



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:45 PM EST

PDB ID : 3J99
EMDB ID : EMD-6209
Title : Structure of 20S supercomplex determined by single particle cryoelectron microscopy (State IIIb)
Authors : Zhao, M.; Wu, S.; Cheng, Y.; Brunger, A.T.
Deposited on : 2014-12-05
Resolution : 8.20 Å (reported)
Based on initial models : 1QCS, 1NSF, 1N7S

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

We welcome your comments at 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>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

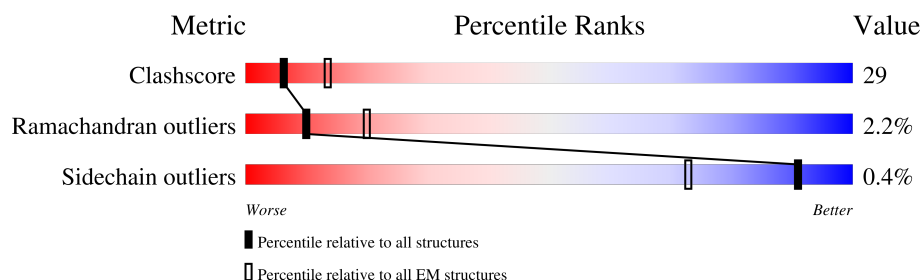
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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 (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 747 | <div> <div>38%</div> <div>47%</div> <div>41%</div> <div>9%</div> </div> |
| 1 | B | 747 | <div> <div>23%</div> <div>48%</div> <div>40%</div> <div>10%</div> </div> |
| 1 | C | 747 | <div> <div>32%</div> <div>47%</div> <div>41%</div> <div>10%</div> </div> |
| 1 | D | 747 | <div> <div>23%</div> <div>47%</div> <div>42%</div> <div>10%</div> </div> |
| 1 | E | 747 | <div> <div>39%</div> <div>45%</div> <div>42%</div> <div>10%</div> </div> |
| 1 | F | 747 | <div> <div>43%</div> <div>46%</div> <div>39%</div> <div>12%</div> </div> |
| 2 | G | 297 | <div> <div>47%</div> <div>51%</div> <div>43%</div> <div></div> </div> |
| 2 | H | 297 | <div> <div>39%</div> <div>51%</div> <div>41%</div> <div></div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | I | 297 | <div><div><div>32%</div><div>59%</div><div>36%</div><div></div><div></div></div></div> |
| 2 | J | 297 | <div><div><div>32%</div><div>52%</div><div>43%</div><div></div><div></div></div></div> |
| 3 | K | 63 | <div><div><div>32%</div><div>33%</div><div>62%</div><div></div><div></div></div></div> |
| 4 | L | 67 | <div><div><div>34%</div><div>40%</div><div>58%</div><div></div><div></div></div></div> |
| 5 | M | 188 | <div><div><div>31%</div><div>27%</div><div>43%</div><div>30%</div><div></div></div></div> |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40976 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 Vesicle-fusing ATPase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 678 | Total | C | N | O | S | 0 | 0 |
| | | | 5039 | 3197 | 876 | 943 | 23 | | |
| 1 | B | 672 | Total | C | N | O | S | 0 | 0 |
| | | | 4995 | 3168 | 863 | 940 | 24 | | |
| 1 | C | 676 | Total | C | N | O | S | 0 | 0 |
| | | | 5027 | 3186 | 871 | 947 | 23 | | |
| 1 | D | 673 | Total | C | N | O | S | 0 | 0 |
| | | | 4976 | 3157 | 856 | 939 | 24 | | |
| 1 | E | 670 | Total | C | N | O | S | 0 | 0 |
| | | | 4992 | 3171 | 860 | 938 | 23 | | |
| 1 | F | 654 | Total | C | N | O | S | 0 | 0 |
| | | | 4903 | 3112 | 849 | 918 | 24 | | |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -2 | GLY | - | EXPRESSION TAG | UNP P18708 |
| A | -1 | ALA | - | EXPRESSION TAG | UNP P18708 |
| A | 0 | HIS | - | EXPRESSION TAG | UNP P18708 |
| B | -2 | GLY | - | EXPRESSION TAG | UNP P18708 |
| B | -1 | ALA | - | EXPRESSION TAG | UNP P18708 |
| B | 0 | HIS | - | EXPRESSION TAG | UNP P18708 |
| C | -2 | GLY | - | EXPRESSION TAG | UNP P18708 |
| C | -1 | ALA | - | EXPRESSION TAG | UNP P18708 |
| C | 0 | HIS | - | EXPRESSION TAG | UNP P18708 |
| D | -2 | GLY | - | EXPRESSION TAG | UNP P18708 |
| D | -1 | ALA | - | EXPRESSION TAG | UNP P18708 |
| D | 0 | HIS | - | EXPRESSION TAG | UNP P18708 |
| E | -2 | GLY | - | EXPRESSION TAG | UNP P18708 |
| E | -1 | ALA | - | EXPRESSION TAG | UNP P18708 |
| E | 0 | HIS | - | EXPRESSION TAG | UNP P18708 |
| F | -2 | GLY | - | EXPRESSION TAG | UNP P18708 |
| F | -1 | ALA | - | EXPRESSION TAG | UNP P18708 |
| F | 0 | HIS | - | EXPRESSION TAG | UNP P18708 |

- Molecule 2 is a protein called Alpha-soluble NSF attachment protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | H | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2246 | 1415 | 373 | 441 | 17 | | |
| 2 | I | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2249 | 1418 | 373 | 441 | 17 | | |
| 2 | J | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2255 | 1424 | 373 | 441 | 17 | | |
| 2 | G | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2249 | 1421 | 370 | 441 | 17 | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| H | -1 | GLY | - | EXPRESSION TAG | UNP P54921 |
| H | 0 | SER | - | EXPRESSION TAG | UNP P54921 |
| I | -1 | GLY | - | EXPRESSION TAG | UNP P54921 |
| I | 0 | SER | - | EXPRESSION TAG | UNP P54921 |
| J | -1 | GLY | - | EXPRESSION TAG | UNP P54921 |
| J | 0 | SER | - | EXPRESSION TAG | UNP P54921 |
| G | -1 | GLY | - | EXPRESSION TAG | UNP P54921 |
| G | 0 | SER | - | EXPRESSION TAG | UNP P54921 |

- Molecule 3 is a protein called Vesicle-associated membrane protein 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 | K | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 480 | 293 | 89 | 97 | 1 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| K | 27 | GLY | - | EXPRESSION TAG | UNP P63045 |

- Molecule 4 is a protein called Syntaxin-1A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 4 | L | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 523 | 320 | 89 | 109 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| L | 190 | MET | - | EXPRESSION TAG | UNP P32851 |

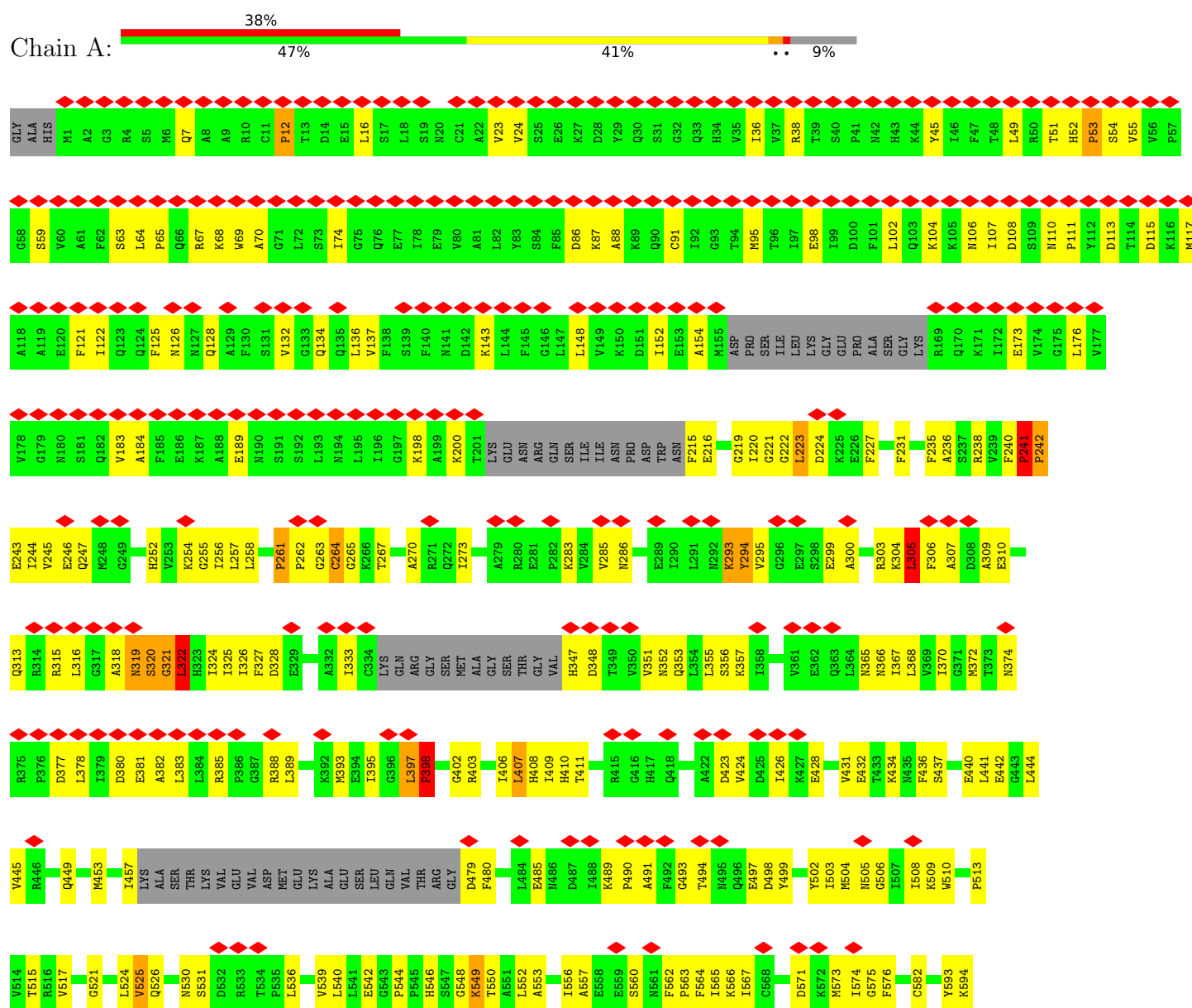
- Molecule 5 is a protein called Synaptosomal-associated protein 25.

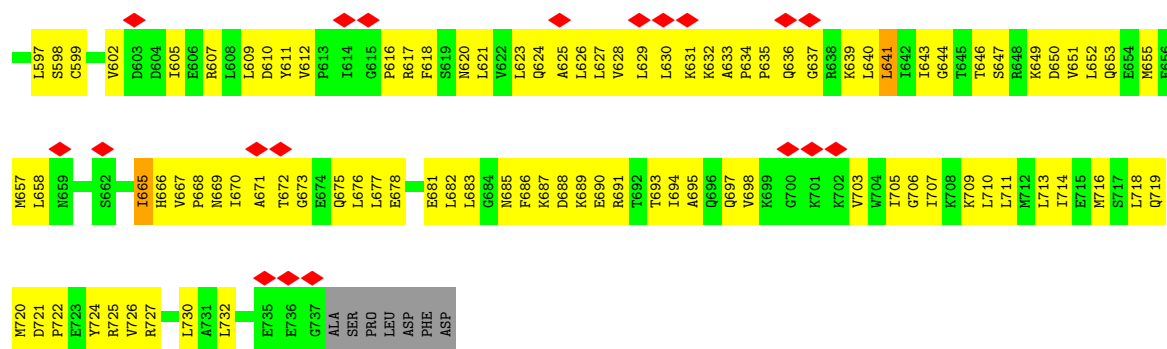
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | M | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1042 | 617 | 195 | 221 | 9 | | |

3 Residue-property plots

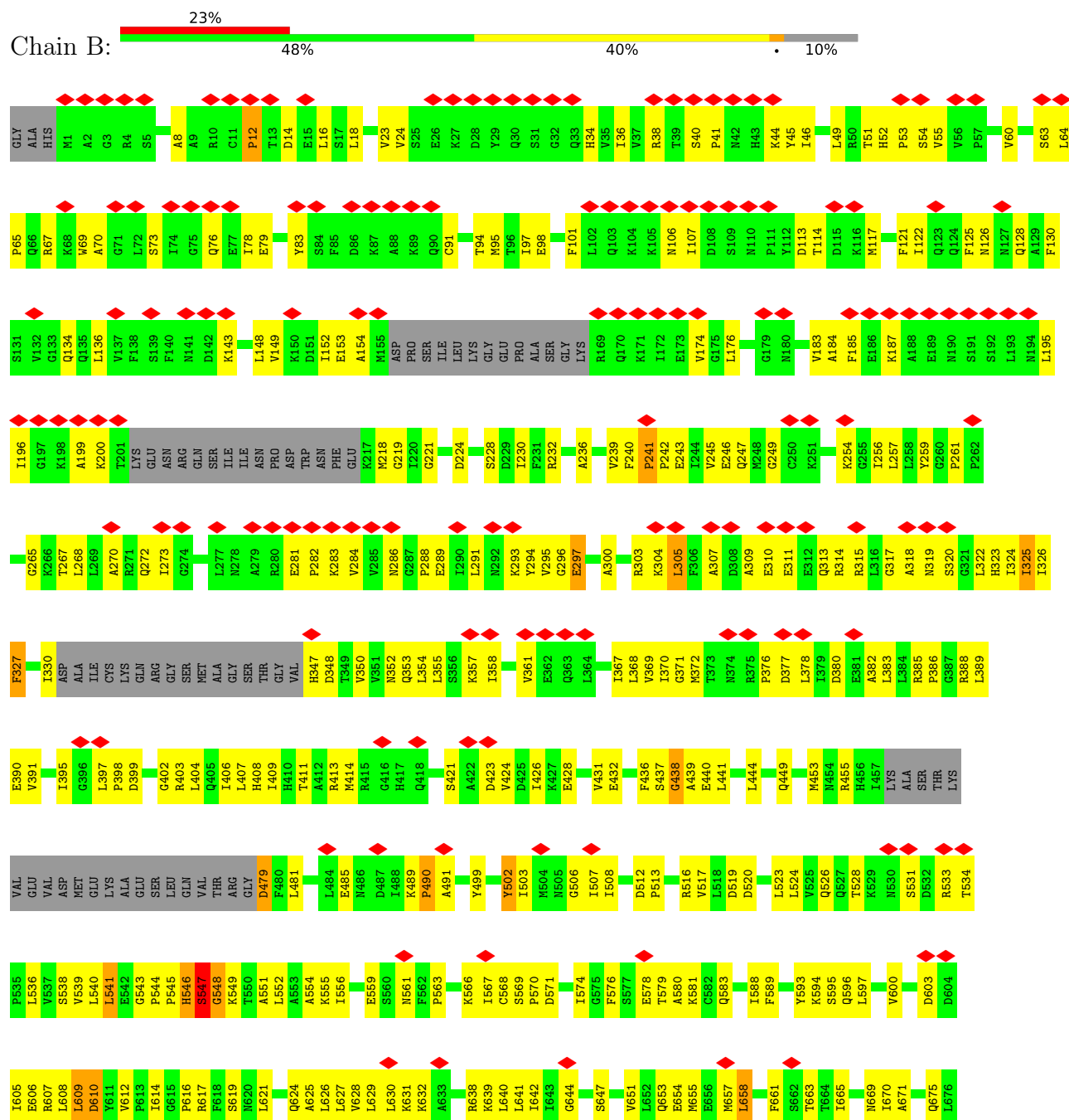
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Vesicle-fusing ATPase



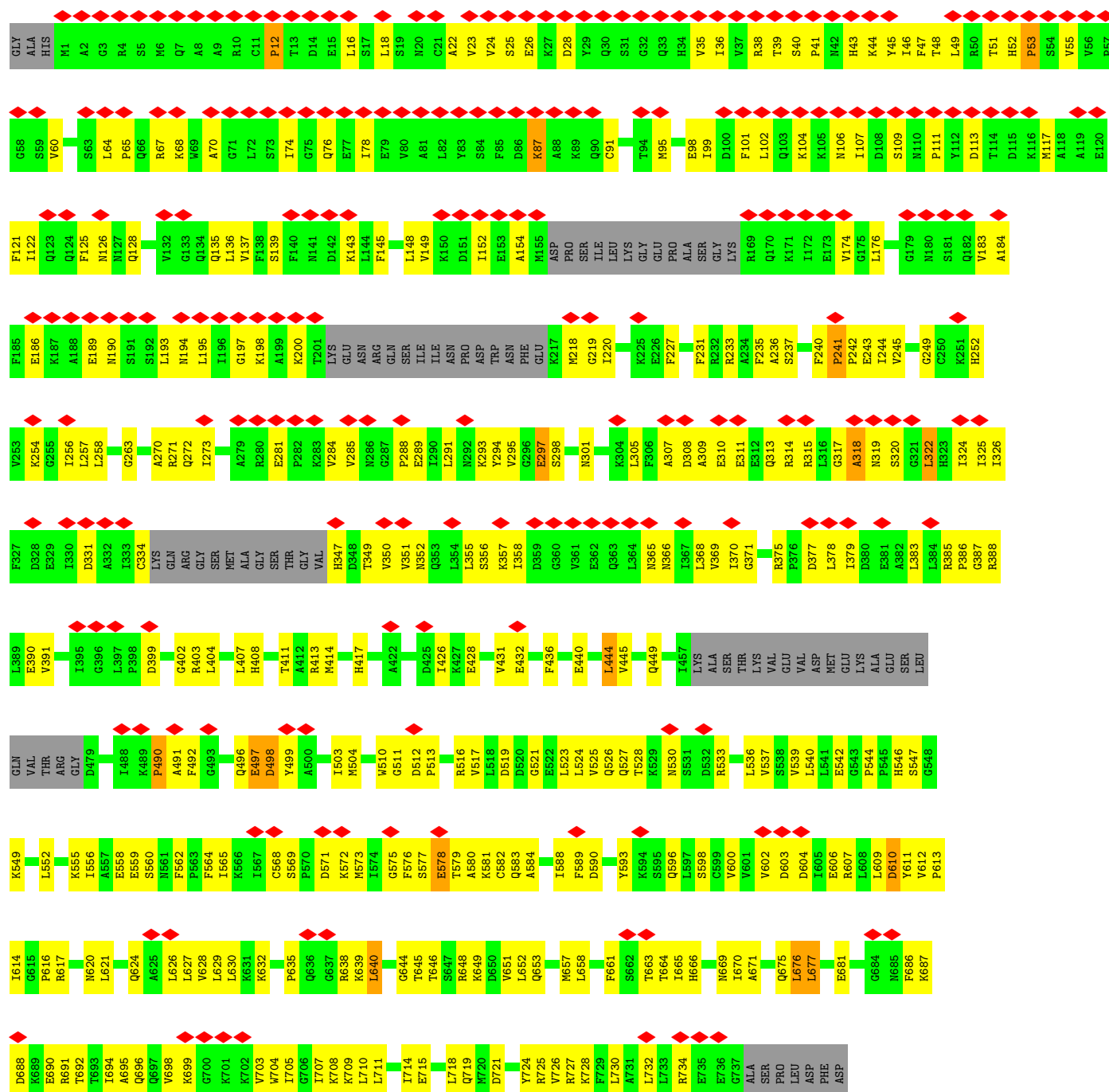


• Molecule 1: Vesicle-fusing ATPase



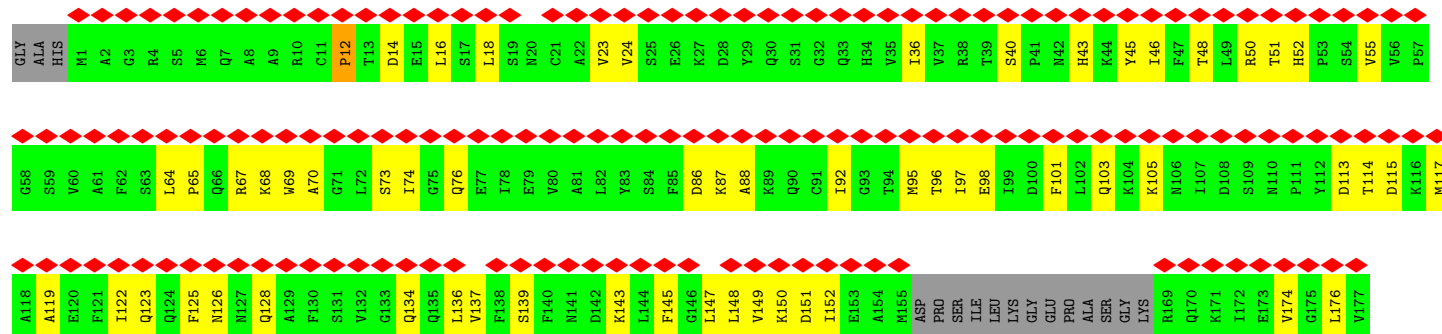


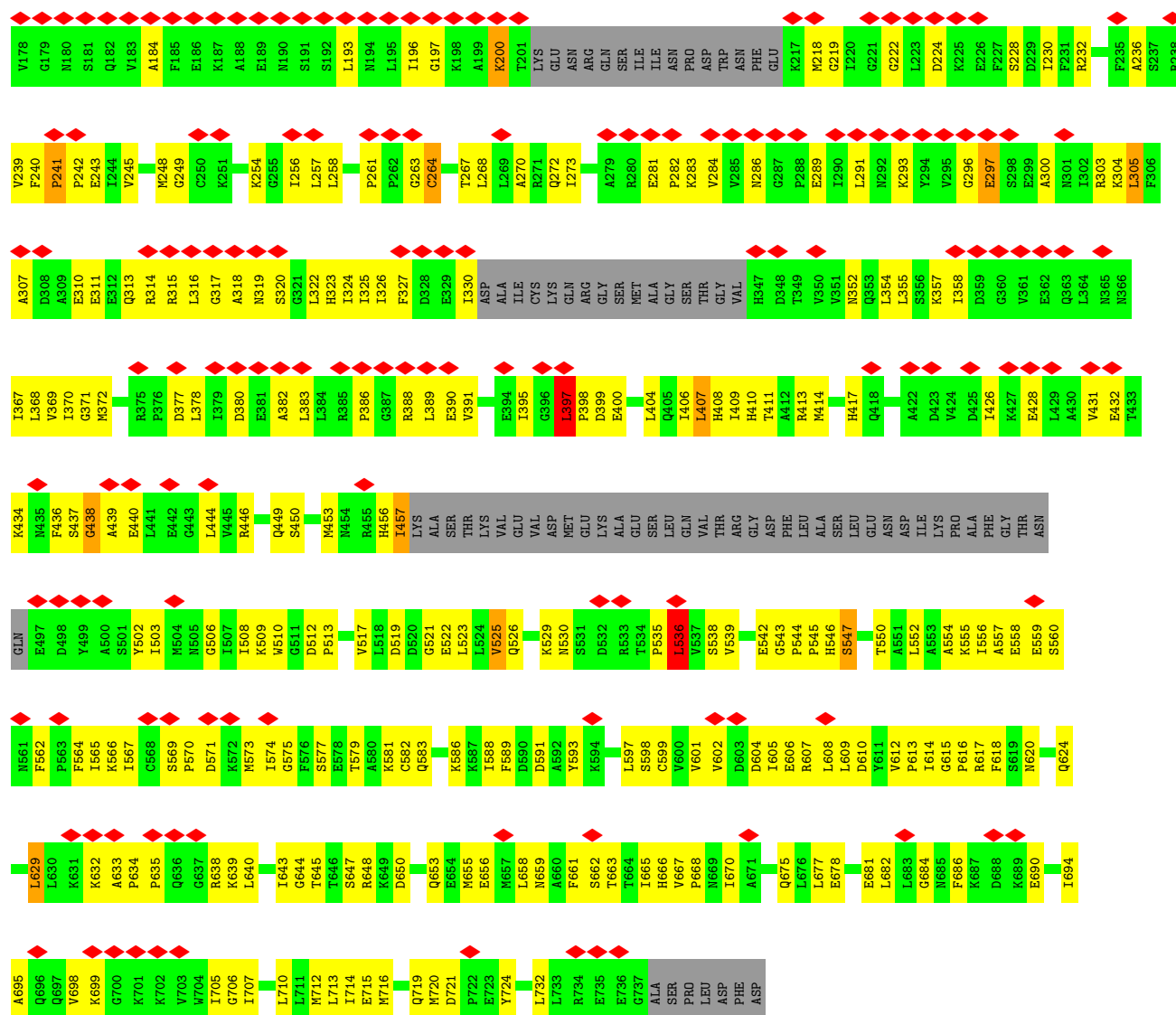
• Molecule 1: Vesicle-fusing ATPase



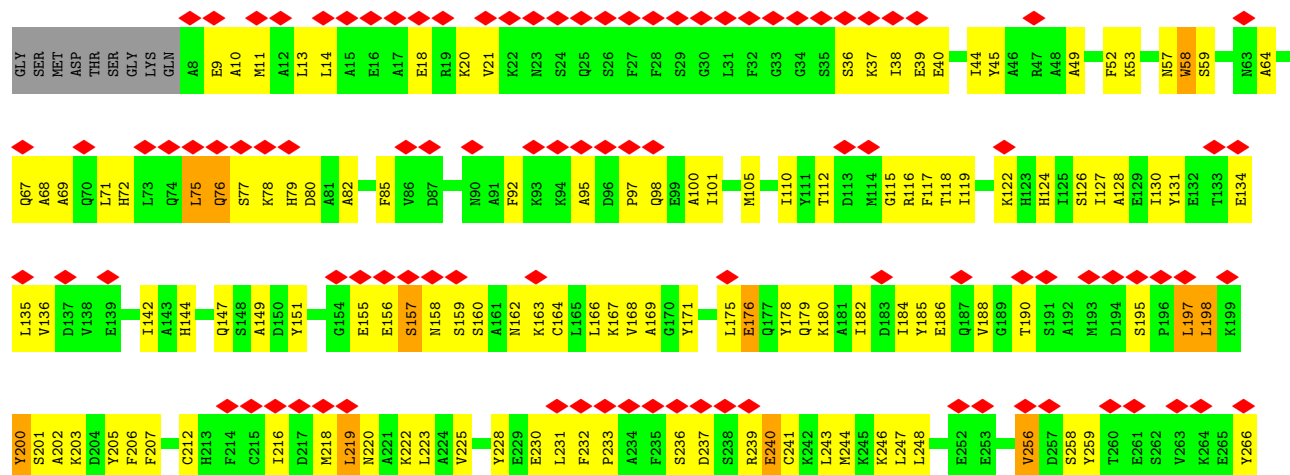
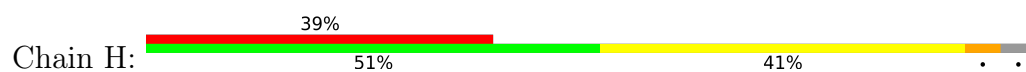
• Molecule 1: Vesicle-fusing ATPase

