAL:HG21 | 12:A4:156:LEU:HD12 | 1.99                     | 0.43              |
| 1:A1:431:ASN:HD21  | 1:h1:414:ASP:HB3   | 1.82                     | 0.43              |
| 1:C1:176:VAL:HB    | 1:C1:212:LEU:HD23  | 2.00                     | 0.43              |
| 1:E1:195:VAL:HG13  | 1:E1:210:VAL:CG2   | 2.48                     | 0.43              |
| 1:N1:197:LEU:HD11  | 1:O1:177:THR:CG2   | 2.47                     | 0.43              |
| 1:Q1:161:LYS:HD2   | 1:Q1:163:SER:HA    | 2.01                     | 0.43              |
| 1:W1:191:ILE:O     | 1:W1:195:VAL:HG23  | 2.18                     | 0.43              |
| 1:W1:244:ARG:HH21  | 1:W1:244:ARG:HG3   | 1.83                     | 0.43              |
| 1:X1:393:TYR:HB3   | 1:X1:402:LEU:N     | 2.33                     | 0.43              |
| 1:d1:188:GLU:HA    | 1:d1:191:ILE:HG12  | 1.99                     | 0.43              |
| 1:g1:125:GLN:O     | 1:g1:128:GLU:HG3   | 2.19                     | 0.43              |
| 2:D2:138:MET:O     | 2:D2:142:THR:HG23  | 2.19                     | 0.43              |
| 4:G2:6:VAL:HA      | 4:G2:9:MET:HG2     | 2.01                     | 0.43              |
| 6:T2:51:LYS:HZ3    | 6:T2:55:ARG:HE     | 1.65                     | 0.43              |
| 7:W2:74:GLU:O      | 7:W2:76:LEU:HD12   | 2.18                     | 0.43              |
| 7:Y2:83:PRO:HG2    | 9:i2:62:LEU:HD23   | 2.01                     | 0.43              |
| 7:a2:112:TYR:O     | 7:a2:116:ILE:HG12  | 2.19                     | 0.43              |
| 8:c2:46:VAL:O      | 8:c2:47:ASP:C      | 2.61                     | 0.43              |
| 8:f2:196:ASP:O     | 8:f2:198:SER:N     | 2.45                     | 0.43              |
| 9:k2:36:ARG:HG3    | 9:k2:80:LEU:HD12   | 2.00                     | 0.43              |
| 9:n2:95:VAL:O      | 9:n2:118:GLY:HA3   | 2.18                     | 0.43              |
| 9:o2:100:GLN:N     | 9:o2:100:GLN:OE1   | 2.51                     | 0.43              |
| 9:p2:249:THR:O     | 9:p2:253:MET:HG3   | 2.18                     | 0.43              |
| 9:s2:189:GLU:HA    | 9:x2:42:GLU:CG     | 2.48                     | 0.43              |
| 9:t2:79:ARG:NH2    | 9:t2:184:LEU:O     | 2.43                     | 0.43              |
| 9:w2:237:GLN:NE2   | 9:22:252:GLN:OE1   | 2.51                     | 0.43              |
| 9:32:156:VAL:HG13  | 9:32:169:GLN:HG2   | 2.00                     | 0.43              |
| 9:32:173:LEU:HD23  | 9:32:214:LEU:HD21  | 1.99                     | 0.43              |
| 10:A3:45:PRO:CG    | 10:B3:60:TYR:HD1   | 2.32                     | 0.43              |
| 10:B3:84:GLU:HG2   | 10:B3:197:SER:OG   | 2.19                     | 0.43              |
| 10:E3:222:LEU:HB2  | 10:F3:231:PRO:HB3  | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:I3:84:GLU:HG2   | 10:I3:197:SER:OG   | 2.19                     | 0.43              |
| 10:J3:50:SER:HB3   | 11:k3:99:GLN:HE21  | 1.82                     | 0.43              |
| 10:K3:106:PHE:O    | 10:K3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:L3:84:GLU:HG2   | 10:L3:197:SER:OG   | 2.19                     | 0.43              |
| 10:L3:101:LYS:HB2  | 10:L3:101:LYS:NZ   | 2.32                     | 0.43              |
| 10:L3:171:ILE:O    | 10:L3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:M3:101:LYS:HB2  | 10:M3:101:LYS:NZ   | 2.32                     | 0.43              |
| 10:R3:65:LEU:HD23  | 11:r3:68:GLN:HG2   | 2.00                     | 0.43              |
| 10:R3:148:LEU:HD13 | 10:R3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:T3:171:ILE:O    | 10:T3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:V3:101:LYS:HB2  | 10:V3:101:LYS:NZ   | 2.32                     | 0.43              |
| 10:W3:90:LYS:HE3   | 10:W3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:Y3:40:ILE:H     | 10:Y3:40:ILE:HG12  | 1.48                     | 0.43              |
| 10:Y3:84:GLU:HG2   | 10:Y3:197:SER:OG   | 2.19                     | 0.43              |
| 11:a3:319:LEU:HD12 | 11:a3:319:LEU:HA   | 1.82                     | 0.43              |
| 11:c3:32:ARG:H     | 11:c3:95:PRO:HB3   | 1.83                     | 0.43              |
| 11:c3:73:VAL:HG11  | 11:c3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:d3:185:ILE:O    | 11:d3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:d3:225:VAL:HG12 | 11:d3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:d3:359:ARG:HD2  | 11:d3:359:ARG:N    | 2.32                     | 0.43              |
| 11:f3:93:TYR:OH    | 11:f3:173:ARG:O    | 2.25                     | 0.43              |
| 11:h3:32:ARG:H     | 11:h3:95:PRO:HB3   | 1.82                     | 0.43              |
| 11:h3:57:PHE:CE1   | 11:h3:110:MET:HE2  | 2.52                     | 0.43              |
| 11:i3:192:GLU:HB2  | 11:i3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:j3:192:GLU:HB2  | 11:j3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:k3:73:VAL:HG11  | 11:k3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:l3:73:VAL:HG11  | 11:l3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:m3:22:ILE:HA    | 11:m3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:m3:141:ILE:HD13 | 11:m3:165:ILE:CD1  | 2.38                     | 0.43              |
| 11:m3:328:LEU:HD21 | 11:n3:273:CYS:HA   | 2.01                     | 0.43              |
| 11:o3:46:ASP:OD1   | 11:p3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:o3:225:VAL:HG12 | 11:o3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:q3:255:ILE:HD12 | 11:q3:362:LEU:HD12 | 2.01                     | 0.43              |
| 11:r3:185:ILE:O    | 11:r3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:s3:123:MET:HE1  | 11:s3:136:LEU:HB3  | 1.98                     | 0.43              |
| 11:s3:185:ILE:O    | 11:s3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:u3:34:ASN:HB2   | 11:u3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:u3:46:ASP:OD1   | 11:v3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:u3:352:MET:O    | 11:u3:356:GLY:O    | 2.35                     | 0.43              |
| 11:w3:225:VAL:HG12 | 11:w3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:x3:22:ILE:HA    | 11:x3:25:LEU:CD2   | 2.48                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:y3:46:ASP:OD1   | 11:z3:160:LEU:HD12 | 2.17                     | 0.43              |
| 11:z3:93:TYR:OH    | 11:z3:173:ARG:O    | 2.25                     | 0.43              |
| 12:D4:75:ASN:OD1   | 12:D4:76:THR:N     | 2.51                     | 0.43              |
| 1:B1:197:LEU:HD11  | 1:C1:177:THR:OG1   | 2.18                     | 0.43              |
| 1:C1:186:LEU:HD22  | 1:C1:190:GLN:HB3   | 2.00                     | 0.43              |
| 1:E1:160:PRO:HD3   | 1:E1:172:PRO:HA    | 2.00                     | 0.43              |
| 1:G1:234:GLN:HB3   | 1:G1:272:PHE:CZ    | 2.52                     | 0.43              |
| 1:J1:263:HIS:HB2   | 1:J1:390:VAL:HG22  | 2.00                     | 0.43              |
| 1:O1:170:LYS:HD2   | 1:O1:170:LYS:C     | 2.43                     | 0.43              |
| 1:T1:165:PHE:CZ    | 3:F2:170:MET:HG2   | 2.53                     | 0.43              |
| 1:T1:280:GLU:HG2   | 1:T1:282:TYR:CE2   | 2.53                     | 0.43              |
| 1:Y1:142:ARG:HB3   | 1:a1:154:ARG:HH22  | 1.83                     | 0.43              |
| 1:e1:267:THR:OG1   | 1:e1:386:SER:HB2   | 2.19                     | 0.43              |
| 1:g1:252:ILE:O     | 1:g1:255:PRO:HD2   | 2.18                     | 0.43              |
| 2:E2:181:THR:O     | 2:E2:185:ILE:HG12  | 2.18                     | 0.43              |
| 5:N2:71:VAL:HG12   | 5:N2:72:MET:HE2    | 2.00                     | 0.43              |
| 6:S2:114:LEU:HD13  | 7:Y2:127:LEU:HD12  | 2.00                     | 0.43              |
| 8:b2:5:ILE:HG13    | 8:b2:234:ILE:HG12  | 1.99                     | 0.43              |
| 8:f2:174:SER:OG    | 8:f2:180:ARG:NH1   | 2.52                     | 0.43              |
| 9:m2:179:MET:HE3   | 9:m2:179:MET:HB3   | 1.85                     | 0.43              |
| 9:u2:153:ARG:NH1   | 9:u2:213:LEU:HD22  | 2.33                     | 0.43              |
| 9:u2:248:SER:OG    | 9:z2:260:LEU:HD13  | 2.18                     | 0.43              |
| 9:v2:27:ALA:O      | 9:12:72:VAL:HG21   | 2.18                     | 0.43              |
| 9:w2:238:ARG:NH2   | 9:32:255:GLN:HE22  | 2.16                     | 0.43              |
| 9:z2:9:LYS:HB3     | 9:z2:9:LYS:HE3     | 1.69                     | 0.43              |
| 10:A3:84:GLU:HG2   | 10:A3:197:SER:OG   | 2.19                     | 0.43              |
| 10:E3:84:GLU:HG2   | 10:E3:197:SER:OG   | 2.19                     | 0.43              |
| 10:G3:90:LYS:HE3   | 10:G3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:J3:171:ILE:O    | 10:J3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:M3:148:LEU:HD13 | 10:M3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:N3:171:ILE:O    | 10:N3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:O3:148:LEU:HD13 | 10:O3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:P3:101:LYS:HB2  | 10:P3:101:LYS:NZ   | 2.32                     | 0.43              |
| 10:Q3:106:PHE:O    | 10:Q3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:T3:84:GLU:HG2   | 10:T3:197:SER:OG   | 2.19                     | 0.43              |
| 10:X3:101:LYS:HB2  | 10:X3:101:LYS:HZ3  | 1.83                     | 0.43              |
| 10:Y3:121:ARG:HB3  | 10:Z3:111:ARG:HB3  | 1.99                     | 0.43              |
| 11:b3:192:GLU:HB2  | 11:b3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:b3:225:VAL:HG12 | 11:b3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:b3:359:ARG:N    | 11:b3:359:ARG:HD2  | 2.32                     | 0.43              |
| 11:g3:22:ILE:HA    | 11:g3:25:LEU:CD2   | 2.48                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:g3:225:VAL:HG12 | 11:g3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:h3:225:VAL:HG12 | 11:h3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:i3:208:ARG:HG3  | 11:i3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:i3:328:LEU:HD21 | 11:j3:273:CYS:HA   | 2.00                     | 0.43              |
| 11:j3:22:ILE:O     | 11:j3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:k3:22:ILE:O     | 11:k3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:k3:192:GLU:HB2  | 11:k3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:o3:101:GLN:OE1  | 11:p3:219:ARG:HD3  | 2.18                     | 0.43              |
| 11:o3:255:ILE:HD12 | 11:o3:362:LEU:HD12 | 2.01                     | 0.43              |
| 11:p3:86:ALA:O     | 11:p3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:p3:93:TYR:OH    | 11:p3:173:ARG:O    | 2.25                     | 0.43              |
| 11:p3:255:ILE:HD12 | 11:p3:362:LEU:HD12 | 2.01                     | 0.43              |
| 11:q3:86:ALA:O     | 11:q3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:q3:101:GLN:OE1  | 11:r3:219:ARG:HD3  | 2.18                     | 0.43              |
| 11:r3:73:VAL:HG11  | 11:r3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:s3:225:VAL:HG12 | 11:s3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:u3:208:ARG:HG3  | 11:u3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:u3:225:VAL:HG12 | 11:u3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:v3:208:ARG:HG3  | 11:v3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:x3:328:LEU:HD21 | 11:y3:273:CYS:HA   | 2.01                     | 0.43              |
| 11:y3:192:GLU:HB2  | 11:y3:219:ARG:HB2  | 1.99                     | 0.43              |
| 12:C4:122:THR:OG1  | 12:C4:165:TRP:O    | 2.35                     | 0.43              |
| 1:H1:261:ASN:O     | 1:H1:392:ASN:N     | 2.42                     | 0.43              |
| 1:I1:164:LEU:O     | 2:B2:148:ALA:HB1   | 2.19                     | 0.43              |
| 1:J1:389:VAL:HB    | 1:J1:432:VAL:HG13  | 2.01                     | 0.43              |
| 1:N1:191:ILE:HD11  | 1:N1:220:LEU:HD13  | 1.99                     | 0.43              |
| 1:O1:202:VAL:HB    | 1:O1:205:LEU:HD22  | 1.99                     | 0.43              |
| 1:O1:231:ASN:OD1   | 1:O1:232:ASP:N     | 2.51                     | 0.43              |
| 1:Q1:129:GLN:O     | 1:Q1:133:GLN:NE2   | 2.50                     | 0.43              |
| 1:Q1:231:ASN:OD1   | 1:Q1:232:ASP:N     | 2.51                     | 0.43              |
| 1:Q1:252:ILE:O     | 1:Q1:255:PRO:HD2   | 2.18                     | 0.43              |
| 1:W1:373:ARG:NH2   | 1:X1:275:LYS:HE2   | 2.34                     | 0.43              |
| 1:c1:256:ILE:HG21  | 1:c1:412:ILE:HD11  | 2.01                     | 0.43              |
| 2:B2:225:LEU:HD11  | 4:H2:77:VAL:HG21   | 2.00                     | 0.43              |
| 2:D2:207:LEU:HD23  | 2:D2:207:LEU:HA    | 1.87                     | 0.43              |
| 2:E2:84:PRO:HG3    | 3:F2:96:ARG:HH11   | 1.83                     | 0.43              |
| 3:F2:108:LEU:C     | 3:F2:121:ASN:HD21  | 2.20                     | 0.43              |
| 6:R2:44:ASP:OD1    | 6:R2:44:ASP:N      | 2.49                     | 0.43              |
| 8:b2:57:VAL:O      | 8:b2:57:VAL:HG12   | 2.19                     | 0.43              |
| 8:e2:187:ALA:O     | 8:e2:188:GLU:HG2   | 2.18                     | 0.43              |
| 9:i2:130:THR:HG23  | 9:i2:130:THR:O     | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:i2:238:ARG:HD3   | 9:i2:238:ARG:HA    | 1.72                     | 0.43              |
| 9:l2:189:GLU:HA    | 9:q2:42:GLU:HG2    | 2.01                     | 0.43              |
| 9:o2:147:LEU:HB2   | 9:o2:160:THR:HG23  | 2.00                     | 0.43              |
| 9:p2:28:ASN:OD1    | 9:u2:72:VAL:HG22   | 2.17                     | 0.43              |
| 9:p2:36:ARG:HE     | 9:p2:80:LEU:HD22   | 1.84                     | 0.43              |
| 9:r2:205:THR:HG23  | 11:m3:80:GLN:OE1   | 2.18                     | 0.43              |
| 9:v2:226:VAL:HG13  | 9:l2:242:ILE:CD1   | 2.48                     | 0.43              |
| 9:x2:18:ASN:HB2    | 9:x2:41:PHE:HZ     | 1.84                     | 0.43              |
| 9:z2:114:TYR:HE1   | 9:z2:178:PHE:HZ    | 1.66                     | 0.43              |
| 9:22:89:THR:HG23   | 9:22:91:ASN:H      | 1.83                     | 0.43              |
| 10:C3:170:ALA:HB3  | 10:D3:206:GLU:HG3  | 2.00                     | 0.43              |
| 10:F3:37:ALA:HB1   | 10:G3:74:ILE:CG2   | 2.48                     | 0.43              |
| 10:F3:90:LYS:HE3   | 10:F3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:H3:90:LYS:HE3   | 10:H3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:J3:148:LEU:HD13 | 10:J3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:K3:222:LEU:HB2  | 10:L3:231:PRO:HB3  | 2.01                     | 0.43              |
| 10:L3:106:PHE:O    | 10:L3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:N3:84:GLU:HG2   | 10:N3:197:SER:OG   | 2.19                     | 0.43              |
| 10:O3:84:GLU:HG2   | 10:O3:197:SER:OG   | 2.19                     | 0.43              |
| 10:P3:82:LEU:HD12  | 10:P3:146:GLY:HA3  | 1.98                     | 0.43              |
| 10:Q3:40:ILE:H     | 10:Q3:40:ILE:HG12  | 1.48                     | 0.43              |
| 10:Q3:148:LEU:HD13 | 10:Q3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:S3:50:SER:HB3   | 11:t3:99:GLN:HE21  | 1.82                     | 0.43              |
| 10:Y3:149:THR:HG22 | 10:Z3:201:ALA:HB2  | 2.00                     | 0.43              |
| 11:a3:73:VAL:HG11  | 11:a3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:b3:352:MET:O    | 11:b3:356:GLY:O    | 2.35                     | 0.43              |
| 11:c3:328:LEU:HD21 | 11:d3:273:CYS:HA   | 2.01                     | 0.43              |
| 11:d3:192:GLU:HB2  | 11:d3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:d3:208:ARG:HG3  | 11:d3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:h3:359:ARG:N    | 11:h3:359:ARG:HD2  | 2.32                     | 0.43              |
| 11:i3:22:ILE:O     | 11:i3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:l3:22:ILE:HA    | 11:l3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:l3:34:ASN:HB2   | 11:l3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:l3:86:ALA:O     | 11:l3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:l3:225:VAL:HG12 | 11:l3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:m3:83:ASN:ND2   | 11:n3:109:SER:OG   | 2.48                     | 0.43              |
| 11:n3:34:ASN:HB2   | 11:n3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:p3:73:VAL:HG11  | 11:p3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:p3:225:VAL:HG12 | 11:p3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:r3:255:ILE:HD12 | 11:r3:362:LEU:HD12 | 2.01                     | 0.43              |
| 11:s3:255:ILE:HD12 | 11:s3:362:LEU:HD12 | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:t3:352:MET:O    | 11:t3:356:GLY:O    | 2.35                     | 0.43              |
| 11:u3:73:VAL:HG11  | 11:u3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:u3:123:MET:CE   | 11:u3:136:LEU:HD22 | 2.38                     | 0.43              |
| 11:x3:73:VAL:HG11  | 11:x3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:y3:208:ARG:HG3  | 11:y3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:z3:208:ARG:HG3  | 11:z3:235:PHE:CZ   | 2.53                     | 0.43              |
| 12:D4:136:VAL:HG21 | 12:D4:156:LEU:HD12 | 2.01                     | 0.43              |
| 1:C1:164:LEU:HD12  | 2:C2:152:ARG:HD2   | 2.01                     | 0.43              |
| 1:E1:420:MET:SD    | 1:E1:422:PHE:HB2   | 2.58                     | 0.43              |
| 1:F1:426:ARG:HH21  | 1:F1:428:ASP:CG    | 2.27                     | 0.43              |
| 1:G1:153:ALA:HA    | 1:G1:178:VAL:HA    | 1.99                     | 0.43              |
| 1:H1:164:LEU:CD2   | 2:B2:148:ALA:HB2   | 2.45                     | 0.43              |
| 1:J1:234:GLN:OE1   | 1:J1:234:GLN:N     | 2.47                     | 0.43              |
| 1:N1:304:VAL:HG22  | 1:O1:356:ARG:O     | 2.18                     | 0.43              |
| 1:d1:186:LEU:HD12  | 1:d1:186:LEU:HA    | 1.86                     | 0.43              |
| 1:f1:191:ILE:HD11  | 1:f1:220:LEU:HD23  | 2.00                     | 0.43              |
| 1:f1:203:ALA:HA    | 1:g1:158:ALA:HB1   | 2.00                     | 0.43              |
| 1:h1:283:SER:HB2   | 1:h1:369:ASP:HB2   | 2.01                     | 0.43              |
| 2:B2:49:THR:HA     | 2:B2:52:THR:HG22   | 2.00                     | 0.43              |
| 2:C2:205:MET:HA    | 2:C2:205:MET:HE3   | 2.00                     | 0.43              |
| 2:D2:125:GLU:OE1   | 2:D2:125:GLU:N     | 2.49                     | 0.43              |
| 2:E2:69:ILE:O      | 2:E2:73:LEU:HG     | 2.19                     | 0.43              |
| 2:E2:185:ILE:O     | 2:E2:189:ILE:HG12  | 2.19                     | 0.43              |
| 8:d2:71:LEU:HB3    | 8:d2:205:VAL:HG11  | 1.99                     | 0.43              |
| 9:g2:189:GLU:HA    | 9:l2:42:GLU:HG3    | 2.00                     | 0.43              |
| 9:g2:230:LEU:HD13  | 9:g2:233:MET:HE3   | 2.01                     | 0.43              |
| 9:k2:255:GLN:O     | 9:k2:259:GLN:HG2   | 2.18                     | 0.43              |
| 9:l2:109:ASP:OD2   | 9:l2:111:THR:HG22  | 2.18                     | 0.43              |
| 9:o2:89:THR:HG21   | 9:o2:94:ASP:HB2    | 2.00                     | 0.43              |
| 9:w2:215:TYR:CE2   | 9:32:189:GLU:HG2   | 2.54                     | 0.43              |
| 9:x2:120:PHE:O     | 9:x2:121:GLN:HG2   | 2.19                     | 0.43              |
| 9:42:186:SER:HA    | 9:42:192:TYR:HD1   | 1.83                     | 0.43              |
| 10:D3:84:GLU:HG2   | 10:D3:197:SER:OG   | 2.19                     | 0.43              |
| 10:I3:148:LEU:HD13 | 10:I3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:K3:148:LEU:HD13 | 10:K3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:L3:37:ALA:HB1   | 10:M3:74:ILE:CG2   | 2.48                     | 0.43              |
| 10:M3:106:PHE:O    | 10:M3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:P3:37:ALA:HB1   | 10:Q3:74:ILE:CG2   | 2.48                     | 0.43              |
| 10:P3:106:PHE:O    | 10:P3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:Q3:65:LEU:HD23  | 11:q3:68:GLN:HG2   | 2.00                     | 0.43              |
| 10:Q3:149:THR:OG1  | 10:R3:198:THR:O    | 2.35                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:Q3:222:LEU:HB2  | 10:R3:231:PRO:HB3  | 2.00                     | 0.43              |
| 10:S3:65:LEU:HD23  | 11:s3:68:GLN:HG2   | 2.00                     | 0.43              |
| 10:S3:106:PHE:O    | 10:S3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:T3:50:SER:HB3   | 11:u3:99:GLN:HE21  | 1.82                     | 0.43              |
| 10:V3:84:GLU:HG2   | 10:V3:197:SER:OG   | 2.19                     | 0.43              |
| 10:V3:90:LYS:HE3   | 10:V3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:X3:90:LYS:HE3   | 10:X3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:Y3:135:LYS:HB2  | 10:Y3:135:LYS:HE2  | 1.76                     | 0.43              |
| 11:a3:46:ASP:OD1   | 11:b3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:d3:22:ILE:HA    | 11:d3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:e3:359:ARG:N    | 11:e3:359:ARG:HD2  | 2.32                     | 0.43              |
| 11:f3:22:ILE:O     | 11:f3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:f3:83:ASN:ND2   | 11:g3:109:SER:OG   | 2.46                     | 0.43              |
| 11:f3:319:LEU:HD12 | 11:f3:319:LEU:HA   | 1.82                     | 0.43              |
| 11:h3:22:ILE:O     | 11:h3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:h3:185:ILE:O    | 11:h3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:k3:83:ASN:ND2   | 11:l3:109:SER:OG   | 2.46                     | 0.43              |
| 11:l3:22:ILE:O     | 11:l3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:m3:34:ASN:HB2   | 11:m3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:m3:185:ILE:O    | 11:m3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:n3:22:ILE:HA    | 11:n3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:n3:141:ILE:HD13 | 11:n3:165:ILE:CD1  | 2.38                     | 0.43              |
| 11:n3:208:ARG:HG3  | 11:n3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:o3:208:ARG:HG3  | 11:o3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:q3:34:ASN:HB2   | 11:q3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:q3:225:VAL:HG12 | 11:q3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:r3:34:ASN:HB2   | 11:r3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:r3:86:ALA:O     | 11:r3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:s3:34:ASN:HB2   | 11:s3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:s3:73:VAL:HG11  | 11:s3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:s3:328:LEU:HD21 | 11:t3:273:CYS:HA   | 2.01                     | 0.43              |
| 11:t3:93:TYR:OH    | 11:t3:173:ARG:O    | 2.25                     | 0.43              |
| 11:u3:22:ILE:HA    | 11:u3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:u3:101:GLN:OE1  | 11:v3:219:ARG:HD3  | 2.19                     | 0.43              |
| 11:u3:328:LEU:HD21 | 11:v3:273:CYS:HA   | 2.01                     | 0.43              |
| 11:v3:46:ASP:OD1   | 11:w3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:x3:185:ILE:O    | 11:x3:223:VAL:HG22 | 2.18                     | 0.43              |
| 1:D1:249:ILE:CD1   | 1:D1:416:THR:HA    | 2.47                     | 0.43              |
| 1:E1:156:HIS:O     | 1:E1:174:ALA:HA    | 2.18                     | 0.43              |
| 1:F1:239:ASN:HA    | 1:F1:242:GLU:OE1   | 2.19                     | 0.43              |
| 1:G1:203:ALA:HA    | 1:H1:158:ALA:HB1   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:K1:181:GLU:HB3  | 1:K1:184:ARG:NH2   | 2.34                     | 0.43              |
| 1:K1:298:LEU:O    | 1:L1:362:GLU:N     | 2.50                     | 0.43              |
| 1:L1:139:GLU:OE2  | 1:N1:154:ARG:NE    | 2.48                     | 0.43              |
| 1:L1:187:ASP:N    | 1:L1:187:ASP:OD1   | 2.50                     | 0.43              |
| 1:O1:165:PHE:CE1  | 3:F2:141:ASN:ND2   | 2.86                     | 0.43              |
| 1:O1:303:GLN:OE1  | 1:O1:303:GLN:N     | 2.51                     | 0.43              |
| 1:O1:411:GLN:O    | 1:O1:415:LEU:HD13  | 2.17                     | 0.43              |
| 1:Q1:269:GLN:HG3  | 1:Q1:384:ARG:NH1   | 2.34                     | 0.43              |
| 1:T1:393:TYR:CE2  | 1:T1:436:PRO:HD3   | 2.54                     | 0.43              |
| 1:W1:166:VAL:O    | 1:W1:167:ARG:HD3   | 2.18                     | 0.43              |
| 2:B2:65:THR:OG1   | 2:B2:178:GLU:HG2   | 2.18                     | 0.43              |
| 2:B2:90:LEU:HD13  | 5:N2:100:MET:HA    | 2.01                     | 0.43              |
| 2:B2:225:LEU:HD21 | 4:H2:77:VAL:HG21   | 2.00                     | 0.43              |
| 2:C2:56:ALA:O     | 2:C2:60:MET:HB2    | 2.17                     | 0.43              |
| 2:D2:125:GLU:H    | 2:D2:125:GLU:CD    | 2.24                     | 0.43              |
| 2:D2:137:PHE:HZ   | 2:D2:243:PHE:CE2   | 2.36                     | 0.43              |
| 5:P2:81:SER:O     | 5:P2:84:MET:HB3    | 2.18                     | 0.43              |
| 5:P2:87:GLN:HE22  | 7:V2:134:GLN:HE21  | 1.64                     | 0.43              |
| 8:d2:217:MET:HE2  | 9:n2:260:LEU:HD12  | 2.00                     | 0.43              |
| 8:e2:110:THR:HA   | 8:e2:131:GLU:OE2   | 2.18                     | 0.43              |
| 9:i2:2:ILE:HD13   | 9:i2:254:LEU:HD21  | 2.00                     | 0.43              |
| 9:i2:194:GLU:OE1  | 9:i2:201:PRO:HD3   | 2.19                     | 0.43              |
| 9:k2:168:VAL:CG2  | 11:f3:114:LYS:HZ1  | 2.09                     | 0.43              |
| 9:m2:238:ARG:HD3  | 9:m2:238:ARG:HA    | 1.66                     | 0.43              |
| 9:p2:101:GLY:HA3  | 9:p2:175:LEU:HD23  | 1.99                     | 0.43              |
| 9:s2:43:ASP:OD2   | 9:s2:43:ASP:N      | 2.52                     | 0.43              |
| 9:s2:216:GLN:HG2  | 9:s2:217:GLY:N     | 2.33                     | 0.43              |
| 9:t2:105:VAL:CG1  | 9:t2:134:PHE:HB3   | 2.49                     | 0.43              |
| 9:u2:153:ARG:NH1  | 9:u2:213:LEU:HD13  | 2.33                     | 0.43              |
| 9:x2:254:LEU:HD23 | 9:x2:254:LEU:HA    | 1.85                     | 0.43              |
| 10:A3:106:PHE:O   | 10:A3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:D3:78:LEU:HD21 | 10:D3:195:VAL:HG11 | 2.01                     | 0.43              |
| 10:F3:171:ILE:O   | 10:F3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:I3:37:ALA:HB1  | 10:J3:74:ILE:CG2   | 2.48                     | 0.43              |
| 10:J3:40:ILE:H    | 10:J3:40:ILE:HG12  | 1.48                     | 0.43              |
| 10:K3:84:GLU:HG2  | 10:K3:197:SER:OG   | 2.19                     | 0.43              |
| 10:L3:82:LEU:HA   | 10:L3:197:SER:CB   | 2.39                     | 0.43              |
| 10:M3:84:GLU:HG2  | 10:M3:197:SER:OG   | 2.19                     | 0.43              |
| 10:N3:106:PHE:O   | 10:N3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:O3:106:PHE:O   | 10:O3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:S3:37:ALA:HB1  | 10:T3:74:ILE:CG2   | 2.48                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:S3:101:LYS:HB2  | 10:S3:101:LYS:HZ3  | 1.83                     | 0.43              |
| 10:S3:148:LEU:HD13 | 10:S3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:X3:65:LEU:HD23  | 11:x3:68:GLN:HG2   | 2.00                     | 0.43              |
| 10:Y3:130:ASN:CG   | 10:Z3:102:THR:HG22 | 2.43                     | 0.43              |
| 10:Z3:106:PHE:O    | 10:Z3:107:ASP:HB2  | 2.18                     | 0.43              |
| 11:b3:22:ILE:O     | 11:b3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:b3:93:TYR:OH    | 11:b3:173:ARG:O    | 2.25                     | 0.43              |
| 11:c3:83:ASN:ND2   | 11:d3:109:SER:OG   | 2.47                     | 0.43              |
| 11:e3:185:ILE:O    | 11:e3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:f3:22:ILE:HA    | 11:f3:25:LEU:CD2   | 2.48                     | 0.43              |
| 11:l3:185:ILE:O    | 11:l3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:n3:46:ASP:OD1   | 11:o3:160:LEU:HD12 | 2.19                     | 0.43              |
| 11:n3:255:ILE:HD12 | 11:n3:362:LEU:HD12 | 2.01                     | 0.43              |
| 11:o3:34:ASN:HB2   | 11:o3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:o3:86:ALA:O     | 11:o3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:p3:34:ASN:HB2   | 11:p3:93:TYR:HB3   | 2.00                     | 0.43              |
| 11:p3:319:LEU:HD12 | 11:p3:319:LEU:HA   | 1.82                     | 0.43              |
| 11:w3:101:GLN:OE1  | 11:x3:219:ARG:HD3  | 2.19                     | 0.43              |
| 11:w3:252:LYS:HB2  | 11:w3:252:LYS:HE3  | 1.52                     | 0.43              |
| 11:y3:114:LYS:HA   | 11:y3:114:LYS:HD2  | 1.77                     | 0.43              |
| 11:y3:217:ASP:OD1  | 11:y3:219:ARG:N    | 2.37                     | 0.43              |
| 12:A4:129:LEU:HD13 | 12:A4:161:HIS:CD2  | 2.52                     | 0.43              |
| 12:D4:56:ASN:C     | 12:D4:56:ASN:HD22  | 2.24                     | 0.43              |
| 12:D4:133:ALA:HB2  | 12:D4:193:LEU:HD12 | 2.01                     | 0.43              |
| 1:A1:392:ASN:ND2   | 1:A1:437:PHE:HB2   | 2.34                     | 0.43              |
| 1:C1:199:SER:HA    | 1:C1:205:LEU:HD23  | 2.00                     | 0.43              |
| 1:F1:249:ILE:HD13  | 1:F1:419:ALA:HB3   | 2.01                     | 0.43              |
| 1:I1:144:ILE:HG22  | 1:I1:150:VAL:HG11  | 2.01                     | 0.43              |
| 1:M1:413:GLU:HA    | 1:M1:416:THR:HG22  | 2.00                     | 0.43              |
| 1:O1:164:LEU:N     | 3:F2:145:TRP:CH2   | 2.51                     | 0.43              |
| 1:Q1:279:GLU:OE1   | 1:Q1:281:HIS:HB2   | 2.19                     | 0.43              |
| 1:U1:161:LYS:NZ    | 2:E2:245:SER:O     | 2.51                     | 0.43              |
| 1:W1:164:LEU:HD13  | 2:E2:143:ARG:CB    | 2.41                     | 0.43              |
| 1:X1:126:PHE:HA    | 1:X1:129:GLN:NE2   | 2.33                     | 0.43              |
| 1:X1:187:ASP:OD1   | 1:X1:190:GLN:HG3   | 2.19                     | 0.43              |
| 1:Y1:382:ILE:HD12  | 1:Y1:382:ILE:H     | 1.84                     | 0.43              |
| 1:a1:139:GLU:HB3   | 1:c1:156:HIS:CE1   | 2.54                     | 0.43              |
| 1:b1:240:ASP:OD2   | 1:b1:244:ARG:NH2   | 2.51                     | 0.43              |
| 1:b1:404:LEU:H     | 1:b1:434:ASN:HD21  | 1.66                     | 0.43              |
| 1:d1:157:LEU:HD13  | 1:d1:174:ALA:HB2   | 2.00                     | 0.43              |
| 2:C2:140:ARG:NH2   | 2:C2:244:TYR:O     | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:C2:163:GLU:H     | 2:C2:163:GLU:CD    | 2.27                     | 0.43              |
| 2:D2:52:THR:HG21   | 5:M2:93:VAL:HG13   | 2.00                     | 0.43              |
| 2:D2:193:PHE:HB3   | 2:D2:222:LYS:NZ    | 2.34                     | 0.43              |
| 2:E2:49:THR:HG22   | 5:L2:89:ARG:HD3    | 2.01                     | 0.43              |
| 3:F2:132:LEU:O     | 3:F2:136:LEU:HD23  | 2.19                     | 0.43              |
| 6:R2:92:GLN:HG2    | 7:X2:22:ASN:HD22   | 1.84                     | 0.43              |
| 8:c2:152:PRO:HB3   | 9:s2:51:GLN:NE2    | 2.34                     | 0.43              |
| 9:j2:231:VAL:HG11  | 9:p2:9:LYS:HB2     | 2.01                     | 0.43              |
| 9:k2:130:THR:HG22  | 9:k2:134:PHE:O     | 2.18                     | 0.43              |
| 9:m2:152:GLY:HA3   | 9:32:56:SER:O      | 2.18                     | 0.43              |
| 9:q2:2:ILE:HG13    | 9:q2:3:SER:N       | 2.33                     | 0.43              |
| 9:s2:130:THR:O     | 9:s2:130:THR:HG23  | 2.19                     | 0.43              |
| 9:x2:52:PRO:HA     | 9:x2:65:GLY:H      | 1.83                     | 0.43              |
| 9:12:107:LEU:HD21  | 9:12:113:ALA:HB2   | 2.00                     | 0.43              |
| 9:22:181:ASP:O     | 9:22:184:LEU:HD23  | 2.18                     | 0.43              |
| 9:32:206:PRO:HG3   | 9:32:214:LEU:HD13  | 2.00                     | 0.43              |
| 9:32:238:ARG:HG3   | 12:B4:55:ASN:HD21  | 1.84                     | 0.43              |
| 9:42:37:GLN:HB2    | 9:42:79:ARG:NH1    | 2.33                     | 0.43              |
| 10:A3:171:ILE:O    | 10:A3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:B3:78:LEU:HD21  | 10:B3:195:VAL:HG11 | 2.01                     | 0.43              |
| 10:C3:78:LEU:HD21  | 10:C3:195:VAL:HG11 | 2.01                     | 0.43              |
| 10:E3:78:LEU:HD21  | 10:E3:195:VAL:HG11 | 2.01                     | 0.43              |
| 10:F3:222:LEU:HB2  | 10:G3:231:PRO:HB3  | 2.01                     | 0.43              |
| 10:G3:45:PRO:CG    | 10:H3:60:TYR:HD1   | 2.32                     | 0.43              |
| 10:L3:148:LEU:HD13 | 10:L3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:L3:170:ALA:HB3  | 10:M3:206:GLU:HG3  | 2.00                     | 0.43              |
| 10:M3:170:ALA:HB3  | 10:N3:206:GLU:HG3  | 2.00                     | 0.43              |
| 10:O3:124:MET:HE3  | 10:O3:124:MET:HB3  | 1.76                     | 0.43              |
| 10:P3:148:LEU:HD13 | 10:P3:167:LYS:HE2  | 2.01                     | 0.43              |
| 10:R3:50:SER:HB3   | 11:s3:99:GLN:HE21  | 1.83                     | 0.43              |
| 10:X3:171:ILE:HD12 | 10:Z3:88:ALA:CB    | 2.35                     | 0.43              |
| 11:a3:192:GLU:HB2  | 11:a3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:a3:328:LEU:HD21 | 11:b3:273:CYS:HA   | 2.01                     | 0.43              |
| 11:c3:93:TYR:OH    | 11:c3:173:ARG:O    | 2.25                     | 0.43              |
| 11:e3:22:ILE:O     | 11:e3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:e3:32:ARG:H     | 11:e3:95:PRO:HB3   | 1.83                     | 0.43              |
| 11:e3:208:ARG:HG3  | 11:e3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:f3:225:VAL:HG12 | 11:f3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:g3:22:ILE:O     | 11:g3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:k3:225:VAL:HG12 | 11:k3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:m3:22:ILE:O     | 11:m3:25:LEU:HD23  | 2.19                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:t3:34:ASN:HB2   | 11:t3:93:TYR:HB3  | 2.00                     | 0.43              |
| 11:t3:101:GLN:OE1  | 11:u3:219:ARG:HD3 | 2.19                     | 0.43              |
| 12:D4:61:GLN:O     | 12:D4:65:ILE:HG12 | 2.19                     | 0.43              |
| 12:D4:156:LEU:HD22 | 12:D4:161:HIS:CG  | 2.53                     | 0.43              |
| 1:B1:253:LEU:HD22  | 1:B1:412:ILE:HD12 | 1.99                     | 0.43              |
| 1:D1:417:ARG:HG3   | 1:D1:422:PHE:CG   | 2.53                     | 0.43              |
| 1:E1:250:GLU:O     | 1:E1:254:SER:OG   | 2.32                     | 0.43              |
| 1:G1:253:LEU:HD23  | 1:G1:253:LEU:HA   | 1.89                     | 0.43              |
| 1:I1:426:ARG:NH2   | 1:I1:428:ASP:OD1  | 2.52                     | 0.43              |
| 1:M1:267:THR:OG1   | 1:M1:386:SER:HB2  | 2.19                     | 0.43              |
| 1:Q1:155:VAL:HG23  | 1:Q1:176:VAL:HG22 | 2.01                     | 0.43              |
| 1:R1:268:ALA:HA    | 1:R1:385:LEU:HD23 | 2.00                     | 0.43              |
| 1:S1:420:MET:SD    | 1:S1:422:PHE:HD1  | 2.42                     | 0.43              |
| 1:V1:263:HIS:HB2   | 1:V1:390:VAL:CG2  | 2.49                     | 0.43              |
| 1:V1:372:ILE:HG23  | 1:V1:372:ILE:O    | 2.19                     | 0.43              |
| 1:X1:420:MET:HE3   | 1:X1:430:LEU:HD13 | 2.00                     | 0.43              |
| 1:Y1:160:PRO:O     | 1:Y1:161:LYS:HB2  | 2.18                     | 0.43              |
| 1:Y1:267:THR:HG1   | 1:Y1:386:SER:HB2  | 1.83                     | 0.43              |
| 1:Z1:363:THR:HG23  | 6:S2:73:ILE:HD11  | 2.00                     | 0.43              |
| 1:a1:148:GLY:O     | 1:a1:150:VAL:N    | 2.44                     | 0.43              |
| 1:a1:158:ALA:HB3   | 1:a1:173:SER:HB3  | 2.00                     | 0.43              |
| 1:c1:408:GLN:O     | 1:c1:412:ILE:HG12 | 2.18                     | 0.43              |
| 1:f1:193:ALA:HA    | 1:g1:219:LEU:HD21 | 2.01                     | 0.43              |
| 1:g1:191:ILE:HG12  | 1:g1:220:LEU:HD13 | 2.00                     | 0.43              |
| 2:B2:85:PRO:C      | 2:B2:87:GLN:H     | 2.25                     | 0.43              |
| 2:C2:75:ARG:HD2    | 2:C2:81:PRO:HA    | 2.01                     | 0.43              |
| 2:D2:180:LYS:HB3   | 2:D2:180:LYS:HE3  | 1.77                     | 0.43              |
| 4:I2:52:ILE:HG13   | 4:J2:25:LEU:HD12  | 2.01                     | 0.43              |
| 5:N2:58:LYS:HB2    | 5:N2:58:LYS:HE2   | 1.57                     | 0.43              |
| 6:Q2:4:ARG:HG2     | 6:Q2:4:ARG:HH11   | 1.84                     | 0.43              |
| 6:Q2:93:PRO:HG2    | 8:b2:46:VAL:HG13  | 2.00                     | 0.43              |
| 6:R2:34:ASP:OD2    | 7:W2:20:ARG:NH1   | 2.52                     | 0.43              |
| 7:V2:93:MET:HA     | 7:V2:93:MET:HE2   | 2.00                     | 0.43              |
| 7:W2:42:TYR:O      | 7:W2:94:PRO:HB3   | 2.19                     | 0.43              |
| 7:Z2:117:GLU:CD    | 7:Z2:117:GLU:C    | 2.86                     | 0.43              |
| 8:c2:217:MET:HE2   | 8:c2:217:MET:HB2  | 1.72                     | 0.43              |
| 9:g2:2:ILE:HD13    | 9:g2:254:LEU:HD21 | 2.00                     | 0.43              |
| 9:i2:102:PHE:CD1   | 9:i2:116:ARG:HG2  | 2.54                     | 0.43              |
| 9:m2:9:LYS:HE3     | 9:m2:9:LYS:HB3    | 1.80                     | 0.43              |
| 9:n2:169:GLN:OE1   | 11:y3:53:THR:OG1  | 2.13                     | 0.43              |
| 9:p2:98:LYS:O      | 9:p2:212:GLY:CA   | 2.66                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:w2:44:LEU:HB2    | 9:w2:70:THR:O      | 2.19                     | 0.43              |
| 9:w2:195:THR:HG23  | 9:w2:197:SER:N     | 2.25                     | 0.43              |
| 9:y2:27:ALA:C      | 9:42:72:VAL:HG21   | 2.43                     | 0.43              |
| 9:z2:49:ILE:HB     | 9:z2:66:LEU:HD23   | 2.00                     | 0.43              |
| 9:12:98:LYS:O      | 9:12:212:GLY:CA    | 2.67                     | 0.43              |
| 9:12:106:MET:HE2   | 9:12:106:MET:HB3   | 1.85                     | 0.43              |
| 9:32:234:ILE:HG23  | 12:B4:55:ASN:ND2   | 2.30                     | 0.43              |
| 10:A3:60:TYR:HD1   | 10:Z3:45:PRO:CG    | 2.32                     | 0.43              |
| 10:A3:231:PRO:HB3  | 10:Z3:222:LEU:HB2  | 2.01                     | 0.43              |
| 10:D3:221:TRP:NE1  | 10:E3:229:LEU:O    | 2.41                     | 0.43              |
| 10:E3:90:LYS:HE3   | 10:E3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:H3:171:ILE:O    | 10:H3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:P3:168:GLN:HG3  | 10:Q3:204:ARG:NE   | 2.34                     | 0.43              |
| 10:P3:171:ILE:O    | 10:P3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:P3:222:LEU:HB2  | 10:Q3:231:PRO:HB3  | 2.00                     | 0.43              |
| 10:R3:106:PHE:O    | 10:R3:107:ASP:HB2  | 2.18                     | 0.43              |
| 10:S3:84:GLU:HG2   | 10:S3:197:SER:OG   | 2.19                     | 0.43              |
| 10:W3:84:GLU:HG2   | 10:W3:197:SER:OG   | 2.19                     | 0.43              |
| 10:Z3:124:MET:HE3  | 10:Z3:124:MET:HB3  | 1.77                     | 0.43              |
| 11:a3:225:VAL:HG12 | 11:a3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:a3:344:ASP:OD1  | 11:a3:344:ASP:N    | 2.52                     | 0.43              |
| 11:a3:359:ARG:HD2  | 11:a3:359:ARG:N    | 2.32                     | 0.43              |
| 11:e3:101:GLN:OE1  | 11:f3:219:ARG:HD3  | 2.19                     | 0.43              |
| 11:f3:32:ARG:H     | 11:f3:95:PRO:HB3   | 1.82                     | 0.43              |
| 11:f3:73:VAL:HG11  | 11:f3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:g3:32:ARG:H     | 11:g3:95:PRO:HB3   | 1.83                     | 0.43              |
| 11:g3:46:ASP:OD1   | 11:h3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:i3:46:ASP:OD1   | 11:j3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:i3:73:VAL:HG11  | 11:i3:79:MET:HE1   | 2.00                     | 0.43              |
| 11:j3:208:ARG:HG3  | 11:j3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:l3:192:GLU:HB2  | 11:l3:219:ARG:HB2  | 1.99                     | 0.43              |
| 11:r3:22:ILE:O     | 11:r3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:t3:86:ALA:O     | 11:t3:110:MET:HB2  | 2.18                     | 0.43              |
| 11:t3:255:ILE:HD12 | 11:t3:362:LEU:HD12 | 2.01                     | 0.43              |
| 11:u3:252:LYS:HB2  | 11:u3:252:LYS:HE3  | 1.52                     | 0.43              |
| 11:w3:22:ILE:O     | 11:w3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:w3:208:ARG:HG3  | 11:w3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:w3:344:ASP:OD1  | 11:w3:344:ASP:N    | 2.52                     | 0.43              |
| 11:x3:22:ILE:O     | 11:x3:25:LEU:HD23  | 2.19                     | 0.43              |
| 12:E4:125:PHE:HD2  | 12:E4:184:ILE:HD11 | 1.84                     | 0.43              |
| 1:B1:186:LEU:HD12  | 1:B1:186:LEU:HA    | 1.72                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C1:143:THR:HG22 | 1:E1:154:ARG:CD    | 2.48                     | 0.43              |
| 1:D1:275:LYS:HB2  | 1:D1:377:MET:HG2   | 2.01                     | 0.43              |
| 1:G1:304:VAL:N    | 1:H1:356:ARG:O     | 2.48                     | 0.43              |
| 1:I1:302:GLU:HA   | 1:I1:357:SER:O     | 2.19                     | 0.43              |
| 1:N1:196:HIS:ND1  | 1:O1:219:LEU:HD11  | 2.34                     | 0.43              |
| 1:R1:125:GLN:HG2  | 2:E2:234:LEU:HD21  | 2.01                     | 0.43              |
| 1:S1:408:GLN:HA   | 1:S1:411:GLN:NE2   | 2.31                     | 0.43              |
| 1:T1:246:GLN:O    | 1:T1:250:GLU:HG3   | 2.19                     | 0.43              |
| 1:Y1:128:GLU:HG2  | 1:Y1:129:GLN:OE1   | 2.19                     | 0.43              |
| 1:Z1:409:MET:HE2  | 1:Z1:409:MET:HB3   | 1.78                     | 0.43              |
| 1:f1:373:ARG:HH21 | 1:g1:275:LYS:HE2   | 1.83                     | 0.43              |
| 1:g1:211:THR:HA   | 1:g1:221:THR:HG21  | 1.99                     | 0.43              |
| 2:A2:63:SER:HB3   | 2:A2:97:THR:OG1    | 2.19                     | 0.43              |
| 3:F2:65:LEU:HD13  | 3:F2:69:ALA:HB3    | 2.00                     | 0.43              |
| 4:I2:70:LEU:HD23  | 4:J2:3:PRO:HB3     | 2.00                     | 0.43              |
| 5:O2:31:THR:HG23  | 5:O2:33:SER:HB3    | 2.00                     | 0.43              |
| 5:P2:72:MET:HB3   | 7:a2:132:LEU:HD23  | 2.01                     | 0.43              |
| 7:a2:123:LYS:HE2  | 8:f2:247:LEU:O     | 2.18                     | 0.43              |
| 8:d2:35:ARG:NH1   | 8:d2:101:ARG:HD3   | 2.34                     | 0.43              |
| 8:e2:35:ARG:HH11  | 8:e2:101:ARG:HG3   | 1.84                     | 0.43              |
| 8:f2:181:LEU:HB2  | 8:f2:186:GLN:HE21  | 1.84                     | 0.43              |
| 9:i2:233:MET:HE1  | 9:o2:245:LYS:HG3   | 2.00                     | 0.43              |
| 9:j2:7:ILE:O      | 9:j2:10:THR:OG1    | 2.32                     | 0.43              |
| 9:m2:44:LEU:HB2   | 9:m2:70:THR:O      | 2.18                     | 0.43              |
| 9:n2:151:ILE:HG12 | 9:n2:157:VAL:HG23  | 2.01                     | 0.43              |
| 9:q2:49:ILE:HB    | 9:q2:66:LEU:HG     | 2.00                     | 0.43              |
| 9:r2:120:PHE:O    | 9:r2:121:GLN:NE2   | 2.50                     | 0.43              |
| 9:r2:123:ASP:OD2  | 9:r2:127:GLN:HB2   | 2.19                     | 0.43              |
| 9:t2:86:LEU:HB3   | 9:t2:218:TYR:HD2   | 1.83                     | 0.43              |
| 9:y2:101:GLY:O    | 9:y2:116:ARG:NH1   | 2.52                     | 0.43              |
| 9:22:102:PHE:HB3  | 9:22:114:TYR:HB3   | 2.00                     | 0.43              |
| 9:32:128:LEU:HD23 | 9:32:128:LEU:HA    | 1.93                     | 0.43              |
| 10:D3:171:ILE:O   | 10:D3:172:ASN:HB3  | 2.18                     | 0.43              |
| 10:I3:82:LEU:HD12 | 10:I3:146:GLY:HA3  | 1.98                     | 0.43              |
| 10:I3:170:ALA:HB3 | 10:J3:206:GLU:HG3  | 2.00                     | 0.43              |
| 10:L3:78:LEU:HD21 | 10:L3:195:VAL:HG11 | 2.01                     | 0.43              |
| 10:M3:45:PRO:CG   | 10:N3:60:TYR:HD1   | 2.32                     | 0.43              |
| 10:M3:78:LEU:HD21 | 10:M3:195:VAL:HG11 | 2.01                     | 0.43              |
| 10:R3:82:LEU:HD12 | 10:R3:146:GLY:HA3  | 1.98                     | 0.43              |
| 10:R3:84:GLU:HG2  | 10:R3:197:SER:OG   | 2.19                     | 0.43              |
| 10:R3:149:THR:OG1 | 10:S3:198:THR:O    | 2.34                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:R3:222:LEU:HB2  | 10:S3:231:PRO:HB3  | 2.01                     | 0.43              |
| 10:V3:82:LEU:HA    | 10:V3:197:SER:CB   | 2.39                     | 0.43              |
| 10:X3:135:LYS:HB2  | 10:X3:135:LYS:HE2  | 1.76                     | 0.43              |
| 10:Y3:90:LYS:HE3   | 10:Y3:138:ALA:HB3  | 2.00                     | 0.43              |
| 10:Z3:65:LEU:HD23  | 11:z3:68:GLN:HG2   | 2.01                     | 0.43              |
| 11:a3:110:MET:HE1  | 11:z3:66:LEU:HD21  | 2.01                     | 0.43              |
| 11:c3:22:ILE:O     | 11:c3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:c3:359:ARG:HD2  | 11:c3:359:ARG:N    | 2.32                     | 0.43              |
| 11:d3:23:ARG:NH1   | 11:e3:249:GLN:O    | 2.52                     | 0.43              |
| 11:d3:46:ASP:OD1   | 11:e3:160:LEU:HD12 | 2.18                     | 0.43              |
| 11:e3:83:ASN:ND2   | 11:f3:109:SER:OG   | 2.46                     | 0.43              |
| 11:i3:185:ILE:O    | 11:i3:223:VAL:HG22 | 2.18                     | 0.43              |
| 11:i3:225:VAL:HG12 | 11:i3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:k3:208:ARG:HG3  | 11:k3:235:PHE:CZ   | 2.53                     | 0.43              |
| 11:m3:255:ILE:HD12 | 11:m3:362:LEU:HD12 | 2.01                     | 0.43              |
| 11:n3:101:GLN:OE1  | 11:o3:219:ARG:HD3  | 2.19                     | 0.43              |
| 11:n3:225:VAL:HG12 | 11:n3:235:PHE:CD1  | 2.53                     | 0.43              |
| 11:r3:114:LYS:HD2  | 11:r3:114:LYS:HA   | 1.77                     | 0.43              |
| 11:r3:344:ASP:N    | 11:r3:344:ASP:OD1  | 2.52                     | 0.43              |
| 11:s3:101:GLN:OE1  | 11:t3:219:ARG:HD3  | 2.19                     | 0.43              |
| 11:s3:344:ASP:N    | 11:s3:344:ASP:OD1  | 2.52                     | 0.43              |
| 11:v3:22:ILE:O     | 11:v3:25:LEU:HD23  | 2.19                     | 0.43              |
| 11:y3:22:ILE:O     | 11:y3:25:LEU:HD23  | 2.19                     | 0.43              |
| 12:A4:207:THR:HB   | 12:A4:214:LEU:HB2  | 2.01                     | 0.43              |
| 12:B4:59:THR:OG1   | 12:C4:43:GLN:NE2   | 2.52                     | 0.43              |
| 12:C4:132:PRO:O    | 12:C4:188:ASN:ND2  | 2.52                     | 0.43              |
| 1:B1:143:THR:HG21  | 1:C1:156:HIS:NE2   | 2.33                     | 0.42              |
| 1:B1:152:SER:O     | 1:B1:178:VAL:HA    | 2.19                     | 0.42              |
| 1:B1:389:VAL:O     | 1:B1:432:VAL:HA    | 2.18                     | 0.42              |
| 1:G1:167:ARG:NH1   | 2:B2:245:SER:HB3   | 2.34                     | 0.42              |
| 1:I1:392:ASN:OD1   | 1:I1:393:TYR:N     | 2.52                     | 0.42              |
| 1:K1:159:MET:SD    | 1:K1:172:PRO:HB3   | 2.59                     | 0.42              |
| 1:L1:141:ALA:HB1   | 1:L1:153:ALA:O     | 2.19                     | 0.42              |
| 1:N1:298:LEU:HD11  | 1:N1:300:ILE:HD11  | 2.01                     | 0.42              |
| 1:P1:258:GLY:HA3   | 1:P1:261:ASN:ND2   | 2.34                     | 0.42              |
| 1:P1:415:LEU:HD13  | 1:Q1:388:ALA:HB1   | 2.01                     | 0.42              |
| 1:S1:254:SER:HB2   | 1:S1:255:PRO:HD3   | 2.02                     | 0.42              |
| 1:T1:203:ALA:CB    | 1:U1:160:PRO:HG3   | 2.49                     | 0.42              |
| 1:U1:287:ASP:OD1   | 1:U1:288:ALA:N     | 2.52                     | 0.42              |
| 1:W1:157:LEU:HD11  | 1:W1:202:VAL:HG21  | 2.01                     | 0.42              |
| 1:Y1:213:VAL:HG12  | 1:Y1:214:ASP:O     | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Y1:301:SER:O     | 1:Y1:359:GLN:N     | 2.45                     | 0.42              |
| 1:a1:415:LEU:HG    | 1:b1:388:ALA:HB1   | 2.01                     | 0.42              |
| 1:f1:248:ARG:HD2   | 1:g1:267:THR:OG1   | 2.19                     | 0.42              |
| 1:f1:413:GLU:CD    | 1:f1:417:ARG:HH12  | 2.27                     | 0.42              |
| 1:g1:256:ILE:HD13  | 1:g1:256:ILE:HA    | 1.91                     | 0.42              |
| 1:h1:148:GLY:O     | 1:h1:150:VAL:N     | 2.47                     | 0.42              |
| 2:C2:150:PHE:O     | 2:C2:169:ILE:HD12  | 2.18                     | 0.42              |
| 2:D2:37:SER:HA     | 2:D2:124:GLN:OE1   | 2.18                     | 0.42              |
| 2:D2:192:PRO:HB3   | 4:J2:77:VAL:HG22   | 2.01                     | 0.42              |
| 3:F2:14:HIS:CE1    | 3:F2:18:TRP:NE1    | 2.87                     | 0.42              |
| 4:J2:26:LEU:O      | 4:J2:30:ILE:HG12   | 2.18                     | 0.42              |
| 6:Q2:97:GLY:O      | 6:Q2:99:THR:HG23   | 2.19                     | 0.42              |
| 7:a2:123:LYS:HD2   | 8:f2:250:MET:SD    | 2.59                     | 0.42              |
| 8:e2:27:ALA:C      | 9:j2:72:VAL:HG11   | 2.44                     | 0.42              |
| 8:e2:223:ASN:OD1   | 8:e2:226:ARG:NH2   | 2.52                     | 0.42              |
| 8:f2:80:VAL:O      | 8:f2:103:GLY:HA3   | 2.19                     | 0.42              |
| 9:i2:121:GLN:HE21  | 9:o2:78:GLU:HB3    | 1.83                     | 0.42              |
| 9:i2:189:GLU:HA    | 9:o2:42:GLU:CG     | 2.49                     | 0.42              |
| 9:n2:238:ARG:HD3   | 9:n2:238:ARG:HA    | 1.75                     | 0.42              |
| 9:p2:227:ALA:HA    | 9:12:257:LEU:HD21  | 2.00                     | 0.42              |
| 9:q2:140:ILE:HD13  | 9:q2:157:VAL:HG11  | 2.01                     | 0.42              |
| 9:s2:91:ASN:ND2    | 9:s2:93:LYS:HB2    | 2.34                     | 0.42              |
| 9:t2:180:ASN:HB3   | 9:t2:198:SER:HA    | 2.01                     | 0.42              |
| 9:w2:237:GLN:O     | 9:w2:241:GLU:HG2   | 2.19                     | 0.42              |
| 9:22:86:LEU:HD12   | 9:22:218:TYR:HB3   | 2.00                     | 0.42              |
| 9:32:102:PHE:HB3   | 9:32:114:TYR:HB3   | 2.01                     | 0.42              |
| 9:32:174:ASN:HA    | 9:32:206:PRO:HD3   | 2.01                     | 0.42              |
| 10:A3:78:LEU:HD21  | 10:A3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:B3:126:ALA:HB3  | 10:Z3:232:MET:HE1  | 2.00                     | 0.42              |
| 10:G3:84:GLU:HG2   | 10:G3:197:SER:OG   | 2.19                     | 0.42              |
| 10:I3:222:LEU:HB2  | 10:J3:231:PRO:HB3  | 2.01                     | 0.42              |
| 10:M3:37:ALA:HB1   | 10:N3:74:ILE:CG2   | 2.48                     | 0.42              |
| 10:M3:222:LEU:HB2  | 10:N3:231:PRO:HB3  | 2.01                     | 0.42              |
| 10:N3:65:LEU:HD23  | 11:n3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:N3:78:LEU:HD21  | 10:N3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:P3:45:PRO:CG    | 10:Q3:60:TYR:HD1   | 2.32                     | 0.42              |
| 10:Q3:82:LEU:HD12  | 10:Q3:146:GLY:HA3  | 1.98                     | 0.42              |
| 10:R3:37:ALA:HB1   | 10:S3:74:ILE:CG2   | 2.49                     | 0.42              |
| 10:S3:222:LEU:HB2  | 10:T3:231:PRO:HB3  | 2.01                     | 0.42              |
| 10:T3:106:PHE:O    | 10:T3:107:ASP:HB2  | 2.18                     | 0.42              |
| 10:T3:148:LEU:HD13 | 10:T3:167:LYS:HE2  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:V3:45:PRO:CG    | 10:W3:60:TYR:HD1   | 2.32                     | 0.42              |
| 10:V3:148:LEU:HD13 | 10:V3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:V3:168:GLN:HG3  | 10:W3:204:ARG:NE   | 2.34                     | 0.42              |
| 10:W3:101:LYS:HB2  | 10:W3:101:LYS:HZ3  | 1.84                     | 0.42              |
| 10:Y3:50:SER:HB3   | 11:z3:99:GLN:HE21  | 1.82                     | 0.42              |
| 11:b3:344:ASP:N    | 11:b3:344:ASP:OD1  | 2.52                     | 0.42              |
| 11:g3:353:GLN:CG   | 11:g3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:h3:82:LYS:HE2   | 11:h3:82:LYS:HB3   | 1.94                     | 0.42              |
| 11:h3:353:GLN:CG   | 11:h3:362:LEU:HD22 | 2.50                     | 0.42              |
| 11:o3:141:ILE:HD13 | 11:o3:165:ILE:CD1  | 2.38                     | 0.42              |
| 11:p3:46:ASP:OD1   | 11:q3:160:LEU:HD12 | 2.18                     | 0.42              |
| 11:p3:185:ILE:O    | 11:p3:223:VAL:HG22 | 2.18                     | 0.42              |
| 11:s3:86:ALA:O     | 11:s3:110:MET:HB2  | 2.18                     | 0.42              |
| 11:t3:46:ASP:OD1   | 11:u3:160:LEU:HD12 | 2.19                     | 0.42              |
| 11:u3:255:ILE:HD12 | 11:u3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:v3:344:ASP:OD1  | 11:v3:344:ASP:N    | 2.52                     | 0.42              |
| 11:x3:225:VAL:HG12 | 11:x3:235:PHE:CD1  | 2.53                     | 0.42              |
| 11:x3:344:ASP:N    | 11:x3:344:ASP:OD1  | 2.52                     | 0.42              |
| 11:x3:353:GLN:CG   | 11:x3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:z3:22:ILE:O     | 11:z3:25:LEU:HD23  | 2.19                     | 0.42              |
| 12:A4:140:ILE:HB   | 12:A4:149:ARG:HB3  | 2.00                     | 0.42              |
| 1:B1:392:ASN:OD1   | 1:B1:393:TYR:N     | 2.50                     | 0.42              |
| 1:C1:164:LEU:CG    | 2:C2:152:ARG:HD2   | 2.49                     | 0.42              |
| 1:E1:363:THR:CG2   | 6:U2:75:ALA:CB     | 2.89                     | 0.42              |
| 1:L1:276:GLU:OE2   | 1:L1:374:HIS:NE2   | 2.52                     | 0.42              |
| 1:N1:132:TYR:O     | 1:N1:136:LEU:HD23  | 2.17                     | 0.42              |
| 1:N1:266:VAL:HG22  | 1:N1:387:VAL:HG22  | 2.01                     | 0.42              |
| 1:O1:250:GLU:OE2   | 1:O1:264:ALA:N     | 2.52                     | 0.42              |
| 1:P1:297:GLN:HB3   | 1:P1:363:THR:HB    | 2.00                     | 0.42              |
| 1:Q1:163:SER:OG    | 1:Q1:164:LEU:N     | 2.51                     | 0.42              |
| 1:T1:290:LYS:O     | 1:T1:290:LYS:HG2   | 2.20                     | 0.42              |
| 1:W1:151:LYS:HG2   | 1:W1:179:THR:O     | 2.19                     | 0.42              |
| 1:W1:385:LEU:N     | 1:W1:428:ASP:OD2   | 2.47                     | 0.42              |
| 1:a1:191:ILE:HD11  | 1:a1:220:LEU:HD12  | 2.01                     | 0.42              |
| 1:b1:407:ASP:OD1   | 1:b1:408:GLN:N     | 2.52                     | 0.42              |
| 1:g1:141:ALA:O     | 1:g1:145:GLU:HG2   | 2.19                     | 0.42              |
| 1:g1:236:LYS:HE3   | 1:g1:236:LYS:HB3   | 1.75                     | 0.42              |
| 1:h1:273:ALA:HB3   | 1:h1:275:LYS:HE3   | 2.00                     | 0.42              |
| 1:h1:407:ASP:O     | 1:h1:410:LYS:HG2   | 2.19                     | 0.42              |
| 2:A2:183:PHE:CZ    | 3:F2:38:ILE:HD11   | 2.54                     | 0.42              |
| 2:B2:181:THR:O     | 2:B2:185:ILE:HG12  | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:G2:50:SER:C      | 4:G2:53:PRO:HD2    | 2.43                     | 0.42              |
| 5:N2:59:PHE:CE2    | 6:S2:118:MET:HE2   | 2.54                     | 0.42              |
| 6:R2:114:LEU:HD11  | 7:X2:126:MET:CB    | 2.49                     | 0.42              |
| 6:T2:17:ASN:HD22   | 6:T2:17:ASN:C      | 2.25                     | 0.42              |
| 8:b2:226:ARG:O     | 8:b2:230:GLN:HG2   | 2.20                     | 0.42              |
| 8:d2:146:LEU:HD13  | 8:d2:155:VAL:HG12  | 2.02                     | 0.42              |
| 8:f2:66:MET:HE1    | 8:f2:87:TRP:CZ2    | 2.55                     | 0.42              |
| 8:f2:177:GLY:C     | 8:f2:178:LEU:HD12  | 2.43                     | 0.42              |
| 9:j2:130:THR:O     | 9:j2:131:ALA:C     | 2.62                     | 0.42              |
| 9:o2:130:THR:HG23  | 9:o2:130:THR:O     | 2.18                     | 0.42              |
| 9:u2:175:LEU:HD13  | 9:u2:206:PRO:HG3   | 2.01                     | 0.42              |
| 10:B3:45:PRO:CG    | 10:C3:60:TYR:HD1   | 2.32                     | 0.42              |
| 10:F3:45:PRO:CG    | 10:G3:60:TYR:HD1   | 2.33                     | 0.42              |
| 10:F3:78:LEU:HD21  | 10:F3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:G3:222:LEU:HB2  | 10:H3:231:PRO:HB3  | 2.01                     | 0.42              |
| 10:H3:148:LEU:HD13 | 10:H3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:P3:84:GLU:HG2   | 10:P3:197:SER:OG   | 2.19                     | 0.42              |