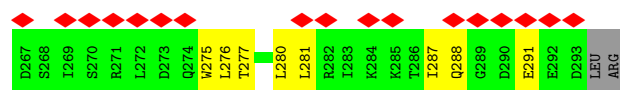




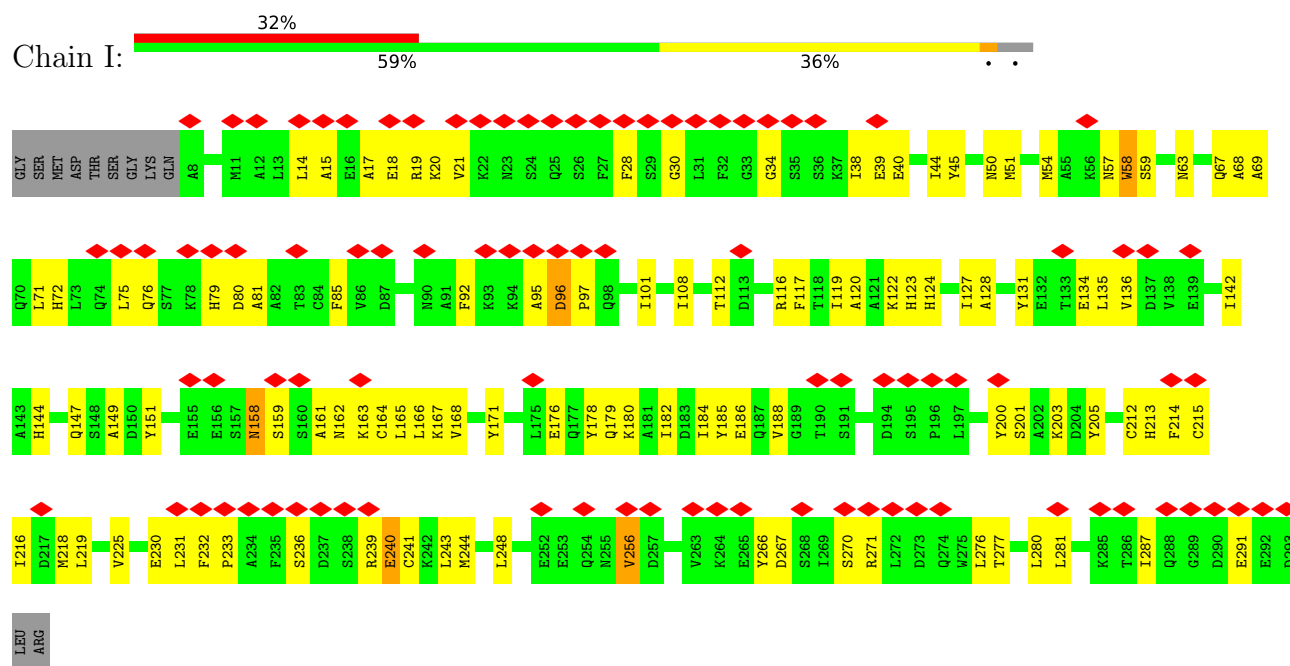


• Molecule 2: Alpha-soluble NSF attachment protein





• Molecule 2: Alpha-soluble NSF attachment protein

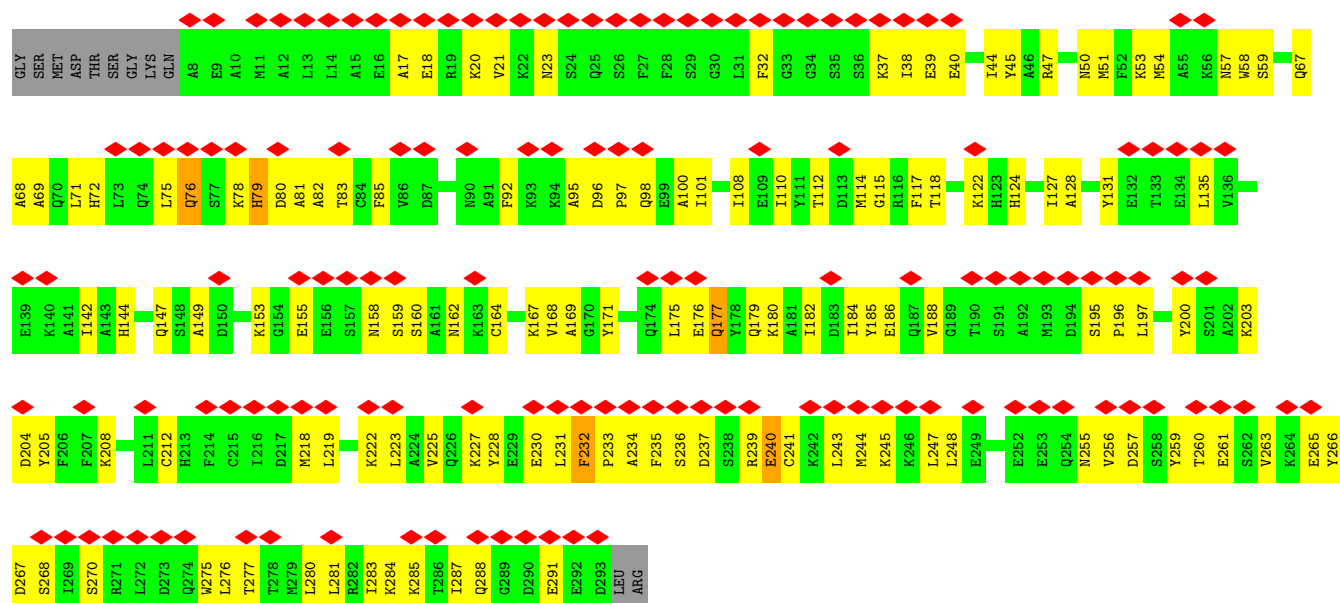


• Molecule 2: Alpha-soluble NSF attachment protein

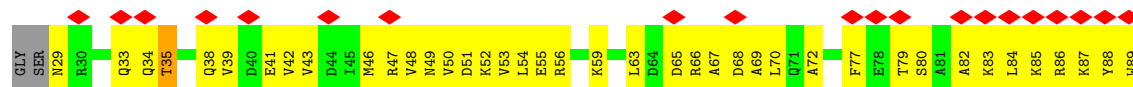


• Molecule 2: Alpha-soluble NSF attachment protein

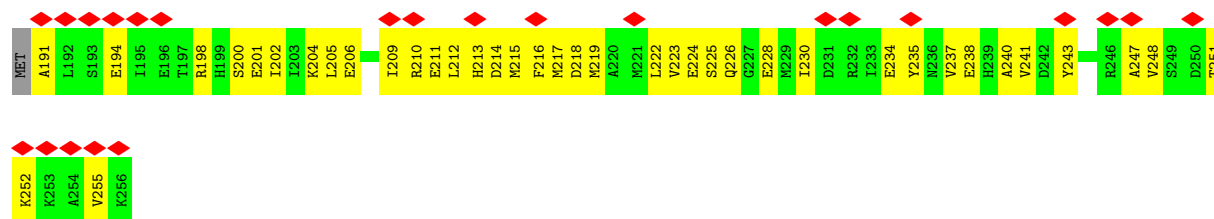




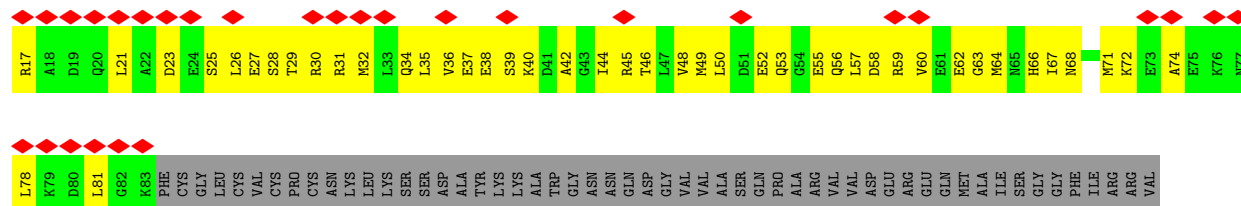
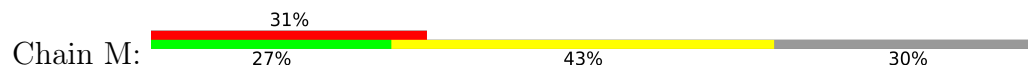
• Molecule 3: Vesicle-associated membrane protein 2



• Molecule 4: Syntaxin-1A



• Molecule 5: Synaptosomal-associated protein 25





4 Experimental information

| Property | Value | Source |
|--------------------------------------|------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 14991 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Each particle | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 44 | Depositor |
| Minimum defocus (nm) | -1800 | Depositor |
| Maximum defocus (nm) | -2800 | Depositor |
| Magnification | 31000 | Depositor |
| Image detector | GATAN K2 (4k x 4k) | Depositor |
| Maximum map value | 10.964 | Depositor |
| Minimum map value | -5.319 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 5.0 | Depositor |
| Map size (\AA) | 311.1936, 311.1936, 311.1936 | wwPDB |
| Map dimensions | 128, 128, 128 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 2.4312, 2.4312, 2.4312 | Depositor |

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.48 | 0/5116 | 0.85 | 14/6925 (0.2%) |
| 1 | B | 0.41 | 1/5069 (0.0%) | 0.77 | 11/6863 (0.2%) |
| 1 | C | 0.40 | 0/5102 | 0.74 | 6/6905 (0.1%) |
| 1 | D | 0.42 | 0/5050 | 0.75 | 7/6840 (0.1%) |
| 1 | E | 0.44 | 0/5068 | 0.81 | 9/6859 (0.1%) |
| 1 | F | 0.43 | 1/4977 (0.0%) | 0.79 | 12/6730 (0.2%) |
| 2 | G | 0.35 | 0/2289 | 0.61 | 0/3079 |
| 2 | H | 0.38 | 0/2285 | 0.63 | 4/3073 (0.1%) |
| 2 | I | 0.34 | 0/2288 | 0.59 | 1/3077 (0.0%) |
| 2 | J | 0.36 | 0/2295 | 0.57 | 0/3086 |
| 3 | K | 0.25 | 0/483 | 0.42 | 0/648 |
| 4 | L | 0.23 | 0/527 | 0.42 | 0/704 |
| 5 | M | 0.22 | 0/1042 | 0.43 | 0/1385 |
| All | All | 0.41 | 2/41591 (0.0%) | 0.74 | 64/56174 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 1 | B | 0 | 1 |
| 1 | E | 0 | 1 |
| 1 | F | 0 | 1 |
| 2 | H | 0 | 1 |
| All | All | 0 | 6 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | F | 264 | CYS | CB-SG | -5.77 | 1.72 | 1.81 |
| 1 | B | 547 | SER | C-O | 5.69 | 1.34 | 1.23 |

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 319 | ASN | N-CA-C | -9.95 | 84.15 | 111.00 |
| 1 | F | 397 | LEU | CA-CB-CG | 9.06 | 136.15 | 115.30 |
| 1 | E | 629 | LEU | CB-CG-CD1 | -8.90 | 95.87 | 111.00 |
| 1 | D | 547 | SER | C-N-CA | -8.85 | 103.72 | 122.30 |
| 1 | C | 322 | LEU | CA-CB-CG | 8.20 | 134.15 | 115.30 |
| 1 | F | 305 | LEU | CA-CB-CG | 7.88 | 133.43 | 115.30 |
| 1 | F | 629 | LEU | CB-CG-CD1 | -7.76 | 97.81 | 111.00 |
| 1 | B | 610 | ASP | CB-CG-OD2 | -7.58 | 111.48 | 118.30 |
| 1 | C | 677 | LEU | CB-CG-CD2 | -7.45 | 98.33 | 111.00 |
| 1 | E | 305 | LEU | CA-CB-CG | 7.41 | 132.34 | 115.30 |
| 1 | B | 305 | LEU | CA-CB-CG | 7.38 | 132.27 | 115.30 |
| 1 | F | 536 | LEU | CA-CB-CG | 7.03 | 131.47 | 115.30 |
| 1 | E | 652 | LEU | CB-CG-CD2 | -6.74 | 99.54 | 111.00 |
| 1 | A | 552 | LEU | CA-CB-CG | 6.62 | 130.54 | 115.30 |
| 1 | B | 395 | ILE | CG1-CB-CG2 | -6.60 | 96.88 | 111.40 |
| 1 | C | 444 | LEU | CA-CB-CG | 6.58 | 130.43 | 115.30 |
| 1 | B | 658 | LEU | CB-CG-CD1 | -6.57 | 99.83 | 111.00 |
| 1 | B | 708 | LYS | CD-CE-NZ | 6.50 | 126.64 | 111.70 |
| 1 | A | 305 | LEU | CA-CB-CG | 6.29 | 129.76 | 115.30 |
| 1 | B | 609 | LEU | CA-CB-CG | -6.25 | 100.93 | 115.30 |
| 2 | I | 96 | ASP | CB-CG-OD1 | 6.23 | 123.90 | 118.30 |
| 1 | C | 387 | GLY | N-CA-C | -6.21 | 97.58 | 113.10 |
| 1 | D | 627 | LEU | CB-CG-CD2 | -6.01 | 100.78 | 111.00 |
| 1 | B | 543 | GLY | N-CA-C | -5.99 | 98.13 | 113.10 |
| 1 | D | 609 | LEU | CA-CB-CG | 5.97 | 129.04 | 115.30 |
| 1 | C | 504 | MET | C-N-CA | -5.95 | 106.82 | 121.70 |
| 2 | H | 198 | LEU | CB-CG-CD2 | -5.93 | 100.92 | 111.00 |
| 1 | A | 549 | LYS | N-CA-C | -5.91 | 95.04 | 111.00 |
| 1 | D | 627 | LEU | CA-CB-CG | -5.90 | 101.73 | 115.30 |
| 1 | F | 525 | VAL | CG1-CB-CG2 | 5.88 | 120.31 | 110.90 |
| 1 | A | 641 | LEU | CA-CB-CG | 5.86 | 128.78 | 115.30 |
| 1 | A | 322 | LEU | CA-CB-CG | 5.85 | 128.75 | 115.30 |
| 1 | D | 643 | ILE | CB-CA-C | -5.85 | 99.91 | 111.60 |
| 1 | A | 525 | VAL | CG1-CB-CG2 | 5.84 | 120.25 | 110.90 |
| 1 | F | 543 | GLY | C-N-CD | 5.79 | 140.56 | 128.40 |
| 1 | A | 407 | LEU | CA-CB-CG | 5.65 | 128.29 | 115.30 |
| 1 | E | 395 | ILE | CG1-CB-CG2 | -5.61 | 99.05 | 111.40 |
| 1 | A | 398 | PRO | CA-N-CD | -5.61 | 103.65 | 111.50 |
| 1 | F | 547 | SER | N-CA-C | -5.46 | 96.27 | 111.00 |
| 1 | B | 548 | GLY | N-CA-C | -5.44 | 99.50 | 113.10 |
| 1 | A | 216 | GLU | N-CA-C | -5.43 | 96.34 | 111.00 |
| 1 | F | 640 | LEU | CA-CB-CG | 5.43 | 127.78 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | D | 404 | LEU | CA-CB-CG | 5.42 | 127.76 | 115.30 |
| 2 | H | 197 | LEU | CB-CG-CD1 | 5.40 | 120.18 | 111.00 |
| 1 | A | 665 | ILE | CG1-CB-CG2 | -5.39 | 99.53 | 111.40 |
| 1 | A | 236 | ALA | N-CA-C | -5.39 | 96.46 | 111.00 |
| 1 | A | 261 | PRO | C-N-CD | -5.37 | 108.78 | 120.60 |
| 1 | D | 416 | GLY | N-CA-C | -5.32 | 99.80 | 113.10 |
| 1 | B | 479 | ASP | N-CA-C | -5.31 | 96.66 | 111.00 |
| 1 | E | 676 | LEU | CA-CB-CG | 5.28 | 127.44 | 115.30 |
| 1 | F | 536 | LEU | CB-CG-CD2 | -5.25 | 102.08 | 111.00 |
| 1 | E | 438 | GLY | N-CA-C | 5.25 | 126.22 | 113.10 |
| 1 | E | 522 | GLU | CA-CB-CG | 5.22 | 124.89 | 113.40 |
| 1 | E | 397 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |
| 1 | F | 268 | LEU | CA-CB-CG | 5.20 | 127.27 | 115.30 |
| 2 | H | 219 | LEU | CA-CB-CG | 5.19 | 127.23 | 115.30 |
| 1 | F | 457 | ILE | CG1-CB-CG2 | -5.15 | 100.06 | 111.40 |
| 1 | B | 541 | LEU | CA-CB-CG | 5.13 | 127.11 | 115.30 |
| 1 | C | 640 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 1 | E | 258 | LEU | CA-CB-CG | 5.09 | 127.01 | 115.30 |
| 2 | H | 75 | LEU | CA-CB-CG | 5.09 | 127.00 | 115.30 |
| 1 | F | 407 | LEU | CA-CB-CG | 5.07 | 126.95 | 115.30 |
| 1 | A | 441 | LEU | CB-CG-CD2 | -5.05 | 102.42 | 111.00 |
| 1 | B | 544 | PRO | N-CA-C | -5.02 | 99.05 | 112.10 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 241 | PRO | Peptide |
| 1 | A | 321 | GLY | Peptide |
| 1 | B | 438 | GLY | Peptide |
| 1 | E | 438 | GLY | Peptide |
| 1 | F | 438 | GLY | Peptide |
| 2 | H | 200 | TYR | Mainchain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 5039 | 0 | 4945 | 309 | 0 |
| 1 | B | 4995 | 0 | 4920 | 281 | 0 |
| 1 | C | 5027 | 0 | 4945 | 329 | 0 |
| 1 | D | 4976 | 0 | 4880 | 318 | 0 |
| 1 | E | 4992 | 0 | 4910 | 318 | 0 |
| 1 | F | 4903 | 0 | 4853 | 308 | 0 |
| 2 | G | 2249 | 0 | 2188 | 114 | 0 |
| 2 | H | 2246 | 0 | 2183 | 128 | 0 |
| 2 | I | 2249 | 0 | 2192 | 99 | 0 |
| 2 | J | 2255 | 0 | 2199 | 129 | 0 |
| 3 | K | 480 | 0 | 465 | 73 | 0 |
| 4 | L | 523 | 0 | 497 | 52 | 0 |
| 5 | M | 1042 | 0 | 1022 | 118 | 0 |
| All | All | 40976 | 0 | 40199 | 2329 | 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 29.

All (2329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:490:PRO:HA | 1:B:491:ALA:HB3 | 1.46 | 0.93 |
| 1:A:490:PRO:HA | 1:A:491:ALA:HB3 | 1.50 | 0.92 |
| 1:C:386:PRO:HA | 1:C:390:GLU:HA | 1.54 | 0.90 |
| 1:C:490:PRO:HA | 1:C:491:ALA:HB3 | 1.51 | 0.90 |
| 1:F:545:PRO:HA | 1:F:547:SER:H | 1.38 | 0.89 |
| 1:F:105:LYS:HZ3 | 2:G:257:ASP:HB2 | 1.39 | 0.87 |
| 1:C:240:PHE:HD2 | 1:C:244:ILE:HG21 | 1.37 | 0.86 |
| 2:I:38:ILE:HD11 | 2:I:71:LEU:HB3 | 1.57 | 0.86 |
| 1:D:628:VAL:HG11 | 1:E:574:ILE:HG21 | 1.57 | 0.86 |
| 2:H:219:LEU:HB2 | 2:H:222:LYS:HB3 | 1.57 | 0.86 |
| 1:B:256:ILE:HG13 | 1:B:370:ILE:HG22 | 1.57 | 0.86 |
| 2:I:80:ASP:OD1 | 5:M:187:SER:OG | 1.93 | 0.86 |
| 3:K:56:ARG:HD2 | 5:M:171:ILE:HG23 | 1.58 | 0.85 |
| 2:J:235:PHE:HB3 | 3:K:38:GLN:HE21 | 1.38 | 0.85 |
| 1:F:539:VAL:HB | 1:F:643:ILE:HG12 | 1.59 | 0.85 |
| 1:B:327:PHE:HB2 | 1:B:330:ILE:HG22 | 1.59 | 0.85 |
| 1:E:386:PRO:HA | 1:E:390:GLU:HA | 1.59 | 0.84 |
| 1:A:264:CYS:SG | 1:A:265:GLY:N | 2.48 | 0.84 |
| 1:A:542:GLU:HG2 | 1:A:649:LYS:HD2 | 1.59 | 0.84 |
| 1:C:497:GLU:O | 1:C:499:TYR:N | 2.09 | 0.84 |
| 1:E:256:ILE:HG13 | 1:E:370:ILE:HG22 | 1.58 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:38:ILE:HG23 | 2:I:75:LEU:HD12 | 1.59 | 0.84 |
| 1:A:305:LEU:HD23 | 1:A:325:ILE:HG21 | 1.59 | 0.84 |
| 1:E:526:GLN:NE2 | 1:F:719:GLN:O | 2.10 | 0.83 |
| 1:E:585:MET:HG3 | 1:E:589:PHE:CZ | 2.13 | 0.83 |
| 1:A:562:PHE:CD2 | 1:A:597:LEU:HD21 | 2.14 | 0.83 |
| 1:E:327:PHE:HB2 | 1:E:330:ILE:HG22 | 1.58 | 0.83 |
| 1:E:527:GLN:O | 1:E:531:SER:OG | 1.97 | 0.83 |
| 1:F:570:PRO:HG2 | 1:F:604:ASP:HB2 | 1.61 | 0.83 |
| 2:G:159:SER:OG | 5:M:48:VAL:HG13 | 1.79 | 0.83 |
| 1:C:111:PRO:HG3 | 1:C:194:ASN:ND2 | 1.94 | 0.83 |
| 1:F:386:PRO:HA | 1:F:390:GLU:HA | 1.60 | 0.83 |
| 1:D:518:LEU:HD21 | 1:D:552:LEU:HD22 | 1.61 | 0.83 |
| 2:G:219:LEU:HB2 | 2:G:222:LYS:HB3 | 1.58 | 0.83 |
| 2:H:157:SER:HA | 4:L:228:GLU:OE1 | 1.79 | 0.82 |
| 2:J:201:SER:HG | 2:J:205:TYR:HE1 | 1.25 | 0.82 |
| 1:D:606:GLU:HA | 1:D:609:LEU:HG | 1.59 | 0.82 |
| 1:A:398:PRO:HG3 | 1:A:436:PHE:O | 1.78 | 0.82 |
| 1:F:327:PHE:HB2 | 1:F:330:ILE:HG22 | 1.59 | 0.82 |
| 1:C:256:ILE:HG13 | 1:C:370:ILE:HG22 | 1.61 | 0.82 |
| 3:K:54:LEU:HD21 | 4:L:222:LEU:HD13 | 1.61 | 0.81 |
| 1:B:566:LYS:HD2 | 1:B:588:ILE:HG23 | 1.62 | 0.81 |
| 1:A:705:ILE:HD13 | 1:A:710:LEU:HD12 | 1.61 | 0.81 |
| 1:D:510:TRP:HE3 | 1:D:675:GLN:HG2 | 1.45 | 0.81 |
| 1:E:490:PRO:HA | 1:E:491:ALA:HB3 | 1.61 | 0.81 |
| 2:H:116:ARG:NH2 | 3:K:68:ASP:OD2 | 2.13 | 0.81 |
| 2:J:201:SER:HB2 | 5:M:165:LEU:HD11 | 1.60 | 0.81 |
| 1:A:502:TYR:HE2 | 1:A:567:ILE:HG21 | 1.45 | 0.80 |
| 1:D:313:GLN:HE22 | 1:D:364:LEU:HA | 1.45 | 0.80 |
| 1:B:386:PRO:HA | 1:B:390:GLU:HA | 1.62 | 0.80 |
| 1:C:687:LYS:N | 1:C:690:GLU:OE2 | 2.14 | 0.80 |
| 1:F:256:ILE:HG13 | 1:F:370:ILE:HG22 | 1.63 | 0.80 |
| 2:J:235:PHE:CZ | 3:K:34:GLN:HG2 | 2.17 | 0.80 |
| 1:D:510:TRP:CD2 | 1:D:670:ILE:HG22 | 2.16 | 0.80 |
| 1:E:240:PHE:HD2 | 1:E:244:ILE:HG21 | 1.46 | 0.80 |
| 1:A:497:GLU:O | 1:A:499:TYR:N | 2.15 | 0.79 |
| 5:M:32:MET:HA | 5:M:35:LEU:HD12 | 1.65 | 0.79 |
| 1:B:407:LEU:HD11 | 1:B:426:ILE:HG23 | 1.64 | 0.79 |
| 2:I:72:HIS:HE1 | 2:I:80:ASP:HB2 | 1.47 | 0.79 |
| 1:E:587:LYS:NZ | 1:E:587:LYS:O | 2.15 | 0.79 |
| 1:E:720:MET:HG3 | 1:E:728:LYS:HE3 | 1.65 | 0.79 |
| 2:J:219:LEU:HB2 | 2:J:222:LYS:HB3 | 1.62 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:527:GLN:HE22 | 1:F:716:MET:HG2 | 1.48 | 0.79 |
| 1:C:627:LEU:HD12 | 1:D:607:ARG:HH12 | 1.47 | 0.79 |
| 1:E:407:LEU:HD11 | 1:E:426:ILE:HG23 | 1.65 | 0.79 |
| 1:E:686:PHE:HE1 | 1:E:714:ILE:HG23 | 1.47 | 0.79 |
| 1:B:589:PHE:HE1 | 1:B:600:VAL:HG11 | 1.48 | 0.78 |
| 1:C:313:GLN:O | 1:C:317:GLY:N | 2.17 | 0.78 |
| 1:C:690:GLU:HB2 | 1:C:726:VAL:HG21 | 1.65 | 0.78 |
| 1:E:589:PHE:CZ | 1:E:629:LEU:HD11 | 2.19 | 0.78 |
| 1:E:618:PHE:HZ | 1:F:612:VAL:HG11 | 1.48 | 0.78 |
| 1:F:525:VAL:HG13 | 1:F:562:PHE:CE1 | 2.18 | 0.78 |
| 1:F:545:PRO:HA | 1:F:547:SER:N | 1.99 | 0.78 |
| 1:A:557:ALA:O | 1:A:560:SER:OG | 2.01 | 0.78 |
| 1:B:526:GLN:HE21 | 1:C:719:GLN:HB3 | 1.48 | 0.78 |
| 5:M:49:MET:HB3 | 5:M:53:GLN:NE2 | 1.99 | 0.78 |
| 1:A:316:LEU:HB3 | 1:A:320:SER:HB2 | 1.65 | 0.77 |
| 1:A:713:LEU:HD21 | 1:A:732:LEU:HB3 | 1.67 | 0.77 |
| 1:F:105:LYS:NZ | 2:G:257:ASP:HB2 | 1.99 | 0.77 |
| 1:D:627:LEU:HD21 | 1:D:657:MET:HG3 | 1.67 | 0.77 |
| 2:H:119:ILE:HD11 | 3:K:65:ASP:OD2 | 1.85 | 0.77 |
| 1:C:676:LEU:HD12 | 1:C:705:ILE:HG21 | 1.64 | 0.77 |
| 1:A:686:PHE:HE2 | 1:A:714:ILE:HG12 | 1.49 | 0.77 |
| 1:A:285:VAL:HG13 | 1:A:326:ILE:HD11 | 1.65 | 0.77 |
| 1:A:353:GLN:HA | 1:B:288:PRO:HG3 | 1.65 | 0.77 |
| 1:F:407:LEU:HD11 | 1:F:426:ILE:HG23 | 1.65 | 0.77 |
| 1:E:246:GLU:O | 1:F:413:ARG:NH1 | 2.14 | 0.76 |
| 1:B:621:LEU:HD11 | 1:C:575:GLY:HA2 | 1.66 | 0.76 |
| 5:M:50:LEU:HB3 | 5:M:170:GLU:HG2 | 1.67 | 0.76 |
| 1:D:399:ASP:O | 1:D:403:ARG:N | 2.19 | 0.76 |
| 1:A:115:ASP:CB | 1:A:242:PRO:HG3 | 2.16 | 0.76 |
| 1:D:106:ASN:HB3 | 1:D:143:LYS:HZ1 | 1.50 | 0.76 |
| 1:D:605:ILE:HD11 | 1:D:644:GLY:HA3 | 1.67 | 0.76 |
| 1:C:496:GLN:O | 1:C:498:ASP:N | 2.19 | 0.76 |
| 1:C:540:LEU:HB3 | 1:C:664:THR:HG22 | 1.68 | 0.76 |
| 1:A:353:GLN:HE21 | 1:A:357:LYS:HG2 | 1.50 | 0.75 |
| 1:A:316:LEU:HB3 | 1:A:320:SER:CB | 2.17 | 0.75 |
| 1:C:407:LEU:HD11 | 1:C:426:ILE:HG23 | 1.66 | 0.75 |
| 1:E:585:MET:HA | 1:E:588:ILE:HD12 | 1.68 | 0.75 |
| 2:H:228:TYR:OH | 2:H:237:ASP:OD1 | 2.05 | 0.75 |
| 1:C:524:LEU:HD21 | 1:C:537:VAL:CG1 | 2.16 | 0.75 |
| 1:A:525:VAL:HG13 | 1:A:562:PHE:CZ | 2.21 | 0.75 |
| 4:L:209:ILE:HG21 | 5:M:32:MET:HG3 | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:386:PRO:HA | 1:D:390:GLU:HA | 1.69 | 0.75 |
| 1:D:728:LYS:HE3 | 1:D:732:LEU:HD11 | 1.69 | 0.75 |
| 1:F:536:LEU:HD11 | 1:F:634:PRO:HD3 | 1.66 | 0.75 |
| 1:D:67:ARG:HD2 | 2:J:218:MET:HE2 | 1.68 | 0.75 |
| 1:F:98:GLU:HB3 | 1:F:148:LEU:HB3 | 1.69 | 0.75 |
| 1:C:331:ASP:HA | 1:C:379:ILE:HD11 | 1.69 | 0.74 |
| 2:J:53:LYS:HE3 | 2:G:117:PHE:HD2 | 1.52 | 0.74 |
| 1:A:221:GLY:HA3 | 1:A:406:ILE:HD11 | 1.70 | 0.74 |
| 1:E:300:ALA:O | 1:E:304:LYS:HG2 | 1.87 | 0.74 |
| 2:H:149:ALA:HB2 | 2:H:164:CYS:HB2 | 1.67 | 0.74 |
| 1:D:711:LEU:HA | 1:D:714:ILE:HD12 | 1.70 | 0.74 |
| 1:E:653:GLN:HA | 1:E:658:LEU:HB2 | 1.67 | 0.74 |
| 1:E:625:ALA:HA | 1:F:574:ILE:HD11 | 1.70 | 0.74 |
| 1:C:544:PRO:O | 1:C:547:SER:OG | 2.06 | 0.73 |
| 1:E:606:GLU:OE2 | 1:E:646:THR:OG1 | 2.06 | 0.73 |
| 2:H:239:ARG:NH1 | 4:L:214:ASP:OD1 | 2.21 | 0.73 |
| 1:E:624:GLN:NE2 | 1:F:610:ASP:OD1 | 2.20 | 0.73 |
| 1:C:98:GLU:HB3 | 1:C:148:LEU:HB3 | 1.70 | 0.73 |
| 1:C:724:TYR:HD2 | 1:C:727:ARG:HH21 | 1.36 | 0.73 |
| 1:F:300:ALA:O | 1:F:304:LYS:HG2 | 1.87 | 0.73 |
| 1:B:540:LEU:HD23 | 1:B:661:PHE:CD1 | 2.23 | 0.73 |
| 1:F:303:ARG:HG3 | 1:F:357:LYS:HE2 | 1.70 | 0.73 |
| 2:I:21:VAL:HG21 | 2:I:71:LEU:HD22 | 1.71 | 0.73 |
| 1:C:524:LEU:HD21 | 1:C:537:VAL:HG11 | 1.70 | 0.73 |
| 1:E:240:PHE:CD2 | 1:E:244:ILE:HG21 | 2.23 | 0.73 |
| 1:B:300:ALA:O | 1:B:304:LYS:HG2 | 1.89 | 0.73 |
| 1:C:611:TYR:CE1 | 1:C:616:PRO:HB2 | 2.23 | 0.73 |
| 1:A:115:ASP:HB2 | 1:A:242:PRO:HG3 | 1.70 | 0.73 |
| 1:E:563:PRO:HG2 | 1:E:595:SER:OG | 1.88 | 0.73 |
| 2:I:200:TYR:HB3 | 3:K:47:ARG:HH22 | 1.54 | 0.73 |
| 1:C:318:ALA:O | 1:C:319:ASN:ND2 | 2.21 | 0.73 |
| 1:C:109:SER:OG | 1:C:315:ARG:HB3 | 1.88 | 0.72 |
| 1:E:553:ALA:HA | 1:E:556:ILE:HD12 | 1.70 | 0.72 |
| 2:H:115:GLY:HA2 | 2:G:50:ASN:ND2 | 2.04 | 0.72 |
| 3:K:53:VAL:HG22 | 4:L:226:GLN:HE22 | 1.54 | 0.72 |
| 1:A:309:ALA:HB1 | 1:A:367:ILE:HG21 | 1.71 | 0.72 |
| 1:F:569:SER:OG | 1:F:571:ASP:OD2 | 2.06 | 0.72 |
| 1:A:549:LYS:NZ | 1:A:647:SER:OG | 2.19 | 0.72 |
| 1:A:602:VAL:HG12 | 1:A:605:ILE:HG12 | 1.71 | 0.72 |
| 1:D:106:ASN:HB3 | 1:D:143:LYS:NZ | 2.04 | 0.72 |
| 1:F:564:PHE:O | 1:F:598:SER:OG | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:175:LEU:HD23 | 2:G:177:GLN:HE21 | 1.55 | 0.72 |
| 1:D:626:LEU:HB3 | 1:D:657:MET:HE3 | 1.72 | 0.72 |
| 1:C:533:ARG:O | 1:D:505:ASN:ND2 | 2.22 | 0.72 |
| 1:D:527:GLN:HE21 | 1:E:715:GLU:HG3 | 1.54 | 0.72 |
| 1:F:606:GLU:OE1 | 1:F:606:GLU:N | 2.22 | 0.72 |
| 2:G:72:HIS:HE1 | 2:G:80:ASP:HB2 | 1.55 | 0.72 |
| 1:A:677:LEU:HD21 | 1:A:695:ALA:HA | 1.70 | 0.72 |
| 1:C:691:ARG:HA | 1:C:694:ILE:HD12 | 1.72 | 0.72 |
| 1:E:686:PHE:HB3 | 1:E:690:GLU:HB2 | 1.71 | 0.72 |
| 1:F:105:LYS:NZ | 2:G:255:ASN:OD1 | 2.21 | 0.72 |
| 1:F:555:LYS:NZ | 1:F:559:GLU:OE2 | 2.14 | 0.72 |
| 3:K:63:LEU:HD22 | 5:M:178:ILE:HG23 | 1.71 | 0.72 |
| 1:D:654:GLU:HB3 | 1:E:614:ILE:HD11 | 1.72 | 0.71 |
| 1:A:125:PHE:HA | 1:A:128:GLN:NE2 | 2.05 | 0.71 |
| 1:D:544:PRO:O | 1:D:547:SER:HB3 | 1.90 | 0.71 |
| 3:K:42:VAL:HG11 | 5:M:160:LEU:HD13 | 1.71 | 0.71 |
| 2:I:72:HIS:CE1 | 2:I:80:ASP:HB2 | 2.25 | 0.71 |
| 1:A:553:ALA:HA | 1:A:556:ILE:HD12 | 1.73 | 0.71 |
| 1:F:634:PRO:HB2 | 1:F:638:ARG:HG3 | 1.70 | 0.71 |
| 1:A:562:PHE:HD2 | 1:A:597:LEU:HD21 | 1.55 | 0.71 |
| 1:B:303:ARG:HG3 | 1:B:357:LYS:HE2 | 1.73 | 0.71 |
| 2:G:228:TYR:OH | 2:G:237:ASP:OD1 | 2.05 | 0.71 |
| 1:A:351:VAL:O | 1:A:355:LEU:HG | 1.90 | 0.71 |
| 1:F:125:PHE:HA | 1:F:128:GLN:NE2 | 2.06 | 0.71 |
| 1:C:718:LEU:O | 1:C:725:ARG:NH1 | 2.24 | 0.71 |
| 1:E:538:SER:OG | 1:E:661:PHE:HA | 1.91 | 0.71 |
| 1:D:301:ASN:HA | 1:D:304:LYS:HD3 | 1.71 | 0.71 |
| 2:G:235:PHE:CG | 5:M:152:GLN:HG2 | 2.25 | 0.71 |
| 5:M:49:MET:HB3 | 5:M:53:GLN:HE21 | 1.54 | 0.70 |
| 1:C:630:LEU:HD11 | 1:C:661:PHE:CE1 | 2.25 | 0.70 |
| 1:C:652:LEU:HD22 | 1:C:657:MET:HG2 | 1.73 | 0.70 |
| 1:F:517:VAL:HG13 | 1:F:665:ILE:HG21 | 1.73 | 0.70 |
| 1:A:326:ILE:HG22 | 1:A:370:ILE:HG12 | 1.73 | 0.70 |
| 1:E:125:PHE:HA | 1:E:128:GLN:NE2 | 2.07 | 0.70 |
| 1:F:264:CYS:SG | 1:F:395:ILE:HG22 | 2.32 | 0.70 |
| 1:C:564:PHE:O | 1:C:598:SER:OG | 2.10 | 0.70 |
| 1:E:303:ARG:HG3 | 1:E:357:LYS:HE2 | 1.73 | 0.70 |
| 1:E:680:LEU:HD13 | 1:E:694:ILE:HD13 | 1.73 | 0.70 |
| 2:J:235:PHE:CE2 | 3:K:34:GLN:HG2 | 2.26 | 0.70 |
| 1:E:253:VAL:N | 1:F:446:ARG:HH12 | 1.89 | 0.70 |
| 1:E:586:LYS:NZ | 1:F:574:ILE:O | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:83:LYS:HD2 | 5:M:203:LEU:HD11 | 1.73 | 0.70 |
| 1:D:620:ASN:O | 1:D:624:GLN:HG2 | 1.92 | 0.70 |
| 1:E:513:PRO:HA | 1:E:516:ARG:HG2 | 1.72 | 0.70 |
| 1:A:564:PHE:CE1 | 1:A:566:LYS:HB2 | 2.27 | 0.70 |
| 1:B:627:LEU:HD21 | 1:B:657:MET:HG3 | 1.74 | 0.70 |
| 1:D:513:PRO:HA | 1:D:516:ARG:HG2 | 1.73 | 0.70 |
| 1:E:510:TRP:CZ3 | 1:E:670:ILE:HG13 | 2.27 | 0.70 |
| 3:K:52:LYS:HB3 | 5:M:171:ILE:HD13 | 1.74 | 0.70 |
| 1:E:397:LEU:HD22 | 1:E:398:PRO:HD2 | 1.73 | 0.69 |
| 1:C:513:PRO:O | 1:C:516:ARG:HG2 | 1.91 | 0.69 |
| 2:H:18:GLU:HA | 2:H:21:VAL:HG12 | 1.74 | 0.69 |
| 1:E:706:GLY:O | 1:E:710:LEU:N | 2.24 | 0.69 |
| 1:E:549:LYS:HA | 1:E:552:LEU:HD12 | 1.75 | 0.69 |
| 1:C:111:PRO:HG3 | 1:C:194:ASN:HD22 | 1.55 | 0.69 |
| 1:F:96:THR:HB | 1:F:151:ASP:H | 1.57 | 0.69 |
| 3:K:63:LEU:HD13 | 5:M:182:MET:HG2 | 1.75 | 0.69 |
| 1:E:603:ASP:OD2 | 1:E:645:THR:OG1 | 2.09 | 0.69 |
| 1:B:581:LYS:NZ | 1:B:608:LEU:O | 2.25 | 0.69 |
| 1:B:713:LEU:HD22 | 1:B:732:LEU:HB3 | 1.74 | 0.69 |
| 1:A:502:TYR:CE2 | 1:A:567:ILE:HG21 | 2.26 | 0.69 |
| 1:D:353:GLN:HE22 | 1:E:288:PRO:HG2 | 1.56 | 0.69 |
| 1:B:533:ARG:HG3 | 1:B:534:THR:H | 1.58 | 0.69 |
| 1:E:625:ALA:O | 1:E:629:LEU:HG | 1.93 | 0.69 |
| 1:E:670:ILE:HG22 | 1:E:672:THR:H | 1.57 | 0.69 |
| 2:J:101:ILE:HG21 | 2:J:135:LEU:HD11 | 1.75 | 0.69 |
| 1:B:98:GLU:HB3 | 1:B:148:LEU:HB3 | 1.73 | 0.68 |
| 1:B:624:GLN:NE2 | 1:C:610:ASP:O | 2.25 | 0.68 |
| 1:E:592:ALA:HB1 | 1:E:640:LEU:HD22 | 1.75 | 0.68 |
| 1:F:513:PRO:O | 1:F:517:VAL:HG23 | 1.94 | 0.68 |
| 2:I:101:ILE:HG21 | 2:I:135:LEU:HD11 | 1.75 | 0.68 |
| 1:B:125:PHE:HA | 1:B:128:GLN:NE2 | 2.08 | 0.68 |
| 1:C:542:GLU:CB | 1:C:649:LYS:HD3 | 2.24 | 0.68 |
| 1:C:578:GLU:HB3 | 1:C:621:LEU:HB3 | 1.75 | 0.68 |
| 1:F:358:ILE:HD12 | 1:F:388:ARG:HB3 | 1.74 | 0.68 |
| 2:J:200:TYR:HE2 | 3:K:41:GLU:HG2 | 1.58 | 0.68 |
| 1:A:653:GLN:NE2 | 1:A:653:GLN:O | 2.26 | 0.68 |
| 1:D:543:GLY:H | 1:D:549:LYS:HD3 | 1.59 | 0.68 |
| 2:H:203:LYS:HD3 | 2:H:236:SER:HB3 | 1.74 | 0.68 |
| 2:J:50:ASN:ND2 | 2:G:115:GLY:HA2 | 2.07 | 0.68 |
| 1:A:503:ILE:HG23 | 1:A:506:GLY:HA2 | 1.75 | 0.68 |
| 1:B:64:LEU:HA | 1:B:67:ARG:HE | 1.58 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:211:GLU:HA | 4:L:214:ASP:OD2 | 1.92 | 0.68 |
| 1:A:258:LEU:HA | 1:A:393:MET:O | 1.94 | 0.68 |
| 1:D:67:ARG:HB3 | 2:J:218:MET:SD | 2.34 | 0.68 |
| 1:D:404:LEU:HA | 1:D:407:LEU:HD12 | 1.74 | 0.68 |
| 1:F:589:PHE:HD2 | 1:F:629:LEU:HD13 | 1.57 | 0.68 |
| 1:C:596:GLN:HA | 1:C:638:ARG:HD3 | 1.74 | 0.68 |