| 10:R3:171:ILE:O    | 10:R3:172:ASN:HB3  | 2.18                     | 0.42              |
| 10:U3:148:LEU:HD13 | 10:U3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:W3:168:GLN:HG3  | 10:X3:204:ARG:NE   | 2.35                     | 0.42              |
| 10:X3:84:GLU:HG2   | 10:X3:197:SER:OG   | 2.19                     | 0.42              |
| 11:a3:22:ILE:O     | 11:a3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:a3:188:GLN:HB3  | 11:z3:101:GLN:NE2  | 2.33                     | 0.42              |
| 11:e3:22:ILE:HA    | 11:e3:25:LEU:CD2   | 2.48                     | 0.42              |
| 11:e3:141:ILE:HD13 | 11:e3:165:ILE:CD1  | 2.38                     | 0.42              |
| 11:e3:225:VAL:HG12 | 11:e3:235:PHE:CD1  | 2.53                     | 0.42              |
| 11:f3:353:GLN:CG   | 11:f3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:g3:208:ARG:HG3  | 11:g3:235:PHE:CZ   | 2.53                     | 0.42              |
| 11:l3:255:ILE:HD12 | 11:l3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:n3:22:ILE:O     | 11:n3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:r3:208:ARG:HG3  | 11:r3:235:PHE:CZ   | 2.53                     | 0.42              |
| 11:t3:225:VAL:HG12 | 11:t3:235:PHE:CD1  | 2.53                     | 0.42              |
| 11:t3:252:LYS:HB2  | 11:t3:252:LYS:HE3  | 1.52                     | 0.42              |
| 11:u3:185:ILE:O    | 11:u3:223:VAL:HG22 | 2.18                     | 0.42              |
| 11:w3:353:GLN:CG   | 11:w3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:y3:353:GLN:CG   | 11:y3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:y3:359:ARG:HD2  | 11:y3:359:ARG:N    | 2.32                     | 0.42              |
| 1:C1:125:GLN:CB    | 4:H2:75:ASP:OD2    | 2.67                     | 0.42              |
| 1:D1:253:LEU:O     | 1:D1:257:VAL:HG22  | 2.20                     | 0.42              |
| 1:E1:283:SER:HB2   | 1:E1:369:ASP:HB2   | 1.99                     | 0.42              |
| 1:E1:367:GLU:OE1   | 6:U2:68:THR:HG23   | 2.17                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:H1:241:VAL:HG22  | 1:I1:235:LEU:HD21  | 2.00                     | 0.42              |
| 1:H1:269:GLN:O     | 1:H1:270:LEU:HD23  | 2.19                     | 0.42              |
| 1:K1:393:TYR:CZ    | 1:K1:436:PRO:HD3   | 2.54                     | 0.42              |
| 1:N1:293:LEU:HD13  | 1:N1:296:ARG:HE    | 1.84                     | 0.42              |
| 1:P1:231:ASN:CG    | 1:P1:232:ASP:H     | 2.27                     | 0.42              |
| 1:Q1:221:THR:HG23  | 1:Q1:223:SER:H     | 1.84                     | 0.42              |
| 1:T1:405:THR:OG1   | 1:T1:408:GLN:HB2   | 2.19                     | 0.42              |
| 1:V1:382:ILE:HG21  | 1:V1:385:LEU:HG    | 2.00                     | 0.42              |
| 1:Y1:147:LEU:HD11  | 1:a1:217:GLY:H     | 1.85                     | 0.42              |
| 1:b1:381:ASP:OD1   | 1:b1:382:ILE:N     | 2.52                     | 0.42              |
| 1:f1:151:LYS:NZ    | 1:f1:182:PRO:HD3   | 2.35                     | 0.42              |
| 1:f1:164:LEU:CG    | 2:D2:152:ARG:HD2   | 2.49                     | 0.42              |
| 2:A2:150:PHE:HA    | 2:A2:153:LEU:HG    | 2.01                     | 0.42              |
| 2:B2:196:ILE:O     | 2:B2:200:ILE:HG12  | 2.19                     | 0.42              |
| 2:E2:134:LEU:O     | 2:E2:138:MET:HG3   | 2.19                     | 0.42              |
| 3:F2:44:LEU:CD1    | 5:P2:102:MET:HG3   | 2.47                     | 0.42              |
| 3:F2:122:MET:HB3   | 3:F2:123:PRO:HD3   | 2.01                     | 0.42              |
| 3:F2:137:PHE:HB2   | 3:F2:244:PHE:CZ    | 2.54                     | 0.42              |
| 5:K2:86:ILE:HG12   | 5:P2:102:MET:CE    | 2.49                     | 0.42              |
| 8:d2:116:GLN:OE1   | 8:d2:116:GLN:N     | 2.53                     | 0.42              |
| 8:e2:99:TYR:OH     | 8:e2:193:LEU:HD13  | 2.19                     | 0.42              |
| 9:h2:189:GLU:HA    | 9:m2:42:GLU:CG     | 2.49                     | 0.42              |
| 9:i2:154:ASP:HA    | 9:i2:206:PRO:HB2   | 2.02                     | 0.42              |
| 9:p2:130:THR:HG23  | 9:p2:130:THR:O     | 2.18                     | 0.42              |
| 9:p2:252:GLN:O     | 9:p2:255:GLN:HB2   | 2.19                     | 0.42              |
| 9:x2:1:MET:HE3     | 9:x2:1:MET:HB3     | 1.85                     | 0.42              |
| 9:y2:136:VAL:O     | 9:y2:137:GLN:NE2   | 2.53                     | 0.42              |
| 9:z2:101:GLY:HA2   | 9:z2:176:THR:O     | 2.19                     | 0.42              |
| 9:12:91:ASN:OD1    | 9:12:92:SER:N      | 2.53                     | 0.42              |
| 9:22:95:VAL:O      | 9:22:118:GLY:HA3   | 2.19                     | 0.42              |
| 10:F3:82:LEU:HA    | 10:F3:197:SER:CB   | 2.39                     | 0.42              |
| 10:G3:148:LEU:HD13 | 10:G3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:K3:78:LEU:HD21  | 10:K3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:S3:45:PRO:CG    | 10:T3:60:TYR:HD1   | 2.32                     | 0.42              |
| 10:T3:65:LEU:HD23  | 11:t3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:U3:106:PHE:O    | 10:U3:107:ASP:HB2  | 2.18                     | 0.42              |
| 10:U3:135:LYS:HB2  | 10:U3:135:LYS:HE2  | 1.76                     | 0.42              |
| 10:Z3:43:PRO:O     | 10:Z3:43:PRO:CD    | 2.66                     | 0.42              |
| 10:Z3:78:LEU:HD21  | 10:Z3:195:VAL:HG11 | 2.01                     | 0.42              |
| 11:a3:255:ILE:HD12 | 11:a3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:a3:273:CYS:HA   | 11:z3:328:LEU:HD21 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:b3:255:ILE:HD12 | 11:b3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:d3:93:TYR:OH    | 11:d3:173:ARG:O    | 2.25                     | 0.42              |
| 11:d3:344:ASP:OD1  | 11:d3:344:ASP:N    | 2.52                     | 0.42              |
| 11:e3:319:LEU:HD12 | 11:e3:319:LEU:HA   | 1.82                     | 0.42              |
| 11:f3:32:ARG:HH11  | 11:f3:32:ARG:HG2   | 1.85                     | 0.42              |
| 11:h3:46:ASP:OD1   | 11:i3:160:LEU:HD12 | 2.19                     | 0.42              |
| 11:i3:101:GLN:OE1  | 11:j3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:m3:86:ALA:O     | 11:m3:110:MET:HB2  | 2.18                     | 0.42              |
| 11:n3:86:ALA:O     | 11:n3:110:MET:HB2  | 2.18                     | 0.42              |
| 11:p3:101:GLN:OE1  | 11:q3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:q3:22:ILE:O     | 11:q3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:r3:136:LEU:HD13 | 11:s3:129:VAL:HG11 | 2.00                     | 0.42              |
| 11:u3:22:ILE:O     | 11:u3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:v3:73:VAL:HG11  | 11:v3:79:MET:HE1   | 2.00                     | 0.42              |
| 11:v3:101:GLN:OE1  | 11:w3:219:ARG:HD3  | 2.19                     | 0.42              |
| 1:D1:287:ASP:HB3   | 1:D1:290:LYS:HG2   | 2.01                     | 0.42              |
| 1:D1:393:TYR:CZ    | 1:D1:436:PRO:HD3   | 2.54                     | 0.42              |
| 1:E1:207:PRO:O     | 1:E1:210:VAL:HG22  | 2.19                     | 0.42              |
| 1:E1:393:TYR:HB3   | 1:E1:402:LEU:N     | 2.35                     | 0.42              |
| 1:E1:416:THR:O     | 1:E1:420:MET:HG3   | 2.18                     | 0.42              |
| 1:G1:167:ARG:HH12  | 2:B2:245:SER:CB    | 2.33                     | 0.42              |
| 1:H1:378:ASN:HB3   | 1:H1:381:ASP:OD2   | 2.18                     | 0.42              |
| 1:K1:370:ARG:HG2   | 1:K1:371:THR:N     | 2.33                     | 0.42              |
| 1:L1:372:ILE:O     | 1:M1:277:GLN:HA    | 2.19                     | 0.42              |
| 1:Q1:187:ASP:O     | 1:Q1:191:ILE:HG12  | 2.19                     | 0.42              |
| 1:R1:408:GLN:O     | 1:R1:412:ILE:HG12  | 2.20                     | 0.42              |
| 1:T1:161:LYS:NZ    | 1:T1:163:SER:HA    | 2.34                     | 0.42              |
| 1:T1:187:ASP:OD1   | 1:T1:187:ASP:N     | 2.44                     | 0.42              |
| 1:V1:275:LYS:HB3   | 1:V1:377:MET:HE2   | 2.00                     | 0.42              |
| 1:W1:142:ARG:HD2   | 1:X1:154:ARG:HH12  | 1.85                     | 0.42              |
| 1:X1:164:LEU:HD12  | 1:X1:169:GLN:NE2   | 2.34                     | 0.42              |
| 1:Y1:367:GLU:HG3   | 1:Z1:368:VAL:HG11  | 2.01                     | 0.42              |
| 1:a1:253:LEU:HD23  | 1:a1:253:LEU:HA    | 1.84                     | 0.42              |
| 1:d1:418:GLU:HB3   | 1:e1:388:ALA:HB2   | 2.00                     | 0.42              |
| 1:d1:423:SER:HB2   | 1:e1:384:ARG:NH1   | 2.35                     | 0.42              |
| 1:e1:417:ARG:HG3   | 1:e1:422:PHE:CB    | 2.50                     | 0.42              |
| 1:f1:158:ALA:C     | 1:f1:159:MET:HE2   | 2.44                     | 0.42              |
| 4:G2:46:GLU:OE2    | 4:G2:49:LEU:HG     | 2.19                     | 0.42              |
| 5:N2:89:ARG:HD2    | 5:N2:89:ARG:C      | 2.45                     | 0.42              |
| 7:Y2:29:ALA:CB     | 8:d2:57:VAL:HG21   | 2.49                     | 0.42              |
| 7:Y2:109:SER:HA    | 8:d2:240:ASN:HD21  | 1.85                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:b2:46:VAL:O      | 8:b2:47:ASP:C      | 2.63                     | 0.42              |
| 8:d2:99:TYR:OH     | 8:d2:193:LEU:HD13  | 2.20                     | 0.42              |
| 9:i2:123:ASP:OD1   | 9:i2:123:ASP:N     | 2.52                     | 0.42              |
| 9:j2:233:MET:HG2   | 9:n2:249:THR:HG21  | 2.01                     | 0.42              |
| 9:n2:14:ALA:HB2    | 9:n2:72:VAL:HG13   | 2.01                     | 0.42              |
| 9:o2:72:VAL:HG22   | 9:o2:72:VAL:O      | 2.19                     | 0.42              |
| 9:t2:233:MET:SD    | 9:y2:246:ALA:HA    | 2.59                     | 0.42              |
| 9:t2:257:LEU:O     | 9:t2:260:LEU:HB3   | 2.19                     | 0.42              |
| 9:y2:238:ARG:NH2   | 12:D4:52:PRO:CA    | 2.80                     | 0.42              |
| 9:42:130:THR:HG23  | 9:42:134:PHE:HD2   | 1.84                     | 0.42              |
| 10:A3:90:LYS:HE3   | 10:A3:138:ALA:HB3  | 2.00                     | 0.42              |
| 10:C3:65:LEU:HD23  | 11:c3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:F3:65:LEU:HD23  | 11:f3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:F3:84:GLU:HG2   | 10:F3:197:SER:OG   | 2.19                     | 0.42              |
| 10:F3:148:LEU:HD13 | 10:F3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:H3:65:LEU:HD23  | 11:h3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:J3:84:GLU:HG2   | 10:J3:197:SER:OG   | 2.19                     | 0.42              |
| 10:K3:65:LEU:HD23  | 11:k3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:L3:45:PRO:CG    | 10:M3:60:TYR:HD1   | 2.33                     | 0.42              |
| 10:L3:222:LEU:HB2  | 10:M3:231:PRO:HB3  | 2.01                     | 0.42              |
| 10:M3:65:LEU:HD23  | 11:m3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:Q3:168:GLN:HG3  | 10:R3:204:ARG:NE   | 2.35                     | 0.42              |
| 10:U3:84:GLU:HG2   | 10:U3:197:SER:OG   | 2.19                     | 0.42              |
| 10:W3:135:LYS:HE2  | 10:W3:135:LYS:HB2  | 1.76                     | 0.42              |
| 10:X3:29:PRO:HB3   | 10:Y3:179:ARG:HH21 | 1.85                     | 0.42              |
| 10:Z3:90:LYS:HE3   | 10:Z3:138:ALA:HB3  | 2.00                     | 0.42              |
| 11:c3:46:ASP:OD1   | 11:d3:160:LEU:HD12 | 2.19                     | 0.42              |
| 11:c3:196:MET:HA   | 11:c3:196:MET:CE   | 2.34                     | 0.42              |
| 11:c3:255:ILE:HD12 | 11:c3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:d3:136:LEU:HD13 | 11:e3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:d3:255:ILE:HD12 | 11:d3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:g3:114:LYS:HD2  | 11:g3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:g3:328:LEU:HD21 | 11:h3:273:CYS:HA   | 2.01                     | 0.42              |
| 11:h3:217:ASP:OD1  | 11:h3:219:ARG:N    | 2.37                     | 0.42              |
| 11:i3:353:GLN:CG   | 11:i3:362:LEU:HD22 | 2.50                     | 0.42              |
| 11:j3:114:LYS:HA   | 11:j3:114:LYS:HD2  | 1.77                     | 0.42              |
| 11:q3:344:ASP:OD1  | 11:q3:344:ASP:N    | 2.52                     | 0.42              |
| 11:s3:22:ILE:O     | 11:s3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:v3:23:ARG:NH1   | 11:w3:249:GLN:O    | 2.52                     | 0.42              |
| 11:v3:353:GLN:CG   | 11:v3:362:LEU:HD22 | 2.49                     | 0.42              |
| 12:A4:75:ASN:C     | 12:A4:75:ASN:HD22  | 2.27                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:D4:165:TRP:CZ2 | 12:D4:175:VAL:HG11 | 2.55                     | 0.42              |
| 1:A1:294:ARG:NE   | 1:A1:367:GLU:OE1   | 2.52                     | 0.42              |
| 1:A1:415:LEU:CD1  | 1:B1:388:ALA:HB1   | 2.49                     | 0.42              |
| 1:E1:134:ARG:HE   | 1:E1:134:ARG:HB3   | 1.70                     | 0.42              |
| 1:E1:186:LEU:HD12 | 1:E1:186:LEU:HA    | 1.82                     | 0.42              |
| 1:H1:141:ALA:O    | 1:H1:144:ILE:N     | 2.52                     | 0.42              |
| 1:J1:408:GLN:O    | 1:J1:411:GLN:HG2   | 2.20                     | 0.42              |
| 1:L1:394:LYS:HG2  | 1:L1:402:LEU:HB2   | 2.01                     | 0.42              |
| 1:T1:186:LEU:HD11 | 1:T1:190:GLN:HB3   | 2.00                     | 0.42              |
| 1:T1:242:GLU:HA   | 1:T1:245:ILE:HG22  | 2.01                     | 0.42              |
| 1:W1:167:ARG:HH21 | 2:E2:142:THR:C     | 2.22                     | 0.42              |
| 1:W1:287:ASP:H    | 1:W1:290:LYS:NZ    | 2.17                     | 0.42              |
| 1:Z1:247:ARG:HA   | 1:Z1:250:GLU:CD    | 2.45                     | 0.42              |
| 1:Z1:271:ASP:O    | 1:Z1:380:GLY:N     | 2.52                     | 0.42              |
| 1:Z1:280:GLU:OE1  | 1:Z1:280:GLU:HA    | 2.19                     | 0.42              |
| 1:a1:186:LEU:HD11 | 1:a1:190:GLN:OE1   | 2.20                     | 0.42              |
| 1:e1:249:ILE:HD13 | 1:e1:419:ALA:HB3   | 2.01                     | 0.42              |
| 1:g1:252:ILE:HG22 | 1:g1:253:LEU:HD22  | 2.02                     | 0.42              |
| 2:A2:107:LYS:HD2  | 2:A2:133:PRO:HG3   | 2.01                     | 0.42              |
| 2:B2:137:PHE:CZ   | 2:B2:243:PHE:CE2   | 3.06                     | 0.42              |
| 4:I2:50:SER:C     | 4:I2:53:PRO:HD2    | 2.44                     | 0.42              |
| 4:I2:60:ILE:O     | 4:I2:64:VAL:HG22   | 2.18                     | 0.42              |
| 5:P2:84:MET:HE2   | 7:V2:130:LEU:HD11  | 2.01                     | 0.42              |
| 6:Q2:111:ASP:OD2  | 7:W2:3:LEU:HA      | 2.17                     | 0.42              |
| 6:R2:93:PRO:HB3   | 8:c2:48:GLY:HA3    | 2.01                     | 0.42              |
| 6:T2:102:MET:O    | 6:T2:106:ARG:HG3   | 2.19                     | 0.42              |
| 6:U2:46:ALA:O     | 6:U2:50:LYS:HG3    | 2.19                     | 0.42              |
| 7:V2:119:LEU:HD23 | 7:V2:119:LEU:HA    | 1.86                     | 0.42              |
| 7:Z2:35:THR:OG1   | 7:Z2:39:GLY:HA2    | 2.19                     | 0.42              |
| 8:d2:26:LEU:HD11  | 9:i2:242:ILE:HG21  | 2.02                     | 0.42              |
| 9:g2:130:THR:O    | 9:g2:131:ALA:C     | 2.63                     | 0.42              |
| 9:g2:160:THR:HG21 | 9:w2:51:GLN:HG2    | 2.00                     | 0.42              |
| 9:h2:130:THR:HG22 | 9:h2:134:PHE:HB2   | 2.00                     | 0.42              |
| 9:j2:91:ASN:HB3   | 9:j2:94:ASP:HB2    | 2.02                     | 0.42              |
| 9:n2:254:LEU:HD23 | 9:n2:254:LEU:HA    | 1.93                     | 0.42              |
| 9:o2:154:ASP:OD1  | 9:42:57:SER:HA     | 2.19                     | 0.42              |
| 9:p2:170:VAL:HA   | 11:c3:53:THR:CG2   | 2.48                     | 0.42              |
| 9:v2:116:ARG:HH21 | 9:v2:220:GLU:CD    | 2.28                     | 0.42              |
| 9:w2:254:LEU:O    | 9:w2:258:THR:HG23  | 2.20                     | 0.42              |
| 10:C3:90:LYS:HE3  | 10:C3:138:ALA:HB3  | 2.00                     | 0.42              |
| 10:D3:90:LYS:HE3  | 10:D3:138:ALA:HB3  | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:G3:78:LEU:HD21  | 10:G3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:I3:65:LEU:HD23  | 11:i3:68:GLN:HG2   | 2.01                     | 0.42              |
| 10:J3:45:PRO:CG    | 10:K3:60:TYR:HD1   | 2.32                     | 0.42              |
| 10:O3:65:LEU:HD23  | 11:o3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:V3:135:LYS:HB2  | 10:V3:135:LYS:HE2  | 1.76                     | 0.42              |
| 10:W3:65:LEU:HD23  | 11:w3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:Z3:84:GLU:HG2   | 10:Z3:197:SER:OG   | 2.19                     | 0.42              |
| 11:a3:83:ASN:ND2   | 11:b3:109:SER:OG   | 2.49                     | 0.42              |
| 11:b3:208:ARG:HG3  | 11:b3:235:PHE:CZ   | 2.53                     | 0.42              |
| 11:c3:101:GLN:OE1  | 11:d3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:d3:42:VAL:CG1   | 11:d3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:e3:123:MET:CE   | 11:e3:136:LEU:HD22 | 2.38                     | 0.42              |
| 11:e3:353:GLN:CG   | 11:e3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:f3:359:ARG:HD2  | 11:f3:359:ARG:N    | 2.32                     | 0.42              |
| 11:h3:101:GLN:OE1  | 11:i3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:h3:136:LEU:HD13 | 11:i3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:i3:166:THR:HG21 | 11:k3:362:LEU:HD23 | 2.01                     | 0.42              |
| 11:j3:23:ARG:NH1   | 11:k3:249:GLN:O    | 2.52                     | 0.42              |
| 11:l3:101:GLN:OE1  | 11:m3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:m3:101:GLN:OE1  | 11:n3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:t3:344:ASP:OD1  | 11:t3:344:ASP:N    | 2.52                     | 0.42              |
| 11:v3:255:ILE:HD12 | 11:v3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:w3:114:LYS:HD2  | 11:w3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:x3:23:ARG:NH1   | 11:y3:249:GLN:O    | 2.53                     | 0.42              |
| 11:z3:255:ILE:HD12 | 11:z3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:z3:344:ASP:OD1  | 11:z3:344:ASP:N    | 2.52                     | 0.42              |
| 11:z3:353:GLN:CG   | 11:z3:362:LEU:HD22 | 2.50                     | 0.42              |
| 1:C1:166:VAL:HG22  | 1:C1:168:GLU:OE1   | 2.19                     | 0.42              |
| 1:D1:373:ARG:HH21  | 1:E1:275:LYS:HZ2   | 1.67                     | 0.42              |
| 1:E1:145:GLU:OE2   | 1:E1:153:ALA:N     | 2.53                     | 0.42              |
| 1:H1:231:ASN:OD1   | 1:H1:232:ASP:N     | 2.51                     | 0.42              |
| 1:H1:262:VAL:HG23  | 1:H1:391:VAL:HG12  | 2.02                     | 0.42              |
| 1:N1:166:VAL:HG22  | 2:A2:161:GLY:O     | 2.12                     | 0.42              |
| 1:O1:187:ASP:OD1   | 1:O1:187:ASP:N     | 2.50                     | 0.42              |
| 1:O1:293:LEU:HD13  | 1:O1:296:ARG:HB2   | 2.01                     | 0.42              |
| 1:Q1:233:ALA:HA    | 1:Q1:236:LYS:HE2   | 2.01                     | 0.42              |
| 1:R1:409:MET:HE1   | 1:R1:434:ASN:HB2   | 1.99                     | 0.42              |
| 1:S1:268:ALA:HA    | 1:S1:385:LEU:HD23  | 2.02                     | 0.42              |
| 1:U1:159:MET:HA    | 1:U1:172:PRO:HB3   | 2.01                     | 0.42              |
| 1:X1:372:ILE:HG23  | 1:X1:372:ILE:O     | 2.20                     | 0.42              |
| 1:f1:420:MET:HE1   | 1:f1:428:ASP:HB3   | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:g1:144:ILE:HD11  | 1:g1:197:LEU:HD22  | 2.02                     | 0.42              |
| 2:A2:115:PRO:CB    | 2:A2:121:ILE:HD12  | 2.43                     | 0.42              |
| 3:F2:104:LEU:HD13  | 3:F2:109:SER:HB3   | 2.02                     | 0.42              |
| 6:S2:17:ASN:C      | 6:S2:17:ASN:HD22   | 2.27                     | 0.42              |
| 7:W2:30:ASN:ND2    | 8:b2:57:VAL:HG22   | 2.35                     | 0.42              |
| 7:W2:39:GLY:O      | 7:W2:40:GLN:HG3    | 2.19                     | 0.42              |
| 8:b2:183:ALA:HA    | 8:b2:186:GLN:HG3   | 2.00                     | 0.42              |
| 8:c2:186:GLN:C     | 8:c2:188:GLU:H     | 2.27                     | 0.42              |
| 8:f2:42:ARG:HD2    | 9:k2:64:SER:CB     | 2.50                     | 0.42              |
| 8:f2:176:ASP:C     | 8:f2:178:LEU:H     | 2.28                     | 0.42              |
| 9:i2:6:TRP:HZ3     | 9:i2:9:LYS:HE3     | 1.77                     | 0.42              |
| 9:m2:98:LYS:HE3    | 9:m2:98:LYS:HB3    | 1.87                     | 0.42              |
| 9:p2:70:THR:O      | 9:p2:70:THR:HG23   | 2.19                     | 0.42              |
| 9:p2:85:ASN:HD22   | 9:12:70:THR:HG21   | 1.84                     | 0.42              |
| 9:t2:116:ARG:NH2   | 9:t2:220:GLU:OE1   | 2.52                     | 0.42              |
| 9:12:178:PHE:CE2   | 9:12:201:PRO:HB3   | 2.54                     | 0.42              |
| 10:A3:37:ALA:HB1   | 10:B3:74:ILE:CG2   | 2.49                     | 0.42              |
| 10:B3:90:LYS:HE3   | 10:B3:138:ALA:HB3  | 2.00                     | 0.42              |
| 10:D3:65:LEU:HD23  | 11:d3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:J3:78:LEU:HD21  | 10:J3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:O3:78:LEU:HD21  | 10:O3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:P3:78:LEU:HD21  | 10:P3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:T3:168:GLN:HG3  | 10:U3:204:ARG:NE   | 2.35                     | 0.42              |
| 10:U3:222:LEU:HB2  | 10:V3:231:PRO:HB3  | 2.02                     | 0.42              |
| 11:a3:353:GLN:CG   | 11:a3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:b3:136:LEU:HD13 | 11:c3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:c3:344:ASP:OD1  | 11:c3:344:ASP:N    | 2.52                     | 0.42              |
| 11:d3:22:ILE:O     | 11:d3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:d3:166:THR:HG21 | 11:f3:362:LEU:HD23 | 2.02                     | 0.42              |
| 11:e3:255:ILE:HD12 | 11:e3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:g3:136:LEU:HD13 | 11:h3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:j3:73:VAL:HG11  | 11:j3:79:MET:HE1   | 2.00                     | 0.42              |
| 11:k3:101:GLN:OE1  | 11:l3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:o3:32:ARG:HH11  | 11:o3:32:ARG:HG2   | 1.85                     | 0.42              |
| 11:o3:208:ARG:NH2  | 11:o3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:o3:353:GLN:CG   | 11:o3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:p3:353:GLN:CG   | 11:p3:362:LEU:HD22 | 2.50                     | 0.42              |
| 11:q3:353:GLN:CG   | 11:q3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:u3:41:LEU:HD23  | 11:u3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:v3:319:LEU:HD12 | 11:v3:319:LEU:HA   | 1.82                     | 0.42              |
| 11:w3:42:VAL:CG1   | 11:w3:45:LEU:HD21  | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:z3:271:ASP:HB3  | 11:z3:357:CYS:CA   | 2.34                     | 0.42              |
| 12:A4:134:ASP:OD2  | 12:A4:189:GLY:N    | 2.50                     | 0.42              |
| 12:C4:100:GLY:HA3  | 12:C4:200:PHE:CZ   | 2.54                     | 0.42              |
| 12:C4:162:THR:HG21 | 12:C4:232:ILE:HD11 | 2.00                     | 0.42              |
| 1:B1:186:LEU:HD11  | 1:B1:190:GLN:HB2   | 2.01                     | 0.42              |
| 1:C1:164:LEU:CD2   | 2:C2:149:LEU:CD1   | 2.85                     | 0.42              |
| 1:C1:369:ASP:OD1   | 1:D1:282:TYR:HB2   | 2.19                     | 0.42              |
| 1:E1:205:LEU:HD12  | 1:E1:206:PRO:HD2   | 2.02                     | 0.42              |
| 1:E1:254:SER:HB2   | 1:E1:255:PRO:HD3   | 2.02                     | 0.42              |
| 1:G1:206:PRO:HG2   | 1:G1:209:ASN:OD1   | 2.19                     | 0.42              |
| 1:G1:405:THR:OG1   | 1:G1:407:ASP:OD1   | 2.21                     | 0.42              |
| 1:K1:269:GLN:O     | 1:K1:382:ILE:HD12  | 2.19                     | 0.42              |
| 1:L1:139:GLU:CD    | 1:N1:154:ARG:HH11  | 2.27                     | 0.42              |
| 1:Q1:245:ILE:HG21  | 1:Q1:266:VAL:HG11  | 2.00                     | 0.42              |
| 1:R1:407:ASP:HA    | 1:R1:410:LYS:HE3   | 2.02                     | 0.42              |
| 1:S1:385:LEU:HD23  | 1:S1:385:LEU:HA    | 1.82                     | 0.42              |
| 1:W1:167:ARG:HB3   | 1:X1:165:PHE:CD1   | 2.55                     | 0.42              |
| 1:Z1:239:ASN:HA    | 1:Z1:242:GLU:OE1   | 2.20                     | 0.42              |
| 1:Z1:280:GLU:HG3   | 1:Z1:282:TYR:HE2   | 1.85                     | 0.42              |
| 1:c1:181:GLU:HB3   | 1:c1:184:ARG:HD3   | 2.02                     | 0.42              |
| 1:c1:411:GLN:O     | 1:c1:415:LEU:HG    | 2.20                     | 0.42              |
| 1:d1:164:LEU:HD21  | 1:f1:165:PHE:HA    | 2.02                     | 0.42              |
| 1:d1:206:PRO:HG2   | 1:d1:209:ASN:OD1   | 2.19                     | 0.42              |
| 1:g1:252:ILE:CG1   | 1:h1:265:GLN:HB2   | 2.49                     | 0.42              |
| 2:A2:52:THR:O      | 2:A2:55:PRO:HD2    | 2.20                     | 0.42              |
| 2:B2:42:VAL:HG13   | 5:O2:42:LEU:HD22   | 2.02                     | 0.42              |
| 2:C2:39:SER:C      | 2:C2:41:SER:H      | 2.28                     | 0.42              |
| 3:F2:229:MET:HG2   | 4:G2:14:MET:HE2    | 2.01                     | 0.42              |
| 6:Q2:103:ASP:OD1   | 7:W2:112:TYR:OH    | 2.24                     | 0.42              |
| 6:T2:92:GLN:NE2    | 7:Z2:19:LYS:HG2    | 2.34                     | 0.42              |
| 6:U2:41:ARG:HB3    | 6:U2:85:LEU:HD22   | 2.02                     | 0.42              |
| 6:U2:92:GLN:NE2    | 7:a2:19:LYS:HG2    | 2.31                     | 0.42              |
| 8:c2:117:GLY:O     | 8:c2:118:HIS:CG    | 2.72                     | 0.42              |
| 8:f2:22:THR:O      | 8:f2:26:LEU:N      | 2.53                     | 0.42              |
| 9:i2:26:LEU:HD21   | 9:o2:242:ILE:HG22  | 2.02                     | 0.42              |
| 9:n2:130:THR:HG23  | 9:n2:130:THR:O     | 2.19                     | 0.42              |
| 9:r2:143:PRO:HD2   | 9:r2:159:VAL:HG21  | 2.01                     | 0.42              |
| 9:s2:127:GLN:HA    | 9:s2:140:ILE:O     | 2.19                     | 0.42              |
| 9:v2:27:ALA:C      | 9:12:72:VAL:HG21   | 2.45                     | 0.42              |
| 9:v2:55:GLN:HA     | 9:v2:61:THR:HA     | 2.02                     | 0.42              |
| 9:w2:136:VAL:O     | 9:w2:137:GLN:NE2   | 2.52                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:y2:238:ARG:HH21  | 12:D4:52:PRO:N     | 2.17                     | 0.42              |
| 9:22:72:VAL:O      | 9:22:73:ARG:C      | 2.63                     | 0.42              |
| 10:A3:148:LEU:HD13 | 10:A3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:A3:170:ALA:HB3  | 10:B3:206:GLU:HG3  | 2.01                     | 0.42              |
| 10:E3:148:LEU:HD13 | 10:E3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:J3:168:GLN:HG3  | 10:K3:204:ARG:NE   | 2.34                     | 0.42              |
| 10:L3:117:PHE:HD1  | 10:L3:122:ALA:CB   | 2.33                     | 0.42              |
| 10:L3:149:THR:OG1  | 10:M3:198:THR:O    | 2.34                     | 0.42              |
| 10:W3:148:LEU:HD13 | 10:W3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:X3:37:ALA:HB1   | 10:Y3:74:ILE:CG2   | 2.48                     | 0.42              |
| 10:Y3:43:PRO:O     | 10:Y3:43:PRO:CD    | 2.67                     | 0.42              |
| 11:b3:46:ASP:OD1   | 11:c3:160:LEU:HD12 | 2.19                     | 0.42              |
| 11:c3:32:ARG:HG2   | 11:c3:32:ARG:HH11  | 1.85                     | 0.42              |
| 11:c3:42:VAL:CG1   | 11:c3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:f3:101:GLN:OE1  | 11:g3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:h3:73:VAL:HG11  | 11:h3:79:MET:HE1   | 2.00                     | 0.42              |
| 11:h3:208:ARG:NH2  | 11:h3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:i3:32:ARG:HH11  | 11:i3:32:ARG:HG2   | 1.85                     | 0.42              |
| 11:j3:353:GLN:CG   | 11:j3:362:LEU:HD22 | 2.50                     | 0.42              |
| 11:k3:344:ASP:N    | 11:k3:344:ASP:OD1  | 2.52                     | 0.42              |
| 11:l3:114:LYS:HD2  | 11:l3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:m3:114:LYS:HD2  | 11:m3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:n3:114:LYS:HD2  | 11:n3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:n3:208:ARG:NH2  | 11:n3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:o3:22:ILE:O     | 11:o3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:o3:344:ASP:OD1  | 11:o3:344:ASP:N    | 2.52                     | 0.42              |
| 11:p3:23:ARG:NH1   | 11:q3:249:GLN:O    | 2.52                     | 0.42              |
| 11:p3:141:ILE:HD13 | 11:p3:165:ILE:CD1  | 2.38                     | 0.42              |
| 11:q3:73:VAL:HG11  | 11:q3:79:MET:HE1   | 2.00                     | 0.42              |
| 11:r3:42:VAL:CG1   | 11:r3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:s3:41:LEU:HD23  | 11:s3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:s3:42:VAL:CG1   | 11:s3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:t3:41:LEU:HD23  | 11:t3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:t3:73:VAL:HG11  | 11:t3:79:MET:HE1   | 2.00                     | 0.42              |
| 11:u3:42:VAL:CG1   | 11:u3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:u3:344:ASP:N    | 11:u3:344:ASP:OD1  | 2.52                     | 0.42              |
| 11:v3:41:LEU:HD23  | 11:v3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:v3:42:VAL:CG1   | 11:v3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:v3:123:MET:CE   | 11:v3:136:LEU:HD22 | 2.38                     | 0.42              |
| 11:w3:136:LEU:HD13 | 11:x3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:y3:32:ARG:HG2   | 11:y3:32:ARG:HH11  | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:y3:271:ASP:HB3 | 11:y3:357:CYS:CA  | 2.34                     | 0.42              |
| 1:C1:142:ARG:HB3  | 1:E1:154:ARG:HH22 | 1.83                     | 0.42              |
| 1:C1:194:VAL:HG13 | 1:C1:212:LEU:HD11 | 2.00                     | 0.42              |
| 1:C1:248:ARG:NH2  | 1:D1:242:GLU:OE1  | 2.53                     | 0.42              |
| 1:C1:409:MET:CE   | 1:C1:434:ASN:HB2  | 2.49                     | 0.42              |
| 1:D1:415:LEU:HD21 | 1:E1:433:VAL:HG11 | 2.01                     | 0.42              |
| 1:E1:181:GLU:HG2  | 1:E1:184:ARG:NH2  | 2.35                     | 0.42              |
| 1:F1:388:ALA:HA   | 1:F1:431:ASN:O    | 2.19                     | 0.42              |
| 1:H1:125:GLN:NE2  | 4:G2:71:ASN:OD1   | 2.52                     | 0.42              |
| 1:H1:154:ARG:HB3  | 1:H1:177:THR:OG1  | 2.19                     | 0.42              |
| 1:M1:387:VAL:HB   | 1:M1:420:MET:HE1  | 2.01                     | 0.42              |
| 1:N1:234:GLN:HB2  | 1:N1:272:PHE:CE2  | 2.55                     | 0.42              |
| 1:O1:393:TYR:HB3  | 1:O1:402:LEU:N    | 2.35                     | 0.42              |
| 1:P1:282:TYR:CE1  | 1:P1:370:ARG:HD3  | 2.55                     | 0.42              |
| 1:T1:293:LEU:HD13 | 1:T1:296:ARG:NH1  | 2.31                     | 0.42              |
| 1:U1:157:LEU:HD11 | 1:U1:202:VAL:HG11 | 2.02                     | 0.42              |
| 1:U1:204:GLY:H    | 1:W1:170:LYS:HZ2  | 1.67                     | 0.42              |
| 1:U1:301:SER:HB3  | 1:U1:359:GLN:HB3  | 2.01                     | 0.42              |
| 1:W1:165:PHE:HZ   | 2:E2:140:ARG:NH2  | 2.17                     | 0.42              |
| 1:X1:232:ASP:OD2  | 1:X1:233:ALA:N    | 2.53                     | 0.42              |
| 1:Y1:245:ILE:HD11 | 1:Y1:420:MET:CA   | 2.50                     | 0.42              |
| 1:a1:143:THR:HG23 | 1:c1:154:ARG:NH2  | 2.34                     | 0.42              |
| 1:a1:214:ASP:HB3  | 1:a1:217:GLY:O    | 2.20                     | 0.42              |
| 1:d1:146:THR:O    | 1:d1:146:THR:OG1  | 2.38                     | 0.42              |
| 1:h1:140:LEU:O    | 1:h1:144:ILE:HG12 | 2.19                     | 0.42              |
| 2:B2:92:LEU:HD12  | 2:B2:92:LEU:HA    | 1.91                     | 0.42              |
| 2:C2:224:MET:SD   | 4:J2:6:VAL:HG21   | 2.60                     | 0.42              |
| 2:D2:42:VAL:O     | 2:D2:46:VAL:HG22  | 2.20                     | 0.42              |
| 2:D2:205:MET:HE2  | 2:D2:205:MET:HB2  | 1.83                     | 0.42              |
| 2:E2:146:ASP:OD2  | 2:E2:177:SER:HB3  | 2.19                     | 0.42              |
| 6:T2:92:GLN:NE2   | 7:Z2:19:LYS:HA    | 2.34                     | 0.42              |
| 7:X2:28:LEU:HA    | 7:X2:28:LEU:HD12  | 1.78                     | 0.42              |
| 7:X2:66:SER:O     | 7:X2:68:ILE:HG23  | 2.19                     | 0.42              |
| 7:Y2:76:LEU:HD23  | 7:Y2:90:TYR:HB3   | 2.02                     | 0.42              |
| 8:d2:74:THR:O     | 8:d2:75:SER:OG    | 2.32                     | 0.42              |
| 8:d2:201:ILE:HD13 | 8:d2:201:ILE:HA   | 1.88                     | 0.42              |
| 8:d2:217:MET:HE1  | 9:i2:245:LYS:HG2  | 2.02                     | 0.42              |
| 9:h2:115:THR:HB   | 9:h2:191:LEU:HD23 | 2.01                     | 0.42              |
| 9:k2:184:LEU:HA   | 9:k2:184:LEU:HD23 | 1.77                     | 0.42              |
| 9:p2:242:ILE:HD13 | 9:p2:242:ILE:HA   | 1.91                     | 0.42              |
| 9:s2:105:VAL:CG1  | 9:s2:134:PHE:HB3  | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:s2:196:GLN:HE22  | 9:x2:61:THR:HG23   | 1.84                     | 0.42              |
| 9:w2:36:ARG:NH2    | 9:w2:80:LEU:HD13   | 2.35                     | 0.42              |
| 9:w2:248:SER:O     | 9:w2:252:GLN:HG2   | 2.20                     | 0.42              |
| 9:x2:26:LEU:HD21   | 9:32:242:ILE:HG22  | 2.02                     | 0.42              |
| 9:x2:174:ASN:HA    | 9:x2:206:PRO:HD3   | 2.00                     | 0.42              |
| 9:z2:121:GLN:HB2   | 9:z2:129:VAL:HG23  | 2.01                     | 0.42              |
| 9:32:95:VAL:O      | 9:32:118:GLY:HA3   | 2.20                     | 0.42              |
| 9:42:36:ARG:HB3    | 9:42:80:LEU:HD23   | 2.00                     | 0.42              |
| 10:C3:84:GLU:HG2   | 10:C3:197:SER:OG   | 2.19                     | 0.42              |
| 10:C3:117:PHE:HD1  | 10:C3:122:ALA:CB   | 2.33                     | 0.42              |
| 10:C3:222:LEU:HB2  | 10:D3:231:PRO:HB3  | 2.02                     | 0.42              |
| 10:G3:65:LEU:HD23  | 11:g3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:H3:45:PRO:CG    | 10:I3:60:TYR:HD1   | 2.32                     | 0.42              |
| 10:J3:117:PHE:HD1  | 10:J3:122:ALA:CB   | 2.33                     | 0.42              |
| 10:M3:232:MET:HE1  | 10:O3:126:ALA:HB3  | 2.02                     | 0.42              |
| 10:N3:221:TRP:NE1  | 10:O3:229:LEU:O    | 2.41                     | 0.42              |
| 10:U3:168:GLN:HG3  | 10:V3:204:ARG:NE   | 2.35                     | 0.42              |
| 10:W3:45:PRO:CG    | 10:X3:60:TYR:HD1   | 2.33                     | 0.42              |
| 11:a3:111:GLY:O    | 11:z3:83:ASN:HB2   | 2.20                     | 0.42              |
| 11:a3:136:LEU:HD13 | 11:b3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:a3:271:ASP:HB3  | 11:a3:357:CYS:CA   | 2.34                     | 0.42              |
| 11:d3:101:GLN:OE1  | 11:e3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:d3:319:LEU:HD12 | 11:d3:319:LEU:HA   | 1.82                     | 0.42              |
| 11:d3:353:GLN:CG   | 11:d3:362:LEU:HD22 | 2.49                     | 0.42              |
| 11:f3:166:THR:HG21 | 11:h3:362:LEU:HD23 | 2.02                     | 0.42              |
| 11:f3:344:ASP:OD1  | 11:f3:344:ASP:N    | 2.52                     | 0.42              |
| 11:g3:208:ARG:NH2  | 11:g3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:h3:166:THR:HG21 | 11:j3:362:LEU:HD23 | 2.02                     | 0.42              |
| 11:i3:83:ASN:ND2   | 11:j3:109:SER:OG   | 2.47                     | 0.42              |
| 11:i3:208:ARG:NH2  | 11:i3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:k3:255:ILE:HD12 | 11:k3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:l3:32:ARG:HH11  | 11:l3:32:ARG:HG2   | 1.85                     | 0.42              |
| 11:m3:73:VAL:HG11  | 11:m3:79:MET:HE1   | 2.00                     | 0.42              |
| 11:p3:32:ARG:HH11  | 11:p3:32:ARG:HG2   | 1.85                     | 0.42              |
| 11:q3:41:LEU:HD23  | 11:q3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:t3:22:ILE:O     | 11:t3:25:LEU:HD23  | 2.19                     | 0.42              |
| 11:t3:114:LYS:HD2  | 11:t3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:u3:208:ARG:NH2  | 11:u3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:w3:208:ARG:NH2  | 11:w3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:y3:255:ILE:HD12 | 11:y3:362:LEU:HD12 | 2.01                     | 0.42              |
| 12:A4:208:LYS:N    | 12:B4:229:ARG:O    | 2.48                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:B4:206:VAL:HG12 | 12:B4:213:ASN:OD1  | 2.20                     | 0.42              |
| 1:A1:382:ILE:H     | 1:A1:382:ILE:HD12  | 1.85                     | 0.42              |
| 1:A1:431:ASN:ND2   | 1:h1:414:ASP:HB3   | 2.35                     | 0.42              |
| 1:D1:275:LYS:HB2   | 1:D1:377:MET:CG    | 2.49                     | 0.42              |
| 1:D1:393:TYR:HB3   | 1:D1:402:LEU:N     | 2.35                     | 0.42              |
| 1:F1:423:SER:HB2   | 1:G1:384:ARG:NH1   | 2.34                     | 0.42              |
| 1:K1:234:GLN:HB3   | 1:K1:272:PHE:CE2   | 2.55                     | 0.42              |
| 1:N1:261:ASN:O     | 1:N1:392:ASN:N     | 2.43                     | 0.42              |
| 1:W1:237:PHE:HE2   | 1:X1:232:ASP:HA    | 1.84                     | 0.42              |
| 1:W1:257:VAL:HG21  | 1:W1:262:VAL:HG13  | 2.02                     | 0.42              |
| 1:X1:189:GLY:O     | 1:X1:192:SER:OG    | 2.37                     | 0.42              |
| 1:g1:268:ALA:HB1   | 1:g1:382:ILE:CD1   | 2.49                     | 0.42              |
| 1:h1:147:LEU:O     | 1:h1:149:PRO:HD2   | 2.20                     | 0.42              |
| 2:A2:175:VAL:CG2   | 3:F2:49:MET:HE1    | 2.49                     | 0.42              |
| 2:C2:80:THR:HB     | 2:C2:81:PRO:HD2    | 2.01                     | 0.42              |
| 2:C2:236:MET:CE    | 2:D2:176:THR:HG23  | 2.50                     | 0.42              |
| 2:E2:45:LEU:O      | 2:E2:49:THR:HG23   | 2.20                     | 0.42              |
| 3:F2:237:ALA:HB3   | 3:F2:238:PRO:HD3   | 2.01                     | 0.42              |
| 4:I2:43:GLN:H      | 4:I2:43:GLN:CD     | 2.28                     | 0.42              |
| 4:J2:47:MET:HG3    | 4:J2:48:THR:N      | 2.34                     | 0.42              |
| 5:N2:82:MET:HE2    | 6:S2:133:VAL:HG22  | 2.02                     | 0.42              |
| 5:P2:61:LEU:HD21   | 6:U2:50:LYS:NZ     | 2.34                     | 0.42              |
| 5:P2:69:ASN:HB3    | 7:V2:112:TYR:OH    | 2.20                     | 0.42              |
| 6:Q2:18:LEU:HD12   | 6:Q2:18:LEU:HA     | 1.84                     | 0.42              |
| 6:R2:85:LEU:HD23   | 6:R2:85:LEU:HA     | 1.81                     | 0.42              |
| 7:V2:93:MET:HA     | 7:V2:94:PRO:HD2    | 1.93                     | 0.42              |
| 8:e2:163:LEU:HD11  | 8:e2:201:ILE:HG12  | 2.01                     | 0.42              |
| 8:f2:49:LEU:HA     | 8:f2:49:LEU:HD23   | 1.75                     | 0.42              |
| 9:h2:77:THR:HG21   | 9:m2:67:GLN:O      | 2.19                     | 0.42              |
| 9:j2:82:SER:OG     | 9:j2:223:ASN:ND2   | 2.41                     | 0.42              |
| 9:p2:26:LEU:HD22   | 9:u2:242:ILE:HG21  | 2.02                     | 0.42              |
| 9:q2:257:LEU:O     | 9:q2:260:LEU:HG    | 2.20                     | 0.42              |
| 9:32:30:SER:O      | 9:32:30:SER:OG     | 2.28                     | 0.42              |
| 10:B3:148:LEU:HD13 | 10:B3:167:LYS:HE2  | 2.01                     | 0.42              |
| 10:G3:232:MET:HE1  | 10:I3:126:ALA:HB3  | 2.02                     | 0.42              |
| 10:I3:78:LEU:HD21  | 10:I3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:N3:83:GLN:O     | 10:N3:83:GLN:HG3   | 2.20                     | 0.42              |
| 10:T3:83:GLN:HG3   | 10:T3:83:GLN:O     | 2.20                     | 0.42              |
| 10:W3:82:LEU:HA    | 10:W3:197:SER:CB   | 2.38                     | 0.42              |
| 10:W3:83:GLN:HG3   | 10:W3:83:GLN:O     | 2.20                     | 0.42              |
| 10:X3:148:LEU:HD13 | 10:X3:167:LYS:HE2  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:Z3:83:GLN:O     | 10:Z3:83:GLN:HG3   | 2.20                     | 0.42              |
| 10:Z3:101:LYS:HB2  | 10:Z3:101:LYS:NZ   | 2.32                     | 0.42              |
| 10:Z3:148:LEU:HD13 | 10:Z3:167:LYS:HE2  | 2.01                     | 0.42              |
| 11:b3:101:GLN:OE1  | 11:c3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:f3:255:ILE:HD12 | 11:f3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:g3:101:GLN:OE1  | 11:h3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:g3:344:ASP:OD1  | 11:g3:344:ASP:N    | 2.52                     | 0.42              |
| 11:j3:101:GLN:OE1  | 11:k3:219:ARG:HD3  | 2.19                     | 0.42              |
| 11:j3:166:THR:HG21 | 11:l3:362:LEU:HD23 | 2.02                     | 0.42              |
| 11:j3:208:ARG:NH2  | 11:j3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:k3:46:ASP:OD1   | 11:l3:160:LEU:HD12 | 2.20                     | 0.42              |
| 11:m3:344:ASP:OD1  | 11:m3:344:ASP:N    | 2.52                     | 0.42              |
| 11:n3:344:ASP:OD1  | 11:n3:344:ASP:N    | 2.52                     | 0.42              |
| 11:o3:114:LYS:HD2  | 11:o3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:o3:252:LYS:HB2  | 11:o3:252:LYS:HE3  | 1.52                     | 0.42              |
| 11:p3:41:LEU:HD23  | 11:p3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:p3:208:ARG:NH2  | 11:p3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:q3:319:LEU:HD12 | 11:q3:319:LEU:HA   | 1.82                     | 0.42              |
| 11:r3:32:ARG:HG2   | 11:r3:32:ARG:HH11  | 1.85                     | 0.42              |
| 11:r3:41:LEU:HD23  | 11:r3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:s3:114:LYS:HD2  | 11:s3:114:LYS:HA   | 1.77                     | 0.42              |
| 11:t3:23:ARG:NH1   | 11:u3:249:GLN:O    | 2.53                     | 0.42              |
| 11:t3:42:VAL:CG1   | 11:t3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:v3:208:ARG:NH2  | 11:v3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:w3:41:LEU:HD23  | 11:w3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:x3:41:LEU:HD23  | 11:x3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:x3:42:VAL:CG1   | 11:x3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:x3:159:GLN:CB   | 11:y3:258:ARG:HG2  | 2.49                     | 0.42              |
| 11:x3:208:ARG:NH2  | 11:x3:238:ASP:OD2  | 2.53                     | 0.42              |
| 12:C4:157:ARG:NH1  | 12:C4:159:GLY:HA3  | 2.34                     | 0.42              |
| 1:B1:301:SER:HA    | 1:C1:359:GLN:HA    | 2.01                     | 0.42              |
| 1:C1:246:GLN:NE2   | 1:C1:264:ALA:O     | 2.52                     | 0.42              |
| 1:E1:294:ARG:HE    | 6:U2:68:THR:HG1    | 1.68                     | 0.42              |
| 1:I1:176:VAL:HG12  | 1:I1:178:VAL:HG23  | 2.02                     | 0.42              |
| 1:J1:242:GLU:HG3   | 1:J1:243:SER:N     | 2.34                     | 0.42              |
| 1:N1:394:LYS:CG    | 1:N1:402:LEU:HB2   | 2.49                     | 0.42              |
| 1:Q1:293:LEU:CD1   | 1:Q1:296:ARG:HE    | 2.33                     | 0.42              |
| 1:R1:167:ARG:O     | 1:R1:169:GLN:NE2   | 2.53                     | 0.42              |
| 1:W1:182:PRO:O     | 1:W1:184:ARG:NH1   | 2.53                     | 0.42              |
| 1:W1:187:ASP:OD1   | 1:W1:190:GLN:HG3   | 2.20                     | 0.42              |
| 1:W1:235:LEU:HD23  | 1:W1:235:LEU:HA    | 1.87                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Y1:126:PHE:HA    | 1:Y1:129:GLN:HE22  | 1.85                     | 0.42              |
| 1:Y1:407:ASP:O     | 1:Y1:411:GLN:HG2   | 2.20                     | 0.42              |
| 2:A2:86:ASN:HA     | 2:A2:90:LEU:HD12   | 2.01                     | 0.42              |
| 2:A2:116:PHE:CE1   | 2:A2:123:MET:HG3   | 2.55                     | 0.42              |
| 2:B2:47:PHE:O      | 2:B2:51:LEU:HD23   | 2.20                     | 0.42              |
| 2:D2:135:ARG:CG    | 2:D2:167:MET:HE2   | 2.49                     | 0.42              |
| 2:E2:39:SER:C      | 2:E2:41:SER:N      | 2.77                     | 0.42              |
| 4:J2:47:MET:HG3    | 4:J2:48:THR:H      | 1.85                     | 0.42              |
| 7:V2:76:LEU:HD23   | 7:V2:90:TYR:CD2    | 2.55                     | 0.42              |
| 8:c2:115:ILE:HG22  | 8:c2:116:GLN:OE1   | 2.20                     | 0.42              |
| 8:d2:121:ILE:O     | 8:d2:162:LYS:HG2   | 2.19                     | 0.42              |
| 8:e2:206:LEU:HA    | 8:e2:206:LEU:HD23  | 1.85                     | 0.42              |
| 9:g2:113:ALA:CB    | 9:g2:191:LEU:HD23  | 2.47                     | 0.42              |
| 9:h2:174:ASN:HA    | 9:h2:206:PRO:HD3   | 2.01                     | 0.42              |
| 9:l2:72:VAL:HG22   | 9:l2:72:VAL:O      | 2.19                     | 0.42              |
| 9:l2:209:ASN:OD1   | 9:l2:209:ASN:O     | 2.38                     | 0.42              |
| 9:o2:6:TRP:O       | 9:o2:10:THR:HG23   | 2.20                     | 0.42              |
| 9:o2:226:VAL:O     | 9:o2:230:LEU:HD23  | 2.19                     | 0.42              |
| 9:p2:167:PRO:HD3   | 9:l2:196:GLN:HB2   | 2.02                     | 0.42              |
| 9:q2:40:VAL:O      | 9:q2:75:VAL:HG12   | 2.20                     | 0.42              |
| 9:s2:257:LEU:O     | 9:s2:260:LEU:HB3   | 2.20                     | 0.42              |
| 9:w2:2:ILE:HD11    | 9:w2:254:LEU:HD21  | 2.02                     | 0.42              |
| 9:x2:72:VAL:O      | 9:x2:73:ARG:C      | 2.63                     | 0.42              |
| 10:A3:65:LEU:HD23  | 11:a3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:A3:222:LEU:HB2  | 10:B3:231:PRO:HB3  | 2.02                     | 0.42              |
| 10:B3:65:LEU:HD23  | 11:b3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:E3:45:PRO:CG    | 10:F3:60:TYR:HD1   | 2.33                     | 0.42              |
| 10:E3:117:PHE:HD1  | 10:E3:122:ALA:CB   | 2.33                     | 0.42              |
| 10:H3:168:GLN:HG3  | 10:I3:204:ARG:NE   | 2.35                     | 0.42              |
| 10:I3:117:PHE:HD1  | 10:I3:122:ALA:CB   | 2.33                     | 0.42              |
| 10:J3:106:PHE:C    | 10:J3:108:THR:H    | 2.28                     | 0.42              |
| 10:O3:83:GLN:HG3   | 10:O3:83:GLN:O     | 2.20                     | 0.42              |
| 10:P3:65:LEU:HD23  | 11:p3:68:GLN:HG2   | 2.00                     | 0.42              |
| 10:Q3:45:PRO:CG    | 10:R3:60:TYR:HD1   | 2.33                     | 0.42              |
| 10:Q3:78:LEU:HD21  | 10:Q3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:Q3:83:GLN:HG3   | 10:Q3:83:GLN:O     | 2.20                     | 0.42              |
| 10:R3:168:GLN:HG3  | 10:S3:204:ARG:NE   | 2.35                     | 0.42              |
| 10:S3:43:PRO:O     | 10:S3:43:PRO:CD    | 2.67                     | 0.42              |
| 10:Y3:78:LEU:HD21  | 10:Y3:195:VAL:HG11 | 2.01                     | 0.42              |
| 10:Z3:117:PHE:HD1  | 10:Z3:122:ALA:CB   | 2.33                     | 0.42              |
| 11:a3:364:ILE:HD12 | 11:y3:142:LEU:HD22 | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:b3:23:ARG:NH1   | 11:c3:249:GLN:O    | 2.53                     | 0.42              |
| 11:b3:42:VAL:CG1   | 11:b3:45:LEU:HD21  | 2.50                     | 0.42              |
| 11:c3:136:LEU:HD13 | 11:d3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:e3:344:ASP:N    | 11:e3:344:ASP:OD1  | 2.52                     | 0.42              |
| 11:f3:208:ARG:NH2  | 11:f3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:h3:83:ASN:ND2   | 11:i3:109:SER:OG   | 2.47                     | 0.42              |
| 11:k3:208:ARG:NH2  | 11:k3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:m3:32:ARG:HG2   | 11:m3:32:ARG:HH11  | 1.85                     | 0.42              |
| 11:n3:353:GLN:CG   | 11:n3:362:LEU:HD22 | 2.50                     | 0.42              |
| 11:o3:41:LEU:HD23  | 11:o3:86:ALA:HA    | 2.02                     | 0.42              |
| 11:r3:353:GLN:CG   | 11:r3:362:LEU:HD22 | 2.50                     | 0.42              |
| 11:t3:208:ARG:NH2  | 11:t3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:v3:136:LEU:HD13 | 11:w3:129:VAL:HG11 | 2.02                     | 0.42              |
| 11:x3:32:ARG:HG2   | 11:x3:32:ARG:HH11  | 1.85                     | 0.42              |
| 11:x3:114:LYS:HA   | 11:x3:114:LYS:HD2  | 1.77                     | 0.42              |
| 11:x3:255:ILE:HD12 | 11:x3:362:LEU:HD12 | 2.01                     | 0.42              |
| 11:x3:259:THR:O    | 11:y3:277:GLN:NE2  | 2.53                     | 0.42              |
| 11:y3:208:ARG:NH2  | 11:y3:238:ASP:OD2  | 2.53                     | 0.42              |
| 11:z3:42:VAL:CG1   | 11:z3:45:LEU:HD21  | 2.50                     | 0.42              |
| 1:A1:253:LEU:HD23  | 1:A1:253:LEU:HA    | 1.72                     | 0.41              |
| 1:B1:211:THR:HG21  | 1:h1:196:HIS:HB3   | 2.02                     | 0.41              |
| 1:B1:269:GLN:O     | 1:B1:270:LEU:HD23  | 2.19                     | 0.41              |
| 1:C1:164:LEU:HG    | 2:C2:152:ARG:HD2   | 2.01                     | 0.41              |
| 1:G1:190:GLN:CG    | 1:H1:217:GLY:HA3   | 2.50                     | 0.41              |
| 1:G1:191:ILE:CD1   | 1:G1:220:LEU:HD13  | 2.50                     | 0.41              |
| 1:G1:422:PHE:HE2   | 1:G1:424:ASP:OD1   | 2.02                     | 0.41              |
| 1:I1:159:MET:SD    | 1:I1:172:PRO:HB3   | 2.60                     | 0.41              |
| 1:N1:254:SER:OG    | 1:N1:255:PRO:HD3   | 2.20                     | 0.41              |
| 1:O1:252:ILE:HG23  | 1:O1:253:LEU:HG    | 2.02                     | 0.41              |
| 1:O1:418:GLU:HB3   | 1:P1:388:ALA:HB2   | 2.02                     | 0.41              |
| 1:T1:128:GLU:OE2   | 1:T1:128:GLU:N     | 2.39                     | 0.41              |
| 1:T1:274:ASN:C     | 1:T1:275:LYS:HD3   | 2.45                     | 0.41              |
| 1:U1:142:ARG:HA    | 1:U1:145:GLU:CD    | 2.45                     | 0.41              |
| 1:Y1:245:ILE:HG23  | 1:Y1:266:VAL:HG21  | 2.02                     | 0.41              |
| 1:d1:393:TYR:CD1   | 1:d1:403:PRO:HA    | 2.55                     | 0.41              |
| 1:g1:140:LEU:HD22  | 1:h1:156:HIS:NE2   | 2.35                     | 0.41              |
| 1:h1:423:SER:OG    | 1:h1:425:LYS:HG2   | 2.20                     | 0.41              |
| 2:D2:129:LYS:HD3   | 2:D2:129:LYS:HA    | 1.84                     | 0.41              |
| 2:E2:55:PRO:O      | 2:E2:59:LEU:HB2    | 2.19                     | 0.41              |
| 4:H2:50:SER:C      | 4:H2:53:PRO:HD2    | 2.45                     | 0.41              |
| 5:N2:60:THR:HB     | 6:S2:118:MET:HE1   | 2.01                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:P2:54:VAL:O      | 5:P2:57:GLU:HB3   | 2.20                     | 0.41              |
| 6:Q2:21:GLN:O      | 6:Q2:25:ILE:HG12  | 2.20                     | 0.41              |
| 6:R2:49:LEU:HA     | 6:R2:52:VAL:HG12  | 2.01                     | 0.41              |
| 6:S2:93:PRO:O      | 8:d2:54:ARG:HD2   | 2.19                     | 0.41              |
| 7:Y2:35:THR:HG23   | 8:d2:42:ARG:HE    | 1.85                     | 0.41              |
| 7:Z2:110:ARG:NH1   | 8:e2:243:ARG:HH12 | 2.18                     | 0.41              |
| 7:a2:127:LEU:HD11  | 8:f2:250:MET:CE   | 2.50                     | 0.41              |
| 8:c2:104:ASN:ND2   | 9:h2:78:GLU:OE2   | 2.50                     | 0.41              |
| 8:f2:175:ASP:HA    | 9:k2:46:TYR:HB2   | 2.03                     | 0.41              |
| 9:g2:79:ARG:HA     | 9:g2:79:ARG:HD3   | 1.88                     | 0.41              |
| 9:h2:24:ASN:HD22   | 9:m2:69:GLY:C     | 2.28                     | 0.41              |
| 9:i2:68:ILE:HG22   | 9:i2:69:GLY:O     | 2.20                     | 0.41              |
| 9:m2:98:LYS:O      | 9:m2:212:GLY:CA   | 2.63                     | 0.41              |
| 9:m2:100:GLN:HA    | 9:m2:116:ARG:NH2  | 2.35                     | 0.41              |
| 9:m2:230:LEU:HD11  | 9:r2:242:ILE:HD12 | 2.02                     | 0.41              |
| 9:u2:72:VAL:O      | 9:u2:73:ARG:C     | 2.63                     | 0.41              |
| 9:22:174:ASN:HB2   | 9:22:204:SER:O    | 2.20                     | 0.41              |
| 9:32:72:VAL:O      | 9:32:73:ARG:C     | 2.62                     | 0.41              |
| 9:42:245:LYS:HE3   | 9:42:245:LYS:HB3  | 1.80                     | 0.41              |
| 10:A3:101:LYS:HB2  | 10:A3:101:LYS:HZ3 | 1.85                     | 0.41              |
| 10:A3:206:GLU:HG3  | 10:Z3:170:ALA:HB3 | 2.01                     | 0.41              |
| 10:C3:148:LEU:HD13 | 10:C3:167:LYS:HE2 | 2.01                     | 0.41              |
| 10:D3:106:PHE:C    | 10:D3:108:THR:H   | 2.28                     | 0.41              |
| 10:D3:148:LEU:HD13 | 10:D3:167:LYS:HE2 | 2.01                     | 0.41              |
| 10:D3:168:GLN:HG3  | 10:E3:204:ARG:NE  | 2.34                     | 0.41              |
| 10:F3:117:PHE:HD1  | 10:F3:122:ALA:CB  | 2.33                     | 0.41              |
| 10:F3:168:GLN:HG3  | 10:G3:204:ARG:NE  | 2.34                     | 0.41              |
| 10:G3:117:PHE:HD1  | 10:G3:122:ALA:CB  | 2.33                     | 0.41              |
| 10:H3:117:PHE:HD1  | 10:H3:122:ALA:CB  | 2.33                     | 0.41              |
| 10:I3:40:ILE:H     | 10:I3:40:ILE:HG12 | 1.48                     | 0.41              |
| 10:K3:45:PRO:CG    | 10:L3:60:TYR:HD1  | 2.33                     | 0.41              |
| 10:K3:83:GLN:O     | 10:K3:83:GLN:HG3  | 2.20                     | 0.41              |
| 10:M3:117:PHE:HD1  | 10:M3:122:ALA:CB  | 2.33                     | 0.41              |
| 10:N3:45:PRO:CG    | 10:O3:60:TYR:HD1  | 2.32                     | 0.41              |
| 10:N3:117:PHE:HD1  | 10:N3:122:ALA:CB  | 2.33                     | 0.41              |
| 10:R3:135:LYS:HE2  | 10:R3:135:LYS:HB2 | 1.76                     | 0.41              |
| 10:R3:232:MET:HE1  | 10:T3:126:ALA:HB3 | 2.02                     | 0.41              |
| 10:T3:45:PRO:CG    | 10:U3:60:TYR:HD1  | 2.32                     | 0.41              |
| 10:V3:83:GLN:O     | 10:V3:83:GLN:HG3  | 2.20                     | 0.41              |
| 10:V3:171:ILE:O    | 10:W3:207:TYR:O   | 2.38                     | 0.41              |
| 10:X3:45:PRO:CG    | 10:Y3:60:TYR:HD1  | 2.33                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:X3:106:PHE:C    | 10:X3:108:THR:H    | 2.28                     | 0.41              |
| 11:a3:109:SER:OG   | 11:z3:83:ASN:ND2   | 2.50                     | 0.41              |
| 11:b3:336:ASN:HD22 | 11:b3:336:ASN:HA   | 1.67                     | 0.41              |
| 11:c3:93:TYR:CZ    | 11:c3:97:ALA:HB3   | 2.55                     | 0.41              |
| 11:e3:42:VAL:CG1   | 11:e3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:h3:344:ASP:N    | 11:h3:344:ASP:OD1  | 2.52                     | 0.41              |
| 11:i3:127:LYS:HA   | 11:i3:132:GLN:O    | 2.20                     | 0.41              |
| 11:j3:255:ILE:HD12 | 11:j3:362:LEU:HD12 | 2.01                     | 0.41              |
| 11:k3:353:GLN:CG   | 11:k3:362:LEU:HD22 | 2.49                     | 0.41              |
| 11:m3:41:LEU:HD23  | 11:m3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:m3:93:TYR:CZ    | 11:m3:97:ALA:HB3   | 2.55                     | 0.41              |
| 11:n3:23:ARG:NH1   | 11:o3:249:GLN:O    | 2.53                     | 0.41              |
| 11:n3:41:LEU:HD23  | 11:n3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:n3:42:VAL:CG1   | 11:n3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:o3:42:VAL:CG1   | 11:o3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:s3:127:LYS:HA   | 11:s3:132:GLN:O    | 2.20                     | 0.41              |
| 11:s3:353:GLN:CG   | 11:s3:362:LEU:HD22 | 2.49                     | 0.41              |
| 1:B1:424:ASP:OD2   | 1:B1:425:LYS:N     | 2.54                     | 0.41              |
| 1:E1:139:GLU:O     | 1:E1:143:THR:HG23  | 2.19                     | 0.41              |
| 1:E1:162:PRO:HA    | 1:E1:169:GLN:CD    | 2.45                     | 0.41              |
| 1:J1:293:LEU:HD13  | 1:J1:296:ARG:HE    | 1.85                     | 0.41              |