| 2:J:228:TYR:OH | 2:J:237:ASP:OD1 | 2.10 | 0.68 |
| 1:A:262:PRO:HG2 | 1:A:374:ASN:OD1 | 1.94 | 0.68 |
| 1:B:538:SER:HB3 | 1:B:661:PHE:CD2 | 2.29 | 0.68 |
| 1:B:12:PRO:HG2 | 1:B:23:VAL:HG11 | 1.75 | 0.67 |
| 1:F:92:ILE:HG21 | 1:F:95:MET:HB2 | 1.75 | 0.67 |
| 1:E:685:ASN:HB3 | 1:E:718:LEU:HD11 | 1.75 | 0.67 |
| 1:B:449:GLN:O | 1:B:453:MET:HG2 | 1.94 | 0.67 |
| 1:D:628:VAL:HG13 | 1:E:571:ASP:OD1 | 1.93 | 0.67 |
| 4:L:216:PHE:CE2 | 5:M:39:SER:HB2 | 2.30 | 0.67 |
| 1:D:358:ILE:HD12 | 1:D:388:ARG:HB3 | 1.76 | 0.67 |
| 1:E:589:PHE:CD2 | 1:E:629:LEU:HD21 | 2.29 | 0.67 |
| 1:F:536:LEU:HD21 | 1:F:632:LYS:O | 1.93 | 0.67 |
| 1:A:64:LEU:HB3 | 1:A:65:PRO:HD3 | 1.77 | 0.67 |
| 2:H:115:GLY:HA2 | 2:G:50:ASN:HD21 | 1.58 | 0.67 |
| 2:H:216:ILE:HG12 | 2:H:218:MET:H | 1.59 | 0.67 |
| 1:E:12:PRO:HG2 | 1:E:23:VAL:HG11 | 1.77 | 0.67 |
| 2:J:271:ARG:NH2 | 2:G:234:ALA:HB2 | 2.10 | 0.67 |
| 1:C:106:ASN:HB3 | 1:C:143:LYS:NZ | 2.10 | 0.67 |
| 1:D:546:HIS:ND1 | 1:D:709:LYS:HD3 | 2.10 | 0.67 |
| 1:E:449:GLN:O | 1:E:453:MET:HG2 | 1.95 | 0.67 |
| 1:B:524:LEU:HD21 | 1:B:663:THR:HG21 | 1.75 | 0.67 |
| 1:D:510:TRP:CE3 | 1:D:670:ILE:HG22 | 2.30 | 0.67 |
| 1:E:311:GLU:OE1 | 1:E:314:ARG:NE | 2.26 | 0.67 |
| 1:A:720:MET:O | 1:A:725:ARG:NE | 2.20 | 0.67 |
| 1:C:125:PHE:HA | 1:C:128:GLN:NE2 | 2.10 | 0.67 |
| 1:F:311:GLU:OE1 | 1:F:314:ARG:NE | 2.26 | 0.67 |
| 3:K:83:LYS:HG2 | 3:K:86:ARG:NH2 | 2.09 | 0.67 |
| 1:B:358:ILE:HD12 | 1:B:388:ARG:HB3 | 1.78 | 0.66 |
| 1:B:654:GLU:O | 1:C:613:PRO:HG3 | 1.95 | 0.66 |
| 1:D:234:ALA:HA | 1:D:253:VAL:HG11 | 1.77 | 0.66 |
| 2:J:230:GLU:HG2 | 2:J:231:LEU:N | 2.09 | 0.66 |
| 1:D:527:GLN:HE22 | 1:E:715:GLU:C | 1.99 | 0.66 |
| 1:F:258:LEU:HB3 | 1:F:395:ILE:HD11 | 1.75 | 0.66 |
| 1:F:535:PRO:HA | 1:F:639:LYS:HG2 | 1.76 | 0.66 |
| 1:F:570:PRO:HA | 1:F:573:MET:HE2 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:563:PRO:HD2 | 1:A:597:LEU:HD22 | 1.76 | 0.66 |
| 1:A:687:LYS:N | 1:A:690:GLU:OE1 | 2.28 | 0.66 |
| 1:E:602:VAL:O | 1:E:644:GLY:HA2 | 1.94 | 0.66 |
| 5:M:40:LYS:O | 5:M:44:ILE:HG13 | 1.96 | 0.66 |
| 1:C:546:HIS:HA | 1:C:708:LYS:HD3 | 1.78 | 0.66 |
| 1:F:605:ILE:HD11 | 1:F:644:GLY:HA3 | 1.76 | 0.66 |
| 1:F:612:VAL:HG12 | 1:F:617:ARG:HB2 | 1.77 | 0.66 |
| 2:H:197:LEU:HD12 | 5:M:45:ARG:HD3 | 1.78 | 0.66 |
| 4:L:240:ALA:HA | 4:L:243:TYR:HD2 | 1.59 | 0.66 |
| 1:F:437:SER:OG | 1:F:440:GLU:HG2 | 1.96 | 0.66 |
| 2:J:53:LYS:HE3 | 2:G:117:PHE:CD2 | 2.31 | 0.66 |
| 2:G:21:VAL:HG21 | 2:G:71:LEU:HD22 | 1.78 | 0.66 |
| 1:A:231:PHE:CD1 | 1:A:235:PHE:HE2 | 2.13 | 0.66 |
| 1:F:635:PRO:O | 1:F:638:ARG:HG2 | 1.96 | 0.66 |
| 1:E:64:LEU:HB3 | 1:E:65:PRO:HD3 | 1.78 | 0.66 |
| 1:C:236:ALA:HB1 | 1:D:453:MET:HB3 | 1.77 | 0.65 |
| 2:H:21:VAL:HG21 | 2:H:71:LEU:HD22 | 1.77 | 0.65 |
| 1:A:607:ARG:HD3 | 1:F:624:GLN:NE2 | 2.11 | 0.65 |
| 1:B:589:PHE:CE1 | 1:B:600:VAL:HG11 | 2.30 | 0.65 |
| 2:H:233:PRO:HB3 | 2:G:268:SER:O | 1.95 | 0.65 |
| 1:B:224:ASP:O | 1:B:228:SER:HB2 | 1.97 | 0.65 |
| 1:E:640:LEU:HD12 | 1:E:641:LEU:N | 2.10 | 0.65 |
| 1:E:652:LEU:CD2 | 1:E:657:MET:HB3 | 2.27 | 0.65 |
| 1:F:570:PRO:HG2 | 1:F:604:ASP:CB | 2.26 | 0.65 |
| 1:F:721:ASP:HB2 | 1:F:724:TYR:HD1 | 1.60 | 0.65 |
| 1:A:240:PHE:HE2 | 1:B:453:MET:HB3 | 1.61 | 0.65 |
| 1:A:562:PHE:HD2 | 1:A:597:LEU:CD2 | 2.10 | 0.65 |
| 1:D:223:LEU:HD11 | 1:D:395:ILE:HG12 | 1.77 | 0.65 |
| 1:E:534:THR:HG23 | 1:F:715:GLU:HG3 | 1.78 | 0.65 |
| 2:J:271:ARG:NH2 | 2:G:231:LEU:HB2 | 2.11 | 0.65 |
| 1:B:40:SER:CB | 1:B:41:PRO:HD2 | 2.27 | 0.65 |
| 1:A:710:LEU:O | 1:A:714:ILE:HG13 | 1.96 | 0.65 |
| 1:D:10:ARG:HG3 | 1:D:67:ARG:HH12 | 1.61 | 0.65 |
| 1:F:184:ALA:HB1 | 1:F:200:LYS:O | 1.97 | 0.65 |
| 1:F:307:ALA:O | 1:F:311:GLU:HG2 | 1.96 | 0.65 |
| 1:D:652:LEU:HB3 | 1:D:658:LEU:HB2 | 1.78 | 0.65 |
| 1:D:695:ALA:HB1 | 1:D:699:LYS:HE3 | 1.77 | 0.65 |
| 1:E:652:LEU:HD23 | 1:E:657:MET:HB3 | 1.79 | 0.65 |
| 2:H:155:GLU:C | 2:H:157:SER:H | 1.99 | 0.65 |
| 1:A:612:VAL:HG11 | 1:F:618:PHE:HZ | 1.60 | 0.65 |
| 1:C:711:LEU:HA | 1:C:714:ILE:HD12 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:528:THR:OG1 | 1:D:641:LEU:HD12 | 1.96 | 0.65 |
| 1:E:358:ILE:HD12 | 1:E:388:ARG:HB3 | 1.77 | 0.65 |
| 5:M:153:VAL:O | 5:M:157:ILE:HG12 | 1.97 | 0.65 |
| 1:A:624:GLN:HG3 | 1:B:610:ASP:OD2 | 1.96 | 0.65 |
| 1:B:538:SER:HB3 | 1:B:661:PHE:HD2 | 1.61 | 0.65 |
| 1:D:12:PRO:HG2 | 1:D:23:VAL:HG11 | 1.79 | 0.65 |
| 1:D:245:VAL:O | 1:D:249:GLY:N | 2.29 | 0.65 |
| 1:E:624:GLN:HA | 1:E:624:GLN:OE1 | 1.95 | 0.65 |
| 1:D:74:ILE:O | 2:J:214:PHE:HE2 | 1.79 | 0.65 |
| 1:D:573:MET:SD | 1:D:581:LYS:HD3 | 2.37 | 0.65 |
| 1:E:14:ASP:O | 1:E:18:LEU:HG | 1.96 | 0.65 |
| 1:F:64:LEU:HB3 | 1:F:65:PRO:HD3 | 1.78 | 0.65 |
| 1:F:224:ASP:O | 1:F:228:SER:HB2 | 1.97 | 0.65 |
| 1:A:671:ALA:HA | 1:A:703:VAL:O | 1.97 | 0.64 |
| 1:E:536:LEU:HD12 | 1:E:640:LEU:O | 1.97 | 0.64 |
| 1:D:64:LEU:HB3 | 1:D:65:PRO:HD3 | 1.79 | 0.64 |
| 1:F:222:GLY:HA3 | 1:F:399:ASP:OD2 | 1.97 | 0.64 |
| 2:G:149:ALA:HB2 | 2:G:164:CYS:HB2 | 1.79 | 0.64 |
| 4:L:234:GLU:O | 4:L:238:GLU:HG2 | 1.97 | 0.64 |
| 1:A:521:GLY:O | 1:A:525:VAL:HG23 | 1.97 | 0.64 |
| 1:B:64:LEU:HB3 | 1:B:65:PRO:HD3 | 1.79 | 0.64 |
| 1:C:649:LYS:HE2 | 1:C:658:LEU:HD13 | 1.78 | 0.64 |
| 2:G:158:ASN:OD1 | 2:G:162:ASN:ND2 | 2.30 | 0.64 |
| 3:K:83:LYS:HG2 | 3:K:86:ARG:HH22 | 1.62 | 0.64 |
| 1:B:326:ILE:HG22 | 1:B:370:ILE:HG13 | 1.79 | 0.64 |
| 1:B:36:ILE:HD11 | 1:B:44:LYS:HB3 | 1.79 | 0.64 |
| 1:F:695:ALA:HB1 | 1:F:699:LYS:HE3 | 1.80 | 0.64 |
| 1:F:670:ILE:HG23 | 1:F:675:GLN:HB2 | 1.79 | 0.64 |
| 4:L:223:VAL:HG21 | 5:M:46:THR:HG23 | 1.79 | 0.64 |
| 5:M:57:LEU:HA | 5:M:60:VAL:HB | 1.79 | 0.64 |
| 2:G:256:VAL:HG21 | 2:G:288:GLN:HG3 | 1.79 | 0.64 |
| 1:E:640:LEU:HD12 | 1:E:641:LEU:H | 1.63 | 0.64 |
| 1:F:713:LEU:HD22 | 1:F:732:LEU:HB3 | 1.80 | 0.64 |
| 5:M:68:ASN:HA | 5:M:188:ASN:OD1 | 1.98 | 0.64 |
| 2:J:128:ALA:HB2 | 2:J:144:HIS:HB2 | 1.80 | 0.63 |
| 1:F:105:LYS:HZ3 | 2:G:257:ASP:CB | 2.11 | 0.63 |
| 2:H:72:HIS:HE1 | 2:H:80:ASP:HB2 | 1.62 | 0.63 |
| 1:B:528:THR:O | 1:B:639:LYS:HD2 | 1.98 | 0.63 |
| 1:D:284:VAL:HG23 | 1:D:324:ILE:O | 1.97 | 0.63 |
| 1:E:604:ASP:HB3 | 1:E:607:ARG:HB3 | 1.80 | 0.63 |
| 1:D:632:LYS:NZ | 1:E:571:ASP:HB3 | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:101:ILE:HG21 | 2:H:135:LEU:HD11 | 1.80 | 0.63 |
| 2:H:128:ALA:HB2 | 2:H:144:HIS:HB2 | 1.80 | 0.63 |
| 5:M:42:ALA:HA | 5:M:45:ARG:NH2 | 2.13 | 0.63 |
| 1:A:111:PRO:HD2 | 1:A:320:SER:C | 2.18 | 0.63 |
| 1:A:256:ILE:HG13 | 1:A:370:ILE:HG22 | 1.79 | 0.63 |
| 1:A:672:THR:OG1 | 1:A:675:GLN:OE1 | 2.12 | 0.63 |
| 1:E:710:LEU:O | 1:E:714:ILE:HG13 | 1.98 | 0.63 |
| 1:F:96:THR:CG2 | 1:F:150:LYS:HB2 | 2.28 | 0.63 |
| 1:F:550:THR:HA | 1:F:645:THR:HG21 | 1.80 | 0.63 |
| 2:G:72:HIS:CE1 | 2:G:80:ASP:HB2 | 2.34 | 0.63 |
| 1:A:508:ILE:HB | 1:A:682:LEU:HD22 | 1.80 | 0.63 |
| 1:C:245:VAL:O | 1:C:249:GLY:N | 2.32 | 0.63 |
| 1:E:681:GLU:HA | 1:E:691:ARG:HE | 1.63 | 0.63 |
| 2:H:216:ILE:HD13 | 2:H:220:ASN:HB2 | 1.79 | 0.63 |
| 2:H:230:GLU:HG3 | 2:H:237:ASP:HB3 | 1.79 | 0.63 |
| 1:C:358:ILE:CB | 1:C:388:ARG:HG3 | 2.28 | 0.63 |
| 1:E:224:ASP:O | 1:E:228:SER:HB2 | 1.98 | 0.63 |
| 2:I:116:ARG:HH21 | 3:K:66:ARG:NH1 | 1.97 | 0.63 |
| 1:B:596:GLN:HA | 1:B:638:ARG:HG2 | 1.79 | 0.62 |
| 1:C:64:LEU:HA | 1:C:67:ARG:HE | 1.64 | 0.62 |
| 1:F:67:ARG:NH1 | 1:F:74:ILE:HD11 | 2.13 | 0.62 |
| 1:F:284:VAL:HG23 | 1:F:324:ILE:O | 1.99 | 0.62 |
| 5:M:170:GLU:HG3 | 5:M:174:GLN:HE21 | 1.64 | 0.62 |
| 1:D:604:ASP:HB3 | 1:D:607:ARG:CB | 2.29 | 0.62 |
| 1:E:404:LEU:O | 1:E:408:HIS:HB2 | 1.98 | 0.62 |
| 1:F:48:THR:HG21 | 1:F:128:GLN:HG2 | 1.81 | 0.62 |
| 1:A:238:ARG:HA | 1:A:252:HIS:CE1 | 2.35 | 0.62 |
| 1:C:590:ASP:HA | 1:C:593:TYR:CD2 | 2.34 | 0.62 |
| 1:D:125:PHE:HA | 1:D:128:GLN:NE2 | 2.14 | 0.62 |
| 1:E:587:LYS:HZ1 | 1:E:591:ASP:CG | 2.03 | 0.62 |
| 1:E:628:VAL:O | 1:E:632:LYS:N | 2.33 | 0.62 |
| 1:F:404:LEU:O | 1:F:408:HIS:HB2 | 1.99 | 0.62 |
| 2:J:235:PHE:CE2 | 3:K:35:THR:HA | 2.34 | 0.62 |
| 1:D:521:GLY:O | 1:D:525:VAL:HG23 | 1.98 | 0.62 |
| 1:E:586:LYS:HA | 1:E:589:PHE:CD2 | 2.34 | 0.62 |
| 1:E:674:GLU:HA | 1:E:677:LEU:HD12 | 1.81 | 0.62 |
| 1:D:319:ASN:HB3 | 1:D:320:SER:HB2 | 1.81 | 0.62 |
| 1:D:545:PRO:HD3 | 1:D:647:SER:OG | 1.99 | 0.62 |
| 2:G:159:SER:HG | 5:M:48:VAL:HG13 | 1.61 | 0.62 |
| 2:G:101:ILE:HG21 | 2:G:135:LEU:HD11 | 1.80 | 0.62 |
| 1:A:397:LEU:CB | 1:A:398:PRO:HD3 | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:235:PHE:CD1 | 5:M:152:GLN:HG2 | 2.35 | 0.62 |
| 1:B:221:GLY:HA3 | 1:B:406:ILE:HG13 | 1.80 | 0.62 |
| 1:D:348:ASP:O | 1:D:352:ASN:ND2 | 2.33 | 0.62 |
| 1:F:538:SER:O | 1:F:663:THR:HG22 | 1.99 | 0.62 |
| 1:B:307:ALA:O | 1:B:311:GLU:HG2 | 2.00 | 0.62 |
| 1:B:311:GLU:OE1 | 1:B:314:ARG:NE | 2.28 | 0.62 |
| 1:B:398:PRO:HG3 | 1:B:436:PHE:O | 2.00 | 0.62 |
| 1:C:289:GLU:O | 1:C:291:LEU:N | 2.24 | 0.62 |
| 1:E:513:PRO:O | 1:E:517:VAL:HG23 | 2.00 | 0.62 |
| 1:D:312:GLU:CG | 1:D:313:GLN:H | 2.13 | 0.62 |
| 1:D:651:VAL:O | 1:D:655:MET:HG2 | 1.99 | 0.62 |
| 1:A:423:ASP:HB2 | 1:A:480:PHE:CB | 2.30 | 0.61 |
| 1:A:610:ASP:HA | 1:F:624:GLN:NE2 | 2.15 | 0.61 |
| 1:D:554:ALA:O | 1:D:558:GLU:HG2 | 2.00 | 0.61 |
| 1:A:678:GLU:O | 1:A:682:LEU:HD12 | 1.99 | 0.61 |
| 1:C:542:GLU:HB3 | 1:C:649:LYS:HD3 | 1.83 | 0.61 |
| 1:C:624:GLN:O | 1:C:628:VAL:HG23 | 1.99 | 0.61 |
| 1:A:270:ALA:O | 1:A:273:ILE:HG22 | 2.00 | 0.61 |
| 1:A:353:GLN:HA | 1:B:288:PRO:CG | 2.30 | 0.61 |
| 1:B:540:LEU:HA | 1:B:644:GLY:O | 2.00 | 0.61 |
| 2:H:20:LYS:HE2 | 2:H:37:LYS:HA | 1.83 | 0.61 |
| 1:A:449:GLN:NE2 | 1:F:248:MET:O | 2.34 | 0.61 |
| 1:C:67:ARG:NH1 | 1:C:74:ILE:HD11 | 2.16 | 0.61 |
| 1:D:353:GLN:HE22 | 1:E:288:PRO:CG | 2.12 | 0.61 |
| 1:E:697:GLN:HG3 | 1:E:730:LEU:HD11 | 1.82 | 0.61 |
| 1:F:566:LYS:HD2 | 1:F:567:ILE:N | 2.16 | 0.61 |
| 4:L:205:LEU:O | 4:L:209:ILE:HG12 | 2.01 | 0.61 |
| 5:M:167:MET:O | 5:M:171:ILE:HG13 | 2.01 | 0.61 |
| 1:A:231:PHE:CE1 | 1:A:235:PHE:HE2 | 2.18 | 0.61 |
| 1:A:549:LYS:HE3 | 1:A:646:THR:C | 2.21 | 0.61 |
| 1:B:236:ALA:HA | 1:B:239:VAL:HG12 | 1.83 | 0.61 |
| 1:C:540:LEU:HD12 | 1:C:644:GLY:O | 2.01 | 0.61 |
| 1:F:95:MET:CE | 1:F:97:ILE:HD11 | 2.30 | 0.61 |
| 1:F:565:ILE:HG23 | 1:F:599:CYS:HB3 | 1.81 | 0.61 |
| 1:E:240:PHE:HB3 | 1:E:244:ILE:HB | 1.83 | 0.61 |
| 1:A:597:LEU:C | 1:A:597:LEU:HD23 | 2.21 | 0.61 |
| 1:D:585:MET:O | 1:D:589:PHE:HD2 | 1.84 | 0.61 |
| 2:I:69:ALA:HB1 | 2:I:85:PHE:CE1 | 2.36 | 0.61 |
| 1:A:628:VAL:HG11 | 1:B:571:ASP:HA | 1.82 | 0.61 |
| 1:B:548:GLY:O | 1:B:552:LEU:HD23 | 2.00 | 0.61 |
| 1:C:64:LEU:HB3 | 1:C:65:PRO:HD3 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:436:PHE:HB3 | 1:C:440:GLU:OE1 | 2.00 | 0.61 |
| 1:D:606:GLU:O | 1:D:610:ASP:N | 2.34 | 0.61 |
| 1:E:284:VAL:HG23 | 1:E:324:ILE:O | 2.00 | 0.61 |
| 1:A:627:LEU:HD13 | 1:B:607:ARG:HH12 | 1.66 | 0.61 |
| 1:B:295:VAL:HB | 1:C:294:TYR:CG | 2.36 | 0.61 |
| 1:B:563:PRO:HD2 | 1:B:597:LEU:HB2 | 1.83 | 0.61 |
| 1:A:382:ALA:O | 1:A:385:ARG:HG2 | 2.02 | 0.60 |
| 1:C:576:PHE:HB2 | 1:C:581:LYS:HE3 | 1.83 | 0.60 |
| 1:C:579:THR:O | 1:C:583:GLN:HG2 | 2.01 | 0.60 |
| 1:D:122:ILE:HD12 | 1:D:181:SER:HB2 | 1.83 | 0.60 |
| 1:D:312:GLU:OE1 | 1:D:323:HIS:ND1 | 2.33 | 0.60 |
| 1:D:436:PHE:HE2 | 1:D:444:LEU:HD12 | 1.66 | 0.60 |
| 1:A:184:ALA:HB1 | 1:A:200:LYS:O | 2.01 | 0.60 |
| 1:B:106:ASN:HB3 | 1:B:143:LYS:NZ | 2.16 | 0.60 |
| 1:C:695:ALA:HB1 | 1:C:699:LYS:HE3 | 1.83 | 0.60 |
| 1:F:96:THR:HG21 | 1:F:150:LYS:HB2 | 1.83 | 0.60 |
| 2:G:200:TYR:O | 2:G:203:LYS:HE2 | 2.01 | 0.60 |
| 1:C:711:LEU:O | 1:C:715:GLU:HG2 | 2.01 | 0.60 |
| 1:D:527:GLN:NE2 | 1:E:715:GLU:O | 2.32 | 0.60 |
| 2:J:57:ASN:O | 2:J:59:SER:N | 2.34 | 0.60 |
| 2:J:200:TYR:O | 2:J:203:LYS:HE2 | 2.01 | 0.60 |
| 1:A:536:LEU:HD23 | 1:A:633:ALA:HA | 1.83 | 0.60 |
| 1:B:625:ALA:O | 1:B:629:LEU:HG | 2.02 | 0.60 |
| 1:C:375:ARG:HH12 | 1:C:378:LEU:HG | 1.66 | 0.60 |
| 1:C:383:LEU:HD22 | 1:C:388:ARG:HD2 | 1.83 | 0.60 |
| 1:C:614:ILE:C | 1:C:616:PRO:HA | 2.22 | 0.60 |
| 1:D:534:THR:OG1 | 1:E:715:GLU:HG2 | 2.01 | 0.60 |
| 1:E:266:LYS:HG2 | 1:E:395:ILE:HG12 | 1.83 | 0.60 |
| 3:K:87:LYS:HD2 | 5:M:204:GLY:OXT | 2.02 | 0.60 |
| 1:B:95:MET:HG3 | 1:B:152:ILE:HG12 | 1.83 | 0.60 |
| 1:C:540:LEU:HB2 | 1:C:661:PHE:CD2 | 2.35 | 0.60 |
| 1:C:658:LEU:HD11 | 1:C:664:THR:HG21 | 1.83 | 0.60 |
| 1:D:171:LYS:NZ | 1:D:171:LYS:HB3 | 2.16 | 0.60 |
| 1:D:256:ILE:O | 1:D:370:ILE:HA | 2.02 | 0.60 |
| 1:D:263:GLY:O | 1:D:439:ALA:N | 2.34 | 0.60 |
| 1:A:617:ARG:HH11 | 1:A:617:ARG:HG3 | 1.65 | 0.60 |
| 1:A:627:LEU:O | 1:A:631:LYS:NZ | 2.35 | 0.60 |
| 1:C:386:PRO:HD2 | 1:D:440:GLU:OE1 | 2.00 | 0.60 |
| 1:D:313:GLN:O | 1:D:317:GLY:N | 2.35 | 0.60 |
| 1:F:397:LEU:HB3 | 1:F:398:PRO:CD | 2.32 | 0.60 |
| 2:H:232:PHE:HB2 | 2:H:233:PRO:HD3 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:96:ASP:OD1 | 2:I:97:PRO:HD3 | 2.02 | 0.60 |
| 5:M:174:GLN:O | 5:M:178:ILE:HG13 | 2.01 | 0.60 |
| 1:A:513:PRO:O | 1:A:517:VAL:HG23 | 2.01 | 0.60 |
| 2:I:51:MET:HA | 2:I:54:MET:HG2 | 1.83 | 0.60 |
| 1:A:540:LEU:HD11 | 1:A:646:THR:HG22 | 1.83 | 0.60 |
| 1:B:245:VAL:O | 1:B:249:GLY:N | 2.35 | 0.60 |
| 1:E:326:ILE:HG22 | 1:E:370:ILE:HG13 | 1.83 | 0.60 |
| 1:F:95:MET:HE2 | 1:F:97:ILE:HD11 | 1.84 | 0.60 |
| 1:D:404:LEU:HD11 | 1:D:427:LYS:HE3 | 1.83 | 0.60 |
| 2:I:34:GLY:O | 2:I:38:ILE:HG22 | 2.02 | 0.60 |
| 2:J:67:GLN:O | 2:J:71:LEU:HG | 2.02 | 0.60 |
| 1:B:526:GLN:NE2 | 1:C:719:GLN:HB3 | 2.17 | 0.60 |
| 1:C:624:GLN:NE2 | 1:D:610:ASP:HB2 | 2.17 | 0.60 |
| 1:E:307:ALA:O | 1:E:311:GLU:HG2 | 2.01 | 0.60 |
| 2:I:225:VAL:HG23 | 2:I:241:CYS:HB2 | 1.84 | 0.60 |
| 1:E:236:ALA:HA | 1:E:239:VAL:HG12 | 1.84 | 0.59 |
| 5:M:58:ASP:O | 5:M:62:GLU:HG3 | 2.01 | 0.59 |
| 5:M:74:ALA:O | 5:M:78:LEU:HG | 2.02 | 0.59 |
| 1:B:571:ASP:OD2 | 1:B:571:ASP:N | 2.34 | 0.59 |
| 1:D:312:GLU:HG2 | 1:D:313:GLN:H | 1.66 | 0.59 |
| 1:E:407:LEU:CD1 | 1:E:426:ILE:HG23 | 2.32 | 0.59 |
| 1:F:197:GLY:O | 1:F:200:LYS:HE2 | 2.01 | 0.59 |
| 1:B:354:LEU:O | 1:B:358:ILE:HG12 | 2.03 | 0.59 |
| 1:D:528:THR:OG1 | 1:D:537:VAL:HG21 | 2.02 | 0.59 |
| 1:D:625:ALA:O | 1:D:629:LEU:HG | 2.02 | 0.59 |
| 2:J:112:THR:HG23 | 2:J:117:PHE:HE1 | 1.66 | 0.59 |
| 4:L:218:ASP:O | 4:L:222:LEU:HG | 2.01 | 0.59 |
| 1:C:577:SER:O | 1:C:580:ALA:N | 2.33 | 0.59 |
| 1:F:612:VAL:CG1 | 1:F:617:ARG:HB2 | 2.32 | 0.59 |
| 2:H:230:GLU:HG2 | 2:H:231:LEU:N | 2.17 | 0.59 |
| 1:A:683:LEU:HB3 | 1:A:685:ASN:ND2 | 2.18 | 0.59 |
| 1:D:513:PRO:HB3 | 1:D:516:ARG:HE | 1.65 | 0.59 |
| 1:E:380:ASP:OD1 | 1:E:382:ALA:N | 2.35 | 0.59 |
| 1:F:242:PRO:HD2 | 1:F:243:GLU:H | 1.67 | 0.59 |
| 1:F:354:LEU:O | 1:F:358:ILE:HG12 | 2.02 | 0.59 |
| 3:K:88:TYR:CD2 | 5:M:81:LEU:HD11 | 2.37 | 0.59 |
| 1:E:721:ASP:O | 1:E:725:ARG:HG3 | 2.02 | 0.59 |
| 3:K:39:VAL:HG11 | 4:L:209:ILE:HD13 | 1.84 | 0.59 |
| 1:A:582:CYS:SG | 1:A:621:LEU:HG | 2.43 | 0.59 |
| 1:B:490:PRO:HA | 1:B:491:ALA:CB | 2.22 | 0.59 |
| 1:C:46:ILE:HD12 | 1:C:174:VAL:HG21 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:256:ILE:HG22 | 1:C:391:VAL:HG11 | 1.84 | 0.59 |
| 1:D:512:ASP:O | 1:D:515:THR:OG1 | 2.18 | 0.59 |
| 1:A:189:GLU:CD | 1:A:189:GLU:H | 2.06 | 0.59 |
| 1:A:560:SER:HB2 | 1:A:562:PHE:CE1 | 2.38 | 0.59 |
| 1:C:198:LYS:HD2 | 1:C:198:LYS:N | 2.17 | 0.59 |
| 1:C:377:ASP:OD2 | 1:C:377:ASP:N | 2.35 | 0.59 |
| 1:D:286:ASN:HB2 | 1:D:327:PHE:HD1 | 1.67 | 0.59 |
| 1:D:604:ASP:HB3 | 1:D:607:ARG:HB3 | 1.85 | 0.59 |
| 1:A:670:ILE:HG23 | 1:A:675:GLN:HB2 | 1.85 | 0.59 |
| 1:B:327:PHE:HB2 | 1:B:330:ILE:CG2 | 2.32 | 0.59 |
| 1:B:407:LEU:CD1 | 1:B:426:ILE:HG23 | 2.32 | 0.59 |
| 1:C:12:PRO:HG2 | 1:C:23:VAL:HG11 | 1.85 | 0.59 |
| 1:C:511:GLY:HA3 | 1:C:513:PRO:HD2 | 1.85 | 0.59 |
| 1:D:67:ARG:CD | 2:J:218:MET:HE2 | 2.33 | 0.59 |
| 1:C:256:ILE:HA | 1:C:391:VAL:HG13 | 1.84 | 0.59 |
| 1:D:299:GLU:OE1 | 1:D:350:VAL:HG13 | 2.03 | 0.59 |
| 1:D:513:PRO:O | 1:D:516:ARG:HG2 | 2.03 | 0.59 |
| 1:A:111:PRO:HD2 | 1:A:321:GLY:N | 2.18 | 0.58 |
| 1:A:562:PHE:CD2 | 1:A:597:LEU:CD2 | 2.85 | 0.58 |
| 1:C:311:GLU:HA | 1:C:314:ARG:HG2 | 1.85 | 0.58 |
| 1:E:532:ASP:OD2 | 1:E:533:ARG:N | 2.35 | 0.58 |
| 1:E:573:MET:SD | 1:E:581:LYS:HG2 | 2.43 | 0.58 |
| 1:F:380:ASP:OD1 | 1:F:382:ALA:N | 2.34 | 0.58 |
| 1:A:67:ARG:NH1 | 1:A:74:ILE:HD11 | 2.18 | 0.58 |
| 1:A:726:VAL:O | 1:A:730:LEU:HG | 2.04 | 0.58 |
| 1:B:128:GLN:O | 1:B:176:LEU:HD12 | 2.04 | 0.58 |
| 1:B:437:SER:O | 1:B:440:GLU:HB2 | 2.03 | 0.58 |
| 1:B:545:PRO:O | 1:B:546:HIS:HB2 | 2.03 | 0.58 |
| 1:A:687:LYS:HB2 | 1:A:690:GLU:HG3 | 1.85 | 0.58 |
| 1:B:296:GLY:H | 1:B:297:GLU:CB | 2.17 | 0.58 |
| 1:E:581:LYS:NZ | 1:E:610:ASP:OD1 | 2.35 | 0.58 |
| 1:E:648:ARG:NE | 1:E:650:ASP:OD1 | 2.31 | 0.58 |
| 2:J:225:VAL:HG23 | 2:J:241:CYS:HB2 | 1.84 | 0.58 |
| 2:G:142:ILE:HG23 | 2:G:168:VAL:HG13 | 1.84 | 0.58 |
| 1:A:598:SER:OG | 1:A:640:LEU:HD12 | 2.02 | 0.58 |
| 1:C:533:ARG:HB2 | 1:D:715:GLU:OE1 | 2.03 | 0.58 |
| 1:D:267:THR:HA | 1:D:372:MET:SD | 2.44 | 0.58 |
| 1:D:383:LEU:O | 1:D:389:LEU:HB2 | 2.03 | 0.58 |
| 1:F:383:LEU:O | 1:F:389:LEU:HB2 | 2.03 | 0.58 |
| 1:F:604:ASP:HB3 | 1:F:607:ARG:HB2 | 1.85 | 0.58 |
| 5:M:176:ARG:HA | 5:M:179:ASP:OD2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:284:VAL:HG23 | 1:B:324:ILE:O | 2.03 | 0.58 |
| 1:D:73:SER:O | 1:D:76:GLN:HG2 | 2.03 | 0.58 |
| 1:D:114:THR:OG1 | 1:D:199:ALA:HB3 | 2.03 | 0.58 |
| 1:B:578:GLU:HG3 | 1:B:619:SER:HB2 | 1.86 | 0.58 |
| 1:B:605:ILE:HD11 | 1:B:644:GLY:HA3 | 1.84 | 0.58 |
| 1:E:296:GLY:H | 1:E:297:GLU:CB | 2.16 | 0.58 |
| 1:E:686:PHE:CE1 | 1:E:714:ILE:HG23 | 2.34 | 0.58 |
| 1:F:326:ILE:HG22 | 1:F:370:ILE:HG13 | 1.85 | 0.58 |
| 1:F:650:ASP:O | 1:F:653:GLN:HG3 | 2.03 | 0.58 |
| 1:A:315:ARG:O | 1:A:316:LEU:HD12 | 2.03 | 0.58 |
| 1:A:539:VAL:HG13 | 1:A:643:ILE:HA | 1.84 | 0.58 |
| 1:B:380:ASP:OD1 | 1:B:382:ALA:N | 2.36 | 0.58 |
| 1:A:694:ILE:O | 1:A:698:VAL:HG13 | 2.04 | 0.58 |
| 1:C:240:PHE:CD2 | 1:C:244:ILE:HG21 | 2.29 | 0.58 |
| 1:D:618:PHE:CE2 | 1:E:614:ILE:HD12 | 2.39 | 0.58 |
| 1:E:713:LEU:HD22 | 1:E:732:LEU:HD13 | 1.85 | 0.58 |
| 1:E:289:GLU:C | 1:E:291:LEU:H | 2.07 | 0.57 |
| 2:G:69:ALA:HB1 | 2:G:85:PHE:CE1 | 2.39 | 0.57 |
| 1:A:242:PRO:HD2 | 1:A:243:GLU:H | 1.69 | 0.57 |
| 1:B:397:LEU:CD2 | 1:B:398:PRO:HD2 | 2.34 | 0.57 |
| 1:C:254:LYS:O | 1:C:368:LEU:HA | 2.04 | 0.57 |
| 1:C:404:LEU:O | 1:C:408:HIS:HB2 | 2.03 | 0.57 |
| 1:C:728:LYS:O | 1:C:732:LEU:HG | 2.03 | 0.57 |
| 1:F:521:GLY:O | 1:F:525:VAL:HG23 | 2.04 | 0.57 |
| 2:I:38:ILE:CD1 | 2:I:71:LEU:HB3 | 2.33 | 0.57 |
| 2:J:21:VAL:HG23 | 2:J:38:ILE:HD12 | 1.86 | 0.57 |
| 1:C:490:PRO:HA | 1:C:491:ALA:CB | 2.28 | 0.57 |
| 1:F:554:ALA:O | 1:F:558:GLU:HG3 | 2.05 | 0.57 |
| 5:M:36:VAL:HG23 | 5:M:156:ILE:HG21 | 1.85 | 0.57 |
| 1:A:257:LEU:HG | 1:A:389:LEU:HD12 | 1.86 | 0.57 |
| 1:B:589:PHE:HE2 | 1:B:629:LEU:HB3 | 1.68 | 0.57 |
| 1:D:284:VAL:HB | 1:D:325:ILE:HA | 1.86 | 0.57 |
| 1:E:399:ASP:HB2 | 1:E:402:GLY:H | 1.69 | 0.57 |
| 1:F:407:LEU:CD1 | 1:F:426:ILE:HG23 | 2.34 | 0.57 |
| 1:B:385:ARG:NH1 | 1:C:263:GLY:HA2 | 2.19 | 0.57 |
| 1:F:522:GLU:OE2 | 1:F:526:GLN:HG2 | 2.05 | 0.57 |
| 3:K:70:LEU:HD13 | 5:M:189:LYS:HB2 | 1.86 | 0.57 |
| 4:L:198:ARG:O | 4:L:202:ILE:HG13 | 2.03 | 0.57 |
| 1:B:670:ILE:HG23 | 1:B:675:GLN:HB2 | 1.86 | 0.57 |
| 1:B:695:ALA:HB1 | 1:B:699:LYS:HE3 | 1.87 | 0.57 |
| 1:C:334:CYS:HA | 1:C:351:VAL:HG22 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:437:SER:O | 1:E:440:GLU:HB2 | 2.05 | 0.57 |
| 2:G:160:SER:OG | 5:M:52:GLU:OE2 | 2.19 | 0.57 |
| 1:A:247:GLN:O | 1:B:413:ARG:NH1 | 2.37 | 0.57 |
| 1:A:313:GLN:NE2 | 1:A:365:ASN:O | 2.36 | 0.57 |
| 1:A:607:ARG:HD3 | 1:F:624:GLN:HE22 | 1.69 | 0.57 |
| 1:B:424:VAL:N | 1:B:479:ASP:N | 2.52 | 0.57 |
| 1:C:606:GLU:HG2 | 1:C:607:ARG:N | 2.18 | 0.57 |
| 1:D:680:LEU:HB2 | 1:D:691:ARG:HH21 | 1.68 | 0.57 |
| 2:I:128:ALA:HB2 | 2:I:144:HIS:HB2 | 1.87 | 0.57 |
| 5:M:200:THR:O | 5:M:203:LEU:HB2 | 2.05 | 0.57 |
| 1:A:322:LEU:HA | 1:A:366:ASN:O | 2.04 | 0.57 |
| 1:E:502:TYR:CZ | 1:E:567:ILE:HG21 | 2.40 | 0.57 |
| 1:A:306:PHE:CD1 | 1:A:357:LYS:HB3 | 2.40 | 0.57 |
| 1:A:307:ALA:O | 1:A:310:GLU:HG3 | 2.05 | 0.57 |
| 1:B:404:LEU:O | 1:B:408:HIS:HB2 | 2.05 | 0.57 |
| 1:D:510:TRP:CE3 | 1:D:675:GLN:HG2 | 2.34 | 0.57 |
| 1:E:289:GLU:O | 1:E:291:LEU:N | 2.25 | 0.57 |
| 5:M:68:ASN:O | 5:M:72:LYS:HG3 | 2.04 | 0.57 |
| 1:C:240:PHE:HZ | 1:D:456:HIS:HB3 | 1.69 | 0.56 |
| 1:C:490:PRO:HB2 | 1:C:492:PHE:N | 2.20 | 0.56 |
| 1:E:672:THR:OG1 | 1:E:675:GLN:HB2 | 2.04 | 0.56 |
| 2:I:75:LEU:O | 2:I:76:GLN:HG2 | 2.04 | 0.56 |
| 1:B:267:THR:HA | 1:B:372:MET:SD | 2.46 | 0.56 |
| 1:C:407:LEU:CD1 | 1:C:426:ILE:HG23 | 2.32 | 0.56 |
| 1:D:312:GLU:CG | 1:D:313:GLN:N | 2.67 | 0.56 |
| 1:D:510:TRP:HB3 | 1:D:679:ALA:HB2 | 1.87 | 0.56 |
| 1:D:686:PHE:CE1 | 1:D:714:ILE:HG23 | 2.40 | 0.56 |
| 1:A:352:ASN:HA | 1:A:355:LEU:HD12 | 1.87 | 0.56 |
| 1:A:449:GLN:O | 1:A:453:MET:HG2 | 2.05 | 0.56 |
| 1:B:353:GLN:HA | 1:C:288:PRO:HG3 | 1.88 | 0.56 |
| 1:C:411:THR:O | 1:C:414:MET:HB2 | 2.06 | 0.56 |
| 1:C:540:LEU:HD23 | 1:C:649:LYS:HE3 | 1.88 | 0.56 |
| 1:D:592:ALA:HB1 | 1:D:640:LEU:HD13 | 1.86 | 0.56 |
| 1:E:240:PHE:HZ | 1:F:456:HIS:HB2 | 1.69 | 0.56 |
| 1:F:562:PHE:HE2 | 1:F:597:LEU:HD12 | 1.69 | 0.56 |
| 2:H:117:PHE:CD2 | 2:G:53:LYS:HE3 | 2.40 | 0.56 |
| 3:K:39:VAL:O | 3:K:43:VAL:HG23 | 2.05 | 0.56 |
| 1:A:267:THR:OG1 | 1:A:328:ASP:OD2 | 2.23 | 0.56 |
| 1:B:533:ARG:HG3 | 1:B:534:THR:HG23 | 1.87 | 0.56 |
| 1:C:694:ILE:O | 1:C:698:VAL:HG22 | 2.06 | 0.56 |
| 1:E:502:TYR:OH | 1:E:569:SER:OG | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:38:ILE:HD11 | 2:H:71:LEU:HB3 | 1.88 | 0.56 |
| 5:M:55:GLU:HA | 5:M:58:ASP:OD2 | 2.06 | 0.56 |
| 1:B:361:VAL:O | 1:C:271:ARG:HD2 | 2.05 | 0.56 |
| 1:B:552:LEU:O | 1:B:556:ILE:HG13 | 2.06 | 0.56 |
| 1:D:648:ARG:HG3 | 1:D:651:VAL:HG23 | 1.87 | 0.56 |
| 1:F:196:ILE:CA | 1:F:200:LYS:HD3 | 2.35 | 0.56 |
| 1:B:73:SER:O | 1:B:76:GLN:HG2 | 2.05 | 0.56 |
| 1:C:95:MET:HG3 | 1:C:152:ILE:HG12 | 1.86 | 0.56 |
| 1:E:684:GLY:HA2 | 1:E:691:ARG:HH21 | 1.70 | 0.56 |
| 1:A:408:HIS:HA | 1:A:426:ILE:HD12 | 1.88 | 0.56 |
| 1:B:383:LEU:O | 1:B:389:LEU:HB2 | 2.06 | 0.56 |
| 1:B:404:LEU:HG | 1:B:426:ILE:HG22 | 1.88 | 0.56 |
| 1:C:524:LEU:HD21 | 1:C:537:VAL:HG12 | 1.87 | 0.56 |
| 1:F:296:GLY:H | 1:F:297:GLU:CB | 2.19 | 0.56 |
| 1:F:327:PHE:HB2 | 1:F:330:ILE:CG2 | 2.35 | 0.56 |
| 1:A:223:LEU:HD12 | 1:A:227:PHE:HB2 | 1.88 | 0.56 |
| 1:B:114:THR:OG1 | 1:B:199:ALA:HB3 | 2.06 | 0.56 |
| 1:B:289:GLU:O | 1:B:291:LEU:N | 2.29 | 0.56 |
| 1:C:690:GLU:CB | 1:C:726:VAL:HG21 | 2.36 | 0.56 |
| 3:K:80:SER:O | 3:K:84:LEU:HG | 2.06 | 0.56 |
| 1:B:559:GLU:O | 1:B:561:ASN:ND2 | 2.38 | 0.56 |
| 1:C:555:LYS:HA | 1:C:558:GLU:OE1 | 2.05 | 0.56 |
| 1:D:242:PRO:HD2 | 1:D:243:GLU:H | 1.69 | 0.56 |
| 1:A:111:PRO:O | 1:A:319:ASN:ND2 | 2.39 | 0.55 |
| 1:C:542:GLU:HB2 | 1:C:649:LYS:HD3 | 1.88 | 0.55 |
| 1:D:303:ARG:HD3 | 1:D:353:GLN:CG | 2.36 | 0.55 |
| 1:D:527:GLN:HE22 | 1:E:716:MET:HA | 1.71 | 0.55 |
| 1:F:96:THR:HB | 1:F:151:ASP:N | 2.19 | 0.55 |
| 2:G:128:ALA:HB2 | 2:G:144:HIS:HB2 | 1.87 | 0.55 |
| 1:A:676:LEU:CD1 | 1:A:710:LEU:HD11 | 2.36 | 0.55 |
| 1:C:527:GLN:HB2 | 1:D:719:GLN:HG3 | 1.88 | 0.55 |
| 1:D:731:ALA:HA | 1:D:734:ARG:NH1 | 2.21 | 0.55 |
| 1:E:573:MET:O | 1:E:576:PHE:HB2 | 2.07 | 0.55 |
| 1:B:549:LYS:HZ3 | 1:B:647:SER:HA | 1.72 | 0.55 |
| 1:E:354:LEU:O | 1:E:358:ILE:HG12 | 2.06 | 0.55 |
| 1:F:437:SER:O | 1:F:440:GLU:HB2 | 2.05 | 0.55 |
| 2:I:116:ARG:HH11 | 2:I:116:ARG:HG3 | 1.71 | 0.55 |
| 2:I:127:ILE:HG23 | 2:I:131:TYR:CE1 | 2.41 | 0.55 |
| 2:G:232:PHE:H | 2:G:233:PRO:HD2 | 1.71 | 0.55 |
| 3:K:77:PHE:HE1 | 5:M:78:LEU:HD11 | 1.70 | 0.55 |
| 5:M:180:ARG:O | 5:M:184:LYS:HD3 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:678:GLU:O | 1:A:681:GLU:HG2 | 2.05 | 0.55 |
| 1:C:40:SER:OG | 1:C:41:PRO:HD2 | 2.07 | 0.55 |
| 1:D:593:TYR:O | 1:D:638:ARG:HG2 | 2.07 | 0.55 |
| 1:F:67:ARG:HH12 | 1:F:74:ILE:HD11 | 1.71 | 0.55 |
| 2:H:233:PRO:HG2 | 2:G:268:SER:HA | 1.87 | 0.55 |
| 5:M:177:GLN:HA | 5:M:180:ARG:NH1 | 2.21 | 0.55 |
| 1:A:121:PHE:CD2 | 1:A:183:VAL:HG21 | 2.40 | 0.55 |
| 1:B:503:ILE:HG12 | 1:B:551:ALA:HA | 1.88 | 0.55 |
| 1:B:576:PHE:HB2 | 1:B:581:LYS:HG3 | 1.89 | 0.55 |
| 1:D:527:GLN:NE2 | 1:E:716:MET:HA | 2.21 | 0.55 |
| 1:E:242:PRO:HD2 | 1:E:243:GLU:H | 1.71 | 0.55 |
| 1:F:18:LEU:HA | 1:F:137:VAL:HG23 | 1.89 | 0.55 |
| 1:F:196:ILE:HA | 1:F:200:LYS:HD3 | 1.89 | 0.55 |
| 1:F:503:ILE:HG22 | 1:F:506:GLY:H | 1.71 | 0.55 |
| 1:F:529:LYS:HG3 | 1:F:597:LEU:HD11 | 1.89 | 0.55 |
| 2:H:40:GLU:O | 2:H:44:ILE:HG12 | 2.07 | 0.55 |
| 1:A:411:THR:OG1 | 1:A:426:ILE:HD11 | 2.07 | 0.55 |
| 1:A:688:ASP:OD1 | 1:A:689:LYS:N | 2.39 | 0.55 |
| 1:A:690:GLU:O | 1:A:694:ILE:HG13 | 2.05 | 0.55 |
| 1:A:709:LYS:HE2 | 1:A:709:LYS:HA | 1.88 | 0.55 |
| 1:D:67:ARG:HB3 | 2:J:218:MET:CG | 2.37 | 0.55 |
| 1:D:315:ARG:C | 1:D:316:LEU:HD12 | 2.27 | 0.55 |
| 1:E:652:LEU:HD22 | 1:E:658:LEU:HD13 | 1.89 | 0.55 |
| 1:F:715:GLU:O | 1:F:719:GLN:HG2 | 2.07 | 0.55 |
| 2:I:149:ALA:HB2 | 2:I:164:CYS:HB2 | 1.89 | 0.55 |
| 5:M:56:GLN:O | 5:M:60:VAL:HG23 | 2.06 | 0.55 |
| 1:A:223:LEU:CD1 | 1:A:227:PHE:HB2 | 2.36 | 0.55 |
| 1:A:242:PRO:HD2 | 1:A:243:GLU:CD | 2.27 | 0.55 |