| 1:K1:367:GLU:C     | 1:K1:367:GLU:CD    | 2.88                     | 0.41              |
| 1:L1:258:GLY:HA3   | 1:L1:261:ASN:ND2   | 2.35                     | 0.41              |
| 1:L1:389:VAL:O     | 1:L1:432:VAL:HA    | 2.19                     | 0.41              |
| 1:N1:136:LEU:HD13  | 1:N1:136:LEU:HA    | 1.88                     | 0.41              |
| 1:O1:144:ILE:HD12  | 1:O1:194:VAL:HG23  | 2.02                     | 0.41              |
| 1:O1:164:LEU:HA    | 3:F2:145:TRP:HH2   | 0.96                     | 0.41              |
| 1:T1:167:ARG:CZ    | 2:E2:106:ASP:HB2   | 2.50                     | 0.41              |
| 1:T1:282:TYR:OH    | 1:T1:370:ARG:HD3   | 2.20                     | 0.41              |
| 1:U1:157:LEU:HD11  | 1:U1:159:MET:HE3   | 2.02                     | 0.41              |
| 1:U1:186:LEU:HD11  | 1:U1:190:GLN:HG2   | 2.02                     | 0.41              |
| 1:U1:282:TYR:CZ    | 1:U1:370:ARG:HD3   | 2.55                     | 0.41              |
| 1:Z1:378:ASN:HB3   | 1:Z1:381:ASP:OD2   | 2.20                     | 0.41              |
| 1:Z1:415:LEU:HD22  | 1:a1:431:ASN:HD21  | 1.84                     | 0.41              |
| 1:a1:392:ASN:OD1   | 1:a1:393:TYR:N     | 2.51                     | 0.41              |
| 1:b1:408:GLN:O     | 1:b1:412:ILE:HG13  | 2.19                     | 0.41              |
| 1:d1:420:MET:HE1   | 1:d1:430:LEU:CB    | 2.48                     | 0.41              |
| 1:f1:282:TYR:CZ    | 1:f1:370:ARG:HD3   | 2.56                     | 0.41              |
| 1:h1:424:ASP:OD2   | 1:h1:425:LYS:N     | 2.54                     | 0.41              |
| 2:B2:204:LEU:HD22  | 2:B2:212:VAL:HG11  | 2.02                     | 0.41              |
| 2:D2:40:LEU:HB3    | 6:R2:130:MET:HE1   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:D2:73:LEU:HD23  | 2:D2:73:LEU:HA     | 1.80                     | 0.41              |
| 2:D2:150:PHE:HA   | 2:D2:153:LEU:HG    | 2.02                     | 0.41              |
| 3:F2:138:LEU:O    | 3:F2:140:PHE:N     | 2.54                     | 0.41              |
| 3:F2:176:GLY:HA2  | 3:F2:178:LEU:N     | 2.35                     | 0.41              |
| 4:G2:45:ASN:OD1   | 4:G2:45:ASN:N      | 2.54                     | 0.41              |
| 4:I2:20:LEU:HD12  | 4:I2:69:MET:HG2    | 2.02                     | 0.41              |
| 6:T2:113:SER:O    | 6:T2:117:GLN:HG3   | 2.19                     | 0.41              |
| 7:W2:123:LYS:HE2  | 8:b2:247:LEU:O     | 2.20                     | 0.41              |
| 8:b2:165:LYS:HB2  | 8:b2:196:ASP:OD1   | 2.19                     | 0.41              |
| 8:c2:42:ARG:HD2   | 9:h2:64:SER:CB     | 2.49                     | 0.41              |
| 8:c2:228:GLU:HB2  | 9:h2:256:LYS:HG2   | 2.02                     | 0.41              |
| 8:d2:115:ILE:O    | 8:d2:116:GLN:C     | 2.63                     | 0.41              |
| 8:d2:206:LEU:HD23 | 8:d2:206:LEU:HA    | 1.89                     | 0.41              |
| 9:i2:73:ARG:O     | 9:i2:73:ARG:HG3    | 2.20                     | 0.41              |
| 9:k2:226:VAL:O    | 9:k2:230:LEU:HD23  | 2.20                     | 0.41              |
| 9:n2:28:ASN:ND2   | 9:t2:43:ASP:HB3    | 2.35                     | 0.41              |
| 9:q2:3:SER:O      | 9:q2:7:ILE:HG12    | 2.20                     | 0.41              |
| 9:t2:28:ASN:HD21  | 9:y2:43:ASP:HB3    | 1.85                     | 0.41              |
| 9:t2:130:THR:HG22 | 9:t2:134:PHE:O     | 2.21                     | 0.41              |
| 9:w2:44:LEU:HD23  | 9:w2:44:LEU:HA     | 1.85                     | 0.41              |
| 9:w2:128:LEU:HD12 | 9:w2:140:ILE:HD13  | 2.03                     | 0.41              |
| 9:y2:180:ASN:HB3  | 9:y2:198:SER:HA    | 2.03                     | 0.41              |
| 9:z2:29:VAL:HG22  | 9:z2:224:VAL:HG11  | 2.02                     | 0.41              |
| 9:12:32:ASN:ND2   | 9:12:219:VAL:HB    | 2.35                     | 0.41              |
| 10:A3:117:PHE:HD1 | 10:A3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:B3:117:PHE:HD1 | 10:B3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:C3:83:GLN:O    | 10:C3:83:GLN:HG3   | 2.20                     | 0.41              |
| 10:D3:45:PRO:CG   | 10:E3:60:TYR:HD1   | 2.32                     | 0.41              |
| 10:D3:117:PHE:HD1 | 10:D3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:D3:171:ILE:O   | 10:E3:207:TYR:O    | 2.38                     | 0.41              |
| 10:E3:171:ILE:O   | 10:F3:207:TYR:O    | 2.38                     | 0.41              |
| 10:G3:106:PHE:C   | 10:G3:108:THR:H    | 2.28                     | 0.41              |
| 10:H3:78:LEU:HD21 | 10:H3:195:VAL:HG11 | 2.01                     | 0.41              |
| 10:I3:43:PRO:O    | 10:I3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:I3:45:PRO:CG   | 10:J3:60:TYR:HD1   | 2.33                     | 0.41              |
| 10:J3:43:PRO:O    | 10:J3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:K3:117:PHE:HD1 | 10:K3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:L3:83:GLN:HG3  | 10:L3:83:GLN:O     | 2.20                     | 0.41              |
| 10:L3:168:GLN:HG3 | 10:M3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:L3:232:MET:HE1 | 10:N3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:O3:106:PHE:C   | 10:O3:108:THR:H    | 2.28                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:O3:222:LEU:HB2  | 10:P3:231:PRO:HB3  | 2.02                     | 0.41              |
| 10:Q3:130:ASN:CG   | 10:R3:102:THR:HG22 | 2.46                     | 0.41              |
| 10:Q3:232:MET:HE1  | 10:S3:126:ALA:HB3  | 2.02                     | 0.41              |
| 10:S3:168:GLN:HG3  | 10:T3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:X3:40:ILE:H     | 10:X3:40:ILE:HG12  | 1.48                     | 0.41              |
| 10:X3:43:PRO:O     | 10:X3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:X3:222:LEU:HB2  | 10:Y3:231:PRO:HB3  | 2.02                     | 0.41              |
| 10:Y3:83:GLN:HG3   | 10:Y3:83:GLN:O     | 2.20                     | 0.41              |
| 10:Y3:148:LEU:HD13 | 10:Y3:167:LYS:HE2  | 2.01                     | 0.41              |
| 11:b3:271:ASP:HB3  | 11:b3:357:CYS:CA   | 2.34                     | 0.41              |
| 11:b3:353:GLN:CG   | 11:b3:362:LEU:HD22 | 2.50                     | 0.41              |
| 11:d3:196:MET:CA   | 11:d3:196:MET:CE   | 2.97                     | 0.41              |
| 11:j3:344:ASP:OD1  | 11:j3:344:ASP:N    | 2.52                     | 0.41              |
| 11:m3:208:ARG:NH2  | 11:m3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:n3:342:PRO:O    | 11:n3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:q3:208:ARG:NH2  | 11:q3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:r3:101:GLN:OE1  | 11:s3:219:ARG:HD3  | 2.21                     | 0.41              |
| 11:t3:127:LYS:HA   | 11:t3:132:GLN:O    | 2.20                     | 0.41              |
| 11:u3:32:ARG:HG2   | 11:u3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:u3:127:LYS:HA   | 11:u3:132:GLN:O    | 2.20                     | 0.41              |
| 11:y3:41:LEU:HD23  | 11:y3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:y3:101:GLN:OE1  | 11:z3:219:ARG:HD3  | 2.20                     | 0.41              |
| 11:z3:208:ARG:NH2  | 11:z3:238:ASP:OD2  | 2.53                     | 0.41              |
| 12:A4:215:LEU:HB3  | 12:A4:223:THR:HB   | 2.01                     | 0.41              |
| 12:E4:156:LEU:HD21 | 12:E4:163:PHE:HZ   | 1.84                     | 0.41              |
| 1:B1:167:ARG:CB    | 2:C2:160:GLN:CD    | 2.92                     | 0.41              |
| 1:C1:191:ILE:O     | 1:C1:195:VAL:HG23  | 2.20                     | 0.41              |
| 1:G1:165:PHE:HB3   | 1:G1:167:ARG:HH21  | 1.86                     | 0.41              |
| 1:H1:369:ASP:OD1   | 1:I1:282:TYR:N     | 2.43                     | 0.41              |
| 1:I1:417:ARG:HG3   | 1:I1:422:PHE:HB3   | 2.02                     | 0.41              |
| 1:J1:249:ILE:HD12  | 1:J1:416:THR:OG1   | 2.20                     | 0.41              |
| 1:K1:151:LYS:HZ3   | 1:K1:182:PRO:HD3   | 1.85                     | 0.41              |
| 1:M1:240:ASP:OD2   | 1:N1:235:LEU:HD13  | 2.20                     | 0.41              |
| 1:M1:275:LYS:HB2   | 1:M1:377:MET:HB2   | 2.01                     | 0.41              |
| 1:N1:125:GLN:HB2   | 3:F2:238:PRO:CG    | 2.50                     | 0.41              |
| 1:N1:249:ILE:O     | 1:N1:252:ILE:HG22  | 2.21                     | 0.41              |
| 1:O1:186:LEU:HD22  | 1:O1:190:GLN:CB    | 2.50                     | 0.41              |
| 1:O1:269:GLN:HG3   | 1:O1:384:ARG:NH1   | 2.35                     | 0.41              |
| 1:T1:159:MET:HA    | 1:T1:172:PRO:HB3   | 2.02                     | 0.41              |
| 1:U1:420:MET:SD    | 1:U1:430:LEU:HD13  | 2.61                     | 0.41              |
| 1:W1:167:ARG:HD2   | 1:X1:165:PHE:CE1   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Y1:149:PRO:HB2  | 1:Y1:186:LEU:HD21 | 2.01                     | 0.41              |
| 1:Z1:245:ILE:HG21 | 1:Z1:266:VAL:HG11 | 2.02                     | 0.41              |
| 1:Z1:302:GLU:HB3  | 1:Z1:358:THR:HG23 | 2.03                     | 0.41              |
| 1:a1:143:THR:HG22 | 1:c1:154:ARG:HD3  | 2.01                     | 0.41              |
| 1:c1:394:LYS:CG   | 1:c1:402:LEU:HB2  | 2.48                     | 0.41              |
| 1:d1:378:ASN:ND2  | 1:d1:381:ASP:OD1  | 2.42                     | 0.41              |
| 1:f1:170:LYS:HE3  | 1:f1:170:LYS:HB3  | 1.84                     | 0.41              |
| 1:g1:373:ARG:HH21 | 1:h1:275:LYS:HD2  | 1.84                     | 0.41              |
| 2:C2:43:GLN:O     | 2:C2:44:THR:OG1   | 2.33                     | 0.41              |
| 2:E2:88:VAL:HG23  | 2:E2:89:LEU:N     | 2.35                     | 0.41              |
| 4:I2:46:GLU:HG2   | 4:I2:47:MET:N     | 2.34                     | 0.41              |
| 4:J2:56:VAL:O     | 4:J2:60:ILE:HG12  | 2.20                     | 0.41              |
| 5:P2:49:GLN:HE21  | 5:P2:82:MET:HB2   | 1.86                     | 0.41              |
| 7:W2:54:ALA:HB3   | 7:W2:55:PRO:HD3   | 2.03                     | 0.41              |
| 7:Y2:43:ARG:HB3   | 7:Y2:69:GLU:OE2   | 2.20                     | 0.41              |
| 8:c2:78:LEU:HD23  | 8:c2:135:ILE:HB   | 2.03                     | 0.41              |
| 8:d2:41:LEU:HD11  | 8:d2:226:ARG:NH1  | 2.35                     | 0.41              |
| 8:d2:60:SER:HB2   | 9:i2:64:SER:HB2   | 2.01                     | 0.41              |
| 9:j2:73:ARG:O     | 9:j2:73:ARG:HG3   | 2.19                     | 0.41              |
| 9:o2:109:ASP:OD1  | 9:o2:111:THR:N    | 2.46                     | 0.41              |
| 9:o2:168:VAL:HG23 | 11:t3:54:GLN:HE21 | 1.83                     | 0.41              |
| 9:r2:130:THR:HG23 | 9:r2:130:THR:O    | 2.21                     | 0.41              |
| 9:r2:141:THR:HG21 | 11:l3:53:THR:HB   | 1.96                     | 0.41              |
| 9:r2:237:GLN:O    | 9:r2:241:GLU:HG2  | 2.20                     | 0.41              |
| 9:t2:147:LEU:HB2  | 9:t2:160:THR:HG23 | 2.02                     | 0.41              |
| 9:u2:138:PRO:HD3  | 9:u2:174:ASN:OD1  | 2.20                     | 0.41              |
| 9:x2:18:ASN:O     | 9:x2:22:ILE:HG12  | 2.20                     | 0.41              |
| 9:x2:230:LEU:HD21 | 9:32:242:ILE:HG23 | 2.02                     | 0.41              |
| 10:G3:149:THR:OG1 | 10:H3:198:THR:O   | 2.34                     | 0.41              |
| 10:I3:168:GLN:HG3 | 10:J3:204:ARG:NE  | 2.35                     | 0.41              |
| 10:J3:124:MET:HE3 | 10:J3:124:MET:HB3 | 1.76                     | 0.41              |
| 10:N3:232:MET:HE1 | 10:P3:126:ALA:HB3 | 2.03                     | 0.41              |
| 10:O3:45:PRO:CG   | 10:P3:60:TYR:HD1  | 2.33                     | 0.41              |
| 10:P3:106:PHE:C   | 10:P3:108:THR:H   | 2.28                     | 0.41              |
| 10:P3:117:PHE:HD1 | 10:P3:122:ALA:CB  | 2.33                     | 0.41              |
| 10:R3:171:ILE:O   | 10:S3:207:TYR:O   | 2.38                     | 0.41              |
| 10:S3:83:GLN:O    | 10:S3:83:GLN:HG3  | 2.20                     | 0.41              |
| 10:T3:106:PHE:C   | 10:T3:108:THR:H   | 2.28                     | 0.41              |
| 10:Y3:117:PHE:HD1 | 10:Y3:122:ALA:CB  | 2.33                     | 0.41              |
| 11:e3:32:ARG:HG2  | 11:e3:32:ARG:HH11 | 1.85                     | 0.41              |
| 11:e3:93:TYR:CZ   | 11:e3:97:ALA:HB3  | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:e3:127:LYS:HA   | 11:e3:132:GLN:O    | 2.20                     | 0.41              |
| 11:e3:208:ARG:NH2  | 11:e3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:f3:93:TYR:CZ    | 11:f3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:f3:127:LYS:HA   | 11:f3:132:GLN:O    | 2.21                     | 0.41              |
| 11:f3:262:VAL:HB   | 11:g3:276:ALA:HB3  | 2.01                     | 0.41              |
| 11:g3:93:TYR:CZ    | 11:g3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:g3:255:ILE:HD12 | 11:g3:362:LEU:HD12 | 2.01                     | 0.41              |
| 11:h3:42:VAL:CG1   | 11:h3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:j3:93:TYR:OH    | 11:j3:173:ARG:O    | 2.25                     | 0.41              |
| 11:j3:136:LEU:HD13 | 11:k3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:l3:208:ARG:NH2  | 11:l3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:l3:344:ASP:OD1  | 11:l3:344:ASP:N    | 2.52                     | 0.41              |
| 11:m3:353:GLN:CG   | 11:m3:362:LEU:HD22 | 2.50                     | 0.41              |
| 11:p3:22:ILE:O     | 11:p3:25:LEU:HD23  | 2.19                     | 0.41              |
| 11:p3:93:TYR:CZ    | 11:p3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:p3:344:ASP:N    | 11:p3:344:ASP:OD1  | 2.52                     | 0.41              |
| 11:q3:46:ASP:OD1   | 11:r3:160:LEU:HD12 | 2.20                     | 0.41              |
| 11:s3:32:ARG:HH11  | 11:s3:32:ARG:HG2   | 1.85                     | 0.41              |
| 11:s3:217:ASP:OD1  | 11:s3:219:ARG:N    | 2.37                     | 0.41              |
| 11:w3:255:ILE:HD12 | 11:w3:362:LEU:HD12 | 2.01                     | 0.41              |
| 11:x3:271:ASP:HB3  | 11:x3:357:CYS:CA   | 2.34                     | 0.41              |
| 11:x3:342:PRO:O    | 11:x3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:y3:42:VAL:CG1   | 11:y3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:y3:344:ASP:OD1  | 11:y3:344:ASP:N    | 2.52                     | 0.41              |
| 11:z3:32:ARG:HG2   | 11:z3:32:ARG:HH11  | 1.85                     | 0.41              |
| 12:B4:63:ALA:HB1   | 12:C4:64:GLN:HG3   | 2.02                     | 0.41              |
| 12:B4:216:ASP:HA   | 12:B4:222:THR:HG22 | 2.02                     | 0.41              |
| 1:C1:181:GLU:HB3   | 1:C1:184:ARG:HH21  | 1.85                     | 0.41              |
| 1:I1:408:GLN:O     | 1:I1:411:GLN:HG2   | 2.20                     | 0.41              |
| 1:I1:423:SER:HB2   | 1:J1:384:ARG:NH1   | 2.36                     | 0.41              |
| 1:L1:155:VAL:HG23  | 1:L1:176:VAL:HG22  | 2.02                     | 0.41              |
| 1:L1:371:THR:OG1   | 1:M1:279:GLU:HG2   | 2.20                     | 0.41              |
| 1:N1:143:THR:HG21  | 1:O1:156:HIS:CD2   | 2.56                     | 0.41              |
| 1:N1:404:LEU:HD13  | 1:N1:434:ASN:HD21  | 1.85                     | 0.41              |
| 1:O1:221:THR:HG22  | 1:O1:223:SER:H     | 1.85                     | 0.41              |
| 1:R1:136:LEU:HD12  | 1:R1:136:LEU:HA    | 1.89                     | 0.41              |
| 1:R1:213:VAL:HG12  | 1:R1:214:ASP:O     | 2.20                     | 0.41              |
| 1:U1:256:ILE:HD11  | 1:V1:390:VAL:HG11  | 2.02                     | 0.41              |
| 1:W1:389:VAL:O     | 1:W1:432:VAL:HA    | 2.20                     | 0.41              |
| 1:X1:142:ARG:O     | 1:X1:146:THR:HG23  | 2.21                     | 0.41              |
| 1:X1:221:THR:HG22  | 1:X1:223:SER:H     | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Y1:279:GLU:OE2   | 1:Y1:281:HIS:N     | 2.43                     | 0.41              |
| 1:c1:164:LEU:CB    | 2:D2:144:GLU:OE1   | 2.65                     | 0.41              |
| 1:c1:297:GLN:CD    | 6:S2:55:ARG:HH21   | 2.20                     | 0.41              |
| 2:A2:194:LEU:HD23  | 2:A2:194:LEU:HA    | 1.90                     | 0.41              |
| 4:I2:44:ILE:HB     | 4:J2:36:SER:HB3    | 2.03                     | 0.41              |
| 6:Q2:16:LEU:HD13   | 6:Q2:123:LEU:HD12  | 2.01                     | 0.41              |
| 7:X2:99:VAL:HG22   | 9:i2:257:LEU:HD13  | 2.02                     | 0.41              |
| 8:c2:115:ILE:O     | 8:c2:116:GLN:C     | 2.64                     | 0.41              |
| 8:c2:169:ASN:OD1   | 8:c2:169:ASN:N     | 2.52                     | 0.41              |
| 9:g2:89:THR:O      | 9:l2:36:ARG:NH2    | 2.54                     | 0.41              |
| 9:m2:26:LEU:HD22   | 9:r2:242:ILE:CG2   | 2.49                     | 0.41              |
| 9:m2:118:GLY:O     | 9:m2:120:PHE:N     | 2.51                     | 0.41              |
| 9:n2:98:LYS:HG3    | 9:z2:45:LEU:CD2    | 2.51                     | 0.41              |
| 9:q2:18:ASN:O      | 9:q2:22:ILE:HG12   | 2.20                     | 0.41              |
| 10:B3:168:GLN:HG3  | 10:C3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:C3:106:PHE:C    | 10:C3:108:THR:H    | 2.28                     | 0.41              |
| 10:E3:65:LEU:HD23  | 11:e3:68:GLN:HG2   | 2.00                     | 0.41              |
| 10:F3:40:ILE:H     | 10:F3:40:ILE:HG12  | 1.48                     | 0.41              |
| 10:H3:43:PRO:O     | 10:H3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:H3:232:MET:HE1  | 10:J3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:J3:65:LEU:HD23  | 11:j3:68:GLN:HG2   | 2.00                     | 0.41              |
| 10:K3:43:PRO:O     | 10:K3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:K3:106:PHE:C    | 10:K3:108:THR:H    | 2.28                     | 0.41              |
| 10:K3:232:MET:HE1  | 10:M3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:L3:65:LEU:HD23  | 11:l3:68:GLN:HG2   | 2.00                     | 0.41              |
| 10:N3:130:ASN:CG   | 10:O3:102:THR:HG22 | 2.46                     | 0.41              |
| 10:O3:117:PHE:HD1  | 10:O3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:O3:135:LYS:HE2  | 10:O3:135:LYS:HB2  | 1.76                     | 0.41              |
| 10:O3:168:GLN:HG3  | 10:P3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:P3:232:MET:HE1  | 10:R3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:R3:78:LEU:HD21  | 10:R3:195:VAL:HG11 | 2.01                     | 0.41              |
| 10:S3:232:MET:HE1  | 10:U3:126:ALA:HB3  | 2.02                     | 0.41              |
| 10:T3:130:ASN:CG   | 10:U3:102:THR:HG22 | 2.46                     | 0.41              |
| 10:U3:45:PRO:CG    | 10:V3:60:TYR:HD1   | 2.33                     | 0.41              |
| 10:X3:121:ARG:HA   | 10:Y3:111:ARG:CB   | 2.50                     | 0.41              |
| 11:a3:42:VAL:CG1   | 11:a3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:a3:129:VAL:HG11 | 11:z3:136:LEU:HD13 | 2.01                     | 0.41              |
| 11:a3:276:ALA:HB3  | 11:z3:262:VAL:HB   | 2.02                     | 0.41              |
| 11:a3:342:PRO:O    | 11:a3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:d3:208:ARG:NH2  | 11:d3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:f3:259:THR:O    | 11:g3:277:GLN:NE2  | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:g3:32:ARG:HG2   | 11:g3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:g3:127:LYS:HA   | 11:g3:132:GLN:O    | 2.20                     | 0.41              |
| 11:h3:23:ARG:NH1   | 11:i3:249:GLN:O    | 2.53                     | 0.41              |
| 11:h3:93:TYR:CZ    | 11:h3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:h3:255:ILE:HD12 | 11:h3:362:LEU:HD12 | 2.01                     | 0.41              |
| 11:i3:93:TYR:CZ    | 11:i3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:j3:32:ARG:HG2   | 11:j3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:k3:32:ARG:HH11  | 11:k3:32:ARG:HG2   | 1.85                     | 0.41              |
| 11:l3:93:TYR:CZ    | 11:l3:97:ALA:HB3   | 2.55                     | 0.41              |
| 11:q3:42:VAL:CG1   | 11:q3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:r3:256:ASN:O    | 11:r3:257:SER:OG   | 2.30                     | 0.41              |
| 11:t3:32:ARG:HG2   | 11:t3:32:ARG:HH11  | 1.85                     | 0.41              |
| 12:B4:223:THR:OG1  | 12:B4:227:GLU:OE2  | 2.38                     | 0.41              |
| 1:C1:212:LEU:HB2   | 1:C1:221:THR:HG23  | 2.01                     | 0.41              |
| 1:H1:126:PHE:HA    | 1:H1:129:GLN:HE22  | 1.86                     | 0.41              |
| 1:H1:157:LEU:HD12  | 1:H1:157:LEU:HA    | 1.85                     | 0.41              |
| 1:K1:167:ARG:CZ    | 2:A2:244:TYR:C     | 2.87                     | 0.41              |
| 1:K1:289:SER:O     | 1:K1:290:LYS:HE2   | 2.20                     | 0.41              |
| 1:L1:170:LYS:HE2   | 1:L1:170:LYS:HB2   | 1.97                     | 0.41              |
| 1:L1:244:ARG:HG3   | 1:L1:247:ARG:HH22  | 1.86                     | 0.41              |
| 1:N1:182:PRO:O     | 1:N1:184:ARG:NH1   | 2.53                     | 0.41              |
| 1:O1:277:GLN:HB2   | 1:O1:377:MET:HE1   | 2.02                     | 0.41              |
| 1:Q1:168:GLU:OE1   | 1:Q1:170:LYS:HG2   | 2.21                     | 0.41              |
| 1:Q1:203:ALA:HA    | 1:R1:158:ALA:HB1   | 2.03                     | 0.41              |
| 1:Q1:266:VAL:HG22  | 1:Q1:387:VAL:HG22  | 2.01                     | 0.41              |
| 1:T1:407:ASP:HA    | 1:T1:410:LYS:NZ    | 2.35                     | 0.41              |
| 1:V1:248:ARG:HD3   | 1:W1:265:GLN:HB3   | 2.01                     | 0.41              |
| 1:W1:205:LEU:HD12  | 1:W1:206:PRO:HD2   | 2.01                     | 0.41              |
| 1:X1:167:ARG:HG3   | 2:E2:160:GLN:HB3   | 1.80                     | 0.41              |
| 1:Y1:287:ASP:HB3   | 1:Y1:290:LYS:HG2   | 2.03                     | 0.41              |
| 1:Y1:418:GLU:HB3   | 1:Z1:388:ALA:HB2   | 2.02                     | 0.41              |
| 1:Z1:247:ARG:HA    | 1:Z1:250:GLU:OE2   | 2.21                     | 0.41              |
| 1:Z1:295:SER:HB3   | 6:S2:66:THR:H      | 1.84                     | 0.41              |
| 1:a1:160:PRO:O     | 1:a1:161:LYS:HB2   | 2.20                     | 0.41              |
| 1:g1:256:ILE:HG22  | 1:g1:257:VAL:HG13  | 2.01                     | 0.41              |
| 1:g1:392:ASN:ND2   | 1:g1:437:PHE:HB2   | 2.36                     | 0.41              |
| 2:A2:75:ARG:HD3    | 2:A2:83:ALA:HB3    | 2.02                     | 0.41              |
| 2:A2:116:PHE:HA    | 2:A2:121:ILE:O     | 2.21                     | 0.41              |
| 2:B2:45:LEU:HD13   | 6:T2:133:VAL:HG13  | 2.02                     | 0.41              |
| 2:D2:162:PRO:O     | 2:D2:165:VAL:HG22  | 2.19                     | 0.41              |
| 5:P2:33:SER:O      | 5:P2:35:ALA:N      | 2.53                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:Z2:75:LYS:HA    | 9:k2:47:GLN:OE1    | 2.21                     | 0.41              |
| 7:a2:78:TYR:HB2   | 7:a2:90:TYR:CE1    | 2.55                     | 0.41              |
| 8:b2:76:ARG:HG2   | 8:b2:77:PRO:HD2    | 2.02                     | 0.41              |
| 8:e2:22:THR:O     | 8:e2:26:LEU:N      | 2.53                     | 0.41              |
| 8:e2:115:ILE:O    | 8:e2:116:GLN:C     | 2.63                     | 0.41              |
| 9:h2:93:LYS:O     | 9:h2:120:PHE:HB2   | 2.20                     | 0.41              |
| 9:h2:98:LYS:HG3   | 9:s2:45:LEU:CD1    | 2.48                     | 0.41              |
| 9:h2:238:ARG:CZ   | 9:o2:255:GLN:HG2   | 2.50                     | 0.41              |
| 9:m2:95:VAL:O     | 9:m2:118:GLY:HA3   | 2.21                     | 0.41              |
| 9:q2:66:LEU:HD23  | 9:q2:66:LEU:H      | 1.85                     | 0.41              |
| 9:q2:141:THR:HB   | 11:g3:80:GLN:OE1   | 2.15                     | 0.41              |
| 9:u2:231:VAL:HG11 | 9:12:9:LYS:CG      | 2.50                     | 0.41              |
| 9:x2:27:ALA:O     | 9:32:72:VAL:HG21   | 2.20                     | 0.41              |
| 9:x2:238:ARG:NH1  | 9:42:251:ASP:OD1   | 2.50                     | 0.41              |
| 9:y2:243:ASN:N    | 9:y2:243:ASN:HD22  | 2.19                     | 0.41              |
| 9:z2:36:ARG:HH21  | 9:z2:80:LEU:HD22   | 1.86                     | 0.41              |
| 9:z2:114:TYR:CE1  | 9:z2:178:PHE:CZ    | 3.08                     | 0.41              |
| 10:A3:106:PHE:C   | 10:A3:108:THR:H    | 2.28                     | 0.41              |
| 10:A3:166:GLU:HG2 | 10:A3:167:LYS:N    | 2.36                     | 0.41              |
| 10:B3:166:GLU:HG2 | 10:B3:167:LYS:N    | 2.36                     | 0.41              |
| 10:C3:166:GLU:HG2 | 10:C3:167:LYS:N    | 2.36                     | 0.41              |
| 10:C3:168:GLN:HG3 | 10:D3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:D3:83:GLN:O    | 10:D3:83:GLN:HG3   | 2.20                     | 0.41              |
| 10:G3:168:GLN:HG3 | 10:H3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:H3:121:ARG:HB3 | 10:I3:111:ARG:HB3  | 2.03                     | 0.41              |
| 10:J3:171:ILE:O   | 10:K3:207:TYR:O    | 2.38                     | 0.41              |
| 10:L3:43:PRO:O    | 10:L3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:M3:82:LEU:HA   | 10:M3:197:SER:CB   | 2.39                     | 0.41              |
| 10:N3:106:PHE:C   | 10:N3:108:THR:H    | 2.28                     | 0.41              |
| 10:R3:83:GLN:HG3  | 10:R3:83:GLN:O     | 2.20                     | 0.41              |
| 10:R3:124:MET:HE3 | 10:R3:124:MET:HB3  | 1.77                     | 0.41              |
| 10:S3:166:GLU:HG2 | 10:S3:167:LYS:N    | 2.36                     | 0.41              |
| 10:T3:166:GLU:HG2 | 10:T3:167:LYS:N    | 2.36                     | 0.41              |
| 10:X3:78:LEU:HD21 | 10:X3:195:VAL:HG11 | 2.01                     | 0.41              |
| 10:X3:117:PHE:HD1 | 10:X3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:Y3:101:LYS:HB2 | 10:Y3:101:LYS:HZ3  | 1.84                     | 0.41              |
| 10:Z3:106:PHE:C   | 10:Z3:108:THR:H    | 2.28                     | 0.41              |
| 11:a3:208:ARG:NH2 | 11:a3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:a3:364:ILE:CD1 | 11:y3:142:LEU:HD22 | 2.50                     | 0.41              |
| 11:b3:342:PRO:O   | 11:b3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:f3:342:PRO:O   | 11:f3:346:MET:HG3  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:h3:32:ARG:HG2   | 11:h3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:h3:127:LYS:HA   | 11:h3:132:GLN:O    | 2.20                     | 0.41              |
| 11:i3:42:VAL:CG1   | 11:i3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:i3:82:LYS:HE2   | 11:i3:82:LYS:HB3   | 1.94                     | 0.41              |
| 11:i3:114:LYS:HA   | 11:i3:114:LYS:HD2  | 1.77                     | 0.41              |
| 11:i3:136:LEU:HD13 | 11:j3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:i3:342:PRO:O    | 11:i3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:j3:93:TYR:CZ    | 11:j3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:k3:93:TYR:CZ    | 11:k3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:m3:42:VAL:CG1   | 11:m3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:m3:127:LYS:HA   | 11:m3:132:GLN:O    | 2.20                     | 0.41              |
| 11:n3:127:LYS:HA   | 11:n3:132:GLN:O    | 2.21                     | 0.41              |
| 11:q3:342:PRO:O    | 11:q3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:r3:127:LYS:HA   | 11:r3:132:GLN:O    | 2.21                     | 0.41              |
| 11:s3:208:ARG:NH2  | 11:s3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:t3:342:PRO:O    | 11:t3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:v3:127:LYS:HA   | 11:v3:132:GLN:O    | 2.20                     | 0.41              |
| 11:w3:127:LYS:HA   | 11:w3:132:GLN:O    | 2.20                     | 0.41              |
| 11:x3:217:ASP:OD1  | 11:x3:219:ARG:N    | 2.37                     | 0.41              |
| 11:z3:41:LEU:HD23  | 11:z3:86:ALA:HA    | 2.02                     | 0.41              |
| 12:A4:88:SER:N     | 12:B4:89:GLN:HE22  | 2.18                     | 0.41              |
| 12:D4:128:GLU:HG3  | 12:D4:160:VAL:HG22 | 2.03                     | 0.41              |
| 1:A1:391:VAL:HG21  | 1:A1:409:MET:HE1   | 2.02                     | 0.41              |
| 1:C1:164:LEU:HD21  | 2:C2:149:LEU:HA    | 2.02                     | 0.41              |
| 1:C1:190:GLN:CD    | 1:E1:217:GLY:HA3   | 2.46                     | 0.41              |
| 1:F1:254:SER:HB2   | 1:F1:255:PRO:HD3   | 2.02                     | 0.41              |
| 1:I1:372:ILE:O     | 1:J1:277:GLN:HA    | 2.20                     | 0.41              |
| 1:I1:410:LYS:HD2   | 1:I1:411:GLN:N     | 2.35                     | 0.41              |
| 1:J1:297:GLN:O     | 1:J1:362:GLU:HA    | 2.20                     | 0.41              |
| 1:L1:212:LEU:HB3   | 1:L1:220:LEU:HB2   | 2.03                     | 0.41              |
| 1:L1:371:THR:HG1   | 1:M1:279:GLU:HG2   | 1.86                     | 0.41              |
| 1:M1:298:LEU:HD13  | 1:M1:362:GLU:HB3   | 2.03                     | 0.41              |
| 1:N1:393:TYR:HB3   | 1:N1:402:LEU:N     | 2.36                     | 0.41              |
| 1:O1:170:LYS:HD2   | 1:O1:171:SER:O     | 2.21                     | 0.41              |
| 1:V1:254:SER:HB2   | 1:V1:255:PRO:HD3   | 2.02                     | 0.41              |
| 1:W1:145:GLU:HG2   | 1:W1:152:SER:HA    | 2.02                     | 0.41              |
| 1:W1:159:MET:HB2   | 1:W1:172:PRO:HB3   | 2.02                     | 0.41              |
| 1:X1:418:GLU:OE2   | 1:Y1:387:VAL:N     | 2.53                     | 0.41              |
| 1:Y1:268:ALA:HA    | 1:Y1:385:LEU:HD23  | 2.02                     | 0.41              |
| 1:b1:241:VAL:HG11  | 1:b1:382:ILE:HD11  | 2.01                     | 0.41              |
| 1:c1:204:GLY:HA3   | 1:d1:160:PRO:HB3   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:g1:143:THR:HG21 | 1:h1:156:HIS:CE1   | 2.55                     | 0.41              |
| 1:h1:167:ARG:HA   | 1:h1:167:ARG:NE    | 2.35                     | 0.41              |
| 2:A2:42:VAL:HG11  | 5:P2:42:LEU:HD22   | 2.03                     | 0.41              |
| 2:A2:90:LEU:HD13  | 5:O2:100:MET:HA    | 2.02                     | 0.41              |
| 2:C2:66:ARG:NH2   | 2:C2:178:GLU:OE2   | 2.51                     | 0.41              |
| 2:C2:205:MET:HE1  | 2:C2:210:MET:HE2   | 2.02                     | 0.41              |
| 2:E2:211:MET:O    | 2:E2:211:MET:HG3   | 2.21                     | 0.41              |
| 3:F2:14:HIS:CE1   | 3:F2:18:TRP:HE1    | 2.39                     | 0.41              |
| 4:G2:52:ILE:HG13  | 4:H2:25:LEU:HD12   | 2.03                     | 0.41              |
| 6:S2:55:ARG:HG3   | 6:S2:56:GLY:N      | 2.36                     | 0.41              |
| 6:U2:69:SER:O     | 6:U2:72:HIS:HB2    | 2.20                     | 0.41              |
| 7:Y2:4:LEU:HD12   | 7:Y2:4:LEU:HA      | 1.89                     | 0.41              |
| 7:Y2:64:VAL:O     | 7:Y2:64:VAL:HG22   | 2.20                     | 0.41              |
| 7:Z2:42:TYR:O     | 7:Z2:94:PRO:HB3    | 2.20                     | 0.41              |
| 8:b2:42:ARG:HE    | 8:b2:42:ARG:HB3    | 1.61                     | 0.41              |
| 8:f2:73:TYR:CE2   | 8:f2:75:SER:HB3    | 2.55                     | 0.41              |
| 9:g2:10:THR:CG2   | 9:g2:71:GLY:HA2    | 2.48                     | 0.41              |
| 9:g2:153:ARG:HH11 | 9:m2:134:PHE:HZ    | 1.69                     | 0.41              |
| 9:j2:113:ALA:HB1  | 9:j2:191:LEU:HB3   | 2.03                     | 0.41              |
| 9:k2:251:ASP:O    | 9:k2:255:GLN:HG3   | 2.21                     | 0.41              |
| 9:m2:100:GLN:H    | 9:m2:100:GLN:HG2   | 1.71                     | 0.41              |
| 9:t2:130:THR:HG23 | 9:t2:130:THR:O     | 2.21                     | 0.41              |
| 9:x2:51:GLN:HB3   | 9:x2:54:ALA:HB2    | 2.03                     | 0.41              |
| 9:32:188:GLY:O    | 9:32:190:ASN:N     | 2.53                     | 0.41              |
| 9:32:240:TYR:OH   | 12:B4:49:PRO:HG3   | 2.20                     | 0.41              |
| 9:42:143:PRO:HD2  | 9:42:159:VAL:HG21  | 2.02                     | 0.41              |
| 9:42:230:LEU:O    | 9:42:234:ILE:HG12  | 2.21                     | 0.41              |
| 10:A3:83:GLN:HG3  | 10:A3:83:GLN:O     | 2.20                     | 0.41              |
| 10:A3:221:TRP:NE1 | 10:B3:229:LEU:O    | 2.43                     | 0.41              |
| 10:A3:232:MET:HE1 | 10:C3:126:ALA:HB3  | 2.02                     | 0.41              |
| 10:C3:101:LYS:HB2 | 10:C3:101:LYS:NZ   | 2.32                     | 0.41              |
| 10:F3:232:MET:HE1 | 10:H3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:H3:83:GLN:O    | 10:H3:83:GLN:HG3   | 2.20                     | 0.41              |
| 10:J3:232:MET:HE1 | 10:L3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:K3:168:GLN:HG3 | 10:L3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:N3:166:GLU:HG2 | 10:N3:167:LYS:N    | 2.36                     | 0.41              |
| 10:Q3:117:PHE:HD1 | 10:Q3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:Q3:171:ILE:O   | 10:R3:207:TYR:O    | 2.38                     | 0.41              |
| 10:T3:78:LEU:HD21 | 10:T3:195:VAL:HG11 | 2.01                     | 0.41              |
| 10:U3:166:GLU:HG2 | 10:U3:167:LYS:N    | 2.36                     | 0.41              |
| 10:W3:43:PRO:O    | 10:W3:43:PRO:CD    | 2.67                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:W3:130:ASN:CG   | 10:X3:102:THR:HG22 | 2.46                     | 0.41              |
| 11:a3:32:ARG:HG2   | 11:a3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:a3:93:TYR:CZ    | 11:a3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:d3:32:ARG:HG2   | 11:d3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:d3:93:TYR:CZ    | 11:d3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:d3:123:MET:CE   | 11:d3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:d3:127:LYS:HA   | 11:d3:132:GLN:O    | 2.21                     | 0.41              |
| 11:d3:141:ILE:HD13 | 11:d3:165:ILE:CD1  | 2.37                     | 0.41              |
| 11:d3:342:PRO:O    | 11:d3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:f3:136:LEU:HD13 | 11:g3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:i3:217:ASP:OD1  | 11:i3:219:ARG:N    | 2.37                     | 0.41              |
| 11:i3:255:ILE:HD12 | 11:i3:362:LEU:HD12 | 2.01                     | 0.41              |
| 11:j3:259:THR:O    | 11:k3:277:GLN:NE2  | 2.54                     | 0.41              |
| 11:k3:159:GLN:CB   | 11:l3:258:ARG:HG2  | 2.51                     | 0.41              |
| 11:l3:41:LEU:HD23  | 11:l3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:l3:42:VAL:CG1   | 11:l3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:m3:252:LYS:HD2  | 11:m3:363:GLU:OE1  | 2.21                     | 0.41              |
| 11:n3:32:ARG:HG2   | 11:n3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:o3:93:TYR:CZ    | 11:o3:97:ALA:HB3   | 2.55                     | 0.41              |
| 11:p3:42:VAL:CG1   | 11:p3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:q3:159:GLN:CB   | 11:r3:258:ARG:HG2  | 2.51                     | 0.41              |
| 11:r3:208:ARG:NH2  | 11:r3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:s3:93:TYR:OH    | 11:s3:173:ARG:O    | 2.25                     | 0.41              |
| 11:w3:89:VAL:CG2   | 11:w3:126:LEU:HD21 | 2.51                     | 0.41              |
| 11:w3:342:PRO:O    | 11:w3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:x3:89:VAL:CG2   | 11:x3:126:LEU:HD21 | 2.50                     | 0.41              |
| 12:A4:156:LEU:HB3  | 12:A4:161:HIS:NE2  | 2.36                     | 0.41              |
| 12:B4:100:GLY:HA3  | 12:B4:200:PHE:CZ   | 2.56                     | 0.41              |
| 12:B4:157:ARG:HB2  | 12:B4:161:HIS:NE2  | 2.36                     | 0.41              |
| 12:C4:112:LYS:HE3  | 12:C4:112:LYS:HB3  | 1.91                     | 0.41              |
| 12:D4:136:VAL:HA   | 12:D4:185:THR:O    | 2.20                     | 0.41              |
| 1:B1:150:VAL:O     | 1:B1:151:LYS:HD3   | 2.21                     | 0.41              |
| 1:B1:250:GLU:O     | 1:B1:254:SER:OG    | 2.34                     | 0.41              |
| 1:H1:239:ASN:HA    | 1:H1:242:GLU:HG2   | 2.03                     | 0.41              |
| 1:I1:180:LEU:H     | 1:I1:215:GLN:CD    | 2.29                     | 0.41              |
| 1:M1:280:GLU:O     | 1:M1:280:GLU:HG2   | 2.21                     | 0.41              |
| 1:O1:128:GLU:OE2   | 1:O1:128:GLU:N     | 2.35                     | 0.41              |
| 1:O1:188:GLU:HA    | 1:O1:191:ILE:HD12  | 2.01                     | 0.41              |
| 1:T1:133:GLN:HE22  | 1:T1:159:MET:HE1   | 1.85                     | 0.41              |
| 1:T1:153:ALA:HB2   | 1:T1:178:VAL:HG23  | 2.02                     | 0.41              |
| 1:T1:164:LEU:HB3   | 2:E2:99:PHE:CE1    | 2.50                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:U1:137:GLU:HB3  | 1:U1:155:VAL:HG13  | 2.03                     | 0.41              |
| 1:Z1:245:ILE:CG2  | 1:Z1:266:VAL:HG11  | 2.51                     | 0.41              |
| 1:a1:194:VAL:O    | 1:a1:198:VAL:HG22  | 2.19                     | 0.41              |
| 1:f1:277:GLN:HB3  | 1:f1:375:THR:HB    | 2.02                     | 0.41              |
| 1:g1:160:PRO:HB3  | 1:g1:170:LYS:NZ    | 2.36                     | 0.41              |
| 1:h1:431:ASN:OD1  | 1:h1:432:VAL:N     | 2.53                     | 0.41              |
| 2:A2:101:MET:HE1  | 2:A2:137:PHE:CE2   | 2.56                     | 0.41              |
| 2:A2:143:ARG:HG3  | 2:A2:180:LYS:HD3   | 2.03                     | 0.41              |
| 2:D2:63:SER:C     | 2:D2:65:THR:H      | 2.27                     | 0.41              |
| 2:D2:143:ARG:HE   | 2:D2:143:ARG:HB2   | 1.74                     | 0.41              |
| 4:G2:18:LEU:O     | 4:G2:22:ALA:HB2    | 2.20                     | 0.41              |
| 5:K2:83:GLN:HG2   | 5:P2:98:GLU:CD     | 2.46                     | 0.41              |
| 6:T2:51:LYS:O     | 6:T2:55:ARG:HG2    | 2.21                     | 0.41              |
| 7:V2:113:GLN:HG3  | 7:a2:128:LYS:HD2   | 2.02                     | 0.41              |
| 7:X2:121:THR:O    | 7:X2:125:MET:HG3   | 2.19                     | 0.41              |
| 7:X2:123:LYS:HE2  | 8:c2:247:LEU:O     | 2.20                     | 0.41              |
| 8:b2:117:GLY:O    | 8:b2:118:HIS:CG    | 2.74                     | 0.41              |
| 8:c2:29:ALA:O     | 8:c2:30:SER:OG     | 2.37                     | 0.41              |
| 8:c2:155:VAL:HG21 | 9:s2:54:ALA:H      | 1.85                     | 0.41              |
| 8:e2:122:GLY:HA3  | 8:e2:127:ILE:HD11  | 2.01                     | 0.41              |
| 9:g2:44:LEU:HD21  | 9:g2:73:ARG:CG     | 2.48                     | 0.41              |
| 9:l2:108:PRO:HB3  | 9:v2:57:SER:OG     | 2.21                     | 0.41              |
| 9:m2:184:LEU:HD12 | 9:m2:184:LEU:H     | 1.84                     | 0.41              |
| 9:n2:115:THR:HB   | 9:n2:191:LEU:HD23  | 2.02                     | 0.41              |
| 9:p2:7:ILE:O      | 9:p2:10:THR:OG1    | 2.33                     | 0.41              |
| 9:t2:230:LEU:HA   | 9:t2:233:MET:HE2   | 2.03                     | 0.41              |
| 9:u2:200:ALA:CB   | 11:b3:54:GLN:OE1   | 2.66                     | 0.41              |
| 9:w2:153:ARG:CZ   | 9:32:134:PHE:HZ    | 2.33                     | 0.41              |
| 9:12:143:PRO:HD3  | 9:12:170:VAL:HG21  | 2.02                     | 0.41              |
| 9:32:154:ASP:C    | 9:32:206:PRO:HG2   | 2.46                     | 0.41              |
| 9:42:19:MET:SD    | 12:C4:44:LEU:HD13  | 2.60                     | 0.41              |
| 10:B3:124:MET:HE3 | 10:B3:124:MET:HB3  | 1.77                     | 0.41              |
| 10:C3:45:PRO:CG   | 10:D3:60:TYR:HD1   | 2.33                     | 0.41              |
| 10:D3:166:GLU:HG2 | 10:D3:167:LYS:N    | 2.36                     | 0.41              |
| 10:F3:171:ILE:O   | 10:G3:207:TYR:O    | 2.39                     | 0.41              |
| 10:G3:171:ILE:O   | 10:H3:207:TYR:O    | 2.39                     | 0.41              |
| 10:K3:130:ASN:CG  | 10:L3:102:THR:HG22 | 2.46                     | 0.41              |
| 10:M3:43:PRO:O    | 10:M3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:M3:106:PHE:C   | 10:M3:108:THR:H    | 2.28                     | 0.41              |
| 10:N3:121:ARG:HB3 | 10:O3:111:ARG:HB3  | 2.03                     | 0.41              |
| 10:O3:166:GLU:HG2 | 10:O3:167:LYS:N    | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:R3:117:PHE:HD1  | 10:R3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:R3:166:GLU:HG2  | 10:R3:167:LYS:N    | 2.36                     | 0.41              |
| 10:S3:78:LEU:HD21  | 10:S3:195:VAL:HG11 | 2.01                     | 0.41              |
| 10:S3:106:PHE:C    | 10:S3:108:THR:H    | 2.28                     | 0.41              |
| 10:U3:106:PHE:C    | 10:U3:108:THR:H    | 2.28                     | 0.41              |
| 10:W3:117:PHE:HD1  | 10:W3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:Y3:166:GLU:HG2  | 10:Y3:167:LYS:N    | 2.36                     | 0.41              |
| 10:Z3:166:GLU:HG2  | 10:Z3:167:LYS:N    | 2.36                     | 0.41              |
| 11:b3:217:ASP:OD1  | 11:b3:219:ARG:N    | 2.37                     | 0.41              |
| 11:c3:196:MET:CA   | 11:c3:196:MET:CE   | 2.97                     | 0.41              |
| 11:c3:208:ARG:NH2  | 11:c3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:c3:342:PRO:O    | 11:c3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:e3:136:LEU:HD13 | 11:f3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:e3:159:GLN:CB   | 11:f3:258:ARG:HG2  | 2.51                     | 0.41              |
| 11:g3:42:VAL:CG1   | 11:g3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:j3:41:LEU:HD23  | 11:j3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:j3:127:LYS:HA   | 11:j3:132:GLN:O    | 2.21                     | 0.41              |
| 11:k3:41:LEU:HD23  | 11:k3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:k3:42:VAL:CG1   | 11:k3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:l3:127:LYS:HA   | 11:l3:132:GLN:O    | 2.20                     | 0.41              |
| 11:m3:217:ASP:OD1  | 11:m3:219:ARG:N    | 2.37                     | 0.41              |
| 11:n3:185:ILE:HD12 | 11:n3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:n3:217:ASP:OD1  | 11:n3:219:ARG:N    | 2.37                     | 0.41              |
| 11:p3:342:PRO:O    | 11:p3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:q3:127:LYS:HA   | 11:q3:132:GLN:O    | 2.20                     | 0.41              |
| 11:s3:342:PRO:O    | 11:s3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:t3:82:LYS:HE2   | 11:t3:82:LYS:HB3   | 1.94                     | 0.41              |
| 11:t3:93:TYR:CZ    | 11:t3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:v3:93:TYR:CZ    | 11:v3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:v3:256:ASN:O    | 11:v3:257:SER:OG   | 2.30                     | 0.41              |
| 11:w3:32:ARG:HG2   | 11:w3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:x3:93:TYR:CZ    | 11:x3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:x3:127:LYS:HA   | 11:x3:132:GLN:O    | 2.20                     | 0.41              |
| 11:y3:127:LYS:HA   | 11:y3:132:GLN:O    | 2.20                     | 0.41              |
| 11:y3:259:THR:O    | 11:z3:277:GLN:NE2  | 2.54                     | 0.41              |
| 11:z3:93:TYR:CZ    | 11:z3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:z3:256:ASN:O    | 11:z3:257:SER:OG   | 2.30                     | 0.41              |
| 12:C4:78:LEU:HD12  | 12:C4:78:LEU:HA    | 1.94                     | 0.41              |
| 12:C4:206:VAL:O    | 12:D4:231:ILE:N    | 2.32                     | 0.41              |
| 1:A1:382:ILE:HG21  | 1:A1:385:LEU:HG    | 2.03                     | 0.41              |
| 1:E1:180:LEU:H     | 1:E1:215:GLN:CD    | 2.26                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G1:164:LEU:HG   | 2:B2:144:GLU:OE1  | 2.20                     | 0.41              |
| 1:H1:279:GLU:OE2  | 1:H1:281:HIS:HB2  | 2.21                     | 0.41              |
| 1:K1:191:ILE:HG21 | 1:K1:220:LEU:O    | 2.21                     | 0.41              |
| 1:L1:419:ALA:O    | 1:M1:267:THR:HG21 | 2.20                     | 0.41              |
| 1:M1:246:GLN:O    | 1:M1:250:GLU:HG2  | 2.20                     | 0.41              |
| 1:N1:133:GLN:O    | 1:N1:137:GLU:OE1  | 2.38                     | 0.41              |
| 1:O1:212:LEU:HB2  | 1:O1:220:LEU:HB2  | 2.03                     | 0.41              |
| 1:Q1:246:GLN:O    | 1:Q1:249:ILE:HG22 | 2.21                     | 0.41              |
| 1:Q1:389:VAL:O    | 1:Q1:432:VAL:HA   | 2.21                     | 0.41              |
| 1:R1:248:ARG:HH11 | 1:S1:267:THR:HG22 | 1.86                     | 0.41              |
| 1:T1:167:ARG:NH1  | 2:E2:107:LYS:HD2  | 2.26                     | 0.41              |
| 1:U1:394:LYS:HG3  | 1:U1:402:LEU:N    | 2.36                     | 0.41              |
| 1:X1:166:VAL:HG13 | 1:X1:169:GLN:H    | 1.85                     | 0.41              |
| 1:Y1:152:SER:N    | 1:Y1:179:THR:OG1  | 2.45                     | 0.41              |
| 1:Z1:375:THR:HG22 | 1:Z1:377:MET:SD   | 2.61                     | 0.41              |
| 1:b1:298:LEU:HD12 | 1:b1:361:ASN:O    | 2.20                     | 0.41              |
| 1:c1:149:PRO:O    | 1:c1:180:LEU:HD23 | 2.20                     | 0.41              |
| 1:d1:165:PHE:CE1  | 2:D2:147:LEU:HB2  | 2.56                     | 0.41              |
| 1:f1:253:LEU:HD23 | 1:f1:253:LEU:HA   | 1.92                     | 0.41              |
| 1:g1:252:ILE:HG12 | 1:h1:265:GLN:HB2  | 2.03                     | 0.41              |
| 1:h1:221:THR:HG22 | 1:h1:223:SER:H    | 1.85                     | 0.41              |
| 1:h1:244:ARG:NH2  | 1:h1:244:ARG:HB3  | 2.35                     | 0.41              |
| 2:A2:41:SER:O     | 2:A2:42:VAL:C     | 2.64                     | 0.41              |
| 2:D2:219:LEU:HD22 | 2:E2:190:PHE:CZ   | 2.56                     | 0.41              |
| 2:E2:39:SER:O     | 2:E2:40:LEU:HB2   | 2.20                     | 0.41              |
| 3:F2:190:VAL:HG22 | 3:F2:228:LEU:CD2  | 2.51                     | 0.41              |
| 4:J2:37:ILE:HD13  | 4:J2:37:ILE:HA    | 1.91                     | 0.41              |
| 6:R2:95:LEU:HB2   | 8:c2:46:VAL:CG1   | 2.51                     | 0.41              |
| 8:b2:71:LEU:HB3   | 8:b2:205:VAL:CG1  | 2.51                     | 0.41              |
| 8:c2:71:LEU:HB3   | 8:c2:205:VAL:CG1  | 2.51                     | 0.41              |
| 8:e2:151:PRO:HA   | 8:e2:152:PRO:HD3  | 1.87                     | 0.41              |
| 9:i2:122:VAL:HA   | 9:i2:127:GLN:O    | 2.21                     | 0.41              |
| 9:i2:156:VAL:HG21 | 9:y2:58:GLU:HG2   | 2.02                     | 0.41              |
| 9:k2:164:GLN:CG   | 11:e3:82:LYS:NZ   | 2.83                     | 0.41              |
| 9:k2:184:LEU:HB3  | 9:k2:192:TYR:HB3  | 2.02                     | 0.41              |
| 9:m2:73:ARG:NH2   | 9:m2:75:VAL:HG12  | 2.35                     | 0.41              |
| 9:r2:10:THR:OG1   | 9:r2:71:GLY:HA2   | 2.21                     | 0.41              |
| 9:r2:94:ASP:O     | 9:r2:217:GLY:N    | 2.45                     | 0.41              |
| 9:12:120:PHE:HB3  | 9:12:128:LEU:HD22 | 2.03                     | 0.41              |
| 9:42:120:PHE:HA   | 9:42:130:THR:HB   | 2.01                     | 0.41              |
| 10:B3:83:GLN:HG3  | 10:B3:83:GLN:O    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:D3:232:MET:HE1  | 10:F3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:E3:121:ARG:HB3  | 10:F3:111:ARG:HB3  | 2.03                     | 0.41              |
| 10:G3:83:GLN:O     | 10:G3:83:GLN:HG3   | 2.20                     | 0.41              |
| 10:H3:106:PHE:C    | 10:H3:108:THR:H    | 2.28                     | 0.41              |
| 10:M3:124:MET:HE3  | 10:M3:124:MET:HB3  | 1.77                     | 0.41              |
| 10:M3:168:GLN:HG3  | 10:N3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:U3:83:GLN:HG3   | 10:U3:83:GLN:O     | 2.20                     | 0.41              |
| 10:Y3:30:LEU:HD23  | 10:Z3:206:GLU:OE1  | 2.20                     | 0.41              |
| 10:Y3:45:PRO:CG    | 10:Z3:60:TYR:HD1   | 2.34                     | 0.41              |
| 11:a3:41:LEU:HD23  | 11:a3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:a3:83:ASN:HB2   | 11:b3:111:GLY:O    | 2.21                     | 0.41              |
| 11:a3:101:GLN:OE1  | 11:b3:219:ARG:HD3  | 2.20                     | 0.41              |
| 11:b3:123:MET:CE   | 11:b3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:b3:208:ARG:NH2  | 11:b3:238:ASP:OD2  | 2.53                     | 0.41              |
| 11:c3:123:MET:CE   | 11:c3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:c3:127:LYS:HA   | 11:c3:132:GLN:O    | 2.20                     | 0.41              |
| 11:e3:23:ARG:NH1   | 11:f3:249:GLN:O    | 2.54                     | 0.41              |
| 11:g3:342:PRO:O    | 11:g3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:i3:344:ASP:OD1  | 11:i3:344:ASP:N    | 2.52                     | 0.41              |
| 11:k3:185:ILE:HD12 | 11:k3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:k3:342:PRO:O    | 11:k3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:l3:252:LYS:HD2  | 11:l3:363:GLU:OE1  | 2.21                     | 0.41              |
| 11:l3:353:GLN:CG   | 11:l3:362:LEU:HD22 | 2.50                     | 0.41              |
| 11:m3:185:ILE:HD12 | 11:m3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:n3:89:VAL:CG2   | 11:n3:126:LEU:HD21 | 2.51                     | 0.41              |
| 11:n3:93:TYR:CZ    | 11:n3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:n3:252:LYS:HD2  | 11:n3:363:GLU:OE1  | 2.21                     | 0.41              |
| 11:p3:136:LEU:HD13 | 11:q3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:s3:93:TYR:CZ    | 11:s3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:t3:353:GLN:CG   | 11:t3:362:LEU:HD22 | 2.50                     | 0.41              |
| 11:u3:93:TYR:CZ    | 11:u3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:v3:89:VAL:CG2   | 11:v3:126:LEU:HD21 | 2.51                     | 0.41              |
| 11:v3:123:MET:HE3  | 11:v3:123:MET:HA   | 2.03                     | 0.41              |
| 11:v3:259:THR:O    | 11:w3:277:GLN:NE2  | 2.54                     | 0.41              |
| 11:w3:93:TYR:CZ    | 11:w3:97:ALA:HB3   | 2.56                     | 0.41              |
| 11:w3:271:ASP:HB3  | 11:w3:357:CYS:CA   | 2.34                     | 0.41              |
| 1:A1:290:LYS:HE2   | 1:A1:290:LYS:HB2   | 1.89                     | 0.41              |
| 1:A1:418:GLU:HB3   | 1:B1:388:ALA:HB2   | 2.03                     | 0.41              |
| 1:C1:151:LYS:HZ1   | 1:C1:182:PRO:HD3   | 1.86                     | 0.41              |
| 1:E1:193:ALA:HA    | 1:G1:219:LEU:CG    | 2.51                     | 0.41              |
| 1:E1:253:LEU:O     | 1:E1:257:VAL:HG22  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E1:374:HIS:HB3  | 1:F1:276:GLU:HB3  | 2.03                     | 0.41              |
| 1:E1:404:LEU:H    | 1:E1:434:ASN:HD21 | 1.68                     | 0.41              |
| 1:E1:409:MET:O    | 1:E1:413:GLU:HG2  | 2.20                     | 0.41              |
| 1:G1:180:LEU:HD21 | 1:G1:186:LEU:HB2  | 2.01                     | 0.41              |
| 1:G1:378:ASN:HD22 | 1:G1:381:ASP:CG   | 2.22                     | 0.41              |
| 1:G1:404:LEU:H    | 1:G1:434:ASN:ND2  | 2.18                     | 0.41              |
| 1:H1:164:LEU:HD21 | 2:B2:148:ALA:HA   | 2.03                     | 0.41              |
| 1:N1:221:THR:HG22 | 1:N1:223:SER:H    | 1.85                     | 0.41              |
| 1:P1:249:ILE:HA   | 1:P1:252:ILE:HG22 | 2.03                     | 0.41              |
| 1:Q1:394:LYS:HG3  | 1:Q1:402:LEU:HB2  | 2.02                     | 0.41              |
| 1:R1:137:GLU:OE1  | 1:R1:155:VAL:HG13 | 2.21                     | 0.41              |
| 1:R1:139:GLU:O    | 1:T1:154:ARG:NH2  | 2.43                     | 0.41              |
| 1:R1:140:LEU:HD12 | 1:R1:198:VAL:HG12 | 2.03                     | 0.41              |
| 1:T1:151:LYS:HG2  | 1:T1:179:THR:O    | 2.21                     | 0.41              |
| 1:T1:197:LEU:HD12 | 1:U1:177:THR:OG1  | 2.21                     | 0.41              |
| 1:T1:244:ARG:NH2  | 1:U1:235:LEU:HB3  | 2.36                     | 0.41              |
| 1:U1:155:VAL:HG23 | 1:U1:176:VAL:HG22 | 2.02                     | 0.41              |
| 1:b1:410:LYS:O    | 1:b1:413:GLU:HG3  | 2.21                     | 0.41              |
| 1:c1:410:LYS:HB3  | 1:c1:410:LYS:HE3  | 1.84                     | 0.41              |
| 1:d1:162:PRO:HB2  | 1:f1:165:PHE:CD2  | 2.54                     | 0.41              |
| 1:d1:423:SER:OG   | 1:d1:425:LYS:NZ   | 2.41                     | 0.41              |
| 1:e1:412:ILE:O    | 1:e1:416:THR:HG23 | 2.21                     | 0.41              |
| 1:f1:268:ALA:HB1  | 1:f1:382:ILE:HD11 | 2.03                     | 0.41              |
| 1:f1:296:ARG:HA   | 1:f1:363:THR:O    | 2.21                     | 0.41              |
| 1:h1:240:ASP:O    | 1:h1:244:ARG:HG3  | 2.21                     | 0.41              |
| 2:A2:43:GLN:C     | 2:A2:45:LEU:H     | 2.29                     | 0.41              |
| 2:A2:73:LEU:HD12  | 2:A2:186:GLY:HA3  | 2.03                     | 0.41              |
| 2:B2:49:THR:O     | 2:B2:53:PHE:HD1   | 2.04                     | 0.41              |
| 2:C2:52:THR:HG21  | 5:N2:93:VAL:HG13  | 2.02                     | 0.41              |
| 2:D2:49:THR:HG22  | 5:M2:89:ARG:HD3   | 2.03                     | 0.41              |
| 4:I2:1:MET:HE1    | 4:I2:87:ILE:O     | 2.21                     | 0.41              |
| 6:T2:114:LEU:HD11 | 7:Z2:126:MET:CB   | 2.51                     | 0.41              |
| 8:b2:60:SER:HB2   | 9:g2:64:SER:HB2   | 2.03                     | 0.41              |
| 8:b2:174:SER:C    | 8:b2:176:ASP:H    | 2.28                     | 0.41              |
| 8:b2:218:THR:HG23 | 9:h2:9:LYS:CE     | 2.50                     | 0.41              |
| 8:d2:186:GLN:C    | 8:d2:188:GLU:H    | 2.28                     | 0.41              |
| 8:d2:189:ARG:HH11 | 8:d2:193:LEU:CD2  | 2.32                     | 0.41              |
| 8:e2:167:GLU:N    | 8:e2:167:GLU:OE1  | 2.54                     | 0.41              |
| 9:i2:185:GLU:HB2  | 9:i2:195:THR:CG2  | 2.50                     | 0.41              |
| 9:j2:230:LEU:HD21 | 9:n2:242:ILE:HD12 | 2.01                     | 0.41              |
| 9:l2:114:TYR:HE1  | 9:l2:176:THR:HG21 | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:m2:72:VAL:O      | 9:m2:72:VAL:HG22   | 2.21                     | 0.41              |
| 9:n2:154:ASP:OD1   | 9:n2:156:VAL:HG12  | 2.20                     | 0.41              |
| 9:p2:114:TYR:CD1   | 9:p2:176:THR:HG21  | 2.56                     | 0.41              |
| 9:r2:36:ARG:NH1    | 9:r2:38:ARG:HB2    | 2.35                     | 0.41              |
| 9:r2:234:ILE:HD11  | 9:32:260:LEU:CD2   | 2.51                     | 0.41              |
| 9:r2:258:THR:C     | 9:r2:260:LEU:H     | 2.29                     | 0.41              |
| 9:s2:196:GLN:NE2   | 9:x2:61:THR:HG23   | 2.36                     | 0.41              |
| 9:s2:231:VAL:HG11  | 9:y2:9:LYS:HG3     | 2.02                     | 0.41              |
| 9:t2:72:VAL:O      | 9:t2:73:ARG:C      | 2.64                     | 0.41              |
| 9:v2:88:GLN:NE2    | 9:v2:90:ASN:OD1    | 2.53                     | 0.41              |
| 9:w2:7:ILE:O       | 9:w2:10:THR:OG1    | 2.33                     | 0.41              |
| 9:w2:51:GLN:HB3    | 9:w2:54:ALA:CB     | 2.51                     | 0.41              |
| 9:w2:227:ALA:O     | 9:w2:231:VAL:HG23  | 2.20                     | 0.41              |
| 9:y2:143:PRO:HD3   | 9:y2:170:VAL:HG21  | 2.03                     | 0.41              |
| 9:y2:150:THR:HA    | 9:y2:216:GLN:NE2   | 2.36                     | 0.41              |
| 9:z2:62:LEU:O      | 9:z2:62:LEU:HD23   | 2.21                     | 0.41              |
| 9:12:230:LEU:HD23  | 9:12:230:LEU:HA    | 1.93                     | 0.41              |
| 9:32:56:SER:OG     | 9:32:57:SER:N      | 2.54                     | 0.41              |
| 9:42:130:THR:HG23  | 9:42:130:THR:O     | 2.21                     | 0.41              |
| 10:A3:113:LEU:HD23 | 10:A3:113:LEU:HA   | 1.96                     | 0.41              |
| 10:B3:121:ARG:HB3  | 10:C3:111:ARG:HB3  | 2.03                     | 0.41              |
| 10:B3:171:ILE:O    | 10:C3:207:TYR:O    | 2.39                     | 0.41              |
| 10:C3:104:PHE:CZ   | 10:Z3:231:PRO:HG2  | 2.55                     | 0.41              |
| 10:D3:149:THR:OG1  | 10:E3:198:THR:O    | 2.35                     | 0.41              |
| 10:E3:168:GLN:HG3  | 10:F3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:E3:232:MET:HE1  | 10:G3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:F3:101:LYS:HB2  | 10:F3:101:LYS:HZ3  | 1.85                     | 0.41              |
| 10:F3:106:PHE:C    | 10:F3:108:THR:H    | 2.28                     | 0.41              |