| 1:A:531:SER:O | 1:A:639:LYS:HE2 | 2.05 | 0.55 |
| 1:B:414:MET:HE2 | 1:B:414:MET:HA | 1.89 | 0.55 |
| 1:D:547:SER:OG | 1:D:549:LYS:HG3 | 2.06 | 0.55 |
| 1:F:632:LYS:HD2 | 1:F:633:ALA:H | 1.71 | 0.55 |
| 2:J:39:GLU:HB2 | 2:J:75:LEU:HD13 | 1.89 | 0.55 |
| 1:C:533:ARG:HD2 | 1:D:505:ASN:OD1 | 2.06 | 0.55 |
| 1:D:686:PHE:HB2 | 1:D:691:ARG:HG2 | 1.89 | 0.55 |
| 1:E:671:ALA:HA | 1:E:703:VAL:O | 2.07 | 0.55 |
| 1:F:542:GLU:O | 1:F:666:HIS:ND1 | 2.39 | 0.55 |
| 2:H:39:GLU:HB2 | 2:H:75:LEU:HD11 | 1.88 | 0.55 |
| 2:H:124:HIS:HE1 | 2:H:147:GLN:HB3 | 1.71 | 0.55 |
| 2:I:179:GLN:O | 2:I:182:ILE:HG12 | 2.07 | 0.55 |
| 2:G:80:ASP:O | 2:G:83:THR:OG1 | 2.24 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:206:GLU:HG3 | 5:M:28:SER:OG | 2.06 | 0.55 |
| 1:A:542:GLU:OE2 | 1:A:666:HIS:NE2 | 2.40 | 0.55 |
| 1:B:242:PRO:HD2 | 1:B:243:GLU:H | 1.71 | 0.55 |
| 1:B:589:PHE:CE2 | 1:B:629:LEU:HB3 | 2.41 | 0.55 |
| 1:E:383:LEU:O | 1:E:389:LEU:HB2 | 2.07 | 0.55 |
| 1:F:613:PRO:HD3 | 1:F:648:ARG:HH12 | 1.72 | 0.55 |
| 2:I:39:GLU:HB2 | 2:I:75:LEU:HD11 | 1.89 | 0.55 |
| 2:I:108:ILE:HD12 | 2:I:127:ILE:HD12 | 1.89 | 0.55 |
| 2:J:35:SER:HB3 | 2:J:75:LEU:HD12 | 1.88 | 0.55 |
| 3:K:46:MET:O | 3:K:50:VAL:HG23 | 2.07 | 0.55 |
| 4:L:200:SER:O | 4:L:204:LYS:HG3 | 2.07 | 0.55 |
| 1:B:289:GLU:C | 1:B:291:LEU:H | 2.09 | 0.55 |
| 1:D:10:ARG:HA | 1:D:67:ARG:NH1 | 2.22 | 0.55 |
| 1:E:516:ARG:O | 1:E:519:ASP:OD1 | 2.24 | 0.55 |
| 1:E:527:GLN:HG3 | 1:F:719:GLN:HG3 | 1.87 | 0.55 |
| 1:F:410:HIS:O | 1:F:414:MET:HG2 | 2.06 | 0.55 |
| 1:A:571:ASP:HA | 1:A:574:ILE:HG23 | 1.89 | 0.54 |
| 1:A:677:LEU:HG | 1:A:695:ALA:HB2 | 1.88 | 0.54 |
| 1:B:310:GLU:OE2 | 1:B:357:LYS:NZ | 2.40 | 0.54 |
| 1:C:536:LEU:HD12 | 1:C:640:LEU:HB3 | 1.89 | 0.54 |
| 1:D:67:ARG:HB3 | 2:J:218:MET:HG2 | 1.88 | 0.54 |
| 1:D:632:LYS:HZ1 | 1:E:571:ASP:HB3 | 1.73 | 0.54 |
| 1:E:673:GLY:HA3 | 1:E:698:VAL:HB | 1.89 | 0.54 |
| 1:A:383:LEU:O | 1:A:389:LEU:HB2 | 2.07 | 0.54 |
| 1:C:577:SER:O | 1:C:579:THR:N | 2.40 | 0.54 |
| 1:C:688:ASP:O | 1:C:692:THR:HG23 | 2.07 | 0.54 |
| 1:F:635:PRO:HD2 | 1:F:638:ARG:HD2 | 1.89 | 0.54 |
| 2:H:195:SER:C | 2:H:197:LEU:H | 2.10 | 0.54 |
| 1:A:300:ALA:O | 1:A:304:LYS:HG3 | 2.08 | 0.54 |
| 1:A:503:ILE:CG2 | 1:A:506:GLY:HA2 | 2.37 | 0.54 |
| 1:A:563:PRO:HG2 | 1:A:597:LEU:O | 2.07 | 0.54 |
| 1:D:663:THR:HG22 | 1:D:664:THR:N | 2.21 | 0.54 |
| 1:E:689:LYS:O | 1:E:692:THR:OG1 | 2.25 | 0.54 |
| 2:G:230:GLU:HG2 | 2:G:231:LEU:N | 2.23 | 0.54 |
| 1:A:625:ALA:O | 1:A:629:LEU:HG | 2.07 | 0.54 |
| 1:C:653:GLN:HG3 | 1:C:658:LEU:HD23 | 1.89 | 0.54 |
| 1:E:552:LEU:HD11 | 1:E:667:VAL:HG11 | 1.88 | 0.54 |
| 4:L:248:VAL:O | 4:L:252:LYS:HG3 | 2.07 | 0.54 |
| 1:C:227:PHE:O | 1:C:231:PHE:HB2 | 2.08 | 0.54 |
| 1:E:604:ASP:O | 1:E:608:LEU:N | 2.38 | 0.54 |
| 1:F:602:VAL:N | 1:F:643:ILE:O | 2.26 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:57:ASN:O | 2:G:59:SER:N | 2.41 | 0.54 |
| 2:G:67:GLN:O | 2:G:71:LEU:HG | 2.08 | 0.54 |
| 1:A:293:LYS:O | 1:A:294:TYR:CG | 2.61 | 0.54 |
| 1:C:18:LEU:HA | 1:C:137:VAL:HG23 | 1.90 | 0.54 |
| 1:C:307:ALA:O | 1:C:310:GLU:HG2 | 2.07 | 0.54 |
| 1:D:380:ASP:OD1 | 1:D:382:ALA:N | 2.37 | 0.54 |
| 1:E:95:MET:HG3 | 1:E:152:ILE:HG12 | 1.90 | 0.54 |
| 1:B:270:ALA:O | 1:B:273:ILE:HG22 | 2.08 | 0.54 |
| 1:C:64:LEU:O | 1:C:68:LYS:HG3 | 2.07 | 0.54 |
| 1:C:106:ASN:HB3 | 1:C:143:LYS:HZ2 | 1.72 | 0.54 |
| 1:D:687:LYS:O | 1:D:691:ARG:HG3 | 2.07 | 0.54 |
| 1:E:670:ILE:H | 1:E:670:ILE:HD12 | 1.73 | 0.54 |
| 2:H:239:ARG:NH2 | 4:L:217:MET:HG3 | 2.23 | 0.54 |
| 2:H:256:VAL:HG11 | 2:H:288:GLN:HG2 | 1.90 | 0.54 |
| 5:M:17:ARG:CZ | 5:M:21:LEU:HD21 | 2.38 | 0.54 |
| 1:A:111:PRO:HD2 | 1:A:320:SER:HA | 1.89 | 0.54 |
| 1:E:104:LYS:HA | 1:E:107:ILE:HD11 | 1.90 | 0.54 |
| 1:E:240:PHE:HZ | 1:F:456:HIS:CB | 2.21 | 0.54 |
| 1:E:550:THR:HA | 1:E:645:THR:HG21 | 1.89 | 0.54 |
| 1:F:105:LYS:CE | 2:G:257:ASP:HB2 | 2.37 | 0.54 |
| 1:F:270:ALA:O | 1:F:273:ILE:HG22 | 2.08 | 0.54 |
| 1:F:544:PRO:HD2 | 1:F:547:SER:OG | 2.08 | 0.54 |
| 5:M:59:ARG:HA | 5:M:62:GLU:OE1 | 2.08 | 0.54 |
| 1:E:284:VAL:O | 1:E:326:ILE:HG12 | 2.06 | 0.54 |
| 1:F:542:GLU:HB2 | 1:F:666:HIS:HA | 1.90 | 0.54 |
| 1:F:555:LYS:HE2 | 1:F:555:LYS:HA | 1.90 | 0.54 |
| 4:L:198:ARG:HG2 | 4:L:202:ILE:HD11 | 1.89 | 0.54 |
| 1:B:570:PRO:HG3 | 1:B:608:LEU:HD23 | 1.89 | 0.54 |
| 1:B:728:LYS:HE3 | 1:B:732:LEU:HD21 | 1.89 | 0.54 |
| 1:D:98:GLU:HB3 | 1:D:148:LEU:HB3 | 1.90 | 0.54 |
| 1:E:508:ILE:HB | 1:E:682:LEU:HD13 | 1.90 | 0.54 |
| 1:F:525:VAL:HG13 | 1:F:562:PHE:HE1 | 1.72 | 0.54 |
| 1:A:424:VAL:HG22 | 1:A:479:ASP:O | 2.08 | 0.53 |
| 1:C:589:PHE:CD2 | 1:C:629:LEU:HD13 | 2.43 | 0.53 |
| 1:D:257:LEU:HG | 1:D:371:GLY:O | 2.07 | 0.53 |
| 1:D:681:GLU:HG2 | 1:D:691:ARG:NH1 | 2.23 | 0.53 |
| 1:A:12:PRO:HG2 | 1:A:23:VAL:HG11 | 1.90 | 0.53 |
| 1:F:606:GLU:OE2 | 1:F:647:SER:HB2 | 2.07 | 0.53 |
| 1:F:710:LEU:O | 1:F:714:ILE:HG13 | 2.08 | 0.53 |
| 3:K:51:ASP:O | 3:K:55:GLU:HG3 | 2.07 | 0.53 |
| 1:B:261:PRO:HB3 | 1:B:594:LYS:NZ | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:397:LEU:HD11 | 1:B:595:SER:HA | 1.89 | 0.53 |
| 1:C:18:LEU:HD13 | 1:C:139:SER:HB2 | 1.90 | 0.53 |
| 1:C:40:SER:HB3 | 1:C:43:HIS:HB2 | 1.88 | 0.53 |
| 1:C:308:ASP:OD1 | 1:C:309:ALA:N | 2.41 | 0.53 |
| 1:C:728:LYS:HE3 | 1:C:732:LEU:HD21 | 1.91 | 0.53 |
| 1:D:657:MET:HG2 | 1:D:661:PHE:CE2 | 2.44 | 0.53 |
| 1:E:310:GLU:OE2 | 1:E:357:LYS:NZ | 2.41 | 0.53 |
| 2:H:95:ALA:HB1 | 2:H:97:PRO:HD2 | 1.90 | 0.53 |
| 2:I:120:ALA:O | 2:I:124:HIS:HB2 | 2.08 | 0.53 |
| 3:K:56:ARG:NH1 | 3:K:56:ARG:HB3 | 2.23 | 0.53 |
| 1:B:626:LEU:O | 1:B:630:LEU:HG | 2.09 | 0.53 |
| 1:C:285:VAL:HG13 | 1:C:326:ILE:HD11 | 1.89 | 0.53 |
| 1:D:64:LEU:N | 1:D:67:ARG:HH21 | 2.06 | 0.53 |
| 1:D:95:MET:HG3 | 1:D:152:ILE:HG12 | 1.91 | 0.53 |
| 1:D:677:LEU:O | 1:D:691:ARG:NH2 | 2.41 | 0.53 |
| 1:E:399:ASP:O | 1:E:403:ARG:N | 2.34 | 0.53 |
| 1:F:245:VAL:O | 1:F:249:GLY:N | 2.37 | 0.53 |
| 2:J:188:VAL:HG13 | 2:J:205:TYR:HD2 | 1.73 | 0.53 |
| 2:G:266:TYR:C | 2:G:268:SER:H | 2.10 | 0.53 |
| 4:L:230:ILE:HD12 | 5:M:53:GLN:OE1 | 2.08 | 0.53 |
| 1:A:406:ILE:O | 1:A:409:ILE:HG22 | 2.09 | 0.53 |
| 1:B:284:VAL:O | 1:B:326:ILE:HG12 | 2.09 | 0.53 |
| 1:D:23:VAL:HG12 | 1:D:55:VAL:HG21 | 1.90 | 0.53 |
| 1:D:524:LEU:O | 1:D:527:GLN:HB3 | 2.08 | 0.53 |
| 1:D:686:PHE:HE1 | 1:D:714:ILE:HG23 | 1.74 | 0.53 |
| 2:I:116:ARG:HH21 | 3:K:66:ARG:HH12 | 1.57 | 0.53 |
| 1:B:546:HIS:O | 1:B:549:LYS:HE3 | 2.08 | 0.53 |
| 1:D:36:ILE:HD11 | 1:D:44:LYS:HB3 | 1.91 | 0.53 |
| 1:E:684:GLY:HA2 | 1:E:691:ARG:NH2 | 2.24 | 0.53 |
| 1:F:559:GLU:HA | 1:F:559:GLU:OE1 | 2.08 | 0.53 |
| 5:M:171:ILE:HG22 | 5:M:175:ASN:HD21 | 1.73 | 0.53 |
| 1:A:724:TYR:HD1 | 1:A:727:ARG:HH12 | 1.56 | 0.53 |
| 1:C:584:ALA:O | 1:C:588:ILE:HG13 | 2.09 | 0.53 |
| 1:C:613:PRO:HD3 | 1:C:648:ARG:NH2 | 2.24 | 0.53 |
| 1:D:539:VAL:HG13 | 1:D:643:ILE:HG13 | 1.91 | 0.53 |
| 1:E:595:SER:HB3 | 1:E:598:SER:HB3 | 1.90 | 0.53 |
| 1:E:666:HIS:CD2 | 1:E:668:PRO:HD3 | 2.44 | 0.53 |
| 1:F:562:PHE:CD1 | 1:F:599:CYS:HB2 | 2.44 | 0.53 |
| 2:H:203:LYS:NZ | 2:H:239:ARG:HH21 | 2.05 | 0.53 |
| 3:K:33:GLN:HG2 | 4:L:201:GLU:HG3 | 1.89 | 0.53 |
| 3:K:42:VAL:HG21 | 5:M:157:ILE:HD12 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:121:PHE:HD2 | 1:A:183:VAL:HG21 | 1.73 | 0.53 |
| 1:F:236:ALA:HA | 1:F:239:VAL:HG12 | 1.91 | 0.53 |
| 1:F:263:GLY:HA3 | 1:F:437:SER:HA | 1.89 | 0.53 |
| 1:F:617:ARG:HH11 | 1:F:617:ARG:HG3 | 1.73 | 0.53 |
| 2:H:72:HIS:CE1 | 2:H:80:ASP:HB2 | 2.44 | 0.53 |
| 2:H:239:ARG:HH22 | 4:L:217:MET:HG3 | 1.73 | 0.53 |
| 3:K:67:ALA:O | 3:K:70:LEU:HB3 | 2.09 | 0.53 |
| 1:A:64:LEU:HA | 1:A:67:ARG:HE | 1.74 | 0.53 |
| 1:A:113:ASP:O | 1:A:117:MET:HG3 | 2.09 | 0.53 |
| 1:A:315:ARG:C | 1:A:316:LEU:HD12 | 2.29 | 0.53 |
| 1:A:544:PRO:HB2 | 1:A:669:ASN:ND2 | 2.24 | 0.53 |
| 1:C:122:ILE:O | 1:C:126:ASN:HB3 | 2.08 | 0.53 |
| 2:J:266:TYR:C | 2:J:268:SER:H | 2.11 | 0.53 |
| 2:G:38:ILE:HD11 | 2:G:71:LEU:HB3 | 1.91 | 0.53 |
| 1:A:136:LEU:N | 1:A:136:LEU:HD23 | 2.24 | 0.53 |
| 1:C:135:GLN:HG2 | 1:C:148:LEU:HD13 | 1.91 | 0.53 |
| 1:D:599:CYS:SG | 1:D:641:LEU:HD22 | 2.49 | 0.53 |
| 1:E:267:THR:HA | 1:E:372:MET:SD | 2.48 | 0.53 |
| 1:F:720:MET:HB3 | 1:F:724:TYR:HB2 | 1.91 | 0.53 |
| 2:H:57:ASN:O | 2:H:59:SER:N | 2.42 | 0.53 |
| 2:J:219:LEU:CB | 2:J:222:LYS:HB3 | 2.36 | 0.53 |
| 1:A:64:LEU:HA | 1:A:67:ARG:HH21 | 1.75 | 0.52 |
| 1:A:286:ASN:HB2 | 1:A:327:PHE:CB | 2.39 | 0.52 |
| 1:D:74:ILE:HG13 | 2:J:218:MET:HE3 | 1.91 | 0.52 |
| 1:E:506:GLY:O | 1:E:508:ILE:N | 2.40 | 0.52 |
| 1:A:536:LEU:HD23 | 1:A:634:PRO:HD3 | 1.91 | 0.52 |
| 1:A:719:GLN:HG2 | 1:F:523:LEU:HG | 1.91 | 0.52 |
| 1:C:388:ARG:NH1 | 1:C:388:ARG:HB2 | 2.24 | 0.52 |
| 1:D:113:ASP:O | 1:D:117:MET:HG3 | 2.09 | 0.52 |
| 1:D:265:GLY:O | 1:D:268:LEU:HG | 2.09 | 0.52 |
| 1:E:122:ILE:O | 1:E:126:ASN:HB3 | 2.09 | 0.52 |
| 2:I:119:ILE:O | 2:I:122:LYS:HB2 | 2.09 | 0.52 |
| 1:F:512:ASP:OD1 | 1:F:513:PRO:HD3 | 2.09 | 0.52 |
| 2:H:207:PHE:HB2 | 2:H:240:GLU:HG2 | 1.91 | 0.52 |
| 2:J:45:TYR:HB2 | 2:J:68:ALA:HB2 | 1.89 | 0.52 |
| 2:G:182:ILE:O | 2:G:186:GLU:HG2 | 2.10 | 0.52 |
| 1:C:242:PRO:HD2 | 1:C:243:GLU:H | 1.74 | 0.52 |
| 1:C:444:LEU:HD12 | 1:C:445:VAL:HG23 | 1.91 | 0.52 |
| 1:C:688:ASP:OD1 | 1:C:691:ARG:NH2 | 2.31 | 0.52 |
| 1:D:64:LEU:O | 1:D:68:LYS:HG3 | 2.09 | 0.52 |
| 1:D:300:ALA:O | 1:D:303:ARG:HB3 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:313:GLN:O | 1:E:317:GLY:N | 2.42 | 0.52 |
| 2:I:147:GLN:HG2 | 2:I:151:TYR:CE2 | 2.44 | 0.52 |
| 2:I:158:ASN:O | 2:I:162:ASN:ND2 | 2.39 | 0.52 |
| 1:A:428:GLU:O | 1:A:432:GLU:HG2 | 2.10 | 0.52 |
| 1:A:525:VAL:HG13 | 1:A:562:PHE:CE1 | 2.43 | 0.52 |
| 1:B:421:SER:HB3 | 1:B:424:VAL:HG23 | 1.91 | 0.52 |
| 1:C:281:GLU:CB | 1:C:324:ILE:HD13 | 2.40 | 0.52 |
| 1:C:521:GLY:HA3 | 1:C:556:ILE:HD13 | 1.92 | 0.52 |
| 1:E:36:ILE:HD11 | 1:E:44:LYS:HB3 | 1.91 | 0.52 |
| 1:E:549:LYS:O | 1:E:552:LEU:HB2 | 2.10 | 0.52 |
| 1:E:666:HIS:HD2 | 1:E:668:PRO:HD3 | 1.75 | 0.52 |
| 1:F:289:GLU:O | 1:F:291:LEU:N | 2.32 | 0.52 |
| 2:H:179:GLN:O | 2:H:182:ILE:HG12 | 2.10 | 0.52 |
| 2:J:175:LEU:HD23 | 2:J:177:GLN:HE21 | 1.74 | 0.52 |
| 2:G:239:ARG:NH2 | 5:M:37:GLU:OE1 | 2.42 | 0.52 |
| 1:B:34:HIS:HB2 | 1:B:83:TYR:O | 2.10 | 0.52 |
| 1:B:113:ASP:O | 1:B:117:MET:HG3 | 2.09 | 0.52 |
| 1:B:606:GLU:OE1 | 1:B:606:GLU:N | 2.43 | 0.52 |
| 1:C:399:ASP:O | 1:C:403:ARG:N | 2.36 | 0.52 |
| 1:C:703:VAL:O | 1:C:704:TRP:HD1 | 1.93 | 0.52 |
| 1:D:94:THR:HA | 1:D:182:GLN:O | 2.09 | 0.52 |
| 1:D:128:GLN:O | 1:D:176:LEU:HD12 | 2.09 | 0.52 |
| 1:F:86:ASP:C | 1:F:88:ALA:H | 2.13 | 0.52 |
| 1:F:128:GLN:O | 1:F:176:LEU:HD12 | 2.09 | 0.52 |
| 1:F:450:SER:O | 1:F:453:MET:HB2 | 2.09 | 0.52 |
| 1:F:635:PRO:HB2 | 1:F:638:ARG:NH1 | 2.25 | 0.52 |
| 2:H:9:GLU:O | 2:H:13:LEU:HG | 2.10 | 0.52 |
| 2:H:243:LEU:HD13 | 2:H:266:TYR:HB2 | 1.92 | 0.52 |
| 2:H:246:LYS:HZ1 | 2:H:258:SER:HB3 | 1.75 | 0.52 |
| 1:A:222:GLY:O | 1:A:224:ASP:N | 2.42 | 0.52 |
| 1:A:716:MET:HG2 | 1:A:732:LEU:HD11 | 1.92 | 0.52 |
| 1:B:106:ASN:HB3 | 1:B:143:LYS:HZ1 | 1.75 | 0.52 |
| 1:D:312:GLU:O | 1:D:316:LEU:N | 2.38 | 0.52 |
| 1:E:18:LEU:HD13 | 1:E:139:SER:OG | 2.10 | 0.52 |
| 1:E:270:ALA:O | 1:E:273:ILE:HG22 | 2.09 | 0.52 |
| 5:M:52:GLU:O | 5:M:56:GLN:HG3 | 2.10 | 0.52 |
| 1:A:227:PHE:CE1 | 1:A:273:ILE:HD13 | 2.45 | 0.52 |
| 1:D:104:LYS:HA | 1:D:107:ILE:HD11 | 1.92 | 0.52 |
| 1:D:528:THR:CB | 1:D:641:LEU:HD12 | 2.40 | 0.52 |
| 1:F:14:ASP:O | 1:F:18:LEU:HG | 2.09 | 0.52 |
| 2:H:244:MET:O | 2:H:248:LEU:HG | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:149:ALA:HB2 | 2:J:164:CYS:HB2 | 1.92 | 0.52 |
| 2:G:40:GLU:O | 2:G:44:ILE:HG12 | 2.09 | 0.52 |
| 5:M:171:ILE:HG22 | 5:M:175:ASN:ND2 | 2.24 | 0.52 |
| 1:A:355:LEU:HB3 | 1:A:388:ARG:NH1 | 2.25 | 0.52 |
| 1:B:576:PHE:HB3 | 1:B:580:ALA:HB3 | 1.90 | 0.52 |
| 1:C:231:PHE:O | 1:C:235:PHE:HB2 | 2.09 | 0.52 |
| 1:C:525:VAL:HG13 | 1:C:562:PHE:CZ | 2.45 | 0.52 |
| 1:D:527:GLN:NE2 | 1:E:715:GLU:HG3 | 2.23 | 0.52 |
| 1:F:96:THR:O | 1:F:149:VAL:HA | 2.10 | 0.52 |
| 1:F:562:PHE:HB2 | 1:F:565:ILE:HG12 | 1.92 | 0.52 |
| 2:H:219:LEU:HD12 | 2:H:223:LEU:HB2 | 1.91 | 0.52 |
| 1:C:326:ILE:HB | 1:C:370:ILE:HD11 | 1.92 | 0.52 |
| 1:C:611:TYR:CZ | 1:C:651:VAL:HG11 | 2.45 | 0.52 |
| 1:D:604:ASP:HB3 | 1:D:607:ARG:HB2 | 1.91 | 0.52 |
| 1:F:655:MET:O | 1:F:656:GLU:CB | 2.58 | 0.52 |
| 2:I:271:ARG:NH2 | 2:J:231:LEU:HB2 | 2.25 | 0.52 |
| 2:G:127:ILE:HG23 | 2:G:131:TYR:CE1 | 2.44 | 0.52 |
| 1:A:300:ALA:HA | 1:A:303:ARG:HG2 | 1.92 | 0.51 |