| 10:G3:43:PRO:O     | 10:G3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:G3:166:GLU:HG2  | 10:G3:167:LYS:N    | 2.36                     | 0.41              |
| 10:H3:171:ILE:O    | 10:I3:207:TYR:O    | 2.38                     | 0.41              |
| 10:I3:106:PHE:C    | 10:I3:108:THR:H    | 2.28                     | 0.41              |
| 10:I3:232:MET:HE1  | 10:K3:126:ALA:HB3  | 2.03                     | 0.41              |
| 10:J3:83:GLN:O     | 10:J3:83:GLN:HG3   | 2.20                     | 0.41              |
| 10:K3:124:MET:HE3  | 10:K3:124:MET:HB3  | 1.77                     | 0.41              |
| 10:K3:135:LYS:HB2  | 10:K3:135:LYS:HE2  | 1.76                     | 0.41              |
| 10:M3:121:ARG:HB3  | 10:N3:111:ARG:HB3  | 2.03                     | 0.41              |
| 10:M3:130:ASN:CG   | 10:N3:102:THR:HG22 | 2.46                     | 0.41              |
| 10:N3:168:GLN:HG3  | 10:O3:204:ARG:NE   | 2.35                     | 0.41              |
| 10:N3:171:ILE:O    | 10:O3:207:TYR:O    | 2.39                     | 0.41              |
| 10:O3:232:MET:HE1  | 10:Q3:126:ALA:HB3  | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:P3:171:ILE:O    | 10:Q3:207:TYR:O    | 2.38                     | 0.41              |
| 10:P3:221:TRP:NE1  | 10:Q3:229:LEU:O    | 2.41                     | 0.41              |
| 10:Q3:221:TRP:NE1  | 10:R3:229:LEU:O    | 2.41                     | 0.41              |
| 10:R3:43:PRO:O     | 10:R3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:R3:130:ASN:CG   | 10:S3:102:THR:HG22 | 2.46                     | 0.41              |
| 10:S3:117:PHE:HD1  | 10:S3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:S3:130:ASN:CG   | 10:T3:102:THR:HG22 | 2.46                     | 0.41              |
| 10:U3:78:LEU:HD21  | 10:U3:195:VAL:HG11 | 2.01                     | 0.41              |
| 10:U3:171:ILE:O    | 10:V3:207:TYR:O    | 2.39                     | 0.41              |
| 10:V3:43:PRO:O     | 10:V3:43:PRO:CD    | 2.66                     | 0.41              |
| 10:V3:117:PHE:HD1  | 10:V3:122:ALA:CB   | 2.33                     | 0.41              |
| 10:V3:166:GLU:HG2  | 10:V3:167:LYS:N    | 2.36                     | 0.41              |
| 10:W3:106:PHE:C    | 10:W3:108:THR:H    | 2.28                     | 0.41              |
| 10:X3:83:GLN:HG3   | 10:X3:83:GLN:O     | 2.20                     | 0.41              |
| 10:X3:166:GLU:HG2  | 10:X3:167:LYS:N    | 2.36                     | 0.41              |
| 11:a3:123:MET:CE   | 11:a3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:a3:219:ARG:HD3  | 11:z3:101:GLN:OE1  | 2.20                     | 0.41              |
| 11:a3:336:ASN:HD22 | 11:a3:336:ASN:HA   | 1.67                     | 0.41              |
| 11:b3:32:ARG:HG2   | 11:b3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:c3:123:MET:HE3  | 11:c3:123:MET:HA   | 2.03                     | 0.41              |
| 11:c3:271:ASP:HB3  | 11:c3:357:CYS:CA   | 2.34                     | 0.41              |
| 11:c3:353:GLN:CG   | 11:c3:362:LEU:HD22 | 2.50                     | 0.41              |
| 11:e3:217:ASP:OD1  | 11:e3:219:ARG:N    | 2.37                     | 0.41              |
| 11:f3:252:LYS:HD2  | 11:f3:363:GLU:OE1  | 2.21                     | 0.41              |
| 11:h3:41:LEU:HD23  | 11:h3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:h3:114:LYS:HD2  | 11:h3:114:LYS:HA   | 1.77                     | 0.41              |
| 11:h3:185:ILE:HD12 | 11:h3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:i3:41:LEU:HD23  | 11:i3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:i3:185:ILE:HD12 | 11:i3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:j3:42:VAL:CG1   | 11:j3:45:LEU:HD21  | 2.50                     | 0.41              |
| 11:j3:185:ILE:HD12 | 11:j3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:k3:252:LYS:HD2  | 11:k3:363:GLU:OE1  | 2.21                     | 0.41              |
| 11:l3:185:ILE:HD12 | 11:l3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:l3:217:ASP:OD1  | 11:l3:219:ARG:N    | 2.37                     | 0.41              |
| 11:l3:252:LYS:HE3  | 11:l3:252:LYS:HB2  | 1.52                     | 0.41              |
| 11:l3:342:PRO:O    | 11:l3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:o3:127:LYS:HA   | 11:o3:132:GLN:O    | 2.21                     | 0.41              |
| 11:p3:259:THR:O    | 11:q3:277:GLN:NE2  | 2.54                     | 0.41              |
| 11:q3:23:ARG:NH1   | 11:r3:249:GLN:O    | 2.54                     | 0.41              |
| 11:q3:136:LEU:HD13 | 11:r3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:r3:93:TYR:CZ    | 11:r3:97:ALA:HB3   | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:s3:136:LEU:HD13 | 11:t3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:u3:83:ASN:ND2   | 11:v3:109:SER:OG   | 2.47                     | 0.41              |
| 11:v3:32:ARG:HG2   | 11:v3:32:ARG:HH11  | 1.85                     | 0.41              |
| 11:w3:23:ARG:NH1   | 11:x3:249:GLN:O    | 2.54                     | 0.41              |
| 11:w3:123:MET:CE   | 11:w3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:x3:123:MET:CE   | 11:x3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:y3:89:VAL:CG2   | 11:y3:126:LEU:HD21 | 2.51                     | 0.41              |
| 11:y3:123:MET:CE   | 11:y3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:z3:123:MET:CE   | 11:z3:136:LEU:HD22 | 2.38                     | 0.41              |
| 11:z3:342:PRO:O    | 11:z3:346:MET:HG3  | 2.21                     | 0.41              |
| 12:C4:110:ALA:HB2  | 12:C4:122:THR:HG22 | 2.02                     | 0.41              |
| 12:C4:223:THR:OG1  | 12:C4:227:GLU:OE2  | 2.34                     | 0.41              |
| 1:B1:125:GLN:HB2   | 4:H2:71:ASN:HD21   | 1.86                     | 0.41              |
| 1:B1:407:ASP:OD1   | 1:B1:407:ASP:N     | 2.54                     | 0.41              |
| 1:E1:410:LYS:HE3   | 1:E1:410:LYS:HB3   | 1.89                     | 0.41              |
| 1:F1:247:ARG:HB2   | 1:F1:247:ARG:CZ    | 2.51                     | 0.41              |
| 1:H1:254:SER:HB2   | 1:H1:255:PRO:HD3   | 2.03                     | 0.41              |
| 1:J1:283:SER:HB2   | 1:J1:369:ASP:HB2   | 2.03                     | 0.41              |
| 1:L1:252:ILE:HB    | 1:M1:265:GLN:HG3   | 2.02                     | 0.41              |
| 1:L1:410:LYS:HA    | 1:L1:413:GLU:HG3   | 2.02                     | 0.41              |
| 1:N1:181:GLU:CB    | 1:N1:184:ARG:HB2   | 2.51                     | 0.41              |
| 1:R1:142:ARG:HB2   | 1:T1:154:ARG:CZ    | 2.51                     | 0.41              |
| 1:R1:180:LEU:H     | 1:R1:215:GLN:CD    | 2.28                     | 0.41              |
| 1:X1:163:SER:OG    | 1:X1:164:LEU:N     | 2.54                     | 0.41              |
| 1:X1:163:SER:O     | 1:Y1:165:PHE:HB3   | 2.20                     | 0.41              |
| 1:Y1:143:THR:HG22  | 1:a1:154:ARG:CD    | 2.51                     | 0.41              |
| 1:Z1:253:LEU:HD22  | 1:Z1:412:ILE:HD12  | 2.03                     | 0.41              |
| 1:Z1:256:ILE:HD12  | 1:a1:435:SER:OG    | 2.21                     | 0.41              |
| 1:Z1:413:GLU:CD    | 1:Z1:432:VAL:HB    | 2.45                     | 0.41              |
| 1:c1:187:ASP:OD1   | 1:c1:190:GLN:HG3   | 2.20                     | 0.41              |
| 1:d1:279:GLU:O     | 1:d1:372:ILE:HA    | 2.20                     | 0.41              |
| 1:f1:147:LEU:O     | 1:f1:149:PRO:HD2   | 2.20                     | 0.41              |
| 1:g1:417:ARG:HG3   | 1:g1:422:PHE:HB3   | 2.03                     | 0.41              |
| 2:B2:43:GLN:HG2    | 2:B2:123:MET:SD    | 2.60                     | 0.41              |
| 2:C2:61:MET:HG3    | 2:C2:171:LEU:HD11  | 2.02                     | 0.41              |
| 3:F2:66:PHE:CD1    | 6:Q2:130:MET:HE1   | 2.55                     | 0.41              |
| 4:G2:42:THR:O      | 4:G2:44:ILE:HG12   | 2.21                     | 0.41              |
| 5:P2:75:MET:HE3    | 5:P2:75:MET:HB2    | 1.72                     | 0.41              |
| 6:S2:104:ARG:O     | 6:S2:108:GLN:HG2   | 2.20                     | 0.41              |
| 8:d2:46:VAL:HG12   | 8:d2:46:VAL:O      | 2.20                     | 0.41              |
| 8:e2:46:VAL:O      | 8:e2:47:ASP:C      | 2.64                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:e2:89:VAL:HG22   | 8:e2:99:TYR:CE2    | 2.56                     | 0.41              |
| 8:f2:89:VAL:HG22   | 8:f2:99:TYR:CE2    | 2.56                     | 0.41              |
| 8:f2:226:ARG:HG2   | 8:f2:230:GLN:HE21  | 1.86                     | 0.41              |
| 9:i2:2:ILE:HD11    | 9:i2:250:THR:CG2   | 2.52                     | 0.41              |
| 9:n2:238:ARG:CZ    | 9:u2:255:GLN:HB3   | 2.51                     | 0.41              |
| 9:o2:109:ASP:OD1   | 9:o2:111:THR:HG22  | 2.20                     | 0.41              |
| 9:q2:2:ILE:CG1     | 9:q2:3:SER:H       | 2.33                     | 0.41              |
| 9:q2:163:GLY:HA2   | 9:22:111:THR:CG2   | 2.50                     | 0.41              |
| 9:r2:6:TRP:O       | 9:r2:10:THR:HG23   | 2.21                     | 0.41              |
| 9:r2:26:LEU:HD21   | 9:w2:242:ILE:HG22  | 2.03                     | 0.41              |
| 9:w2:98:LYS:O      | 9:w2:212:GLY:HA3   | 2.21                     | 0.41              |
| 9:y2:143:PRO:HG2   | 9:y2:159:VAL:HG21  | 2.02                     | 0.41              |
| 9:22:52:PRO:HA     | 9:22:65:GLY:H      | 1.86                     | 0.41              |
| 9:32:238:ARG:HG3   | 12:C4:46:ASN:HB3   | 1.36                     | 0.41              |
| 9:42:26:LEU:HA     | 9:42:29:VAL:HG13   | 2.02                     | 0.41              |
| 9:42:42:GLU:HB2    | 9:42:75:VAL:HG13   | 2.03                     | 0.41              |
| 10:A3:179:ARG:HH21 | 10:Z3:29:PRO:HB3   | 1.86                     | 0.41              |
| 10:E3:106:PHE:C    | 10:E3:108:THR:H    | 2.28                     | 0.41              |
| 10:E3:166:GLU:HG2  | 10:E3:167:LYS:N    | 2.36                     | 0.41              |
| 10:G3:82:LEU:HA    | 10:G3:197:SER:CB   | 2.39                     | 0.41              |
| 10:I3:121:ARG:HB3  | 10:J3:111:ARG:HB3  | 2.03                     | 0.41              |
| 10:K3:121:ARG:HB3  | 10:L3:111:ARG:HB3  | 2.03                     | 0.41              |
| 10:K3:171:ILE:O    | 10:L3:207:TYR:O    | 2.38                     | 0.41              |
| 10:N3:43:PRO:O     | 10:N3:43:PRO:CD    | 2.67                     | 0.41              |
| 10:O3:101:LYS:HB2  | 10:O3:101:LYS:NZ   | 2.32                     | 0.41              |
| 10:Q3:106:PHE:C    | 10:Q3:108:THR:H    | 2.29                     | 0.41              |
| 10:Q3:231:PRO:HG2  | 10:T3:104:PHE:CZ   | 2.56                     | 0.41              |
| 10:T3:171:ILE:O    | 10:U3:207:TYR:O    | 2.39                     | 0.41              |
| 10:W3:78:LEU:HD21  | 10:W3:195:VAL:HG11 | 2.01                     | 0.41              |
| 10:W3:166:GLU:HG2  | 10:W3:167:LYS:N    | 2.36                     | 0.41              |
| 10:Z3:113:LEU:HD23 | 10:Z3:113:LEU:HA   | 1.96                     | 0.41              |
| 11:a3:66:LEU:HD21  | 11:b3:110:MET:HE1  | 2.02                     | 0.41              |
| 11:e3:41:LEU:HD23  | 11:e3:86:ALA:HA    | 2.02                     | 0.41              |
| 11:e3:166:THR:HG21 | 11:g3:362:LEU:HD23 | 2.01                     | 0.41              |
| 11:g3:83:ASN:ND2   | 11:h3:109:SER:OG   | 2.48                     | 0.41              |
| 11:g3:252:LYS:HD2  | 11:g3:363:GLU:OE1  | 2.21                     | 0.41              |
| 11:h3:252:LYS:HD2  | 11:h3:363:GLU:OE1  | 2.21                     | 0.41              |
| 11:k3:127:LYS:HA   | 11:k3:132:GLN:O    | 2.20                     | 0.41              |
| 11:n3:136:LEU:HD13 | 11:o3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:o3:185:ILE:HD12 | 11:o3:225:VAL:HG21 | 2.03                     | 0.41              |
| 11:o3:252:LYS:HD2  | 11:o3:363:GLU:OE1  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:o3:342:PRO:O    | 11:o3:346:MET:HG3  | 2.21                     | 0.41              |
| 11:s3:123:MET:HE3  | 11:s3:123:MET:HA   | 2.03                     | 0.41              |
| 11:t3:136:LEU:HD13 | 11:u3:129:VAL:HG11 | 2.02                     | 0.41              |
| 11:w3:101:GLN:HE22 | 11:x3:219:ARG:CD   | 2.32                     | 0.41              |
| 11:w3:319:LEU:HD12 | 11:w3:319:LEU:HA   | 1.82                     | 0.41              |
| 12:C4:94:THR:HG21  | 12:D4:97:ILE:HD13  | 2.03                     | 0.41              |
| 1:B1:133:GLN:O     | 1:B1:137:GLU:HG3   | 2.21                     | 0.40              |
| 1:B1:370:ARG:HE    | 1:B1:370:ARG:HB3   | 1.69                     | 0.40              |
| 1:C1:139:GLU:HG2   | 1:E1:156:HIS:CE1   | 2.47                     | 0.40              |
| 1:C1:372:ILE:HG23  | 1:C1:372:ILE:O     | 2.21                     | 0.40              |
| 1:D1:378:ASN:HB3   | 1:D1:381:ASP:OD2   | 2.20                     | 0.40              |
| 1:F1:277:GLN:HB3   | 1:F1:375:THR:HB    | 2.04                     | 0.40              |
| 1:O1:206:PRO:HG2   | 1:O1:209:ASN:OD1   | 2.21                     | 0.40              |
| 1:P1:246:GLN:OE1   | 1:P1:265:GLN:HA    | 2.21                     | 0.40              |
| 1:P1:385:LEU:HD23  | 1:P1:385:LEU:HA    | 1.80                     | 0.40              |
| 1:U1:126:PHE:HA    | 1:U1:129:GLN:NE2   | 2.36                     | 0.40              |
| 1:V1:244:ARG:CZ    | 1:W1:235:LEU:HB3   | 2.51                     | 0.40              |
| 1:V1:269:GLN:HB3   | 1:V1:383:GLU:OE2   | 2.21                     | 0.40              |
| 1:V1:417:ARG:HA    | 1:V1:420:MET:CE    | 2.49                     | 0.40              |
| 1:a1:302:GLU:HA    | 1:a1:357:SER:O     | 2.21                     | 0.40              |
| 1:b1:246:GLN:HE22  | 1:b1:265:GLN:NE2   | 2.19                     | 0.40              |
| 1:d1:234:GLN:HB3   | 1:d1:272:PHE:CZ    | 2.56                     | 0.40              |
| 1:d1:404:LEU:H     | 1:d1:434:ASN:ND2   | 2.19                     | 0.40              |
| 1:e1:372:ILE:O     | 1:f1:277:GLN:HA    | 2.21                     | 0.40              |
| 1:f1:394:LYS:HG2   | 1:f1:402:LEU:HB2   | 2.03                     | 0.40              |
| 2:D2:41:SER:HB2    | 5:M2:82:MET:SD     | 2.61                     | 0.40              |
| 2:D2:196:ILE:HD13  | 2:D2:196:ILE:HA    | 1.92                     | 0.40              |
| 5:L2:99:VAL:HA     | 5:L2:102:MET:HE3   | 2.03                     | 0.40              |
| 7:W2:64:VAL:HG22   | 7:W2:64:VAL:O      | 2.21                     | 0.40              |
| 7:a2:19:LYS:HE3    | 7:a2:64:VAL:CG1    | 2.51                     | 0.40              |
| 8:d2:122:GLY:HA3   | 8:d2:127:ILE:HD11  | 2.03                     | 0.40              |
| 9:g2:44:LEU:CD1    | 9:g2:71:GLY:HA3    | 2.45                     | 0.40              |
| 9:i2:19:MET:HB2    | 9:i2:236:VAL:HG11  | 2.03                     | 0.40              |
| 9:m2:41:PHE:CD1    | 9:m2:74:PRO:HB3    | 2.55                     | 0.40              |
| 9:m2:68:ILE:HD13   | 9:m2:68:ILE:HA     | 1.82                     | 0.40              |
| 9:t2:94:ASP:HA     | 9:t2:118:GLY:O     | 2.21                     | 0.40              |
| 9:u2:83:GLN:NE2    | 9:u2:97:ILE:O      | 2.48                     | 0.40              |
| 9:v2:88:GLN:HE21   | 9:v2:90:ASN:CG     | 2.27                     | 0.40              |
| 9:x2:36:ARG:HE     | 9:x2:36:ARG:HB3    | 1.83                     | 0.40              |
| 9:z2:44:LEU:CD1    | 9:z2:71:GLY:HA3    | 2.51                     | 0.40              |
| 9:12:153:ARG:HH21  | 9:12:213:LEU:HD13  | 1.85                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:42:42:GLU:CB     | 9:42:75:VAL:HG13   | 2.51                     | 0.40              |
| 10:C3:121:ARG:HB3  | 10:D3:111:ARG:HB3  | 2.03                     | 0.40              |
| 10:D3:121:ARG:HB3  | 10:E3:111:ARG:HB3  | 2.03                     | 0.40              |
| 10:E3:101:LYS:HB2  | 10:E3:101:LYS:NZ   | 2.32                     | 0.40              |
| 10:F3:83:GLN:O     | 10:F3:83:GLN:HG3   | 2.20                     | 0.40              |
| 10:L3:135:LYS:HB2  | 10:L3:135:LYS:HE2  | 1.76                     | 0.40              |
| 10:N3:101:LYS:HB2  | 10:N3:101:LYS:NZ   | 2.32                     | 0.40              |
| 10:N3:135:LYS:HE2  | 10:N3:135:LYS:HB2  | 1.76                     | 0.40              |
| 10:Q3:166:GLU:HG2  | 10:Q3:167:LYS:N    | 2.36                     | 0.40              |
| 10:T3:117:PHE:HD1  | 10:T3:122:ALA:CB   | 2.33                     | 0.40              |
| 10:V3:78:LEU:HD21  | 10:V3:195:VAL:HG11 | 2.01                     | 0.40              |
| 10:X3:82:LEU:HA    | 10:X3:197:SER:CB   | 2.39                     | 0.40              |
| 11:a3:365:ILE:HG23 | 11:z3:164:ARG:CZ   | 2.51                     | 0.40              |
| 11:b3:41:LEU:HD23  | 11:b3:86:ALA:HA    | 2.02                     | 0.40              |
| 11:c3:41:LEU:HD23  | 11:c3:86:ALA:HA    | 2.02                     | 0.40              |
| 11:c3:262:VAL:HB   | 11:d3:276:ALA:HB3  | 2.04                     | 0.40              |
| 11:d3:41:LEU:HD23  | 11:d3:86:ALA:HA    | 2.02                     | 0.40              |
| 11:e3:46:ASP:OD1   | 11:f3:160:LEU:HD12 | 2.20                     | 0.40              |
| 11:f3:41:LEU:HD23  | 11:f3:86:ALA:HA    | 2.02                     | 0.40              |
| 11:f3:123:MET:HE3  | 11:f3:123:MET:HA   | 2.04                     | 0.40              |
| 11:f3:185:ILE:HD12 | 11:f3:225:VAL:HG21 | 2.03                     | 0.40              |
| 11:g3:41:LEU:HD23  | 11:g3:86:ALA:HA    | 2.02                     | 0.40              |
| 11:h3:342:PRO:O    | 11:h3:346:MET:HG3  | 2.21                     | 0.40              |
| 11:i3:252:LYS:HD2  | 11:i3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:j3:252:LYS:HD2  | 11:j3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:k3:23:ARG:NH1   | 11:l3:249:GLN:O    | 2.54                     | 0.40              |
| 11:m3:136:LEU:HD13 | 11:n3:129:VAL:HG11 | 2.02                     | 0.40              |
| 11:n3:52:THR:CG2   | 11:n3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:n3:336:ASN:HD22 | 11:n3:336:ASN:HA   | 1.67                     | 0.40              |
| 11:o3:93:TYR:OH    | 11:o3:173:ARG:O    | 2.25                     | 0.40              |
| 11:q3:32:ARG:HH11  | 11:q3:32:ARG:HG2   | 1.85                     | 0.40              |
| 11:t3:101:GLN:HE22 | 11:u3:219:ARG:CD   | 2.33                     | 0.40              |
| 11:u3:66:LEU:HD21  | 11:v3:110:MET:HE1  | 2.03                     | 0.40              |
| 11:u3:342:PRO:O    | 11:u3:346:MET:HG3  | 2.21                     | 0.40              |
| 11:w3:46:ASP:OD1   | 11:x3:160:LEU:HD12 | 2.20                     | 0.40              |
| 11:w3:123:MET:HE3  | 11:w3:123:MET:HA   | 2.03                     | 0.40              |
| 11:y3:123:MET:HE3  | 11:y3:123:MET:HA   | 2.03                     | 0.40              |
| 11:y3:342:PRO:O    | 11:y3:346:MET:HG3  | 2.21                     | 0.40              |
| 11:z3:89:VAL:CG2   | 11:z3:126:LEU:HD21 | 2.51                     | 0.40              |
| 11:z3:127:LYS:HA   | 11:z3:132:GLN:O    | 2.20                     | 0.40              |
| 12:A4:112:LYS:HB2  | 12:A4:177:ASN:HD21 | 1.86                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A1:301:SER:HB2  | 1:B1:359:GLN:OE1  | 2.22                     | 0.40              |
| 1:C1:212:LEU:HD23 | 1:C1:212:LEU:HA   | 1.88                     | 0.40              |
| 1:E1:269:GLN:O    | 1:E1:270:LEU:HD23 | 2.21                     | 0.40              |
| 1:F1:404:LEU:HD23 | 1:F1:434:ASN:ND2  | 2.30                     | 0.40              |
| 1:H1:293:LEU:O    | 1:I1:285:ASN:ND2  | 2.39                     | 0.40              |
| 1:I1:180:LEU:HB2  | 1:I1:215:GLN:HE22 | 1.87                     | 0.40              |
| 1:K1:249:ILE:O    | 1:K1:252:ILE:HG22 | 2.22                     | 0.40              |
| 1:M1:261:ASN:O    | 1:M1:392:ASN:N    | 2.44                     | 0.40              |
| 1:M1:290:LYS:HE2  | 1:M1:290:LYS:HB2  | 1.88                     | 0.40              |
| 1:N1:143:THR:HG23 | 1:O1:154:ARG:NH2  | 2.29                     | 0.40              |
| 1:N1:369:ASP:OD1  | 1:O1:282:TYR:N    | 2.51                     | 0.40              |
| 1:P1:393:TYR:CZ   | 1:P1:436:PRO:HD3  | 2.56                     | 0.40              |
| 1:R1:237:PHE:HE1  | 1:S1:232:ASP:HA   | 1.87                     | 0.40              |
| 1:R1:420:MET:SD   | 1:R1:430:LEU:HB2  | 2.60                     | 0.40              |
| 1:T1:304:VAL:HG22 | 1:T1:356:ARG:HG2  | 2.03                     | 0.40              |
| 1:U1:172:PRO:HG2  | 1:U1:204:GLY:O    | 2.21                     | 0.40              |
| 1:U1:372:ILE:O    | 1:U1:372:ILE:HG23 | 2.21                     | 0.40              |
| 1:W1:234:GLN:HB3  | 1:W1:272:PHE:CE2  | 2.57                     | 0.40              |
| 1:b1:414:ASP:HB3  | 1:c1:431:ASN:HD22 | 1.86                     | 0.40              |
| 1:c1:184:ARG:N    | 1:c1:184:ARG:HD2  | 2.35                     | 0.40              |
| 1:g1:157:LEU:HD21 | 1:g1:159:MET:HE3  | 2.02                     | 0.40              |
| 1:h1:263:HIS:HB2  | 1:h1:390:VAL:CG2  | 2.50                     | 0.40              |
| 2:B2:74:LEU:HD22  | 2:B2:235:LEU:HD22 | 2.03                     | 0.40              |
| 5:P2:69:ASN:OD1   | 5:P2:70:ASP:N     | 2.55                     | 0.40              |
| 7:V2:98:VAL:O     | 7:V2:102:MET:HG2  | 2.21                     | 0.40              |
| 7:W2:95:ASN:O     | 7:W2:95:ASN:CG    | 2.65                     | 0.40              |
| 7:Y2:28:LEU:HD13  | 7:Y2:101:GLU:HB2  | 2.03                     | 0.40              |
| 7:Z2:113:GLN:HG3  | 8:e2:243:ARG:HD3  | 2.03                     | 0.40              |
| 8:b2:16:LEU:HD23  | 8:b2:16:LEU:HA    | 1.97                     | 0.40              |
| 8:d2:27:ALA:O     | 9:i2:72:VAL:HG11  | 2.21                     | 0.40              |
| 8:d2:107:VAL:HG12 | 8:d2:113:LEU:HD23 | 2.02                     | 0.40              |
| 9:h2:127:GLN:OE1  | 9:h2:135:GLN:HG2  | 2.21                     | 0.40              |
| 9:i2:129:VAL:CG2  | 9:s2:63:PRO:HG3   | 2.51                     | 0.40              |
| 9:j2:189:GLU:HA   | 9:n2:42:GLU:CG    | 2.52                     | 0.40              |
| 9:m2:175:LEU:HD23 | 9:m2:175:LEU:HA   | 1.94                     | 0.40              |
| 9:p2:101:GLY:O    | 9:p2:116:ARG:NH1  | 2.54                     | 0.40              |
| 9:p2:143:PRO:HG2  | 9:p2:159:VAL:HG21 | 2.03                     | 0.40              |
| 9:r2:35:LYS:NZ    | 9:r2:220:GLU:OE2  | 2.52                     | 0.40              |
| 9:t2:189:GLU:O    | 9:t2:191:LEU:HG   | 2.21                     | 0.40              |
| 9:t2:238:ARG:O    | 9:t2:242:ILE:HG13 | 2.21                     | 0.40              |
| 9:z2:230:LEU:HD23 | 9:z2:230:LEU:HA   | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:A3:74:ILE:CG2   | 10:Z3:37:ALA:HB1   | 2.49                     | 0.40              |
| 10:C3:171:ILE:O    | 10:D3:207:TYR:O    | 2.39                     | 0.40              |
| 10:F3:43:PRO:O     | 10:F3:43:PRO:CD    | 2.67                     | 0.40              |
| 10:I3:83:GLN:O     | 10:I3:83:GLN:HG3   | 2.20                     | 0.40              |
| 10:I3:171:ILE:O    | 10:J3:207:TYR:O    | 2.39                     | 0.40              |
| 10:J3:121:ARG:HB3  | 10:K3:111:ARG:HB3  | 2.04                     | 0.40              |
| 10:J3:135:LYS:HB2  | 10:J3:135:LYS:HE2  | 1.76                     | 0.40              |
| 10:M3:83:GLN:O     | 10:M3:83:GLN:HG3   | 2.20                     | 0.40              |
| 10:O3:171:ILE:O    | 10:P3:207:TYR:O    | 2.39                     | 0.40              |
| 10:P3:83:GLN:HG3   | 10:P3:83:GLN:O     | 2.20                     | 0.40              |
| 10:P3:166:GLU:HG2  | 10:P3:167:LYS:N    | 2.36                     | 0.40              |
| 10:S3:171:ILE:O    | 10:T3:207:TYR:O    | 2.39                     | 0.40              |
| 10:U3:117:PHE:HD1  | 10:U3:122:ALA:CB   | 2.33                     | 0.40              |
| 10:W3:124:MET:HE3  | 10:W3:124:MET:HB3  | 1.77                     | 0.40              |
| 11:b3:93:TYR:CZ    | 11:b3:97:ALA:HB3   | 2.56                     | 0.40              |
| 11:b3:127:LYS:HA   | 11:b3:132:GLN:O    | 2.20                     | 0.40              |
| 11:b3:196:MET:CA   | 11:b3:196:MET:CE   | 2.97                     | 0.40              |
| 11:c3:82:LYS:HE2   | 11:c3:82:LYS:HB3   | 1.94                     | 0.40              |
| 11:d3:52:THR:CG2   | 11:d3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:e3:185:ILE:HD12 | 11:e3:225:VAL:HG21 | 2.03                     | 0.40              |
| 11:e3:252:LYS:HD2  | 11:e3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:e3:342:PRO:O    | 11:e3:346:MET:HG3  | 2.21                     | 0.40              |
| 11:f3:42:VAL:CG1   | 11:f3:45:LEU:HD21  | 2.50                     | 0.40              |
| 11:f3:52:THR:CG2   | 11:f3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:g3:185:ILE:HD12 | 11:g3:225:VAL:HG21 | 2.03                     | 0.40              |
| 11:h3:101:GLN:HE22 | 11:i3:219:ARG:CD   | 2.33                     | 0.40              |
| 11:i3:123:MET:HE3  | 11:i3:123:MET:HA   | 2.03                     | 0.40              |
| 11:k3:52:THR:CG2   | 11:k3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:m3:52:THR:CG2   | 11:m3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:o3:126:LEU:HB2  | 11:o3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:o3:217:ASP:OD1  | 11:o3:219:ARG:N    | 2.37                     | 0.40              |
| 11:p3:123:MET:HE3  | 11:p3:123:MET:HA   | 2.03                     | 0.40              |
| 11:p3:126:LEU:HB2  | 11:p3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:q3:93:TYR:CZ    | 11:q3:97:ALA:HB3   | 2.55                     | 0.40              |
| 11:r3:52:THR:CG2   | 11:r3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:t3:123:MET:HE3  | 11:t3:123:MET:HA   | 2.03                     | 0.40              |
| 11:u3:101:GLN:HE22 | 11:v3:219:ARG:CD   | 2.33                     | 0.40              |
| 11:u3:262:VAL:HB   | 11:v3:276:ALA:HB3  | 2.04                     | 0.40              |
| 11:u3:353:GLN:CG   | 11:u3:362:LEU:HD22 | 2.50                     | 0.40              |
| 11:v3:252:LYS:HD2  | 11:v3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:v3:342:PRO:O    | 11:v3:346:MET:HG3  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:y3:93:TYR:CZ   | 11:y3:97:ALA:HB3  | 2.56                     | 0.40              |
| 11:z3:123:MET:HE3 | 11:z3:123:MET:HA  | 2.03                     | 0.40              |
| 12:D4:56:ASN:OD1  | 12:E4:55:ASN:HB3  | 2.21                     | 0.40              |
| 1:A1:246:GLN:OE1  | 1:A1:265:GLN:HA   | 2.21                     | 0.40              |
| 1:B1:245:ILE:O    | 1:B1:249:ILE:HG13 | 2.21                     | 0.40              |
| 1:B1:269:GLN:HG3  | 1:B1:384:ARG:NH1  | 2.35                     | 0.40              |
| 1:C1:269:GLN:O    | 1:C1:270:LEU:HD23 | 2.21                     | 0.40              |
| 1:E1:141:ALA:O    | 1:E1:145:GLU:HG2  | 2.22                     | 0.40              |
| 1:G1:188:GLU:O    | 1:G1:191:ILE:HB   | 2.22                     | 0.40              |
| 1:G1:234:GLN:HB3  | 1:G1:272:PHE:CE2  | 2.57                     | 0.40              |
| 1:K1:231:ASN:OD1  | 1:K1:232:ASP:N    | 2.54                     | 0.40              |
| 1:N1:151:LYS:N    | 1:N1:151:LYS:HD2  | 2.36                     | 0.40              |
| 1:R1:159:MET:SD   | 1:R1:172:PRO:HB3  | 2.61                     | 0.40              |
| 1:T1:382:ILE:HG21 | 1:T1:385:LEU:HG   | 2.03                     | 0.40              |
| 1:W1:142:ARG:CG   | 1:X1:154:ARG:HH12 | 2.33                     | 0.40              |
| 1:X1:252:ILE:HD13 | 1:X1:252:ILE:HA   | 1.92                     | 0.40              |
| 1:Y1:191:ILE:HG21 | 1:Y1:220:LEU:O    | 2.21                     | 0.40              |
| 1:h1:137:GLU:OE2  | 1:h1:157:LEU:N    | 2.54                     | 0.40              |
| 2:A2:51:LEU:HB3   | 5:O2:91:LYS:HB3   | 2.02                     | 0.40              |
| 2:A2:143:ARG:H    | 2:A2:177:SER:CB   | 2.34                     | 0.40              |
| 2:C2:119:GLN:O    | 2:C2:120:LYS:HG2  | 2.20                     | 0.40              |
| 2:D2:73:LEU:O     | 2:D2:190:PHE:HE1  | 2.04                     | 0.40              |
| 3:F2:39:PRO:HG2   | 3:F2:42:VAL:CG2   | 2.51                     | 0.40              |
| 4:H2:54:LYS:O     | 4:H2:58:VAL:HG23  | 2.22                     | 0.40              |
| 5:K2:68:LEU:HD11  | 5:P2:84:MET:HE3   | 2.03                     | 0.40              |
| 6:U2:109:PHE:CD2  | 8:f2:248:LEU:HD22 | 2.57                     | 0.40              |
| 7:a2:115:ASN:O    | 7:a2:118:VAL:HG12 | 2.20                     | 0.40              |
| 9:n2:94:ASP:OD1   | 9:n2:119:SER:HA   | 2.21                     | 0.40              |
| 9:p2:16:GLN:NE2   | 9:u2:2:ILE:HG23   | 2.36                     | 0.40              |
| 9:q2:89:THR:HG21  | 9:q2:94:ASP:HB2   | 2.03                     | 0.40              |
| 9:s2:51:GLN:HB3   | 9:s2:54:ALA:HB2   | 2.04                     | 0.40              |
| 9:s2:98:LYS:HD2   | 9:42:45:LEU:CD1   | 2.51                     | 0.40              |
| 9:s2:140:ILE:HD13 | 9:s2:157:VAL:HG11 | 2.02                     | 0.40              |
| 9:s2:156:VAL:HG23 | 9:s2:156:VAL:O    | 2.21                     | 0.40              |
| 9:s2:209:ASN:HA   | 11:s3:54:GLN:HE22 | 1.86                     | 0.40              |
| 9:u2:44:LEU:HD23  | 9:u2:44:LEU:HA    | 1.93                     | 0.40              |
| 9:u2:150:THR:HA   | 9:u2:216:GLN:NE2  | 2.32                     | 0.40              |
| 9:y2:233:MET:HA   | 9:y2:236:VAL:HG22 | 2.03                     | 0.40              |
| 9:32:251:ASP:OD1  | 9:32:255:GLN:NE2  | 2.54                     | 0.40              |
| 10:B3:232:MET:HE1 | 10:D3:126:ALA:HB3 | 2.03                     | 0.40              |
| 10:F3:166:GLU:HG2 | 10:F3:167:LYS:N   | 2.36                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:O3:43:PRO:O     | 10:O3:43:PRO:CD    | 2.67                     | 0.40              |
| 10:P3:130:ASN:CG   | 10:Q3:102:THR:HG22 | 2.47                     | 0.40              |
| 10:R3:106:PHE:C    | 10:R3:108:THR:H    | 2.28                     | 0.40              |
| 11:a3:126:LEU:HB2  | 11:a3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:a3:127:LYS:HA   | 11:a3:132:GLN:O    | 2.20                     | 0.40              |
| 11:b3:126:LEU:HB2  | 11:b3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:h3:123:MET:HE3  | 11:h3:123:MET:HA   | 2.03                     | 0.40              |
| 11:i3:52:THR:CG2   | 11:i3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:i3:101:GLN:HE22 | 11:j3:219:ARG:CD   | 2.33                     | 0.40              |
| 11:k3:136:LEU:HD13 | 11:l3:129:VAL:HG11 | 2.02                     | 0.40              |
| 11:m3:126:LEU:HB2  | 11:m3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:n3:123:MET:HE3  | 11:n3:123:MET:HA   | 2.03                     | 0.40              |
| 11:n3:126:LEU:HB2  | 11:n3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:o3:66:LEU:HD21  | 11:p3:110:MET:HE1  | 2.03                     | 0.40              |
| 11:o3:89:VAL:CG2   | 11:o3:126:LEU:HD21 | 2.51                     | 0.40              |
| 11:p3:52:THR:CG2   | 11:p3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:q3:123:MET:HE3  | 11:q3:123:MET:HA   | 2.03                     | 0.40              |
| 11:q3:126:LEU:HB2  | 11:q3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:q3:256:ASN:O    | 11:q3:257:SER:OG   | 2.30                     | 0.40              |
| 11:r3:83:ASN:HB2   | 11:s3:111:GLY:O    | 2.22                     | 0.40              |
| 11:w3:252:LYS:HD2  | 11:w3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:y3:126:LEU:HB2  | 11:y3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:z3:126:LEU:HB2  | 11:z3:135:ALA:HB3  | 2.04                     | 0.40              |
| 12:C4:204:GLN:HG3  | 12:C4:218:GLY:HA3  | 2.04                     | 0.40              |
| 12:D4:47:GLN:HG2   | 12:D4:52:PRO:HG2   | 2.04                     | 0.40              |
| 1:B1:370:ARG:HD2   | 1:B1:372:ILE:HD11  | 2.04                     | 0.40              |
| 1:F1:408:GLN:O     | 1:F1:411:GLN:HG2   | 2.21                     | 0.40              |
| 1:H1:145:GLU:OE2   | 1:H1:153:ALA:N     | 2.39                     | 0.40              |
| 1:I1:214:ASP:OD1   | 1:I1:220:LEU:HD11  | 2.21                     | 0.40              |
| 1:J1:385:LEU:HB3   | 1:J1:420:MET:HE2   | 2.03                     | 0.40              |
| 1:J1:393:TYR:HB3   | 1:J1:402:LEU:N     | 2.37                     | 0.40              |
| 1:K1:378:ASN:HB3   | 1:K1:381:ASP:OD2   | 2.21                     | 0.40              |
| 1:M1:273:ALA:HB3   | 1:M1:275:LYS:NZ    | 2.37                     | 0.40              |
| 1:M1:280:GLU:HA    | 1:M1:371:THR:O     | 2.22                     | 0.40              |
| 1:N1:359:GLN:OE1   | 7:V2:55:PRO:CG     | 2.70                     | 0.40              |
| 1:N1:407:ASP:O     | 1:N1:410:LYS:HG3   | 2.22                     | 0.40              |
| 1:O1:287:ASP:HB3   | 1:O1:290:LYS:HG2   | 2.03                     | 0.40              |
| 1:R1:145:GLU:HA    | 1:R1:150:VAL:HG11  | 2.03                     | 0.40              |
| 1:R1:266:VAL:HG22  | 1:R1:387:VAL:HG22  | 2.04                     | 0.40              |
| 1:T1:167:ARG:NH1   | 2:E2:107:LYS:HA    | 2.35                     | 0.40              |
| 1:U1:187:ASP:O     | 1:U1:191:ILE:HG12  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:V1:279:GLU:OE2  | 1:V1:373:ARG:HB2  | 2.22                     | 0.40              |
| 1:V1:393:TYR:CE1  | 1:V1:403:PRO:HB3  | 2.57                     | 0.40              |
| 1:V1:421:GLY:HA3  | 1:W1:267:THR:HG21 | 2.04                     | 0.40              |
| 1:Y1:212:LEU:HD23 | 1:Y1:212:LEU:HA   | 1.85                     | 0.40              |
| 1:Y1:297:GLN:HB2  | 6:S2:73:ILE:HD12  | 2.02                     | 0.40              |
| 1:a1:168:GLU:CG   | 1:a1:169:GLN:H    | 2.27                     | 0.40              |
| 1:b1:239:ASN:HA   | 1:b1:242:GLU:HG2  | 2.03                     | 0.40              |
| 1:b1:423:SER:HB3  | 1:b1:426:ARG:HG3  | 2.03                     | 0.40              |
| 1:d1:249:ILE:O    | 1:d1:252:ILE:HG22 | 2.21                     | 0.40              |
| 2:B2:121:ILE:HG23 | 2:B2:125:GLU:HG2  | 2.04                     | 0.40              |
| 2:D2:242:SER:CB   | 4:J2:85:PRO:HA    | 2.52                     | 0.40              |
| 2:E2:92:LEU:HD21  | 3:F2:90:PHE:CZ    | 2.57                     | 0.40              |
| 3:F2:24:LEU:HD23  | 3:F2:24:LEU:HA    | 1.84                     | 0.40              |
| 3:F2:48:ILE:O     | 3:F2:52:LEU:HG    | 2.21                     | 0.40              |
| 3:F2:123:PRO:HA   | 3:F2:127:ARG:CD   | 2.39                     | 0.40              |
| 5:N2:99:VAL:O     | 5:N2:102:MET:HG2  | 2.20                     | 0.40              |
| 6:Q2:48:GLU:O     | 6:Q2:52:VAL:HG23  | 2.22                     | 0.40              |
| 6:S2:51:LYS:HE2   | 6:S2:51:LYS:HB2   | 1.77                     | 0.40              |
| 6:U2:114:LEU:HD11 | 7:a2:126:MET:HB3  | 2.04                     | 0.40              |
| 7:V2:130:LEU:HA   | 7:V2:130:LEU:HD13 | 1.87                     | 0.40              |
| 7:Z2:78:TYR:CZ    | 7:Z2:80:PRO:HG3   | 2.56                     | 0.40              |
| 8:c2:42:ARG:HE    | 8:c2:42:ARG:HB3   | 1.74                     | 0.40              |
| 8:c2:70:GLN:CD    | 9:o2:3:SER:HB2    | 2.47                     | 0.40              |
| 8:d2:122:GLY:HA2  | 8:d2:162:LYS:HB3  | 2.04                     | 0.40              |
| 8:e2:116:GLN:OE1  | 8:e2:116:GLN:N    | 2.55                     | 0.40              |
| 9:g2:24:ASN:OD1   | 9:g2:28:ASN:ND2   | 2.54                     | 0.40              |
| 9:g2:156:VAL:O    | 9:g2:156:VAL:HG13 | 2.22                     | 0.40              |
| 9:g2:226:VAL:O    | 9:g2:230:LEU:HD23 | 2.22                     | 0.40              |
| 9:j2:98:LYS:O     | 9:j2:212:GLY:HA3  | 2.21                     | 0.40              |
| 9:j2:130:THR:O    | 9:j2:130:THR:HG23 | 2.22                     | 0.40              |
| 9:m2:2:ILE:HG23   | 9:m2:3:SER:N      | 2.32                     | 0.40              |
| 9:p2:141:THR:CG2  | 11:c3:54:GLN:CD   | 2.94                     | 0.40              |
| 9:q2:185:GLU:HB2  | 9:v2:52:PRO:HG2   | 2.02                     | 0.40              |
| 9:r2:149:ILE:O    | 9:r2:216:GLN:NE2  | 2.50                     | 0.40              |
| 9:s2:72:VAL:O     | 9:s2:73:ARG:C     | 2.64                     | 0.40              |
| 9:t2:36:ARG:HE    | 9:t2:36:ARG:HB3   | 1.81                     | 0.40              |
| 9:u2:230:LEU:HD12 | 12:E4:49:PRO:HG2  | 2.04                     | 0.40              |
| 9:z2:7:ILE:O      | 9:z2:10:THR:OG1   | 2.31                     | 0.40              |
| 9:32:43:ASP:N     | 9:32:43:ASP:OD2   | 2.46                     | 0.40              |
| 9:32:143:PRO:HD2  | 9:32:159:VAL:HG21 | 2.03                     | 0.40              |
| 9:32:189:GLU:HB2  | 9:32:191:LEU:HD22 | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:H3:130:ASN:CG   | 10:I3:102:THR:HG22 | 2.46                     | 0.40              |
| 10:L3:121:ARG:HB3  | 10:M3:111:ARG:HB3  | 2.04                     | 0.40              |
| 10:R3:221:TRP:NE1  | 10:S3:229:LEU:O    | 2.42                     | 0.40              |
| 10:T3:232:MET:HE1  | 10:V3:126:ALA:HB3  | 2.03                     | 0.40              |
| 10:V3:106:PHE:C    | 10:V3:108:THR:H    | 2.28                     | 0.40              |
| 10:X3:168:GLN:HG3  | 10:Y3:204:ARG:NE   | 2.37                     | 0.40              |
| 10:Y3:106:PHE:C    | 10:Y3:108:THR:H    | 2.28                     | 0.40              |
| 11:b3:123:MET:HE3  | 11:b3:123:MET:HA   | 2.03                     | 0.40              |
| 11:g3:83:ASN:HB2   | 11:h3:111:GLY:O    | 2.22                     | 0.40              |
| 11:h3:52:THR:CG2   | 11:h3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:k3:123:MET:HE3  | 11:k3:123:MET:HA   | 2.03                     | 0.40              |
| 11:l3:104:ASP:OD1  | 11:l3:166:THR:HA   | 2.22                     | 0.40              |
| 11:l3:126:LEU:HB2  | 11:l3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:m3:104:ASP:OD1  | 11:m3:166:THR:HA   | 2.22                     | 0.40              |
| 11:r3:342:PRO:O    | 11:r3:346:MET:HG3  | 2.21                     | 0.40              |
| 11:s3:83:ASN:HB2   | 11:t3:111:GLY:O    | 2.22                     | 0.40              |
| 11:u3:136:LEU:HD13 | 11:v3:129:VAL:HG11 | 2.03                     | 0.40              |
| 11:u3:252:LYS:HD2  | 11:u3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:v3:142:LEU:HD22 | 11:x3:364:ILE:CD1  | 2.52                     | 0.40              |
| 11:x3:252:LYS:HD2  | 11:x3:363:GLU:OE1  | 2.21                     | 0.40              |
| 12:B4:132:PRO:HD3  | 12:B4:158:ALA:HB2  | 2.04                     | 0.40              |
| 1:E1:167:ARG:HB2   | 2:B2:140:ARG:CZ    | 2.35                     | 0.40              |
| 1:I1:142:ARG:CD    | 1:K1:154:ARG:HH12  | 2.35                     | 0.40              |
| 1:I1:284:PRO:O     | 1:I1:290:LYS:NZ    | 2.54                     | 0.40              |
| 1:J1:279:GLU:OE2   | 1:J1:281:HIS:N     | 2.53                     | 0.40              |
| 1:N1:187:ASP:O     | 1:N1:191:ILE:HG12  | 2.22                     | 0.40              |
| 1:N1:394:LYS:HE2   | 1:N1:402:LEU:HD13  | 2.03                     | 0.40              |
| 1:O1:139:GLU:OE2   | 1:Q1:154:ARG:NE    | 2.34                     | 0.40              |
| 1:O1:393:TYR:CD1   | 1:O1:403:PRO:HA    | 2.55                     | 0.40              |
| 1:P1:299:ASN:HD22  | 1:P1:361:ASN:HD22  | 1.69                     | 0.40              |
| 1:P1:416:THR:O     | 1:P1:420:MET:HG3   | 2.22                     | 0.40              |
| 1:Q1:287:ASP:HB3   | 1:Q1:290:LYS:HG2   | 2.04                     | 0.40              |
| 1:Q1:413:GLU:O     | 1:Q1:416:THR:OG1   | 2.34                     | 0.40              |
| 1:R1:292:THR:HB    | 1:R1:367:GLU:O     | 2.21                     | 0.40              |
| 1:X1:199:SER:HA    | 1:X1:205:LEU:HB3   | 2.04                     | 0.40              |
| 1:c1:144:ILE:HD12  | 1:c1:194:VAL:HG23  | 2.03                     | 0.40              |
| 1:c1:219:LEU:HD23  | 1:c1:219:LEU:HA    | 1.90                     | 0.40              |
| 1:d1:158:ALA:O     | 1:d1:159:MET:HE2   | 2.22                     | 0.40              |
| 1:d1:269:GLN:O     | 1:d1:383:GLU:HG2   | 2.22                     | 0.40              |
| 1:g1:143:THR:CG2   | 1:h1:156:HIS:HE1   | 2.35                     | 0.40              |
| 1:h1:145:GLU:HA    | 1:h1:150:VAL:HG12  | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:h1:191:ILE:HG12  | 1:h1:220:LEU:HB3   | 2.04                     | 0.40              |
| 2:A2:59:LEU:HD23   | 2:A2:59:LEU:HA     | 1.77                     | 0.40              |
| 2:B2:81:PRO:O      | 2:B2:83:ALA:N      | 2.55                     | 0.40              |
| 2:E2:75:ARG:HH12   | 2:E2:85:PRO:HG3    | 1.85                     | 0.40              |
| 6:Q2:93:PRO:O      | 8:b2:54:ARG:HD2    | 2.22                     | 0.40              |
| 7:Y2:76:LEU:HD12   | 9:j2:47:GLN:NE2    | 2.37                     | 0.40              |
| 8:e2:57:VAL:HG12   | 8:e2:57:VAL:O      | 2.21                     | 0.40              |
| 8:e2:70:GLN:CD     | 9:p2:3:SER:HB2     | 2.46                     | 0.40              |
| 8:e2:83:GLN:HA     | 9:p2:45:LEU:HD13   | 2.03                     | 0.40              |
| 9:g2:86:LEU:HD11   | 9:r2:45:LEU:HD12   | 2.04                     | 0.40              |
| 9:g2:178:PHE:CE1   | 9:g2:201:PRO:HB3   | 2.57                     | 0.40              |
| 9:k2:172:GLN:OE1   | 9:k2:173:LEU:N     | 2.55                     | 0.40              |
| 9:l2:95:VAL:O      | 9:l2:118:GLY:HA3   | 2.21                     | 0.40              |
| 9:o2:26:LEU:CD1    | 9:o2:233:MET:HE3   | 2.52                     | 0.40              |
| 9:o2:164:GLN:HE22  | 11:s3:80:GLN:CB    | 2.27                     | 0.40              |
| 9:s2:209:ASN:CB    | 11:s3:54:GLN:NE2   | 2.80                     | 0.40              |
| 9:t2:43:ASP:N      | 9:t2:43:ASP:OD2    | 2.51                     | 0.40              |
| 9:t2:227:ALA:O     | 9:t2:231:VAL:HG23  | 2.22                     | 0.40              |
| 9:12:2:ILE:HD13    | 9:12:2:ILE:HA      | 1.97                     | 0.40              |
| 9:42:178:PHE:CE1   | 9:42:201:PRO:HB3   | 2.56                     | 0.40              |
| 10:B3:106:PHE:C    | 10:B3:108:THR:H    | 2.28                     | 0.40              |
| 10:B3:113:LEU:HD23 | 10:B3:113:LEU:HA   | 1.96                     | 0.40              |
| 10:C3:232:MET:HE1  | 10:E3:126:ALA:HB3  | 2.03                     | 0.40              |
| 10:G3:121:ARG:HB3  | 10:H3:111:ARG:HB3  | 2.04                     | 0.40              |
| 10:Q3:121:ARG:HB3  | 10:R3:111:ARG:HB3  | 2.03                     | 0.40              |
| 10:S3:171:ILE:HD12 | 10:U3:88:ALA:CB    | 2.36                     | 0.40              |
| 10:U3:43:PRO:O     | 10:U3:43:PRO:CD    | 2.67                     | 0.40              |
| 10:W3:171:ILE:O    | 10:X3:207:TYR:O    | 2.38                     | 0.40              |
| 11:b3:52:THR:CG2   | 11:b3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:c3:126:LEU:HB2  | 11:c3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:d3:89:VAL:CG2   | 11:d3:126:LEU:HD21 | 2.51                     | 0.40              |
| 11:d3:185:ILE:HD12 | 11:d3:225:VAL:HG21 | 2.03                     | 0.40              |
| 11:d3:252:LYS:HD2  | 11:d3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:e3:126:LEU:HB2  | 11:e3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:k3:104:ASP:OD1  | 11:k3:166:THR:HA   | 2.22                     | 0.40              |
| 11:m3:40:GLY:HA3   | 11:m3:124:THR:CG2  | 2.52                     | 0.40              |
| 11:m3:342:PRO:O    | 11:m3:346:MET:HG3  | 2.21                     | 0.40              |
| 11:o3:52:THR:CG2   | 11:o3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:p3:185:ILE:HD12 | 11:p3:225:VAL:HG21 | 2.03                     | 0.40              |
| 11:p3:252:LYS:HD2  | 11:p3:363:GLU:OE1  | 2.21                     | 0.40              |
| 11:q3:52:THR:CG2   | 11:q3:59:THR:HG23  | 2.52                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:r3:93:TYR:OH    | 11:r3:173:ARG:O    | 2.25                     | 0.40              |
| 11:r3:126:LEU:HB2  | 11:r3:135:ALA:HB3  | 2.04                     | 0.40              |
| 11:t3:52:THR:CG2   | 11:t3:59:THR:HG23  | 2.52                     | 0.40              |
| 11:w3:166:THR:HG21 | 11:y3:362:LEU:HD23 | 2.00                     | 0.40              |
| 11:x3:126:LEU:HB2  | 11:x3:135:ALA:HB3  | 2.04                     | 0.40              |
| 12:A4:224:THR:O    | 12:A4:227:GLU:HG2  | 2.22                     | 0.40              |
| 12:D4:85:ILE:O     | 12:D4:89:GLN:OE1   | 2.40                     | 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   | A1    | 145/560 (26%) | 143 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | B1    | 242/560 (43%) | 227 (94%) | 15 (6%) | 0        | 100         | 100 |
| 1   | C1    | 242/560 (43%) | 230 (95%) | 11 (4%) | 1 (0%)   | 30          | 60  |
| 1   | D1    | 145/560 (26%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | E1    | 242/560 (43%) | 226 (93%) | 16 (7%) | 0        | 100         | 100 |
| 1   | F1    | 145/560 (26%) | 141 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | G1    | 242/560 (43%) | 225 (93%) | 16 (7%) | 1 (0%)   | 30          | 60  |
| 1   | H1    | 242/560 (43%) | 221 (91%) | 19 (8%) | 2 (1%)   | 16          | 48  |
| 1   | I1    | 242/560 (43%) | 229 (95%) | 12 (5%) | 1 (0%)   | 30          | 60  |
| 1   | J1    | 145/560 (26%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | K1    | 242/560 (43%) | 230 (95%) | 11 (4%) | 1 (0%)   | 30          | 60  |
| 1   | L1    | 242/560 (43%) | 224 (93%) | 18 (7%) | 0        | 100         | 100 |
| 1   | M1    | 145/560 (26%) | 141 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | N1    | 242/560 (43%) | 223 (92%) | 19 (8%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | O1    | 242/560 (43%) | 231 (96%) | 10 (4%)  | 1 (0%)   | 30          | 60  |
| 1   | P1    | 145/560 (26%) | 142 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 1   | Q1    | 242/560 (43%) | 224 (93%) | 17 (7%)  | 1 (0%)   | 30          | 60  |
| 1   | R1    | 242/560 (43%) | 229 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 1   | S1    | 145/560 (26%) | 142 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 1   | T1    | 242/560 (43%) | 230 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 1   | U1    | 242/560 (43%) | 231 (96%) | 11 (4%)  | 0        | 100         | 100 |
| 1   | V1    | 145/560 (26%) | 141 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 1   | W1    | 242/560 (43%) | 227 (94%) | 14 (6%)  | 1 (0%)   | 30          | 60  |
| 1   | X1    | 242/560 (43%) | 225 (93%) | 17 (7%)  | 0        | 100         | 100 |
| 1   | Y1    | 242/560 (43%) | 228 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 1   | Z1    | 145/560 (26%) | 142 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 1   | a1    | 242/560 (43%) | 227 (94%) | 14 (6%)  | 1 (0%)   | 30          | 60  |
| 1   | b1    | 145/560 (26%) | 140 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 1   | c1    | 242/560 (43%) | 225 (93%) | 16 (7%)  | 1 (0%)   | 30          | 60  |
| 1   | d1    | 242/560 (43%) | 225 (93%) | 16 (7%)  | 1 (0%)   | 30          | 60  |
| 1   | e1    | 145/560 (26%) | 144 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 1   | f1    | 242/560 (43%) | 229 (95%) | 12 (5%)  | 1 (0%)   | 30          | 60  |
| 1   | g1    | 242/560 (43%) | 226 (93%) | 15 (6%)  | 1 (0%)   | 30          | 60  |
| 1   | h1    | 242/560 (43%) | 232 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 2   | A2    | 207/245 (84%) | 182 (88%) | 23 (11%) | 2 (1%)   | 12          | 43  |
| 2   | B2    | 207/245 (84%) | 183 (88%) | 22 (11%) | 2 (1%)   | 12          | 43  |
| 2   | C2    | 207/245 (84%) | 177 (86%) | 29 (14%) | 1 (0%)   | 24          | 56  |
| 2   | D2    | 207/245 (84%) | 181 (87%) | 25 (12%) | 1 (0%)   | 24          | 56  |
| 2   | E2    | 207/245 (84%) | 183 (88%) | 22 (11%) | 2 (1%)   | 12          | 43  |
| 3   | F2    | 254/264 (96%) | 223 (88%) | 30 (12%) | 1 (0%)   | 30          | 60  |
| 4   | G2    | 87/89 (98%)   | 75 (86%)  | 12 (14%) | 0        | 100         | 100 |
| 4   | H2    | 87/89 (98%)   | 77 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 4   | I2    | 87/89 (98%)   | 78 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 4   | J2    | 87/89 (98%)   | 77 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 5   | K2    | 37/104 (36%)  | 37 (100%) | 0        | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 5   | L2    | 73/104 (70%)  | 68 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 5   | M2    | 73/104 (70%)  | 68 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 5   | N2    | 73/104 (70%)  | 69 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 5   | O2    | 73/104 (70%)  | 69 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 5   | P2    | 73/104 (70%)  | 68 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 6   | Q2    | 131/138 (95%) | 115 (88%) | 16 (12%) | 0        | 100         | 100 |
| 6   | R2    | 114/138 (83%) | 98 (86%)  | 16 (14%) | 0        | 100         | 100 |
| 6   | S2    | 116/138 (84%) | 104 (90%) | 12 (10%) | 0        | 100         | 100 |
| 6   | T2    | 102/138 (74%) | 95 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 6   | U2    | 113/138 (82%) | 102 (90%) | 11 (10%) | 0        | 100         | 100 |
| 7   | V2    | 131/134 (98%) | 112 (86%) | 18 (14%) | 1 (1%)   | 16          | 48  |
| 7   | W2    | 130/134 (97%) | 108 (83%) | 22 (17%) | 0        | 100         | 100 |
| 7   | X2    | 130/134 (97%) | 107 (82%) | 22 (17%) | 1 (1%)   | 16          | 48  |
| 7   | Y2    | 130/134 (97%) | 109 (84%) | 21 (16%) | 0        | 100         | 100 |
| 7   | Z2    | 130/134 (97%) | 113 (87%) | 17 (13%) | 0        | 100         | 100 |
| 7   | a2    | 130/134 (97%) | 109 (84%) | 21 (16%) | 0        | 100         | 100 |
| 8   | b2    | 247/251 (98%) | 217 (88%) | 29 (12%) | 1 (0%)   | 30          | 60  |
| 8   | c2    | 247/251 (98%) | 212 (86%) | 35 (14%) | 0        | 100         | 100 |
| 8   | d2    | 247/251 (98%) | 215 (87%) | 32 (13%) | 0        | 100         | 100 |
| 8   | e2    | 247/251 (98%) | 212 (86%) | 35 (14%) | 0        | 100         | 100 |
| 8   | f2    | 247/251 (98%) | 210 (85%) | 37 (15%) | 0        | 100         | 100 |
| 9   | 12    | 258/260 (99%) | 231 (90%) | 27 (10%) | 0        | 100         | 100 |
| 9   | 22    | 258/260 (99%) | 231 (90%) | 27 (10%) | 0        | 100         | 100 |
| 9   | 32    | 256/260 (98%) | 230 (90%) | 26 (10%) | 0        | 100         | 100 |
| 9   | 42    | 258/260 (99%) | 239 (93%) | 19 (7%)  | 0        | 100         | 100 |
| 9   | g2    | 258/260 (99%) | 240 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 9   | h2    | 258/260 (99%) | 239 (93%) | 19 (7%)  | 0        | 100         | 100 |
| 9   | i2    | 258/260 (99%) | 240 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 9   | j2    | 258/260 (99%) | 240 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 9   | k2    | 258/260 (99%) | 242 (94%) | 16 (6%)  | 0        | 100         | 100 |
| 9   | l2    | 245/260 (94%) | 229 (94%) | 16 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9   | m2    | 245/260 (94%) | 230 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 9   | n2    | 245/260 (94%) | 232 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 9   | o2    | 245/260 (94%) | 230 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 9   | p2    | 245/260 (94%) | 232 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 9   | q2    | 247/260 (95%) | 233 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 9   | r2    | 258/260 (99%) | 233 (90%) | 25 (10%) | 0        | 100         | 100 |
| 9   | s2    | 258/260 (99%) | 230 (89%) | 28 (11%) | 0        | 100         | 100 |
| 9   | t2    | 258/260 (99%) | 236 (92%) | 22 (8%)  | 0        | 100         | 100 |
| 9   | u2    | 258/260 (99%) | 234 (91%) | 24 (9%)  | 0        | 100         | 100 |
| 9   | v2    | 258/260 (99%) | 233 (90%) | 25 (10%) | 0        | 100         | 100 |
| 9   | w2    | 258/260 (99%) | 232 (90%) | 26 (10%) | 0        | 100         | 100 |
| 9   | x2    | 258/260 (99%) | 236 (92%) | 22 (8%)  | 0        | 100         | 100 |
| 9   | y2    | 258/260 (99%) | 238 (92%) | 20 (8%)  | 0        | 100         | 100 |
| 9   | z2    | 258/260 (99%) | 240 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 10  | A3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | B3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | C3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | D3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | E3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | F3    | 209/232 (90%) | 192 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 10  | G3    | 209/232 (90%) | 192 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 10  | H3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | I3    | 209/232 (90%) | 192 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 10  | J3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | K3    | 209/232 (90%) | 192 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 10  | L3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | M3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | N3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | O3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | P3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 10  | Q3    | 209/232 (90%) | 193 (92%) | 16 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 10  | R3    | 209/232 (90%) | 193 (92%) | 16 (8%) | 0        | 100         | 100 |
| 10  | S3    | 209/232 (90%) | 193 (92%) | 16 (8%) | 0        | 100         | 100 |
| 10  | T3    | 209/232 (90%) | 192 (92%) | 17 (8%) | 0        | 100         | 100 |
| 10  | U3    | 209/232 (90%) | 192 (92%) | 17 (8%) | 0        | 100         | 100 |
| 10  | V3    | 209/232 (90%) | 193 (92%) | 16 (8%) | 0        | 100         | 100 |
| 10  | W3    | 208/232 (90%) | 192 (92%) | 16 (8%) | 0        | 100         | 100 |
| 10  | X3    | 209/232 (90%) | 193 (92%) | 16 (8%) | 0        | 100         | 100 |
| 10  | Y3    | 209/232 (90%) | 193 (92%) | 16 (8%) | 0        | 100         | 100 |
| 10  | Z3    | 209/232 (90%) | 193 (92%) | 16 (8%) | 0        | 100         | 100 |
| 11  | a3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | b3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | c3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | d3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | e3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | f3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | g3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | h3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | i3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | j3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | k3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | l3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | m3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | n3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | o3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | p3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | q3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | r3    | 299/365 (82%) | 288 (96%) | 11 (4%) | 0        | 100         | 100 |
| 11  | s3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | t3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | u3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |
| 11  | v3    | 300/365 (82%) | 288 (96%) | 12 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 11  | w3    | 300/365 (82%)     | 288 (96%)   | 12 (4%)   | 0        | 100         | 100 |
| 11  | x3    | 300/365 (82%)     | 288 (96%)   | 12 (4%)   | 0        | 100         | 100 |
| 11  | y3    | 300/365 (82%)     | 288 (96%)   | 12 (4%)   | 0        | 100         | 100 |
| 11  | z3    | 300/365 (82%)     | 288 (96%)   | 12 (4%)   | 0        | 100         | 100 |
| 12  | A4    | 199/232 (86%)     | 194 (98%)   | 5 (2%)    | 0        | 100         | 100 |
| 12  | B4    | 202/232 (87%)     | 200 (99%)   | 2 (1%)    | 0        | 100         | 100 |
| 12  | C4    | 197/232 (85%)     | 185 (94%)   | 12 (6%)   | 0        | 100         | 100 |
| 12  | D4    | 200/232 (86%)     | 194 (97%)   | 6 (3%)    | 0        | 100         | 100 |
| 12  | E4    | 202/232 (87%)     | 197 (98%)   | 5 (2%)    | 0        | 100         | 100 |
| All | All   | 32138/47180 (68%) | 29936 (93%) | 2176 (7%) | 26 (0%)  | 49          | 78  |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B2    | 42  | VAL  |
| 2   | C2    | 42  | VAL  |
| 2   | D2    | 42  | VAL  |
| 2   | A2    | 42  | VAL  |
| 2   | E2    | 42  | VAL  |
| 1   | H1    | 160 | PRO  |
| 1   | O1    | 160 | PRO  |
| 1   | g1    | 160 | PRO  |
| 2   | E2    | 41  | SER  |
| 1   | K1    | 160 | PRO  |
| 1   | a1    | 160 | PRO  |
| 2   | A2    | 41  | SER  |
| 2   | B2    | 41  | SER  |
| 7   | V2    | 58  | ALA  |
| 1   | C1    | 160 | PRO  |
| 1   | H1    | 166 | VAL  |
| 1   | Q1    | 160 | PRO  |
| 1   | f1    | 160 | PRO  |
| 3   | F2    | 158 | PRO  |
| 8   | b2    | 117 | GLY  |
| 1   | G1    | 160 | PRO  |
| 1   | I1    | 160 | PRO  |
| 1   | W1    | 160 | PRO  |
| 1   | d1    | 160 | PRO  |
| 1   | c1    | 160 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | X2    | 93  | MET  |

### 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   | A1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | B1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | C1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | D1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | E1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | F1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | G1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | H1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | I1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | J1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | K1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | L1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | M1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | N1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | O1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | P1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | Q1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | R1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | S1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | T1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | U1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | V1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | W1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | X1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | Y1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | Z1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | a1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | b1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | c1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | d1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | e1    | 134/467 (29%) | 134 (100%) | 0        | 100         | 100 |
| 1   | f1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | g1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 1   | h1    | 217/467 (46%) | 217 (100%) | 0        | 100         | 100 |
| 2   | A2    | 179/204 (88%) | 179 (100%) | 0        | 100         | 100 |
| 2   | B2    | 179/204 (88%) | 179 (100%) | 0        | 100         | 100 |
| 2   | C2    | 179/204 (88%) | 178 (99%)  | 1 (1%)   | 78          | 79  |
| 2   | D2    | 179/204 (88%) | 179 (100%) | 0        | 100         | 100 |
| 2   | E2    | 179/204 (88%) | 179 (100%) | 0        | 100         | 100 |
| 3   | F2    | 215/221 (97%) | 215 (100%) | 0        | 100         | 100 |
| 4   | G2    | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 4   | H2    | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 4   | I2    | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 4   | J2    | 74/74 (100%)  | 74 (100%)  | 0        | 100         | 100 |
| 5   | K2    | 33/79 (42%)   | 33 (100%)  | 0        | 100         | 100 |
| 5   | L2    | 59/79 (75%)   | 59 (100%)  | 0        | 100         | 100 |
| 5   | M2    | 59/79 (75%)   | 59 (100%)  | 0        | 100         | 100 |
| 5   | N2    | 59/79 (75%)   | 59 (100%)  | 0        | 100         | 100 |
| 5   | O2    | 59/79 (75%)   | 59 (100%)  | 0        | 100         | 100 |
| 5   | P2    | 59/79 (75%)   | 59 (100%)  | 0        | 100         | 100 |
| 6   | Q2    | 109/113 (96%) | 109 (100%) | 0        | 100         | 100 |
| 6   | R2    | 100/113 (88%) | 100 (100%) | 0        | 100         | 100 |
| 6   | S2    | 100/113 (88%) | 100 (100%) | 0        | 100         | 100 |
| 6   | T2    | 89/113 (79%)  | 89 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 6   | U2    | 99/113 (88%)   | 98 (99%)   | 1 (1%)   | 68          | 74  |
| 7   | V2    | 104/105 (99%)  | 103 (99%)  | 1 (1%)   | 68          | 74  |
| 7   | W2    | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 7   | X2    | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 7   | Y2    | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 7   | Z2    | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 7   | a2    | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 8   | b2    | 191/193 (99%)  | 191 (100%) | 0        | 100         | 100 |
| 8   | c2    | 191/193 (99%)  | 191 (100%) | 0        | 100         | 100 |
| 8   | d2    | 191/193 (99%)  | 191 (100%) | 0        | 100         | 100 |
| 8   | e2    | 191/193 (99%)  | 191 (100%) | 0        | 100         | 100 |
| 8   | f2    | 191/193 (99%)  | 191 (100%) | 0        | 100         | 100 |
| 9   | 12    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | 22    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | 32    | 214/215 (100%) | 214 (100%) | 0        | 100         | 100 |
| 9   | 42    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | g2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | h2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | i2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | j2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | k2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | l2    | 206/215 (96%)  | 206 (100%) | 0        | 100         | 100 |
| 9   | m2    | 206/215 (96%)  | 206 (100%) | 0        | 100         | 100 |
| 9   | n2    | 206/215 (96%)  | 205 (100%) | 1 (0%)   | 81          | 80  |
| 9   | o2    | 206/215 (96%)  | 206 (100%) | 0        | 100         | 100 |
| 9   | p2    | 206/215 (96%)  | 206 (100%) | 0        | 100         | 100 |
| 9   | q2    | 207/215 (96%)  | 207 (100%) | 0        | 100         | 100 |
| 9   | r2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | s2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | t2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | u2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 9   | v2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | w2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | x2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | y2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 9   | z2    | 215/215 (100%) | 215 (100%) | 0        | 100         | 100 |
| 10  | A3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | B3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | C3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | D3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | E3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | F3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | G3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | H3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | I3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | J3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | K3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | L3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | M3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | N3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | O3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | P3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | Q3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | R3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | S3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | T3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | U3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | V3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | W3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | X3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | Y3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |
| 10  | Z3    | 170/186 (91%)  | 168 (99%)  | 2 (1%)   | 63          | 72  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 11  | a3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | b3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | c3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | d3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | e3    | 251/294 (85%) | 244 (97%)  | 7 (3%)   | 38          | 58  |
| 11  | f3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | g3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | h3    | 251/294 (85%) | 244 (97%)  | 7 (3%)   | 38          | 58  |
| 11  | i3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | j3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | k3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | l3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | m3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | n3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | o3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | p3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | q3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | r3    | 250/294 (85%) | 244 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | s3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | t3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | u3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | v3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | w3    | 251/294 (85%) | 243 (97%)  | 8 (3%)   | 34          | 56  |
| 11  | x3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | y3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 11  | z3    | 251/294 (85%) | 245 (98%)  | 6 (2%)   | 43          | 61  |
| 12  | A4    | 164/188 (87%) | 164 (100%) | 0        | 100         | 100 |
| 12  | B4    | 165/188 (88%) | 165 (100%) | 0        | 100         | 100 |
| 12  | C4    | 162/188 (86%) | 162 (100%) | 0        | 100         | 100 |
| 12  | D4    | 164/188 (87%) | 164 (100%) | 0        | 100         | 100 |
| 12  | E4    | 165/188 (88%) | 165 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| All | All   | 27146/38629 (70%) | 26930 (99%) | 216 (1%) | 70          | 76 |