| 1:A:407:LEU:HD12 | 1:A:426:ILE:HG23 | 1.92 | 0.51 |
| 1:A:607:ARG:NH1 | 1:F:624:GLN:OE1 | 2.42 | 0.51 |
| 1:E:705:ILE:HD13 | 1:E:710:LEU:HD13 | 1.91 | 0.51 |
| 1:A:565:ILE:HA | 1:A:599:CYS:O | 2.09 | 0.51 |
| 1:A:646:THR:HG21 | 1:A:652:LEU:HD22 | 1.93 | 0.51 |
| 1:E:527:GLN:NE2 | 1:F:716:MET:HG2 | 2.20 | 0.51 |
| 1:E:664:THR:C | 1:E:665:ILE:HD13 | 2.29 | 0.51 |
| 2:I:116:ARG:NH1 | 5:M:186:ASP:OD2 | 2.43 | 0.51 |
| 2:G:51:MET:HA | 2:G:54:MET:HG2 | 1.93 | 0.51 |
| 1:A:598:SER:O | 1:A:640:LEU:HA | 2.11 | 0.51 |
| 1:C:612:VAL:CG1 | 1:C:617:ARG:HB3 | 2.40 | 0.51 |
| 1:D:43:HIS:HB3 | 1:D:45:TYR:HE1 | 1.74 | 0.51 |
| 1:D:260:GLY:N | 1:D:266:LYS:HD3 | 2.25 | 0.51 |
| 1:E:611:TYR:CE1 | 1:E:616:PRO:HB2 | 2.44 | 0.51 |
| 1:F:313:GLN:O | 1:F:317:GLY:N | 2.43 | 0.51 |
| 2:H:112:THR:HG23 | 2:H:117:PHE:CE1 | 2.45 | 0.51 |
| 2:J:167:LYS:HE2 | 2:J:171:TYR:HE2 | 1.75 | 0.51 |
| 2:G:266:TYR:CZ | 2:G:270:SER:HB2 | 2.44 | 0.51 |
| 5:M:25:SER:O | 5:M:29:THR:HG23 | 2.11 | 0.51 |
| 1:A:102:LEU:HD22 | 1:A:137:VAL:HG12 | 1.91 | 0.51 |
| 1:A:546:HIS:NE2 | 1:F:659:ASN:OD1 | 2.43 | 0.51 |
| 1:D:512:ASP:N | 1:D:513:PRO:CD | 2.74 | 0.51 |
| 1:D:560:SER:HB2 | 1:D:562:PHE:CD1 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:657:MET:HG2 | 1:D:661:PHE:HE2 | 1.76 | 0.51 |
| 1:E:428:GLU:O | 1:E:432:GLU:HG2 | 2.10 | 0.51 |
| 1:E:612:VAL:HG22 | 1:E:613:PRO:HD2 | 1.92 | 0.51 |
| 1:F:517:VAL:HG13 | 1:F:665:ILE:CG2 | 2.40 | 0.51 |
| 1:F:544:PRO:O | 1:F:547:SER:OG | 2.25 | 0.51 |
| 2:H:69:ALA:HB1 | 2:H:85:PHE:CE1 | 2.45 | 0.51 |
| 2:J:243:LEU:HD13 | 2:J:266:TYR:HB2 | 1.92 | 0.51 |
| 1:A:283:LYS:HA | 1:A:324:ILE:O | 2.11 | 0.51 |
| 1:A:326:ILE:HG22 | 1:A:370:ILE:CG1 | 2.41 | 0.51 |
| 1:C:310:GLU:OE2 | 1:C:357:LYS:NZ | 2.27 | 0.51 |
| 1:C:614:ILE:O | 1:C:616:PRO:HA | 2.10 | 0.51 |
| 1:D:618:PHE:HE1 | 1:E:612:VAL:HG21 | 1.76 | 0.51 |
| 1:E:247:GLN:HA | 1:F:417:HIS:ND1 | 2.26 | 0.51 |
| 2:H:49:ALA:HB2 | 2:H:64:ALA:HB3 | 1.93 | 0.51 |
| 2:H:155:GLU:C | 2:H:157:SER:N | 2.64 | 0.51 |
| 2:J:243:LEU:HD22 | 2:J:266:TYR:CD2 | 2.45 | 0.51 |
| 5:M:179:ASP:O | 5:M:183:GLU:HG2 | 2.11 | 0.51 |
| 1:B:570:PRO:HD3 | 1:B:603:ASP:HB3 | 1.93 | 0.51 |
| 1:D:221:GLY:HA3 | 1:D:406:ILE:HD13 | 1.93 | 0.51 |
| 1:D:313:GLN:OE1 | 1:D:365:ASN:O | 2.29 | 0.51 |
| 2:I:124:HIS:HE1 | 2:I:147:GLN:HB3 | 1.76 | 0.51 |
| 2:I:200:TYR:C | 3:K:47:ARG:HH12 | 2.14 | 0.51 |
| 2:J:69:ALA:HB1 | 2:J:85:PHE:CE1 | 2.46 | 0.51 |
| 2:G:260:THR:HG21 | 2:G:284:LYS:HE3 | 1.93 | 0.51 |
| 5:M:44:ILE:O | 5:M:48:VAL:HG23 | 2.11 | 0.51 |
| 5:M:177:GLN:O | 5:M:181:ILE:HG13 | 2.11 | 0.51 |
| 1:A:198:LYS:O | 1:A:198:LYS:HD3 | 2.10 | 0.51 |
| 1:A:521:GLY:HA2 | 1:A:524:LEU:HD12 | 1.93 | 0.51 |
| 1:C:136:LEU:N | 1:C:136:LEU:HD23 | 2.26 | 0.51 |
| 1:C:573:MET:HB3 | 1:C:576:PHE:CD2 | 2.46 | 0.51 |
| 1:D:522:GLU:OE2 | 1:D:556:ILE:HA | 2.10 | 0.51 |
| 1:D:656:GLU:OE1 | 1:E:613:PRO:HB3 | 2.10 | 0.51 |
| 1:E:46:ILE:HD12 | 1:E:174:VAL:HG21 | 1.92 | 0.51 |
| 1:E:674:GLU:O | 1:E:677:LEU:HB2 | 2.11 | 0.51 |
| 1:F:653:GLN:HB3 | 1:F:658:LEU:HD23 | 1.93 | 0.51 |
| 2:H:67:GLN:O | 2:H:71:LEU:HG | 2.10 | 0.51 |
| 1:A:686:PHE:CE2 | 1:A:714:ILE:HG12 | 2.37 | 0.51 |
| 1:B:136:LEU:N | 1:B:136:LEU:HD23 | 2.26 | 0.51 |
| 1:C:236:ALA:HB1 | 1:D:453:MET:CB | 2.41 | 0.51 |
| 1:E:327:PHE:CZ | 1:E:369:VAL:HG21 | 2.46 | 0.51 |
| 2:H:45:TYR:HE2 | 2:H:71:LEU:HD11 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:163:LYS:O | 2:I:167:LYS:HG2 | 2.10 | 0.51 |
| 2:J:235:PHE:CB | 3:K:38:GLN:HE21 | 2.17 | 0.51 |
| 1:C:404:LEU:HG | 1:C:426:ILE:HG22 | 1.93 | 0.51 |
| 1:C:596:GLN:HA | 1:C:638:ARG:CD | 2.40 | 0.51 |
| 2:I:67:GLN:O | 2:I:71:LEU:HG | 2.11 | 0.51 |
| 2:J:230:GLU:HG3 | 2:J:237:ASP:CB | 2.41 | 0.51 |
| 1:A:673:GLY:O | 1:A:677:LEU:HD22 | 2.11 | 0.51 |
| 1:C:295:VAL:O | 1:D:294:TYR:HB2 | 2.10 | 0.51 |
| 1:C:375:ARG:NH1 | 1:C:378:LEU:HG | 2.26 | 0.51 |
| 1:E:230:ILE:HD11 | 1:E:391:VAL:HG11 | 1.93 | 0.51 |
| 1:E:303:ARG:CG | 1:E:357:LYS:HE2 | 2.41 | 0.51 |
| 1:F:113:ASP:O | 1:F:117:MET:HG3 | 2.11 | 0.51 |
| 1:F:538:SER:H | 1:F:662:SER:CB | 2.24 | 0.51 |
| 2:G:153:LYS:HE2 | 2:G:158:ASN:HD22 | 1.76 | 0.51 |
| 2:G:185:TYR:HA | 2:G:188:VAL:HG12 | 1.92 | 0.51 |
| 1:A:546:HIS:CE1 | 1:A:709:LYS:HE3 | 2.46 | 0.50 |
| 1:B:24:VAL:HG12 | 1:B:60:VAL:HG13 | 1.92 | 0.50 |
| 1:B:539:VAL:HG21 | 1:B:665:ILE:HD12 | 1.93 | 0.50 |
| 1:D:528:THR:HG22 | 1:D:597:LEU:HD11 | 1.93 | 0.50 |
| 1:E:64:LEU:HA | 1:E:67:ARG:HE | 1.75 | 0.50 |
| 1:E:590:ASP:O | 1:E:593:TYR:HB2 | 2.11 | 0.50 |
| 1:F:258:LEU:CB | 1:F:395:ILE:HD11 | 2.40 | 0.50 |
| 1:F:721:ASP:HB2 | 1:F:724:TYR:CD1 | 2.44 | 0.50 |
| 5:M:26:LEU:HG | 5:M:30:ARG:HH12 | 1.75 | 0.50 |
| 1:B:303:ARG:CG | 1:B:357:LYS:HE2 | 2.41 | 0.50 |
| 1:C:399:ASP:O | 1:C:402:GLY:N | 2.45 | 0.50 |
| 1:C:524:LEU:CD2 | 1:C:537:VAL:HG11 | 2.37 | 0.50 |
| 1:C:730:LEU:O | 1:C:734:ARG:HG3 | 2.11 | 0.50 |
| 1:D:136:LEU:N | 1:D:136:LEU:HD23 | 2.26 | 0.50 |
| 1:D:618:PHE:CE1 | 1:E:612:VAL:HG21 | 2.47 | 0.50 |
| 1:E:245:VAL:O | 1:E:249:GLY:N | 2.39 | 0.50 |
| 1:F:281:GLU:N | 1:F:282:PRO:HA | 2.26 | 0.50 |
| 2:H:197:LEU:HD12 | 5:M:45:ARG:CD | 2.41 | 0.50 |
| 1:A:315:ARG:HG2 | 1:A:316:LEU:CD1 | 2.40 | 0.50 |
| 1:A:347:HIS:N | 1:A:348:ASP:HA | 2.25 | 0.50 |
| 1:A:565:ILE:HG13 | 1:A:599:CYS:HB3 | 1.92 | 0.50 |
| 1:B:295:VAL:C | 1:C:294:TYR:HB2 | 2.31 | 0.50 |
| 1:B:571:ASP:O | 1:B:574:ILE:HG13 | 2.11 | 0.50 |
| 1:C:233:ARG:CZ | 1:C:233:ARG:HB2 | 2.41 | 0.50 |
| 1:C:612:VAL:HG12 | 1:C:617:ARG:HB3 | 1.93 | 0.50 |
| 1:C:691:ARG:HH11 | 1:C:691:ARG:HB2 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:284:VAL:O | 1:F:326:ILE:HG12 | 2.12 | 0.50 |
| 2:H:158:ASN:N | 4:L:228:GLU:OE1 | 2.43 | 0.50 |
| 2:G:20:LYS:HE2 | 2:G:37:LYS:HA | 1.93 | 0.50 |
| 5:M:171:ILE:CG2 | 5:M:175:ASN:HD21 | 2.24 | 0.50 |
| 1:B:651:VAL:CG1 | 1:B:655:MET:CE | 2.90 | 0.50 |
| 1:C:24:VAL:O | 1:C:51:THR:HA | 2.12 | 0.50 |
| 1:C:284:VAL:HG11 | 1:C:305:LEU:HD11 | 1.93 | 0.50 |
| 1:C:677:LEU:HD21 | 1:C:695:ALA:CB | 2.42 | 0.50 |
| 1:C:686:PHE:HE1 | 1:C:714:ILE:HG23 | 1.76 | 0.50 |
| 1:D:89:LYS:NZ | 1:D:170:GLN:HE22 | 2.10 | 0.50 |
| 1:D:593:TYR:OH | 1:D:632:LYS:HD2 | 2.11 | 0.50 |
| 1:E:136:LEU:N | 1:E:136:LEU:HD23 | 2.25 | 0.50 |
| 1:F:267:THR:HA | 1:F:372:MET:SD | 2.52 | 0.50 |
| 2:J:200:TYR:HE2 | 3:K:41:GLU:CG | 2.23 | 0.50 |
| 2:G:235:PHE:CD2 | 5:M:152:GLN:HG2 | 2.46 | 0.50 |
| 1:A:95:MET:HG3 | 1:A:152:ILE:HG12 | 1.92 | 0.50 |
| 1:A:650:ASP:OD1 | 1:A:650:ASP:N | 2.45 | 0.50 |
| 1:B:499:TYR:HA | 1:B:502:TYR:CD2 | 2.46 | 0.50 |
| 1:B:589:PHE:HD2 | 1:B:629:LEU:HD22 | 1.76 | 0.50 |
| 1:C:560:SER:HB2 | 1:C:562:PHE:CE1 | 2.46 | 0.50 |
| 1:E:585:MET:HG3 | 1:E:589:PHE:HZ | 1.69 | 0.50 |
| 1:E:593:TYR:CD2 | 1:E:635:PRO:HD3 | 2.47 | 0.50 |
| 1:E:654:GLU:CD | 1:F:614:ILE:HD11 | 2.32 | 0.50 |
| 1:F:436:PHE:HB3 | 1:F:440:GLU:CB | 2.41 | 0.50 |
| 1:F:589:PHE:CD2 | 1:F:629:LEU:HD22 | 2.47 | 0.50 |
| 2:G:244:MET:O | 2:G:248:LEU:HG | 2.12 | 0.50 |
| 5:M:142:ARG:HG2 | 5:M:142:ARG:HH11 | 1.76 | 0.50 |
| 1:C:428:GLU:O | 1:C:432:GLU:HG2 | 2.12 | 0.50 |
| 1:C:533:ARG:C | 1:D:505:ASN:HD21 | 2.14 | 0.50 |
| 1:D:298:SER:O | 1:D:301:ASN:HB3 | 2.12 | 0.50 |
| 1:D:331:ASP:HA | 1:D:379:ILE:HD11 | 1.92 | 0.50 |
| 1:D:690:GLU:O | 1:D:693:THR:OG1 | 2.22 | 0.50 |
| 1:E:327:PHE:HB2 | 1:E:330:ILE:CG2 | 2.35 | 0.50 |
| 2:I:200:TYR:CB | 3:K:47:ARG:HH12 | 2.25 | 0.50 |
| 5:M:149:ASN:HA | 5:M:152:GLN:NE2 | 2.27 | 0.50 |
| 1:A:258:LEU:O | 1:A:372:MET:HA | 2.11 | 0.50 |
| 1:A:398:PRO:HD2 | 1:A:434:LYS:O | 2.12 | 0.50 |
| 1:B:249:GLY:HA2 | 1:C:413:ARG:NH1 | 2.26 | 0.50 |
| 1:B:533:ARG:HG3 | 1:B:534:THR:N | 2.26 | 0.50 |
| 1:C:375:ARG:NH2 | 1:C:377:ASP:OD1 | 2.44 | 0.50 |
| 1:D:114:THR:HG21 | 1:D:200:LYS:HG2 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:64:LEU:HA | 1:F:67:ARG:HE | 1.77 | 0.50 |
| 1:F:508:ILE:C | 1:F:509:LYS:HD3 | 2.32 | 0.50 |
| 2:H:20:LYS:HG2 | 2:H:37:LYS:HB3 | 1.92 | 0.50 |
| 2:H:38:ILE:HG23 | 2:H:75:LEU:HD12 | 1.94 | 0.50 |
| 2:J:18:GLU:HA | 2:J:21:VAL:HG12 | 1.94 | 0.50 |
| 3:K:46:MET:SD | 3:K:49:ASN:ND2 | 2.85 | 0.50 |
| 1:A:286:ASN:HB2 | 1:A:327:PHE:HB3 | 1.93 | 0.50 |
| 1:B:195:LEU:HB2 | 1:B:200:LYS:HE3 | 1.94 | 0.50 |
| 1:B:353:GLN:HE21 | 1:B:357:LYS:HG2 | 1.77 | 0.50 |
| 1:B:428:GLU:O | 1:B:432:GLU:HG2 | 2.11 | 0.50 |
| 1:B:485:GLU:O | 1:B:490:PRO:HD3 | 2.11 | 0.50 |
| 1:B:503:ILE:HD11 | 1:B:554:ALA:HB3 | 1.94 | 0.50 |
| 1:B:628:VAL:CG1 | 1:C:571:ASP:HA | 2.42 | 0.50 |
| 1:B:651:VAL:HG12 | 1:B:655:MET:CE | 2.42 | 0.50 |
| 1:D:310:GLU:O | 1:D:313:GLN:NE2 | 2.45 | 0.50 |
| 1:D:589:PHE:CE2 | 1:D:629:LEU:HD13 | 2.46 | 0.50 |
| 1:D:616:PRO:HG2 | 1:E:614:ILE:HG21 | 1.93 | 0.50 |
| 1:E:258:LEU:HB3 | 1:E:395:ILE:HD11 | 1.94 | 0.50 |
| 1:F:114:THR:HG21 | 1:F:200:LYS:HA | 1.93 | 0.50 |
| 1:F:136:LEU:N | 1:F:136:LEU:HD23 | 2.26 | 0.50 |
| 1:F:570:PRO:CG | 1:F:604:ASP:HB2 | 2.39 | 0.50 |
| 2:G:256:VAL:HG22 | 2:G:256:VAL:O | 2.12 | 0.50 |
| 1:C:36:ILE:HD11 | 1:C:44:LYS:HB3 | 1.92 | 0.50 |
| 1:C:113:ASP:O | 1:C:117:MET:HG3 | 2.12 | 0.50 |
| 2:H:98:GLN:H | 2:H:98:GLN:CD | 2.15 | 0.50 |
| 1:A:132:VAL:HG23 | 1:A:173:GLU:O | 2.12 | 0.49 |
| 1:A:540:LEU:HD12 | 1:A:644:GLY:O | 2.12 | 0.49 |
| 1:D:330:ILE:HD12 | 1:D:331:ASP:N | 2.27 | 0.49 |
| 1:D:581:LYS:O | 1:D:585:MET:HG2 | 2.12 | 0.49 |
| 2:H:112:THR:HG23 | 2:H:117:PHE:HE1 | 1.76 | 0.49 |
| 2:H:243:LEU:HD22 | 2:H:266:TYR:CD2 | 2.47 | 0.49 |
| 2:G:243:LEU:HD13 | 2:G:266:TYR:HB2 | 1.94 | 0.49 |
| 5:M:46:THR:O | 5:M:50:LEU:HG | 2.11 | 0.49 |
| 1:A:397:LEU:CB | 1:A:398:PRO:CD | 2.89 | 0.49 |
| 1:A:493:GLY:HA2 | 1:A:494:THR:CB | 2.41 | 0.49 |
| 1:B:230:ILE:HD11 | 1:B:391:VAL:HG11 | 1.93 | 0.49 |
| 1:B:614:ILE:O | 1:B:616:PRO:HA | 2.12 | 0.49 |
| 1:C:510:TRP:CE3 | 1:C:670:ILE:HG12 | 2.46 | 0.49 |
| 1:D:508:ILE:HG12 | 1:D:683:LEU:HD21 | 1.93 | 0.49 |
| 1:D:540:LEU:HD12 | 1:D:661:PHE:CE1 | 2.47 | 0.49 |
| 1:F:64:LEU:O | 1:F:68:LYS:HG2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:327:PHE:CZ | 1:F:369:VAL:HG21 | 2.47 | 0.49 |
| 2:H:239:ARG:HH22 | 4:L:213:HIS:CE1 | 2.30 | 0.49 |
| 2:I:214:PHE:CE1 | 2:I:216:ILE:HB | 2.47 | 0.49 |
| 3:K:85:LYS:HG3 | 3:K:89:TRP:HE3 | 1.77 | 0.49 |
| 4:L:240:ALA:HA | 4:L:243:TYR:CD2 | 2.44 | 0.49 |
| 1:A:411:THR:HG21 | 1:A:426:ILE:HD11 | 1.93 | 0.49 |
| 1:A:683:LEU:HB3 | 1:A:685:ASN:HD22 | 1.75 | 0.49 |
| 1:B:14:ASP:O | 1:B:18:LEU:HD13 | 2.11 | 0.49 |
| 1:B:63:SER:O | 1:B:67:ARG:HG3 | 2.12 | 0.49 |
| 1:B:569:SER:HA | 1:B:603:ASP:HB3 | 1.95 | 0.49 |
| 1:C:331:ASP:HA | 1:C:379:ILE:CD1 | 2.39 | 0.49 |
| 1:D:26:GLU:HG2 | 1:D:51:THR:HB | 1.93 | 0.49 |
| 1:D:48:THR:HG21 | 1:D:128:GLN:HG2 | 1.95 | 0.49 |
| 1:D:627:LEU:HD13 | 1:E:607:ARG:HH12 | 1.78 | 0.49 |
| 1:F:712:MET:O | 1:F:716:MET:HG3 | 2.11 | 0.49 |
| 5:M:190:THR:HG22 | 5:M:194:GLU:OE2 | 2.12 | 0.49 |
| 1:A:445:VAL:O | 1:A:449:GLN:HG2 | 2.12 | 0.49 |
| 1:B:568:CYS:SG | 1:B:588:ILE:HD12 | 2.53 | 0.49 |
| 1:C:589:PHE:CE1 | 1:C:600:VAL:HG11 | 2.48 | 0.49 |
| 1:E:653:GLN:OE1 | 1:E:658:LEU:HD23 | 2.13 | 0.49 |
| 5:M:31:ARG:O | 5:M:35:LEU:HG | 2.13 | 0.49 |
| 1:A:299:GLU:HG3 | 1:B:289:GLU:CB | 2.41 | 0.49 |
| 1:D:602:VAL:O | 1:D:644:GLY:HA2 | 2.13 | 0.49 |
| 1:E:697:GLN:HG3 | 1:E:730:LEU:CD1 | 2.41 | 0.49 |
| 2:H:142:ILE:HG23 | 2:H:168:VAL:HG13 | 1.94 | 0.49 |
| 2:I:92:PHE:HD1 | 2:I:97:PRO:HG2 | 1.77 | 0.49 |
| 2:G:17:ALA:O | 2:G:21:VAL:HG12 | 2.11 | 0.49 |
| 1:A:505:ASN:OD1 | 1:A:711:LEU:HD13 | 2.13 | 0.49 |
| 1:D:721:ASP:O | 1:D:725:ARG:HG3 | 2.13 | 0.49 |
| 1:E:352:ASN:HA | 1:E:355:LEU:HD12 | 1.95 | 0.49 |
| 1:F:352:ASN:HA | 1:F:355:LEU:HD12 | 1.93 | 0.49 |
| 2:I:20:LYS:NZ | 2:I:40:GLU:HG2 | 2.28 | 0.49 |
| 2:G:162:ASN:OD1 | 2:G:188:VAL:HG23 | 2.13 | 0.49 |
| 5:M:149:ASN:HA | 5:M:152:GLN:HE21 | 1.77 | 0.49 |
| 1:A:295:VAL:HB | 1:B:294:TYR:CB | 2.43 | 0.49 |
| 1:B:272:GLN:OE1 | 1:B:272:GLN:HA | 2.13 | 0.49 |
| 1:B:499:TYR:HA | 1:B:502:TYR:CE2 | 2.47 | 0.49 |
| 1:C:347:HIS:O | 1:C:350:VAL:HG22 | 2.13 | 0.49 |
| 1:D:325:ILE:O | 1:D:369:VAL:HA | 2.13 | 0.49 |
| 1:D:681:GLU:HG2 | 1:D:691:ARG:CZ | 2.43 | 0.49 |
| 1:F:411:THR:O | 1:F:414:MET:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:18:GLU:HA | 2:I:21:VAL:HG12 | 1.94 | 0.49 |
| 2:J:40:GLU:O | 2:J:44:ILE:HG12 | 2.13 | 0.49 |
| 2:J:120:ALA:O | 2:J:124:HIS:HB2 | 2.12 | 0.49 |
| 2:G:95:ALA:HB1 | 2:G:97:PRO:HD2 | 1.95 | 0.49 |
| 1:C:101:PHE:CD2 | 1:C:107:ILE:HA | 2.48 | 0.49 |
| 1:C:609:LEU:O | 1:C:610:ASP:HB2 | 2.11 | 0.49 |
| 1:E:256:ILE:O | 1:E:370:ILE:HA | 2.13 | 0.49 |
| 2:H:203:LYS:O | 2:H:206:PHE:N | 2.46 | 0.49 |