All (216) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C2    | 236 | MET  |
| 6   | U2    | 117 | GLN  |
| 7   | V2    | 59  | THR  |
| 9   | n2    | 172 | GLN  |
| 10  | A3    | 36  | THR  |
| 10  | A3    | 40  | ILE  |
| 10  | B3    | 36  | THR  |
| 10  | B3    | 40  | ILE  |
| 10  | C3    | 36  | THR  |
| 10  | C3    | 40  | ILE  |
| 10  | D3    | 36  | THR  |
| 10  | D3    | 40  | ILE  |
| 10  | E3    | 36  | THR  |
| 10  | E3    | 40  | ILE  |
| 10  | F3    | 36  | THR  |
| 10  | F3    | 40  | ILE  |
| 10  | G3    | 36  | THR  |
| 10  | G3    | 40  | ILE  |
| 10  | H3    | 36  | THR  |
| 10  | H3    | 40  | ILE  |
| 10  | I3    | 36  | THR  |
| 10  | I3    | 40  | ILE  |
| 10  | J3    | 36  | THR  |
| 10  | J3    | 40  | ILE  |
| 10  | K3    | 36  | THR  |
| 10  | K3    | 40  | ILE  |
| 10  | L3    | 36  | THR  |
| 10  | L3    | 40  | ILE  |
| 10  | M3    | 36  | THR  |
| 10  | M3    | 40  | ILE  |
| 10  | N3    | 36  | THR  |
| 10  | N3    | 40  | ILE  |
| 10  | O3    | 36  | THR  |
| 10  | O3    | 40  | ILE  |
| 10  | P3    | 36  | THR  |
| 10  | P3    | 40  | ILE  |
| 10  | Q3    | 36  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | Q3    | 40  | ILE  |
| 10  | R3    | 36  | THR  |
| 10  | R3    | 40  | ILE  |
| 10  | S3    | 36  | THR  |
| 10  | S3    | 40  | ILE  |
| 10  | T3    | 36  | THR  |
| 10  | T3    | 40  | ILE  |
| 10  | U3    | 36  | THR  |
| 10  | U3    | 40  | ILE  |
| 10  | V3    | 36  | THR  |
| 10  | V3    | 40  | ILE  |
| 10  | W3    | 36  | THR  |
| 10  | W3    | 40  | ILE  |
| 10  | X3    | 36  | THR  |
| 10  | X3    | 40  | ILE  |
| 10  | Y3    | 36  | THR  |
| 10  | Y3    | 40  | ILE  |
| 10  | Z3    | 36  | THR  |
| 10  | Z3    | 40  | ILE  |
| 11  | a3    | 84  | VAL  |
| 11  | a3    | 124 | THR  |
| 11  | a3    | 190 | ASN  |
| 11  | a3    | 245 | ASN  |
| 11  | a3    | 252 | LYS  |
| 11  | a3    | 325 | SER  |
| 11  | b3    | 84  | VAL  |
| 11  | b3    | 124 | THR  |
| 11  | b3    | 190 | ASN  |
| 11  | b3    | 245 | ASN  |
| 11  | b3    | 252 | LYS  |
| 11  | b3    | 325 | SER  |
| 11  | c3    | 84  | VAL  |
| 11  | c3    | 124 | THR  |
| 11  | c3    | 190 | ASN  |
| 11  | c3    | 245 | ASN  |
| 11  | c3    | 252 | LYS  |
| 11  | c3    | 325 | SER  |
| 11  | d3    | 84  | VAL  |
| 11  | d3    | 124 | THR  |
| 11  | d3    | 190 | ASN  |
| 11  | d3    | 245 | ASN  |
| 11  | d3    | 252 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | d3    | 325 | SER  |
| 11  | e3    | 84  | VAL  |
| 11  | e3    | 124 | THR  |
| 11  | e3    | 190 | ASN  |
| 11  | e3    | 242 | MET  |
| 11  | e3    | 245 | ASN  |
| 11  | e3    | 252 | LYS  |
| 11  | e3    | 325 | SER  |
| 11  | f3    | 84  | VAL  |
| 11  | f3    | 124 | THR  |
| 11  | f3    | 190 | ASN  |
| 11  | f3    | 245 | ASN  |
| 11  | f3    | 252 | LYS  |
| 11  | f3    | 325 | SER  |
| 11  | g3    | 84  | VAL  |
| 11  | g3    | 124 | THR  |
| 11  | g3    | 190 | ASN  |
| 11  | g3    | 245 | ASN  |
| 11  | g3    | 252 | LYS  |
| 11  | g3    | 325 | SER  |
| 11  | h3    | 84  | VAL  |
| 11  | h3    | 124 | THR  |
| 11  | h3    | 190 | ASN  |
| 11  | h3    | 242 | MET  |
| 11  | h3    | 245 | ASN  |
| 11  | h3    | 252 | LYS  |
| 11  | h3    | 325 | SER  |
| 11  | i3    | 84  | VAL  |
| 11  | i3    | 124 | THR  |
| 11  | i3    | 190 | ASN  |
| 11  | i3    | 245 | ASN  |
| 11  | i3    | 252 | LYS  |
| 11  | i3    | 325 | SER  |
| 11  | j3    | 84  | VAL  |
| 11  | j3    | 124 | THR  |
| 11  | j3    | 190 | ASN  |
| 11  | j3    | 245 | ASN  |
| 11  | j3    | 252 | LYS  |
| 11  | j3    | 325 | SER  |
| 11  | k3    | 84  | VAL  |
| 11  | k3    | 124 | THR  |
| 11  | k3    | 190 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | k3    | 245 | ASN  |
| 11  | k3    | 252 | LYS  |
| 11  | k3    | 325 | SER  |
| 11  | l3    | 84  | VAL  |
| 11  | l3    | 124 | THR  |
| 11  | l3    | 190 | ASN  |
| 11  | l3    | 245 | ASN  |
| 11  | l3    | 252 | LYS  |
| 11  | l3    | 325 | SER  |
| 11  | m3    | 84  | VAL  |
| 11  | m3    | 124 | THR  |
| 11  | m3    | 190 | ASN  |
| 11  | m3    | 245 | ASN  |
| 11  | m3    | 252 | LYS  |
| 11  | m3    | 325 | SER  |
| 11  | n3    | 84  | VAL  |
| 11  | n3    | 124 | THR  |
| 11  | n3    | 190 | ASN  |
| 11  | n3    | 245 | ASN  |
| 11  | n3    | 252 | LYS  |
| 11  | n3    | 325 | SER  |
| 11  | o3    | 84  | VAL  |
| 11  | o3    | 124 | THR  |
| 11  | o3    | 190 | ASN  |
| 11  | o3    | 245 | ASN  |
| 11  | o3    | 252 | LYS  |
| 11  | o3    | 325 | SER  |
| 11  | p3    | 84  | VAL  |
| 11  | p3    | 124 | THR  |
| 11  | p3    | 190 | ASN  |
| 11  | p3    | 245 | ASN  |
| 11  | p3    | 252 | LYS  |
| 11  | p3    | 325 | SER  |
| 11  | q3    | 84  | VAL  |
| 11  | q3    | 124 | THR  |
| 11  | q3    | 190 | ASN  |
| 11  | q3    | 245 | ASN  |
| 11  | q3    | 252 | LYS  |
| 11  | q3    | 325 | SER  |
| 11  | r3    | 84  | VAL  |
| 11  | r3    | 124 | THR  |
| 11  | r3    | 190 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | r3    | 245 | ASN  |
| 11  | r3    | 252 | LYS  |
| 11  | r3    | 325 | SER  |
| 11  | s3    | 84  | VAL  |
| 11  | s3    | 124 | THR  |
| 11  | s3    | 190 | ASN  |
| 11  | s3    | 245 | ASN  |
| 11  | s3    | 252 | LYS  |
| 11  | s3    | 325 | SER  |
| 11  | t3    | 84  | VAL  |
| 11  | t3    | 124 | THR  |
| 11  | t3    | 190 | ASN  |
| 11  | t3    | 245 | ASN  |
| 11  | t3    | 252 | LYS  |
| 11  | t3    | 325 | SER  |
| 11  | u3    | 84  | VAL  |
| 11  | u3    | 124 | THR  |
| 11  | u3    | 190 | ASN  |
| 11  | u3    | 245 | ASN  |
| 11  | u3    | 252 | LYS  |
| 11  | u3    | 325 | SER  |
| 11  | v3    | 84  | VAL  |
| 11  | v3    | 124 | THR  |
| 11  | v3    | 190 | ASN  |
| 11  | v3    | 245 | ASN  |
| 11  | v3    | 252 | LYS  |
| 11  | v3    | 325 | SER  |
| 11  | w3    | 78  | ASN  |
| 11  | w3    | 84  | VAL  |
| 11  | w3    | 124 | THR  |
| 11  | w3    | 190 | ASN  |
| 11  | w3    | 242 | MET  |
| 11  | w3    | 245 | ASN  |
| 11  | w3    | 252 | LYS  |
| 11  | w3    | 325 | SER  |
| 11  | x3    | 84  | VAL  |
| 11  | x3    | 124 | THR  |
| 11  | x3    | 190 | ASN  |
| 11  | x3    | 245 | ASN  |
| 11  | x3    | 252 | LYS  |
| 11  | x3    | 325 | SER  |
| 11  | y3    | 84  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | y3    | 124 | THR  |
| 11  | y3    | 190 | ASN  |
| 11  | y3    | 245 | ASN  |
| 11  | y3    | 252 | LYS  |
| 11  | y3    | 325 | SER  |
| 11  | z3    | 84  | VAL  |
| 11  | z3    | 124 | THR  |
| 11  | z3    | 190 | ASN  |
| 11  | z3    | 245 | ASN  |
| 11  | z3    | 252 | LYS  |
| 11  | z3    | 325 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (514) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 263 | HIS  |
| 1   | A1    | 365 | ASN  |
| 1   | A1    | 378 | ASN  |
| 1   | A1    | 431 | ASN  |
| 1   | A1    | 434 | ASN  |
| 1   | B1    | 156 | HIS  |
| 1   | B1    | 234 | GLN  |
| 1   | B1    | 378 | ASN  |
| 1   | B1    | 434 | ASN  |
| 1   | C1    | 218 | HIS  |
| 1   | C1    | 234 | GLN  |
| 1   | C1    | 246 | GLN  |
| 1   | D1    | 303 | GLN  |
| 1   | D1    | 434 | ASN  |
| 1   | E1    | 169 | GLN  |
| 1   | E1    | 281 | HIS  |
| 1   | E1    | 297 | GLN  |
| 1   | E1    | 365 | ASN  |
| 1   | F1    | 263 | HIS  |
| 1   | G1    | 156 | HIS  |
| 1   | G1    | 169 | GLN  |
| 1   | G1    | 263 | HIS  |
| 1   | G1    | 281 | HIS  |
| 1   | G1    | 434 | ASN  |
| 1   | H1    | 434 | ASN  |
| 1   | I1    | 169 | GLN  |
| 1   | J1    | 263 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J1    | 281 | HIS  |
| 1   | K1    | 133 | GLN  |
| 1   | K1    | 378 | ASN  |
| 1   | L1    | 209 | ASN  |
| 1   | L1    | 234 | GLN  |
| 1   | L1    | 365 | ASN  |
| 1   | M1    | 277 | GLN  |
| 1   | M1    | 431 | ASN  |
| 1   | M1    | 434 | ASN  |
| 1   | N1    | 156 | HIS  |
| 1   | N1    | 190 | GLN  |
| 1   | N1    | 277 | GLN  |
| 1   | N1    | 297 | GLN  |
| 1   | O1    | 156 | HIS  |
| 1   | O1    | 361 | ASN  |
| 1   | P1    | 299 | ASN  |
| 1   | P1    | 359 | GLN  |
| 1   | P1    | 365 | ASN  |
| 1   | P1    | 374 | HIS  |
| 1   | P1    | 431 | ASN  |
| 1   | Q1    | 299 | ASN  |
| 1   | R1    | 169 | GLN  |
| 1   | R1    | 299 | ASN  |
| 1   | S1    | 263 | HIS  |
| 1   | S1    | 374 | HIS  |
| 1   | S1    | 411 | GLN  |
| 1   | T1    | 131 | ASN  |
| 1   | T1    | 169 | GLN  |
| 1   | U1    | 125 | GLN  |
| 1   | V1    | 359 | GLN  |
| 1   | W1    | 156 | HIS  |
| 1   | W1    | 222 | GLN  |
| 1   | W1    | 263 | HIS  |
| 1   | W1    | 269 | GLN  |
| 1   | W1    | 281 | HIS  |
| 1   | X1    | 222 | GLN  |
| 1   | X1    | 277 | GLN  |
| 1   | X1    | 281 | HIS  |
| 1   | Y1    | 378 | ASN  |
| 1   | Z1    | 234 | GLN  |
| 1   | Z1    | 263 | HIS  |
| 1   | Z1    | 281 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z1    | 297 | GLN  |
| 1   | Z1    | 299 | ASN  |
| 1   | a1    | 269 | GLN  |
| 1   | a1    | 299 | ASN  |
| 1   | b1    | 265 | GLN  |
| 1   | b1    | 297 | GLN  |
| 1   | c1    | 277 | GLN  |
| 1   | d1    | 133 | GLN  |
| 1   | d1    | 218 | HIS  |
| 1   | d1    | 411 | GLN  |
| 1   | e1    | 263 | HIS  |
| 1   | e1    | 274 | ASN  |
| 1   | e1    | 277 | GLN  |
| 1   | e1    | 434 | ASN  |
| 1   | f1    | 133 | GLN  |
| 1   | g1    | 263 | HIS  |
| 1   | h1    | 277 | GLN  |
| 1   | h1    | 299 | ASN  |
| 2   | A2    | 86  | ASN  |
| 2   | A2    | 119 | GLN  |
| 2   | B2    | 233 | GLN  |
| 2   | C2    | 86  | ASN  |
| 2   | C2    | 119 | GLN  |
| 2   | D2    | 233 | GLN  |
| 2   | E2    | 141 | GLN  |
| 3   | F2    | 105 | GLN  |
| 3   | F2    | 141 | ASN  |
| 3   | F2    | 143 | HIS  |
| 4   | H2    | 39  | GLN  |
| 5   | M2    | 39  | HIS  |
| 5   | N2    | 83  | GLN  |
| 5   | P2    | 55  | GLN  |
| 6   | Q2    | 13  | GLN  |
| 6   | Q2    | 92  | GLN  |
| 6   | Q2    | 126 | GLN  |
| 6   | S2    | 92  | GLN  |
| 6   | T2    | 17  | ASN  |
| 6   | T2    | 92  | GLN  |
| 6   | U2    | 112 | ASN  |
| 7   | V2    | 50  | GLN  |
| 7   | V2    | 134 | GLN  |
| 7   | W2    | 17  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | W2    | 22  | ASN  |
| 7   | X2    | 22  | ASN  |
| 7   | X2    | 115 | ASN  |
| 7   | Y2    | 17  | GLN  |
| 7   | Y2    | 50  | GLN  |
| 7   | Y2    | 115 | ASN  |
| 7   | Z2    | 5   | ASN  |
| 7   | Z2    | 17  | GLN  |
| 7   | Z2    | 50  | GLN  |
| 7   | a2    | 95  | ASN  |
| 8   | b2    | 14  | GLN  |
| 8   | b2    | 37  | GLN  |
| 8   | b2    | 91  | GLN  |
| 8   | b2    | 106 | GLN  |
| 8   | c2    | 106 | GLN  |
| 8   | c2    | 230 | GLN  |
| 8   | d2    | 14  | GLN  |
| 8   | d2    | 230 | GLN  |
| 8   | d2    | 240 | ASN  |
| 8   | e2    | 14  | GLN  |
| 8   | e2    | 37  | GLN  |
| 8   | e2    | 83  | GLN  |
| 8   | e2    | 91  | GLN  |
| 8   | e2    | 230 | GLN  |
| 8   | f2    | 19  | GLN  |
| 8   | f2    | 37  | GLN  |
| 9   | g2    | 15  | GLN  |
| 9   | g2    | 28  | ASN  |
| 9   | g2    | 32  | ASN  |
| 9   | g2    | 47  | GLN  |
| 9   | g2    | 67  | GLN  |
| 9   | g2    | 88  | GLN  |
| 9   | h2    | 15  | GLN  |
| 9   | h2    | 47  | GLN  |
| 9   | h2    | 67  | GLN  |
| 9   | h2    | 91  | ASN  |
| 9   | i2    | 16  | GLN  |
| 9   | i2    | 32  | ASN  |
| 9   | i2    | 121 | GLN  |
| 9   | j2    | 37  | GLN  |
| 9   | j2    | 169 | GLN  |
| 9   | j2    | 172 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | k2    | 15  | GLN  |
| 9   | k2    | 28  | ASN  |
| 9   | k2    | 32  | ASN  |
| 9   | k2    | 85  | ASN  |
| 9   | k2    | 88  | GLN  |
| 9   | k2    | 135 | GLN  |
| 9   | k2    | 252 | GLN  |
| 9   | l2    | 15  | GLN  |
| 9   | l2    | 161 | GLN  |
| 9   | l2    | 172 | GLN  |
| 9   | l2    | 202 | ASN  |
| 9   | m2    | 28  | ASN  |
| 9   | m2    | 67  | GLN  |
| 9   | m2    | 88  | GLN  |
| 9   | m2    | 164 | GLN  |
| 9   | m2    | 180 | ASN  |
| 9   | m2    | 243 | ASN  |
| 9   | n2    | 15  | GLN  |
| 9   | n2    | 28  | ASN  |
| 9   | n2    | 47  | GLN  |
| 9   | n2    | 135 | GLN  |
| 9   | n2    | 137 | GLN  |
| 9   | n2    | 169 | GLN  |
| 9   | n2    | 209 | ASN  |
| 9   | o2    | 67  | GLN  |
| 9   | o2    | 127 | GLN  |
| 9   | o2    | 161 | GLN  |
| 9   | o2    | 164 | GLN  |
| 9   | o2    | 169 | GLN  |
| 9   | o2    | 202 | ASN  |
| 9   | o2    | 235 | GLN  |
| 9   | p2    | 15  | GLN  |
| 9   | p2    | 28  | ASN  |
| 9   | p2    | 83  | GLN  |
| 9   | p2    | 85  | ASN  |
| 9   | p2    | 88  | GLN  |
| 9   | p2    | 137 | GLN  |
| 9   | p2    | 145 | ASN  |
| 9   | p2    | 172 | GLN  |
| 9   | q2    | 15  | GLN  |
| 9   | q2    | 161 | GLN  |
| 9   | r2    | 15  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | r2    | 100 | GLN  |
| 9   | r2    | 104 | GLN  |
| 9   | r2    | 124 | GLN  |
| 9   | r2    | 180 | ASN  |
| 9   | s2    | 15  | GLN  |
| 9   | s2    | 16  | GLN  |
| 9   | s2    | 24  | ASN  |
| 9   | s2    | 55  | GLN  |
| 9   | s2    | 127 | GLN  |
| 9   | s2    | 235 | GLN  |
| 9   | t2    | 55  | GLN  |
| 9   | t2    | 67  | GLN  |
| 9   | t2    | 104 | GLN  |
| 9   | t2    | 127 | GLN  |
| 9   | u2    | 55  | GLN  |
| 9   | u2    | 202 | ASN  |
| 9   | v2    | 15  | GLN  |
| 9   | v2    | 16  | GLN  |
| 9   | v2    | 24  | ASN  |
| 9   | v2    | 67  | GLN  |
| 9   | v2    | 88  | GLN  |
| 9   | v2    | 100 | GLN  |
| 9   | v2    | 104 | GLN  |
| 9   | v2    | 121 | GLN  |
| 9   | v2    | 180 | ASN  |
| 9   | w2    | 15  | GLN  |
| 9   | w2    | 83  | GLN  |
| 9   | w2    | 135 | GLN  |
| 9   | w2    | 137 | GLN  |
| 9   | w2    | 172 | GLN  |
| 9   | w2    | 235 | GLN  |
| 9   | x2    | 28  | ASN  |
| 9   | x2    | 59  | GLN  |
| 9   | x2    | 172 | GLN  |
| 9   | y2    | 16  | GLN  |
| 9   | y2    | 37  | GLN  |
| 9   | y2    | 67  | GLN  |
| 9   | y2    | 88  | GLN  |
| 9   | z2    | 16  | GLN  |
| 9   | z2    | 28  | ASN  |
| 9   | z2    | 237 | GLN  |
| 9   | z2    | 252 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | 12    | 88  | GLN  |
| 9   | 12    | 164 | GLN  |
| 9   | 12    | 172 | GLN  |
| 9   | 12    | 209 | ASN  |
| 9   | 12    | 237 | GLN  |
| 9   | 22    | 202 | ASN  |
| 9   | 22    | 237 | GLN  |
| 9   | 22    | 259 | GLN  |
| 9   | 32    | 67  | GLN  |
| 9   | 32    | 100 | GLN  |
| 9   | 32    | 104 | GLN  |
| 9   | 32    | 164 | GLN  |
| 9   | 32    | 255 | GLN  |
| 9   | 42    | 37  | GLN  |
| 9   | 42    | 47  | GLN  |
| 9   | 42    | 55  | GLN  |
| 9   | 42    | 164 | GLN  |
| 9   | 42    | 172 | GLN  |
| 9   | 42    | 202 | ASN  |
| 9   | 42    | 255 | GLN  |
| 10  | A3    | 223 | GLN  |
| 10  | B3    | 218 | ASN  |
| 10  | B3    | 223 | GLN  |
| 10  | C3    | 218 | ASN  |
| 10  | C3    | 223 | GLN  |
| 10  | D3    | 218 | ASN  |
| 10  | D3    | 223 | GLN  |
| 10  | E3    | 223 | GLN  |
| 10  | F3    | 223 | GLN  |
| 10  | G3    | 218 | ASN  |
| 10  | G3    | 223 | GLN  |
| 10  | H3    | 218 | ASN  |
| 10  | H3    | 223 | GLN  |
| 10  | I3    | 223 | GLN  |
| 10  | J3    | 218 | ASN  |
| 10  | J3    | 223 | GLN  |
| 10  | K3    | 218 | ASN  |
| 10  | K3    | 223 | GLN  |
| 10  | L3    | 223 | GLN  |
| 10  | M3    | 218 | ASN  |
| 10  | M3    | 223 | GLN  |
| 10  | N3    | 223 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | O3    | 223 | GLN  |
| 10  | P3    | 218 | ASN  |
| 10  | P3    | 223 | GLN  |
| 10  | Q3    | 218 | ASN  |
| 10  | Q3    | 223 | GLN  |
| 10  | R3    | 218 | ASN  |
| 10  | R3    | 223 | GLN  |
| 10  | S3    | 218 | ASN  |
| 10  | S3    | 223 | GLN  |
| 10  | T3    | 223 | GLN  |
| 10  | U3    | 218 | ASN  |
| 10  | U3    | 223 | GLN  |
| 10  | V3    | 218 | ASN  |
| 10  | W3    | 218 | ASN  |
| 10  | W3    | 223 | GLN  |
| 10  | X3    | 218 | ASN  |
| 10  | X3    | 223 | GLN  |
| 10  | Y3    | 83  | GLN  |
| 10  | Y3    | 223 | GLN  |
| 10  | Z3    | 218 | ASN  |
| 10  | Z3    | 223 | GLN  |
| 11  | a3    | 54  | GLN  |
| 11  | a3    | 99  | GLN  |
| 11  | a3    | 159 | GLN  |
| 11  | a3    | 161 | ASN  |
| 11  | a3    | 190 | ASN  |
| 11  | a3    | 198 | GLN  |
| 11  | a3    | 350 | GLN  |
| 11  | b3    | 78  | ASN  |
| 11  | b3    | 99  | GLN  |
| 11  | b3    | 159 | GLN  |
| 11  | b3    | 161 | ASN  |
| 11  | b3    | 190 | ASN  |
| 11  | b3    | 198 | GLN  |
| 11  | b3    | 240 | GLN  |
| 11  | b3    | 350 | GLN  |
| 11  | c3    | 51  | GLN  |
| 11  | c3    | 54  | GLN  |
| 11  | c3    | 80  | GLN  |
| 11  | c3    | 99  | GLN  |
| 11  | c3    | 159 | GLN  |
| 11  | c3    | 161 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | c3    | 190 | ASN  |
| 11  | c3    | 198 | GLN  |
| 11  | c3    | 240 | GLN  |
| 11  | d3    | 78  | ASN  |
| 11  | d3    | 99  | GLN  |
| 11  | d3    | 159 | GLN  |
| 11  | d3    | 161 | ASN  |
| 11  | d3    | 190 | ASN  |
| 11  | d3    | 198 | GLN  |
| 11  | d3    | 240 | GLN  |
| 11  | d3    | 350 | GLN  |
| 11  | e3    | 54  | GLN  |
| 11  | e3    | 78  | ASN  |
| 11  | e3    | 99  | GLN  |
| 11  | e3    | 159 | GLN  |
| 11  | e3    | 161 | ASN  |
| 11  | e3    | 190 | ASN  |
| 11  | e3    | 198 | GLN  |
| 11  | e3    | 240 | GLN  |
| 11  | e3    | 350 | GLN  |
| 11  | f3    | 78  | ASN  |
| 11  | f3    | 99  | GLN  |
| 11  | f3    | 159 | GLN  |
| 11  | f3    | 161 | ASN  |
| 11  | f3    | 190 | ASN  |
| 11  | f3    | 198 | GLN  |
| 11  | f3    | 240 | GLN  |
| 11  | f3    | 350 | GLN  |
| 11  | g3    | 99  | GLN  |
| 11  | g3    | 159 | GLN  |
| 11  | g3    | 161 | ASN  |
| 11  | g3    | 190 | ASN  |
| 11  | g3    | 198 | GLN  |
| 11  | g3    | 240 | GLN  |
| 11  | h3    | 99  | GLN  |
| 11  | h3    | 159 | GLN  |
| 11  | h3    | 161 | ASN  |
| 11  | h3    | 183 | ASN  |
| 11  | h3    | 190 | ASN  |
| 11  | h3    | 198 | GLN  |
| 11  | h3    | 240 | GLN  |
| 11  | h3    | 350 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | i3    | 99  | GLN  |
| 11  | i3    | 159 | GLN  |
| 11  | i3    | 161 | ASN  |
| 11  | i3    | 190 | ASN  |
| 11  | i3    | 198 | GLN  |
| 11  | i3    | 350 | GLN  |
| 11  | j3    | 99  | GLN  |
| 11  | j3    | 159 | GLN  |
| 11  | j3    | 161 | ASN  |
| 11  | j3    | 190 | ASN  |
| 11  | j3    | 198 | GLN  |
| 11  | j3    | 350 | GLN  |
| 11  | k3    | 78  | ASN  |
| 11  | k3    | 99  | GLN  |
| 11  | k3    | 159 | GLN  |
| 11  | k3    | 161 | ASN  |
| 11  | k3    | 190 | ASN  |
| 11  | k3    | 198 | GLN  |
| 11  | k3    | 350 | GLN  |
| 11  | l3    | 54  | GLN  |
| 11  | l3    | 78  | ASN  |
| 11  | l3    | 99  | GLN  |
| 11  | l3    | 159 | GLN  |
| 11  | l3    | 161 | ASN  |
| 11  | l3    | 183 | ASN  |
| 11  | l3    | 190 | ASN  |
| 11  | l3    | 198 | GLN  |
| 11  | l3    | 350 | GLN  |
| 11  | m3    | 54  | GLN  |
| 11  | m3    | 99  | GLN  |
| 11  | m3    | 159 | GLN  |
| 11  | m3    | 161 | ASN  |
| 11  | m3    | 183 | ASN  |
| 11  | m3    | 190 | ASN  |
| 11  | m3    | 198 | GLN  |
| 11  | m3    | 350 | GLN  |
| 11  | n3    | 99  | GLN  |
| 11  | n3    | 159 | GLN  |
| 11  | n3    | 161 | ASN  |
| 11  | n3    | 190 | ASN  |
| 11  | n3    | 198 | GLN  |
| 11  | n3    | 350 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | o3    | 80  | GLN  |
| 11  | o3    | 99  | GLN  |
| 11  | o3    | 159 | GLN  |
| 11  | o3    | 161 | ASN  |
| 11  | o3    | 183 | ASN  |
| 11  | o3    | 190 | ASN  |
| 11  | o3    | 198 | GLN  |
| 11  | p3    | 78  | ASN  |
| 11  | p3    | 99  | GLN  |
| 11  | p3    | 159 | GLN  |
| 11  | p3    | 161 | ASN  |
| 11  | p3    | 183 | ASN  |
| 11  | p3    | 190 | ASN  |
| 11  | p3    | 198 | GLN  |
| 11  | p3    | 350 | GLN  |
| 11  | q3    | 54  | GLN  |
| 11  | q3    | 99  | GLN  |
| 11  | q3    | 159 | GLN  |
| 11  | q3    | 161 | ASN  |
| 11  | q3    | 190 | ASN  |
| 11  | q3    | 198 | GLN  |
| 11  | q3    | 350 | GLN  |
| 11  | r3    | 78  | ASN  |
| 11  | r3    | 99  | GLN  |
| 11  | r3    | 159 | GLN  |
| 11  | r3    | 161 | ASN  |
| 11  | r3    | 190 | ASN  |
| 11  | r3    | 198 | GLN  |
| 11  | r3    | 240 | GLN  |
| 11  | r3    | 350 | GLN  |
| 11  | s3    | 54  | GLN  |
| 11  | s3    | 78  | ASN  |
| 11  | s3    | 80  | GLN  |
| 11  | s3    | 99  | GLN  |
| 11  | s3    | 159 | GLN  |
| 11  | s3    | 161 | ASN  |
| 11  | s3    | 190 | ASN  |
| 11  | s3    | 198 | GLN  |
| 11  | s3    | 350 | GLN  |
| 11  | t3    | 99  | GLN  |
| 11  | t3    | 159 | GLN  |
| 11  | t3    | 161 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | t3    | 190 | ASN  |
| 11  | t3    | 240 | GLN  |
| 11  | t3    | 350 | GLN  |
| 11  | u3    | 78  | ASN  |
| 11  | u3    | 80  | GLN  |
| 11  | u3    | 99  | GLN  |
| 11  | u3    | 159 | GLN  |
| 11  | u3    | 161 | ASN  |
| 11  | u3    | 190 | ASN  |
| 11  | u3    | 198 | GLN  |
| 11  | u3    | 350 | GLN  |
| 11  | v3    | 54  | GLN  |
| 11  | v3    | 78  | ASN  |
| 11  | v3    | 80  | GLN  |
| 11  | v3    | 99  | GLN  |
| 11  | v3    | 159 | GLN  |
| 11  | v3    | 161 | ASN  |
| 11  | v3    | 190 | ASN  |
| 11  | v3    | 198 | GLN  |
| 11  | v3    | 240 | GLN  |
| 11  | v3    | 350 | GLN  |
| 11  | w3    | 99  | GLN  |
| 11  | w3    | 159 | GLN  |
| 11  | w3    | 161 | ASN  |
| 11  | w3    | 190 | ASN  |
| 11  | w3    | 198 | GLN  |
| 11  | w3    | 240 | GLN  |
| 11  | w3    | 350 | GLN  |
| 11  | x3    | 78  | ASN  |
| 11  | x3    | 99  | GLN  |
| 11  | x3    | 159 | GLN  |
| 11  | x3    | 161 | ASN  |
| 11  | x3    | 190 | ASN  |
| 11  | x3    | 198 | GLN  |
| 11  | x3    | 240 | GLN  |
| 11  | x3    | 350 | GLN  |
| 11  | y3    | 159 | GLN  |
| 11  | y3    | 161 | ASN  |
| 11  | y3    | 190 | ASN  |
| 11  | y3    | 198 | GLN  |
| 11  | y3    | 240 | GLN  |
| 11  | y3    | 350 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | z3    | 78  | ASN  |
| 11  | z3    | 80  | GLN  |
| 11  | z3    | 99  | GLN  |
| 11  | z3    | 161 | ASN  |
| 11  | z3    | 190 | ASN  |
| 11  | z3    | 198 | GLN  |
| 11  | z3    | 350 | GLN  |
| 12  | A4    | 55  | ASN  |
| 12  | A4    | 75  | ASN  |
| 12  | A4    | 188 | ASN  |
| 12  | A4    | 192 | GLN  |
| 12  | A4    | 204 | GLN  |
| 12  | A4    | 213 | ASN  |
| 12  | A4    | 230 | GLN  |
| 12  | B4    | 46  | ASN  |
| 12  | B4    | 55  | ASN  |
| 12  | B4    | 64  | GLN  |
| 12  | B4    | 188 | ASN  |
| 12  | B4    | 192 | GLN  |
| 12  | C4    | 84  | GLN  |
| 12  | C4    | 177 | ASN  |
| 12  | D4    | 181 | ASN  |
| 12  | D4    | 188 | ASN  |
| 12  | E4    | 54  | GLN  |
| 12  | E4    | 56  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | F2    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | F2    | 115:ASP   | C      | 116:PRO   | N      | 5.09         |

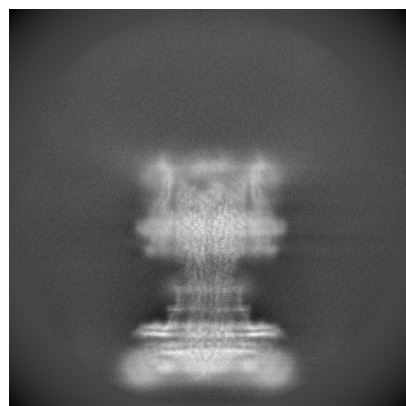
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12603. These allow visual inspection of the internal detail of the map and identification of artifacts.

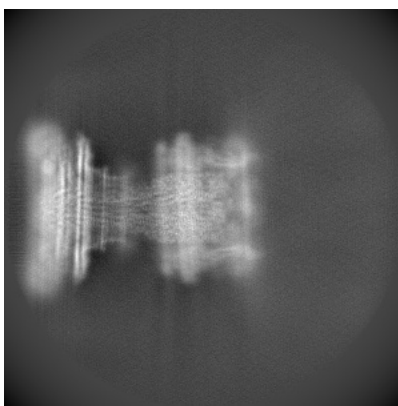
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

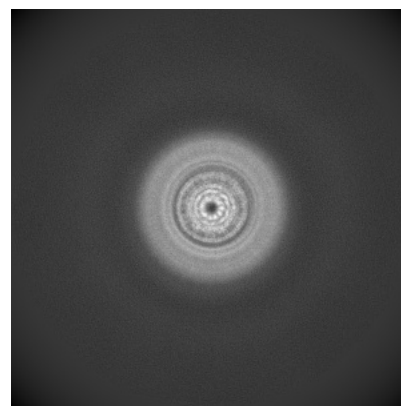
#### 6.1.1 Primary map



X

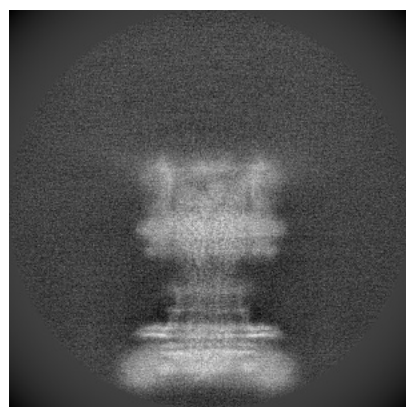


Y

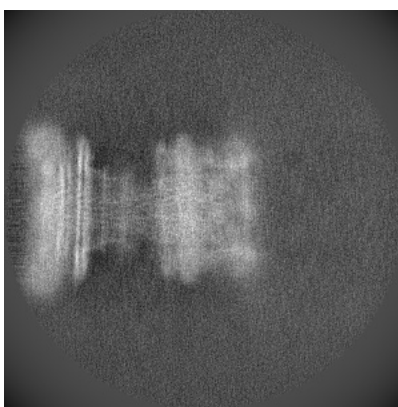


Z

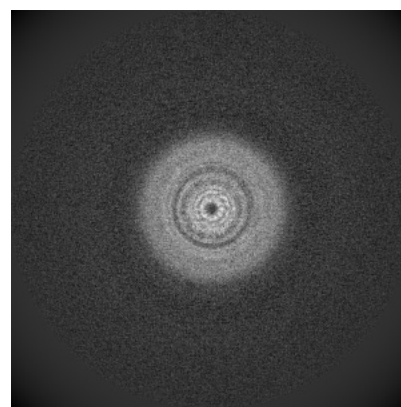
#### 6.1.2 Raw map



X



Y

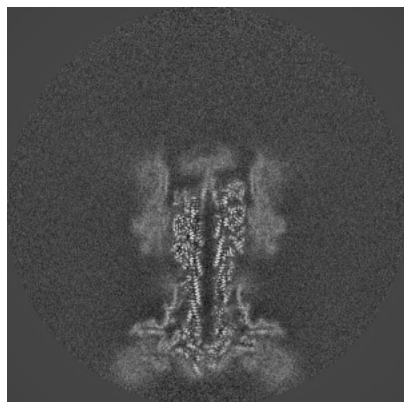


Z

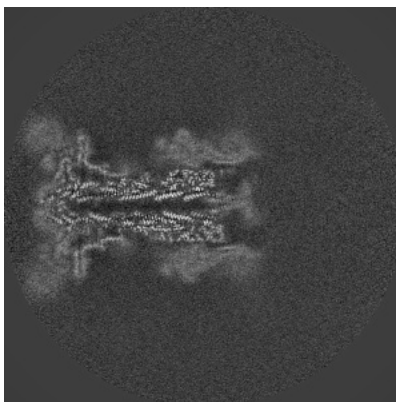
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

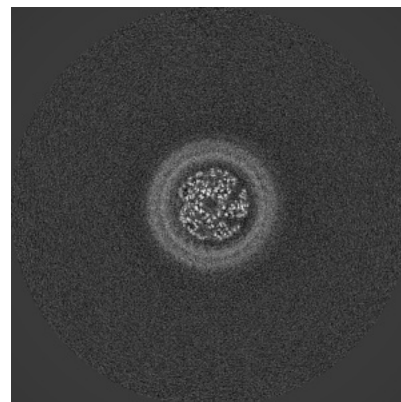
### 6.2.1 Primary map



X Index: 384

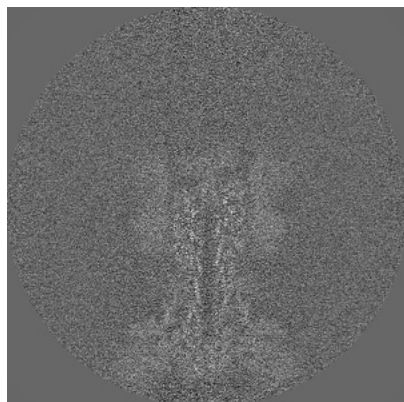


Y Index: 384

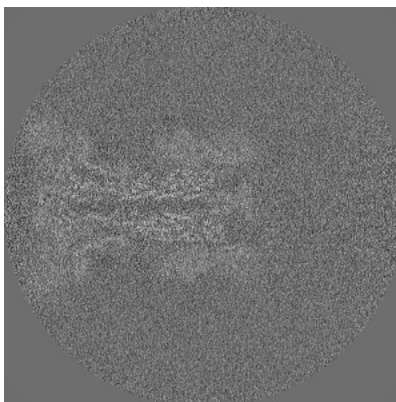


Z Index: 384

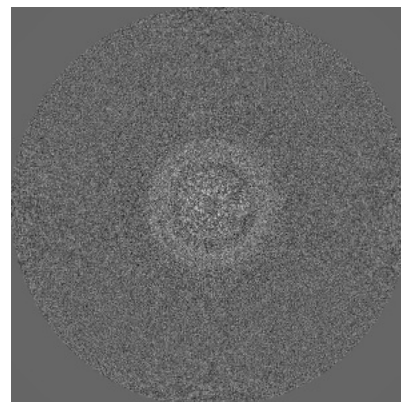
### 6.2.2 Raw map



X Index: 384



Y Index: 384

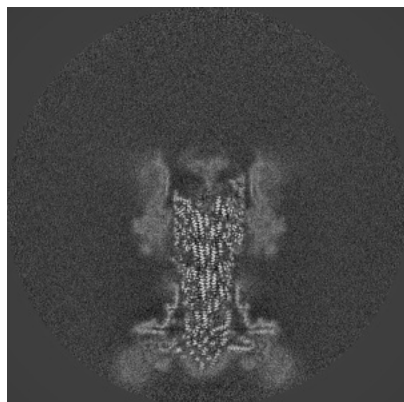


Z Index: 384

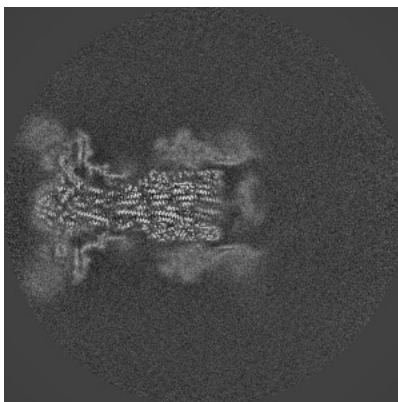
The images above show central slices of the map in three orthogonal directions.

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

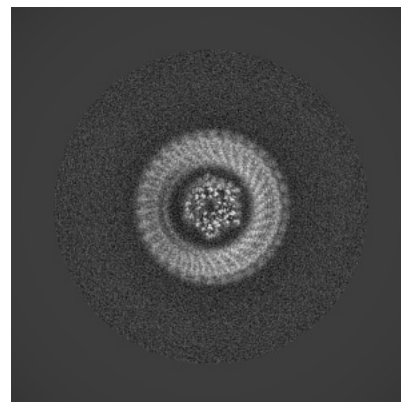
### 6.3.1 Primary map



X Index: 402

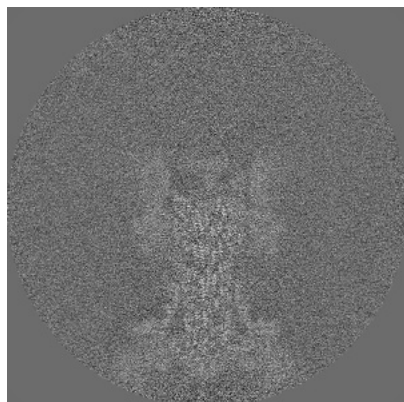


Y Index: 371

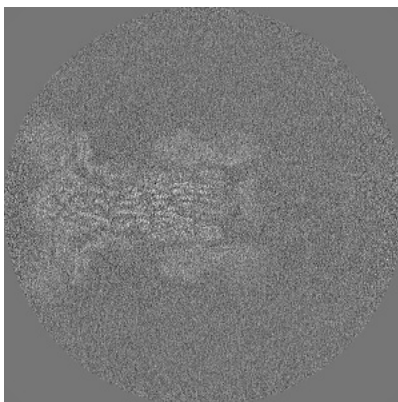


Z Index: 144

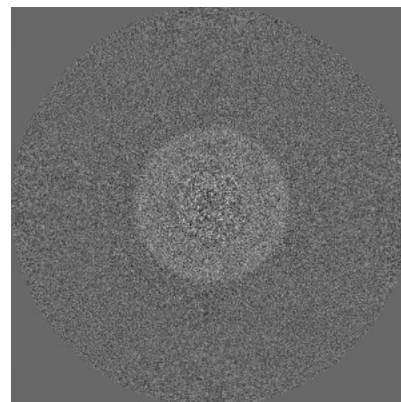
### 6.3.2 Raw map



X Index: 402



Y Index: 371



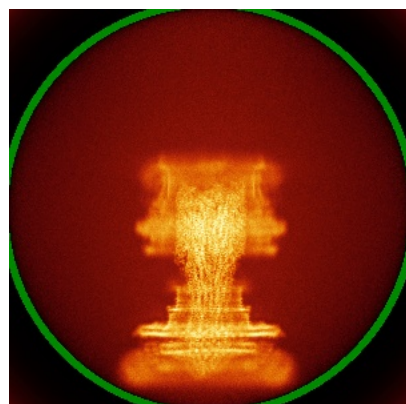
Z Index: 350

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

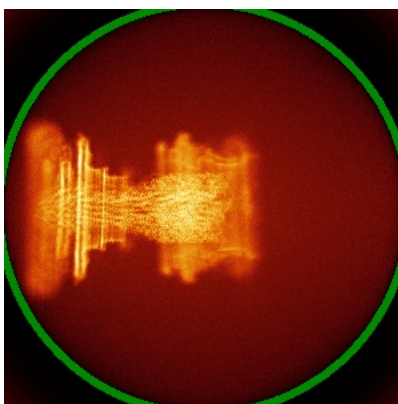


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

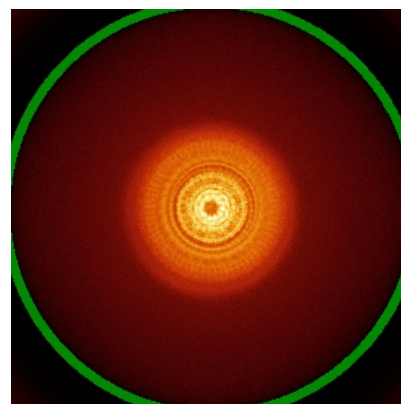
### 6.4.1 Primary map



X

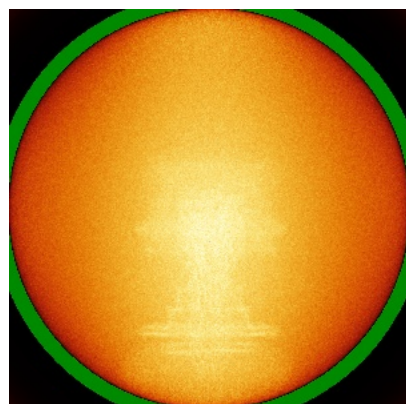


Y

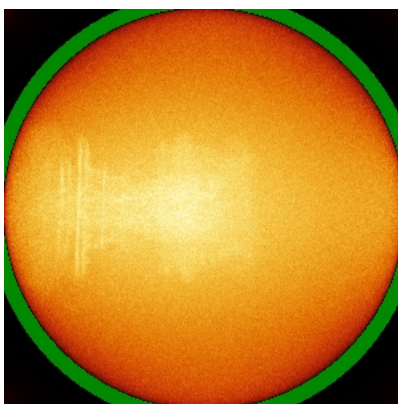


Z

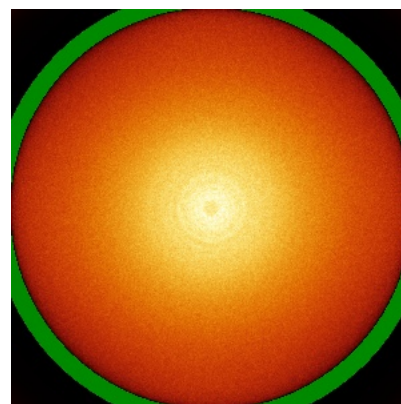
### 6.4.2 Raw map



X



Y



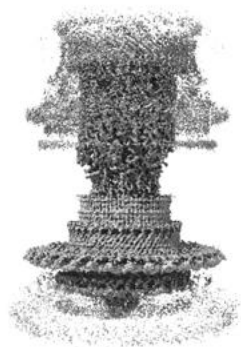
Z

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.

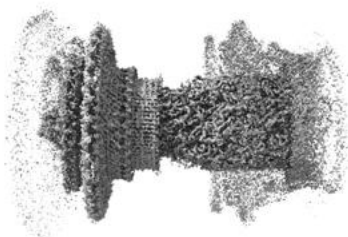


## 6.5 Orthogonal surface views [i](#)

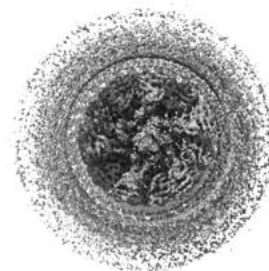
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

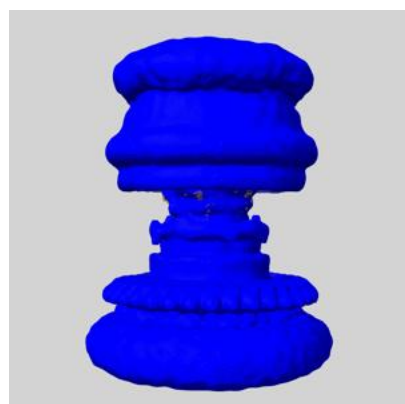
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

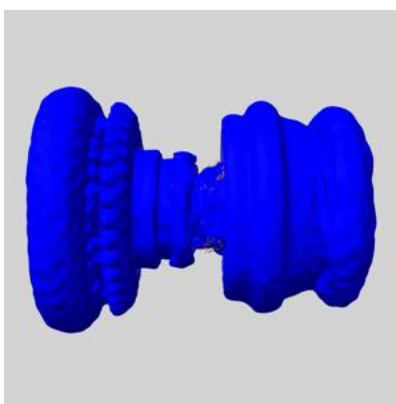
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

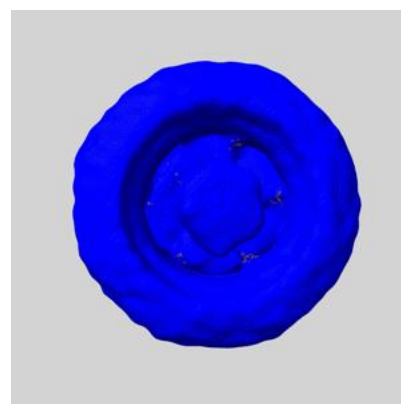
### 6.6.1 emd\_12603\_msk\_1.map [i](#)



X



Y

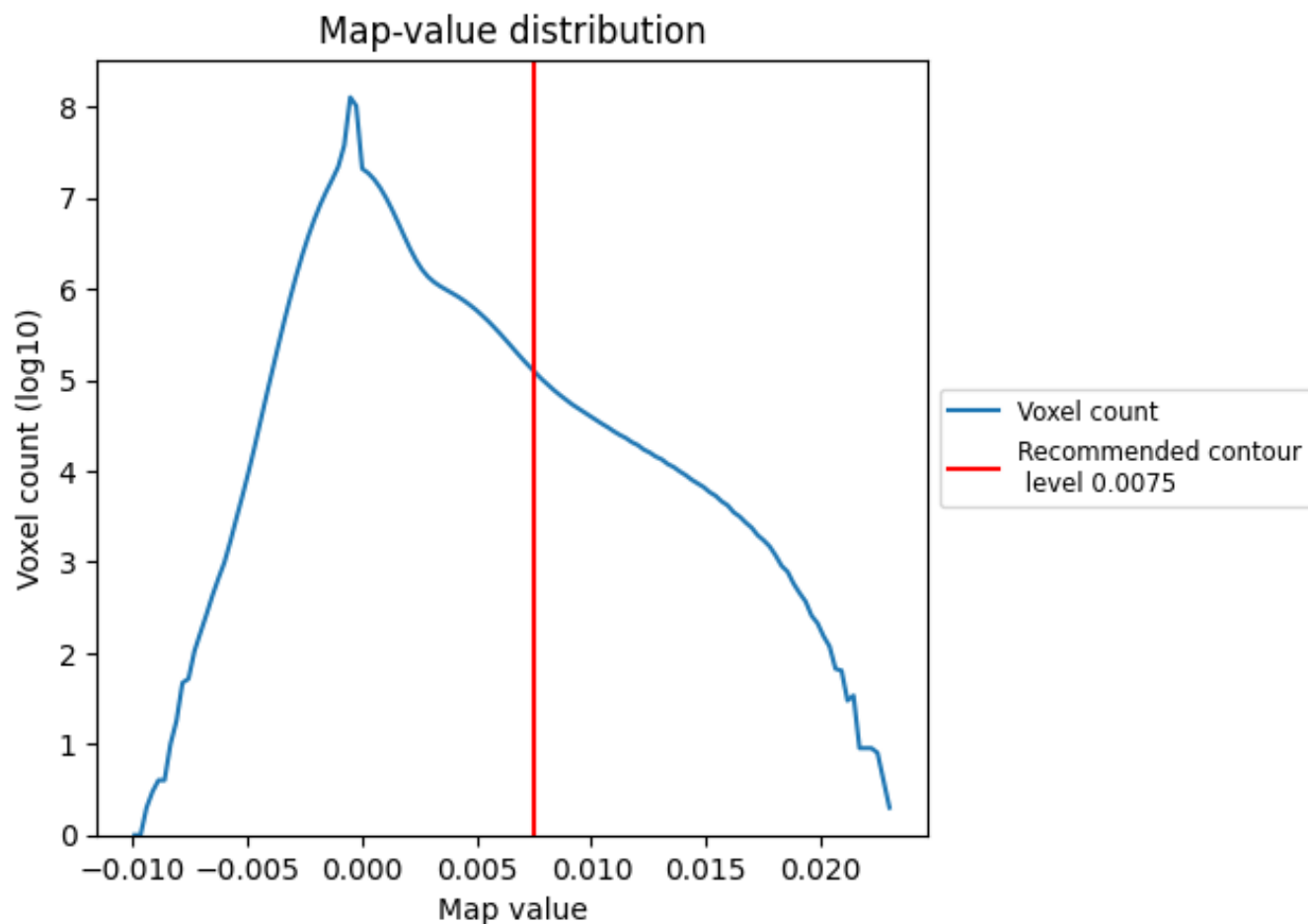


Z

## 7 Map analysis [i](#)

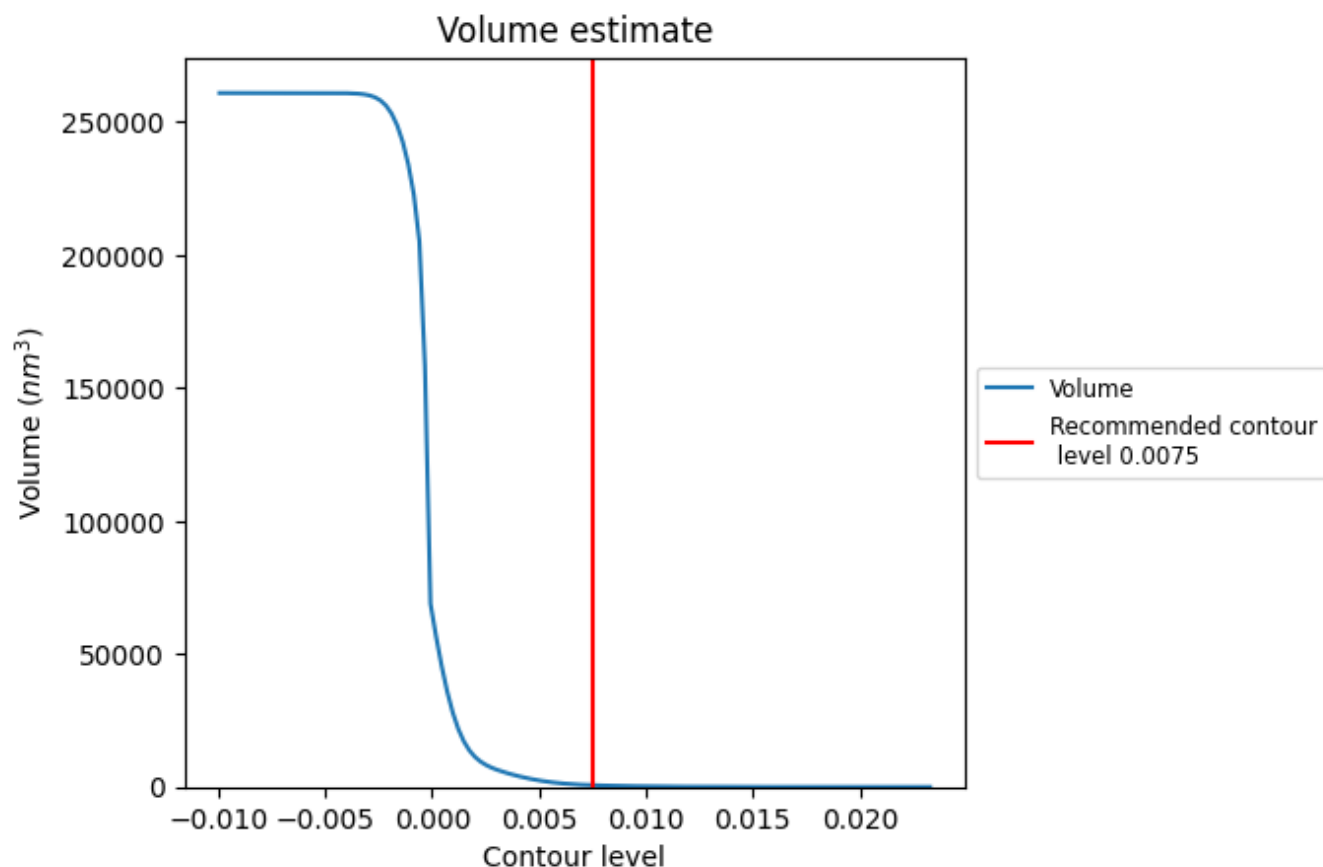
This section contains the results of statistical analysis of the map.

### 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.

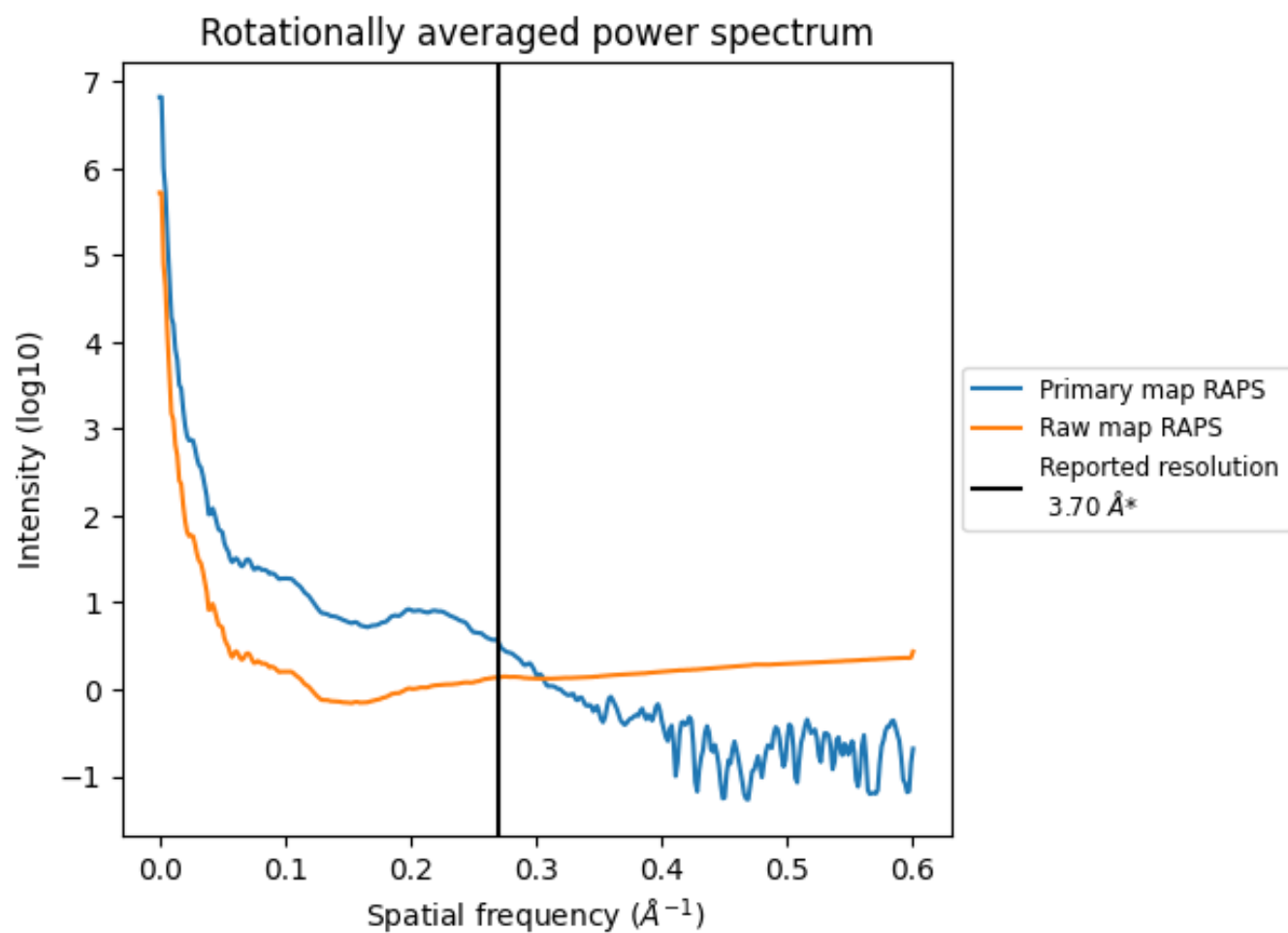
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 648  $\text{nm}^3$ ; this corresponds to an approximate mass of 586 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 ⓘ

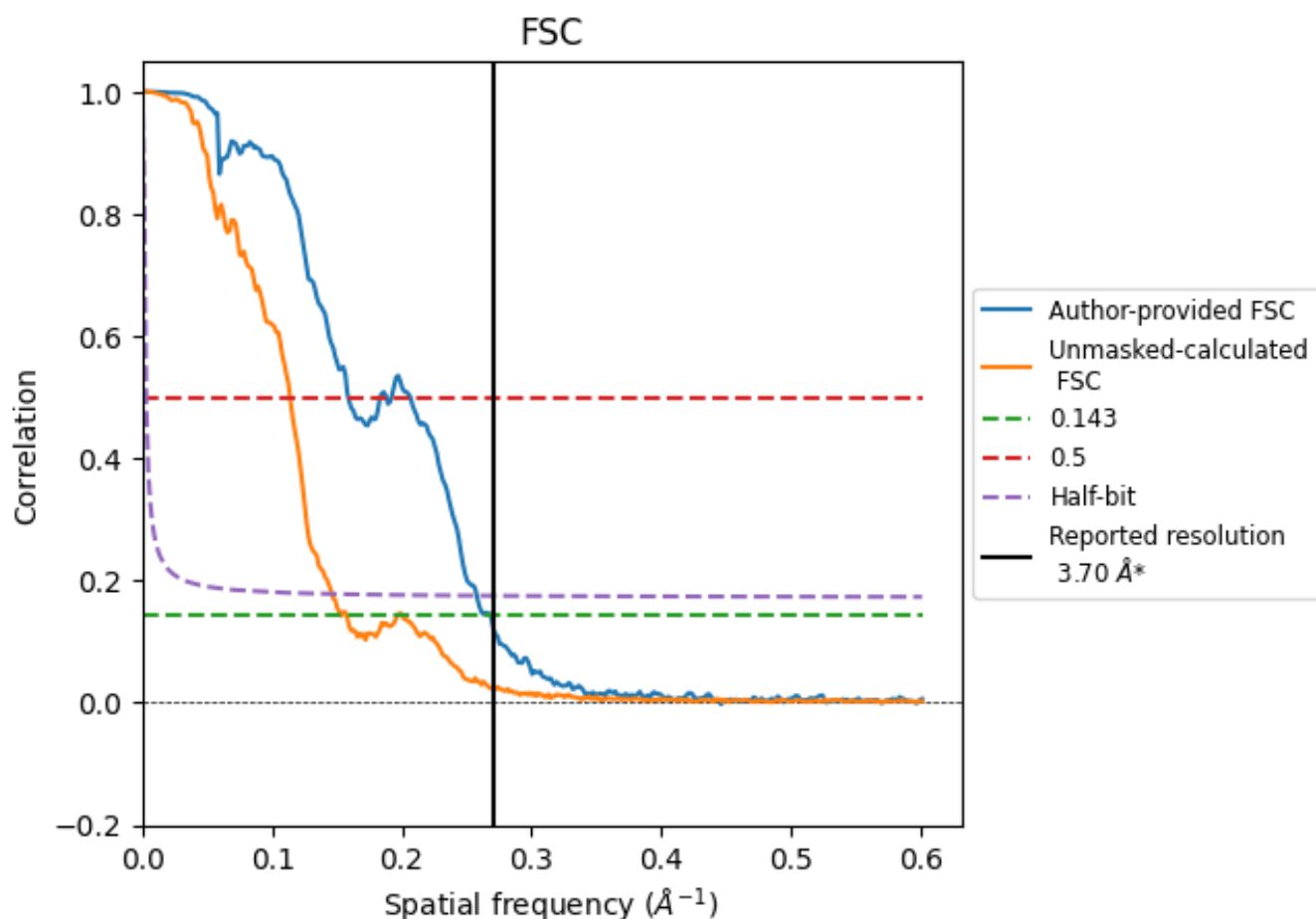


\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.70                               | -    | -        |
| Author-provided FSC curve | 3.73                               | 6.30 | 3.88     |
| Unmasked-calculated*      | 6.53                               | 8.78 | 6.84     |

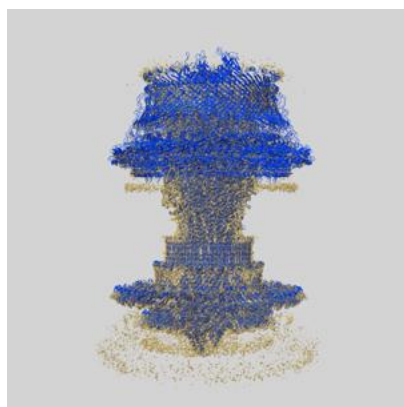
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.53 differs from the reported value 3.7 by more than 10 %



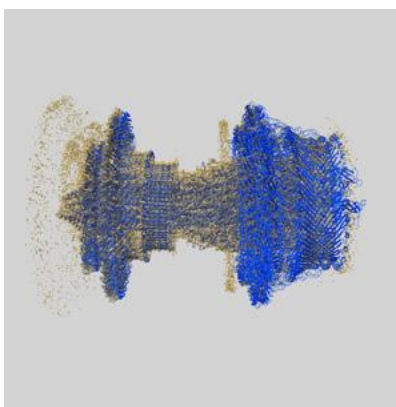
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12603 and PDB model 7NVG. Per-residue inclusion information can be found in section [3](#) on page [18](#).

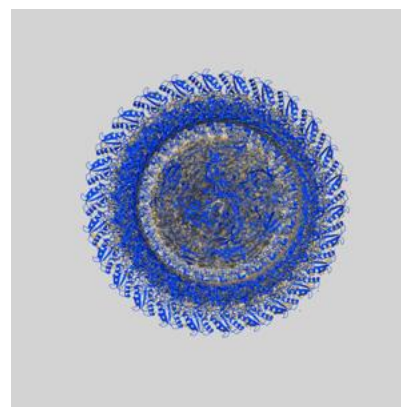
### 9.1 Map-model overlay [i](#)



X



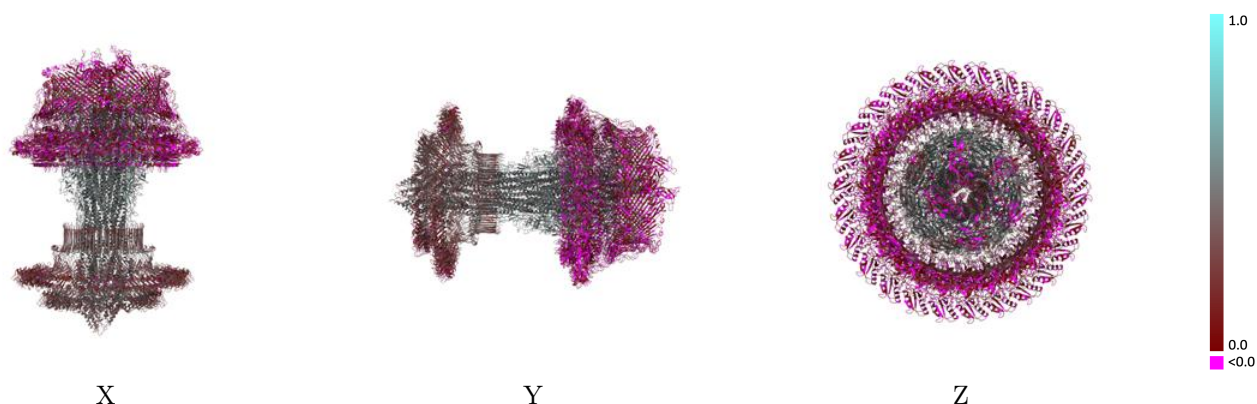
Y



Z

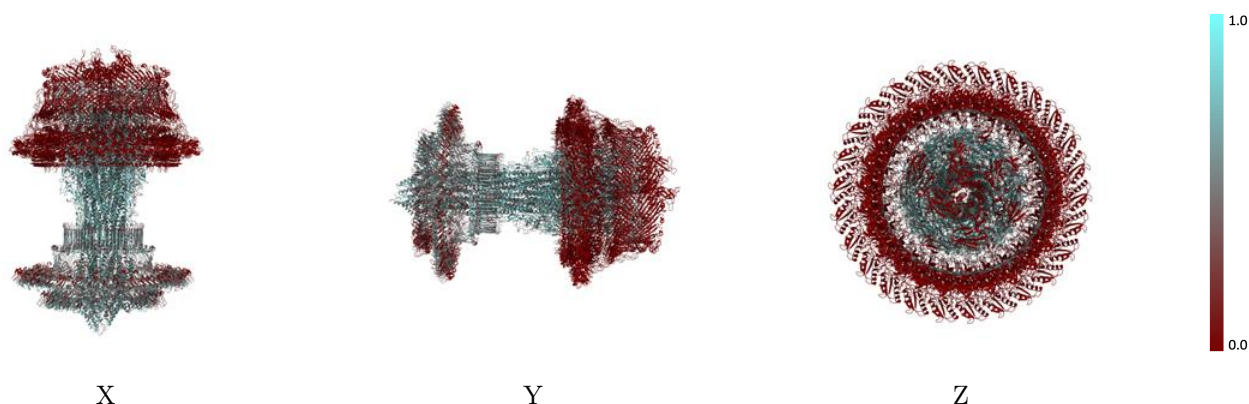
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



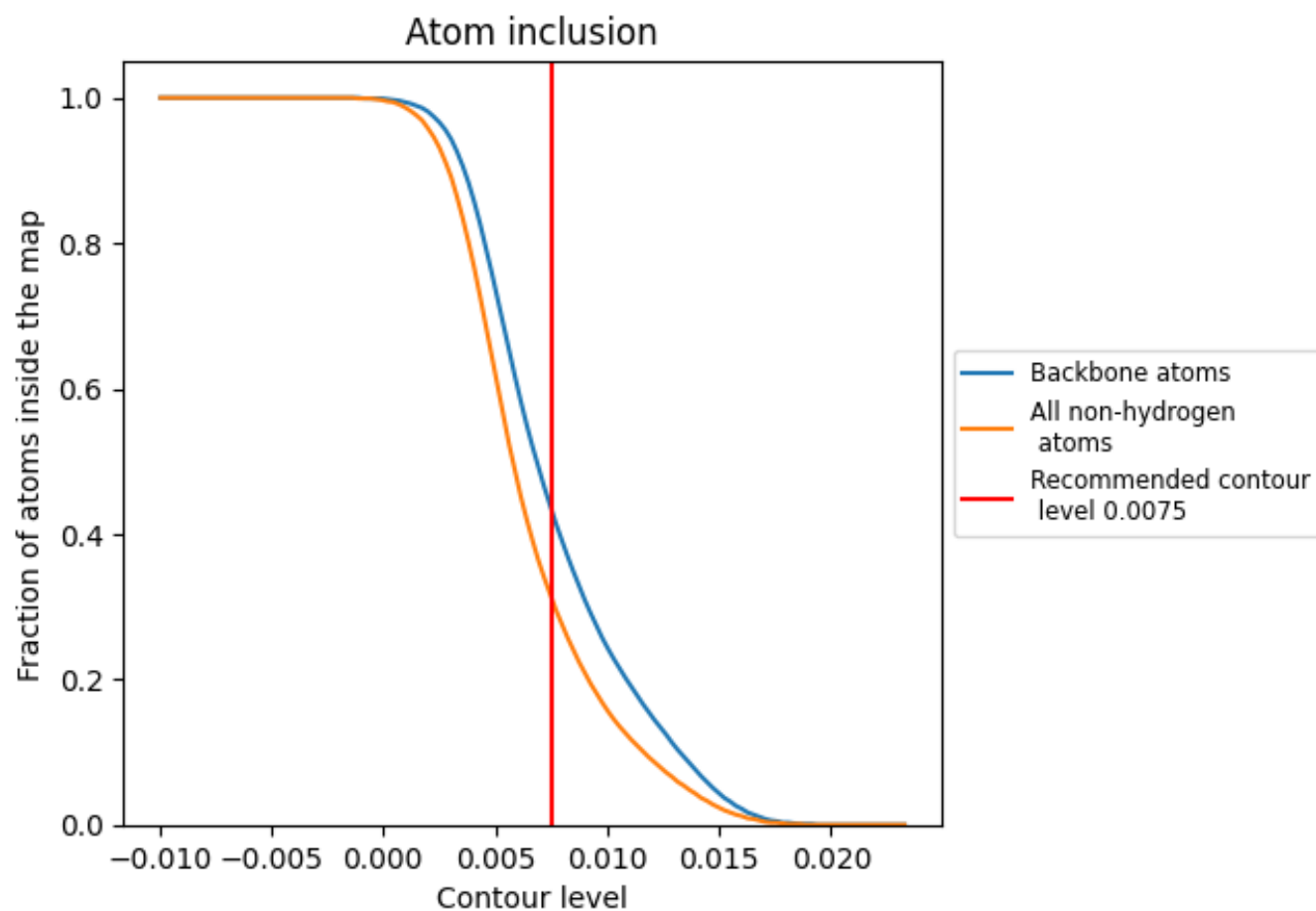
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 44% of all backbone atoms, 31% 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 (0.0075) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.3140   |  0.2600   |
| 12    |  0.5820   |  0.4540   |
| 22    |  0.5740   |  0.4590   |
| 32    |  0.5370   |  0.4490   |
| 42    |  0.2200   |  0.3100   |
| A1    |  0.4300   |  0.2750   |
| A2    |  0.5380   |  0.4390   |
| A3    |  0.0690   |  0.0910   |
| A4    |  0.0850   |  0.1010   |
| B1    |  0.4340   |  0.3030   |
| B2    |  0.5800   |  0.4430   |
| B3    |  0.0710   |  0.1080   |
| B4    |  0.1010   |  0.0920   |
| C1    |  0.4640   |  0.3060   |
| C2    |  0.6100  |  0.4410  |
| C3    |  0.0720 |  0.1010 |
| C4    |  0.0760 |  0.1210 |
| D1    |  0.4240 |  0.2850 |
| D2    |  0.5880 |  0.4330 |
| D3    |  0.0710 |  0.0870 |
| D4    |  0.0690 |  0.0820 |
| E1    |  0.4420 |  0.3140 |
| E2    |  0.5410 |  0.4190 |
| E3    |  0.0840 |  0.1060 |
| E4    |  0.0870 |  0.1120 |
| F1    |  0.4230 |  0.3020 |
| F2    |  0.4960 |  0.4070 |
| F3    |  0.0740 |  0.1080 |
| G1    |  0.4420 |  0.3180 |
| G2    |  0.5370 |  0.3880 |
| G3    |  0.0820 |  0.1110 |
| H1    |  0.4500 |  0.3230 |
| H2    |  0.6050 |  0.4120 |
| H3    |  0.0790 |  0.1110 |
| I1    |  0.4290 |  0.3090 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| I2    |  0.5700   |  0.4000   |
| I3    |  0.0710   |  0.1020   |
| J1    |  0.4160   |  0.2950   |
| J2    |  0.4990   |  0.3730   |
| J3    |  0.0770   |  0.1060   |
| K1    |  0.4060   |  0.2910   |
| K2    |  0.5490   |  0.4530   |
| K3    |  0.0600   |  0.0850   |
| L1    |  0.3980   |  0.3000   |
| L2    |  0.5450   |  0.4600   |
| L3    |  0.0660   |  0.0880   |
| M1    |  0.4170   |  0.2860   |
| M2    |  0.5960   |  0.4700   |
| M3    |  0.0580   |  0.0840   |
| N1    |  0.3840   |  0.2760   |
| N2    |  0.6070   |  0.4750   |
| N3    |  0.0690   |  0.0920   |
| O1    |  0.3940  |  0.2840  |
| O2    |  0.5720 |  0.4610 |
| O3    |  0.0650 |  0.0800 |
| P1    |  0.4130 |  0.2780 |
| P2    |  0.5520 |  0.4700 |
| P3    |  0.0530 |  0.0860 |
| Q1    |  0.3510 |  0.2740 |
| Q2    |  0.5120 |  0.4850 |
| Q3    |  0.0510 |  0.1000 |
| R1    |  0.3270 |  0.2640 |
| R2    |  0.6080 |  0.4760 |
| R3    |  0.0490 |  0.0760 |
| S1    |  0.3950 |  0.2700 |
| S2    |  0.6050 |  0.4750 |
| S3    |  0.0430 |  0.0760 |
| T1    |  0.2860 |  0.2480 |
| T2    |  0.6450 |  0.4990 |
| T3    |  0.0480 |  0.0960 |
| U1    |  0.2810 |  0.2090 |
| U2    |  0.5750 |  0.4800 |
| U3    |  0.0520 |  0.0880 |
| V1    |  0.3510 |  0.2380 |
| V2    |  0.5560 |  0.4590 |
| V3    |  0.0550 |  0.0850 |
| W1    |  0.2980 |  0.2380 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| W2    |  0.6130   |  0.4770   |
| W3    |  0.0580   |  0.0740   |
| X1    |  0.3350   |  0.2480   |
| X2    |  0.6340   |  0.4930   |
| X3    |  0.0430   |  0.0870   |
| Y1    |  0.3600   |  0.2720   |
| Y2    |  0.6360   |  0.4890   |
| Y3    |  0.0570   |  0.0980   |
| Z1    |  0.3890   |  0.2530   |
| Z2    |  0.6360   |  0.4810   |
| Z3    |  0.0700   |  0.1080   |
| a1    |  0.4160   |  0.2790   |
| a2    |  0.6140   |  0.4580   |
| a3    |  0.0180   |  0.0990   |
| b1    |  0.4100   |  0.2630   |
| b2    |  0.6010   |  0.5010   |
| b3    |  0.0240   |  0.0990   |
| c1    |  0.4270   |  0.2960   |
| c2    |  0.6670  |  0.5000  |
| c3    |  0.0260 |  0.0820 |
| d1    |  0.4540 |  0.2960 |
| d2    |  0.6980 |  0.5070 |
| d3    |  0.0270 |  0.1050 |
| e1    |  0.4590 |  0.2880 |
| e2    |  0.6820 |  0.5060 |
| e3    |  0.0210 |  0.0810 |
| f1    |  0.4580 |  0.3080 |
| f2    |  0.6650 |  0.5050 |
| f3    |  0.0300 |  0.1040 |
| g1    |  0.4720 |  0.3040 |
| g2    |  0.6390 |  0.4990 |
| g3    |  0.0280 |  0.0810 |
| h1    |  0.4570 |  0.3010 |
| h2    |  0.6560 |  0.5060 |
| h3    |  0.0230 |  0.0980 |
| i2    |  0.6690 |  0.5130 |
| i3    |  0.0300 |  0.0890 |
| j2    |  0.6560 |  0.5050 |
| j3    |  0.0150 |  0.0810 |
| k2    |  0.6640 |  0.5070 |
| k3    |  0.0160 |  0.0840 |
| l2    |  0.6570 |  0.5090 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| l3    |  0.0110   |  0.0710   |
| m2    |  0.6610   |  0.5130   |
| m3    |  0.0060   |  0.0480   |
| n2    |  0.6630   |  0.5160   |
| n3    |  0.0120   |  0.0500   |
| o2    |  0.6640   |  0.5040   |
| o3    |  0.0140   |  0.0610   |
| p2    |  0.6600   |  0.5020   |
| p3    |  0.0070   |  0.0430   |
| q2    |  0.6710   |  0.5110   |
| q3    |  0.0050   |  0.0530   |
| r2    |  0.6620   |  0.5030   |
| r3    |  0.0060   |  0.0570   |
| s2    |  0.6590   |  0.5030   |
| s3    |  0.0060   |  0.0580   |
| t2    |  0.6570   |  0.4970   |
| t3    |  0.0110   |  0.0570   |
| u2    |  0.6580   |  0.4910   |
| u3    |  0.0080  |  0.0530  |
| v2    |  0.6700 |  0.4960 |
| v3    |  0.0060 |  0.0640 |
| w2    |  0.6740 |  0.4930 |
| w3    |  0.0110 |  0.0690 |
| x2    |  0.6430 |  0.4870 |
| x3    |  0.0160 |  0.0790 |
| y2    |  0.5760 |  0.4470 |
| y3    |  0.0170 |  0.0750 |
| z2    |  0.5250 |  0.4040 |
| z3    |  0.0170 |  0.0910 |