| 2:I:50:ASN:ND2 | 2:J:115:GLY:HA2 | 2.27 | 0.49 |
| 2:I:142:ILE:HG23 | 2:I:168:VAL:HG13 | 1.95 | 0.49 |
| 2:J:118:THR:O | 2:J:122:LYS:HG2 | 2.13 | 0.49 |
| 2:J:124:HIS:HE1 | 2:J:147:GLN:HB3 | 1.77 | 0.49 |
| 1:D:268:LEU:HA | 1:D:271:ARG:HD2 | 1.95 | 0.49 |
| 1:D:284:VAL:HG21 | 1:D:325:ILE:HG22 | 1.95 | 0.49 |
| 1:D:564:PHE:HD2 | 1:D:598:SER:HB2 | 1.78 | 0.49 |
| 1:E:510:TRP:CE3 | 1:E:670:ILE:HG13 | 2.47 | 0.49 |
| 3:K:66:ARG:NH2 | 5:M:182:MET:HB3 | 2.26 | 0.49 |
| 3:K:69:ALA:O | 3:K:72:ALA:HB3 | 2.12 | 0.49 |
| 5:M:178:ILE:O | 5:M:182:MET:HG3 | 2.12 | 0.49 |
| 1:A:128:GLN:O | 1:A:176:LEU:HD12 | 2.11 | 0.49 |
| 1:B:669:ASN:CG | 1:B:706:GLY:HA2 | 2.33 | 0.49 |
| 1:C:705:ILE:HD11 | 1:C:710:LEU:HA | 1.94 | 0.49 |
| 1:E:236:ALA:O | 1:E:239:VAL:HG12 | 2.13 | 0.49 |
| 1:F:45:TYR:CE2 | 1:F:70:ALA:HA | 2.48 | 0.49 |
| 1:F:103:GLN:C | 1:F:105:LYS:H | 2.15 | 0.49 |
| 1:F:105:LYS:HE2 | 2:G:257:ASP:HB2 | 1.95 | 0.49 |
| 1:F:535:PRO:HB2 | 1:F:536:LEU:HD13 | 1.93 | 0.49 |
| 2:H:243:LEU:HD22 | 2:H:266:TYR:CG | 2.48 | 0.49 |
| 2:I:17:ALA:O | 2:I:21:VAL:HG12 | 2.12 | 0.49 |
| 2:I:45:TYR:HB2 | 2:I:68:ALA:HB2 | 1.94 | 0.49 |
| 2:I:266:TYR:CZ | 2:I:270:SER:HB2 | 2.48 | 0.49 |
| 2:J:127:ILE:HG23 | 2:J:131:TYR:CE1 | 2.48 | 0.49 |
| 2:G:223:LEU:O | 2:G:227:LYS:HG3 | 2.13 | 0.49 |
| 1:B:256:ILE:O | 1:B:370:ILE:HA | 2.13 | 0.48 |
| 1:C:349:THR:O | 1:C:352:ASN:HB3 | 2.13 | 0.48 |
| 1:C:677:LEU:HD11 | 1:C:698:VAL:CG2 | 2.42 | 0.48 |
| 1:E:696:GLN:HB3 | 1:E:697:GLN:NE2 | 2.28 | 0.48 |
| 1:F:95:MET:HG3 | 1:F:152:ILE:HG12 | 1.95 | 0.48 |
| 1:F:428:GLU:O | 1:F:432:GLU:HG2 | 2.13 | 0.48 |
| 2:H:36:SER:OG | 5:M:201:LYS:HE2 | 2.13 | 0.48 |
| 2:H:185:TYR:HA | 2:H:188:VAL:HG12 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:262:PRO:HA | 1:A:263:GLY:HA2 | 1.71 | 0.48 |
| 1:B:45:TYR:CE2 | 1:B:70:ALA:HA | 2.48 | 0.48 |
| 1:D:242:PRO:HD2 | 1:D:243:GLU:N | 2.28 | 0.48 |
| 1:D:254:LYS:O | 1:D:368:LEU:HA | 2.13 | 0.48 |
| 1:E:596:GLN:O | 1:E:638:ARG:HA | 2.13 | 0.48 |
| 2:H:45:TYR:HB2 | 2:H:68:ALA:HB2 | 1.94 | 0.48 |
| 5:M:170:GLU:HG3 | 5:M:174:GLN:NE2 | 2.27 | 0.48 |
| 1:A:609:LEU:O | 1:A:610:ASP:HB3 | 2.13 | 0.48 |
| 1:C:193:LEU:HD21 | 1:C:195:LEU:HD21 | 1.95 | 0.48 |
| 1:C:611:TYR:HE1 | 1:C:616:PRO:HB2 | 1.76 | 0.48 |
| 1:D:310:GLU:O | 1:D:313:GLN:HG2 | 2.13 | 0.48 |
| 1:D:663:THR:CG2 | 1:D:664:THR:N | 2.76 | 0.48 |
| 1:D:670:ILE:HD11 | 1:D:705:ILE:HG23 | 1.94 | 0.48 |
| 1:E:257:LEU:HG | 1:E:371:GLY:O | 2.13 | 0.48 |
| 1:E:538:SER:OG | 1:E:662:SER:N | 2.43 | 0.48 |
| 3:K:56:ARG:HD2 | 5:M:171:ILE:HG12 | 1.95 | 0.48 |
| 1:A:490:PRO:HA | 1:A:491:ALA:CB | 2.23 | 0.48 |
| 1:A:611:TYR:CE2 | 1:A:651:VAL:HG11 | 2.48 | 0.48 |
| 1:B:38:ARG:HB3 | 1:B:79:GLU:HB2 | 1.95 | 0.48 |
| 1:B:265:GLY:O | 1:B:268:LEU:HG | 2.13 | 0.48 |
| 1:B:710:LEU:O | 1:B:714:ILE:HG13 | 2.12 | 0.48 |
| 1:C:436:PHE:CD1 | 1:C:436:PHE:N | 2.81 | 0.48 |
| 1:E:404:LEU:HG | 1:E:426:ILE:HG22 | 1.96 | 0.48 |
| 1:F:114:THR:HG21 | 1:F:200:LYS:HG2 | 1.94 | 0.48 |
| 1:F:404:LEU:HG | 1:F:426:ILE:HG22 | 1.96 | 0.48 |
| 2:J:72:HIS:CE1 | 2:J:80:ASP:HB2 | 2.49 | 0.48 |
| 1:A:612:VAL:HG12 | 1:A:617:ARG:HB2 | 1.94 | 0.48 |
| 1:B:236:ALA:O | 1:B:239:VAL:HG12 | 2.14 | 0.48 |
| 1:C:616:PRO:HG2 | 1:D:614:ILE:HD13 | 1.95 | 0.48 |
| 1:D:304:LYS:HA | 1:D:307:ALA:HB3 | 1.95 | 0.48 |
| 1:D:652:LEU:HD13 | 1:D:657:MET:HB3 | 1.96 | 0.48 |
| 2:H:182:ILE:O | 2:H:186:GLU:HG2 | 2.14 | 0.48 |
| 1:A:388:ARG:O | 1:A:389:LEU:HD22 | 2.13 | 0.48 |
| 1:A:620:ASN:ND2 | 1:B:610:ASP:OD1 | 2.46 | 0.48 |
| 1:B:578:GLU:CG | 1:B:619:SER:HB2 | 2.44 | 0.48 |
| 1:C:184:ALA:HB1 | 1:C:200:LYS:O | 2.14 | 0.48 |
| 1:D:326:ILE:HG22 | 1:D:370:ILE:HG13 | 1.95 | 0.48 |
| 1:D:618:PHE:HE2 | 1:E:614:ILE:HD12 | 1.78 | 0.48 |
| 1:E:281:GLU:N | 1:E:282:PRO:HA | 2.28 | 0.48 |
| 1:E:598:SER:OG | 1:E:639:LYS:O | 2.16 | 0.48 |
| 1:E:654:GLU:CG | 1:F:614:ILE:HD11 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:714:ILE:O | 1:E:718:LEU:HG | 2.12 | 0.48 |
| 1:F:236:ALA:O | 1:F:239:VAL:HG12 | 2.13 | 0.48 |
| 2:J:235:PHE:CD2 | 3:K:38:GLN:HB2 | 2.49 | 0.48 |
| 3:K:33:GLN:HG2 | 4:L:201:GLU:CB | 2.44 | 0.48 |
| 1:A:299:GLU:HG2 | 1:A:353:GLN:HG2 | 1.95 | 0.48 |
| 1:A:428:GLU:O | 1:A:431:VAL:HG12 | 2.14 | 0.48 |
| 1:A:575:GLY:HA3 | 1:F:586:LYS:HZ1 | 1.79 | 0.48 |
| 1:B:531:SER:HA | 1:B:639:LYS:HD3 | 1.96 | 0.48 |
| 1:D:375:ARG:NH2 | 1:D:377:ASP:OD2 | 2.47 | 0.48 |
| 1:E:658:LEU:HD12 | 1:E:658:LEU:HA | 1.62 | 0.48 |
| 1:E:670:ILE:HG22 | 1:E:672:THR:N | 2.27 | 0.48 |
| 1:F:136:LEU:HD23 | 1:F:136:LEU:H | 1.79 | 0.48 |
| 2:J:182:ILE:O | 2:J:186:GLU:HG2 | 2.13 | 0.48 |
| 2:J:201:SER:CB | 5:M:165:LEU:HD11 | 2.37 | 0.48 |
| 1:A:403:ARG:O | 1:A:407:LEU:HG | 2.14 | 0.48 |
| 1:B:352:ASN:HA | 1:B:355:LEU:HD12 | 1.95 | 0.48 |
| 1:B:516:ARG:O | 1:B:519:ASP:OD1 | 2.31 | 0.48 |
| 1:B:628:VAL:HG13 | 1:C:571:ASP:HA | 1.95 | 0.48 |
| 1:C:677:LEU:HD11 | 1:C:698:VAL:HG21 | 1.96 | 0.48 |
| 1:D:184:ALA:HA | 1:D:199:ALA:O | 2.14 | 0.48 |
| 1:D:315:ARG:O | 1:D:316:LEU:HD12 | 2.14 | 0.48 |
| 1:E:705:ILE:HG13 | 1:E:709:LYS:HG3 | 1.95 | 0.48 |
| 2:I:201:SER:N | 3:K:47:ARG:NH1 | 2.61 | 0.48 |
| 1:A:104:LYS:HA | 1:A:107:ILE:HD11 | 1.96 | 0.48 |
| 1:A:423:ASP:HB2 | 1:A:480:PHE:N | 2.29 | 0.48 |
| 1:A:485:GLU:O | 1:A:489:LYS:CB | 2.62 | 0.48 |
| 1:A:593:TYR:HB3 | 1:A:635:PRO:HD3 | 1.96 | 0.48 |
| 1:B:249:GLY:HA3 | 1:C:414:MET:CE | 2.44 | 0.48 |
| 1:B:399:ASP:O | 1:B:403:ARG:N | 2.42 | 0.48 |
| 1:C:322:LEU:HD22 | 1:C:366:ASN:O | 2.14 | 0.48 |
| 1:D:402:GLY:HA2 | 1:D:405:GLN:OE1 | 2.12 | 0.48 |
| 1:D:570:PRO:HA | 1:D:573:MET:HB3 | 1.96 | 0.48 |
| 1:D:578:GLU:OE1 | 1:D:621:LEU:HD13 | 2.13 | 0.48 |
| 1:E:526:GLN:HA | 1:E:529:LYS:HG2 | 1.96 | 0.48 |
| 1:E:693:THR:O | 1:E:697:GLN:NE2 | 2.22 | 0.48 |
| 1:F:18:LEU:HD13 | 1:F:139:SER:OG | 2.13 | 0.48 |
| 2:H:201:SER:O | 2:H:203:LYS:N | 2.47 | 0.48 |
| 2:H:230:GLU:HG3 | 2:H:237:ASP:CB | 2.41 | 0.48 |
| 2:I:57:ASN:O | 2:I:59:SER:N | 2.46 | 0.48 |
| 2:G:256:VAL:HG11 | 2:G:288:GLN:HG2 | 1.96 | 0.48 |
| 1:A:222:GLY:HA3 | 1:A:402:GLY:HA3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:325:ILE:HG13 | 1:B:369:VAL:HB | 1.95 | 0.48 |
| 1:C:270:ALA:O | 1:C:273:ILE:HG22 | 2.14 | 0.48 |
| 1:C:612:VAL:CG2 | 1:C:613:PRO:HD2 | 2.44 | 0.48 |
| 1:E:605:ILE:HA | 1:E:608:LEU:HB3 | 1.96 | 0.48 |
| 2:G:177:GLN:HB3 | 2:G:180:LYS:HB2 | 1.96 | 0.48 |
| 3:K:29:ASN:CB | 4:L:198:ARG:HH12 | 2.26 | 0.48 |
| 3:K:42:VAL:HG11 | 5:M:160:LEU:CD1 | 2.41 | 0.48 |
| 3:K:83:LYS:HD2 | 5:M:203:LEU:CD1 | 2.43 | 0.48 |
| 1:A:255:GLY:HA3 | 1:A:389:LEU:HD13 | 1.96 | 0.47 |
| 1:B:91:CYS:O | 1:B:154:ALA:HA | 2.14 | 0.47 |
| 1:B:185:PHE:O | 1:B:200:LYS:HA | 2.14 | 0.47 |
| 1:B:327:PHE:CZ | 1:B:369:VAL:HG21 | 2.50 | 0.47 |
| 1:C:576:PHE:HB3 | 1:C:580:ALA:HB3 | 1.96 | 0.47 |
| 1:E:428:GLU:O | 1:E:431:VAL:HG12 | 2.13 | 0.47 |
| 1:F:579:THR:O | 1:F:583:GLN:HG2 | 2.13 | 0.47 |
| 2:H:127:ILE:HG23 | 2:H:131:TYR:CE1 | 2.48 | 0.47 |
| 1:B:319:ASN:HB3 | 1:B:320:SER:HB2 | 1.96 | 0.47 |
| 1:B:406:ILE:HB | 1:B:441:LEU:HD13 | 1.96 | 0.47 |
| 1:C:26:GLU:HG2 | 1:C:51:THR:HB | 1.95 | 0.47 |
| 1:C:36:ILE:O | 1:C:36:ILE:HG23 | 2.13 | 0.47 |
| 1:D:531:SER:OG | 1:D:534:THR:OG1 | 2.29 | 0.47 |
| 1:E:319:ASN:HB3 | 1:E:320:SER:HB2 | 1.95 | 0.47 |
| 1:F:257:LEU:HG | 1:F:371:GLY:O | 2.12 | 0.47 |
| 1:F:286:ASN:OD1 | 1:F:327:PHE:HD1 | 1.97 | 0.47 |
| 1:F:303:ARG:CG | 1:F:357:LYS:HE2 | 2.39 | 0.47 |
| 2:H:167:LYS:HE2 | 2:H:171:TYR:HE2 | 1.80 | 0.47 |
| 5:M:26:LEU:HG | 5:M:30:ARG:NH1 | 2.29 | 0.47 |
| 5:M:45:ARG:O | 5:M:49:MET:HG3 | 2.14 | 0.47 |
| 1:B:36:ILE:HG23 | 1:B:36:ILE:O | 2.14 | 0.47 |
| 1:B:428:GLU:O | 1:B:431:VAL:HG12 | 2.14 | 0.47 |
| 1:C:18:LEU:HA | 1:C:137:VAL:CG2 | 2.44 | 0.47 |
| 1:C:91:CYS:O | 1:C:154:ALA:HA | 2.14 | 0.47 |
| 1:D:95:MET:CE | 1:D:97:ILE:HD11 | 2.44 | 0.47 |
| 1:E:104:LYS:HA | 1:E:107:ILE:CD1 | 2.44 | 0.47 |
| 1:E:153:GLU:OE1 | 1:E:169:ARG:HD3 | 2.14 | 0.47 |
| 1:E:315:ARG:HG3 | 1:E:316:LEU:HD12 | 1.94 | 0.47 |
| 1:F:653:GLN:HA | 1:F:658:LEU:HB3 | 1.94 | 0.47 |
| 2:H:203:LYS:HZ1 | 2:H:239:ARG:HH21 | 1.63 | 0.47 |
| 2:I:14:LEU:O | 2:I:17:ALA:HB3 | 2.14 | 0.47 |
| 1:B:436:PHE:HB3 | 1:B:440:GLU:CB | 2.44 | 0.47 |
| 1:D:257:LEU:HB2 | 1:D:389:LEU:HD13 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:286:ASN:OD1 | 1:E:327:PHE:HD1 | 1.97 | 0.47 |
| 2:J:256:VAL:HG21 | 2:J:288:GLN:HG3 | 1.95 | 0.47 |
| 2:G:179:GLN:O | 2:G:182:ILE:HG12 | 2.13 | 0.47 |
| 2:G:243:LEU:HD22 | 2:G:266:TYR:CG | 2.49 | 0.47 |
| 2:G:243:LEU:HD22 | 2:G:266:TYR:CD2 | 2.49 | 0.47 |
| 1:B:579:THR:O | 1:B:583:GLN:HG2 | 2.14 | 0.47 |
| 1:C:681:GLU:HG3 | 1:C:691:ARG:HD2 | 1.97 | 0.47 |
| 1:C:686:PHE:CE1 | 1:C:714:ILE:HG23 | 2.49 | 0.47 |
| 1:D:655:MET:O | 1:D:656:GLU:HB2 | 2.14 | 0.47 |
| 1:F:256:ILE:O | 1:F:370:ILE:HA | 2.14 | 0.47 |
| 2:J:212:CYS:HA | 2:J:279:MET:HE2 | 1.95 | 0.47 |
| 4:L:216:PHE:CD2 | 5:M:39:SER:HB2 | 2.49 | 0.47 |
| 5:M:64:MET:HG3 | 5:M:181:ILE:HG23 | 1.95 | 0.47 |
| 1:A:489:LYS:H | 1:A:490:PRO:HD2 | 1.80 | 0.47 |
| 1:B:297:GLU:O | 1:B:300:ALA:HB3 | 2.14 | 0.47 |
| 1:C:18:LEU:HD23 | 1:C:137:VAL:HG21 | 1.97 | 0.47 |
| 1:C:512:ASP:N | 1:C:513:PRO:CD | 2.77 | 0.47 |
| 1:D:281:GLU:N | 1:D:282:PRO:HA | 2.29 | 0.47 |
| 1:E:128:GLN:O | 1:E:176:LEU:HD12 | 2.14 | 0.47 |
| 1:E:257:LEU:HB2 | 1:E:389:LEU:HD13 | 1.96 | 0.47 |
| 2:H:162:ASN:ND2 | 2:H:188:VAL:HG23 | 2.29 | 0.47 |
| 2:I:162:ASN:O | 2:I:166:LEU:HG | 2.14 | 0.47 |
| 2:I:167:LYS:HE2 | 2:I:171:TYR:HE2 | 1.79 | 0.47 |
| 2:J:96:ASP:H | 2:J:97:PRO:HD2 | 1.80 | 0.47 |
| 4:L:222:LEU:O | 4:L:226:GLN:HG3 | 2.15 | 0.47 |
| 1:A:630:LEU:HD11 | 1:A:657:MET:HE3 | 1.95 | 0.47 |
| 1:B:455:ARG:HH21 | 1:B:481:LEU:CB | 2.28 | 0.47 |
| 1:C:40:SER:HB3 | 1:C:43:HIS:CG | 2.49 | 0.47 |
| 1:C:325:ILE:HG13 | 1:C:369:VAL:HG23 | 1.96 | 0.47 |
| 1:C:445:VAL:HG12 | 1:C:449:GLN:HE22 | 1.79 | 0.47 |
| 1:C:562:PHE:O | 1:C:565:ILE:HD11 | 2.15 | 0.47 |
| 1:C:593:TYR:CE2 | 1:C:632:LYS:NZ | 2.83 | 0.47 |
| 1:C:626:LEU:HD13 | 1:C:657:MET:HE2 | 1.96 | 0.47 |
| 1:D:564:PHE:HB3 | 1:D:598:SER:HB3 | 1.95 | 0.47 |
| 1:D:635:PRO:O | 1:D:638:ARG:HB2 | 2.14 | 0.47 |
| 1:D:694:ILE:O | 1:D:698:VAL:HG22 | 2.15 | 0.47 |
| 1:E:26:GLU:HG2 | 1:E:51:THR:HB | 1.95 | 0.47 |
| 1:E:612:VAL:CG2 | 1:E:613:PRO:HD2 | 2.45 | 0.47 |
| 2:H:276:LEU:O | 2:H:280:LEU:HG | 2.14 | 0.47 |
| 2:J:201:SER:OG | 2:J:205:TYR:HE1 | 1.92 | 0.47 |
| 2:J:219:LEU:HD23 | 2:J:219:LEU:H | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:263:VAL:HG23 | 2:J:280:LEU:HD13 | 1.96 | 0.47 |
| 2:G:82:ALA:HB2 | 2:G:110:ILE:HG21 | 1.95 | 0.47 |
| 1:A:687:LYS:NZ | 1:A:722:PRO:HB3 | 2.29 | 0.47 |
| 1:B:257:LEU:HG | 1:B:371:GLY:O | 2.15 | 0.47 |
| 1:B:640:LEU:CD2 | 1:B:642:ILE:HG13 | 2.44 | 0.47 |
| 1:C:356:SER:HB3 | 1:D:288:PRO:HG3 | 1.97 | 0.47 |
| 1:C:721:ASP:O | 1:C:725:ARG:HG3 | 2.14 | 0.47 |
| 1:E:106:ASN:HB3 | 1:E:143:LYS:NZ | 2.29 | 0.47 |
| 1:F:323:HIS:HB2 | 1:F:367:ILE:HG22 | 1.97 | 0.47 |
| 3:K:46:MET:HA | 3:K:49:ASN:HB2 | 1.95 | 0.47 |
| 1:A:242:PRO:HD2 | 1:A:243:GLU:N | 2.29 | 0.47 |
| 1:A:510:TRP:CE3 | 1:A:675:GLN:HG2 | 2.50 | 0.47 |
| 1:C:311:GLU:O | 1:C:314:ARG:HG2 | 2.15 | 0.47 |
| 1:C:322:LEU:HD12 | 1:C:324:ILE:HD11 | 1.97 | 0.47 |
| 1:D:246:GLU:HG2 | 1:D:247:GLN:N | 2.30 | 0.47 |
| 1:D:611:TYR:CE2 | 1:D:613:PRO:HA | 2.50 | 0.47 |
| 1:D:688:ASP:O | 1:D:692:THR:HG23 | 2.15 | 0.47 |
| 1:E:240:PHE:HE1 | 1:F:457:ILE:CD1 | 2.28 | 0.47 |
| 1:A:111:PRO:CD | 1:A:320:SER:HA | 2.45 | 0.47 |
| 1:A:256:ILE:CG1 | 1:A:370:ILE:HG22 | 2.44 | 0.47 |
| 1:B:323:HIS:HB2 | 1:B:367:ILE:HG22 | 1.97 | 0.47 |
| 1:B:397:LEU:HD22 | 1:B:398:PRO:HD2 | 1.97 | 0.47 |
| 1:B:627:LEU:HB3 | 1:C:607:ARG:NH2 | 2.29 | 0.47 |
| 1:D:453:MET:O | 1:D:457:ILE:HG13 | 2.15 | 0.47 |
| 1:E:16:LEU:HD11 | 1:E:52:HIS:CD2 | 2.50 | 0.47 |
| 1:E:113:ASP:O | 1:E:117:MET:HG3 | 2.15 | 0.47 |
| 2:J:147:GLN:HG2 | 2:J:151:TYR:CE2 | 2.50 | 0.47 |
| 3:K:50:VAL:O | 3:K:54:LEU:HG | 2.15 | 0.47 |
| 1:A:564:PHE:CZ | 1:A:566:LYS:HB2 | 2.50 | 0.46 |
| 1:B:307:ALA:HA | 1:B:310:GLU:HG2 | 1.97 | 0.46 |
| 1:C:707:ILE:O | 1:C:711:LEU:HG | 2.15 | 0.46 |
| 1:D:45:TYR:CE2 | 1:D:70:ALA:HA | 2.49 | 0.46 |
| 1:D:89:LYS:NZ | 1:D:89:LYS:HB3 | 2.29 | 0.46 |
| 1:E:40:SER:OG | 1:E:43:HIS:HB2 | 2.15 | 0.46 |
| 1:F:40:SER:HB3 | 1:F:43:HIS:ND1 | 2.30 | 0.46 |
| 1:F:686:PHE:HE1 | 1:F:714:ILE:HG23 | 1.79 | 0.46 |
| 2:H:180:LYS:O | 2:H:184:ILE:HG13 | 2.15 | 0.46 |
| 2:I:230:GLU:HG2 | 2:I:231:LEU:N | 2.30 | 0.46 |
| 2:I:244:MET:O | 2:I:248:LEU:HG | 2.15 | 0.46 |
| 2:G:188:VAL:HG13 | 2:G:205:TYR:HD2 | 1.80 | 0.46 |
| 2:G:260:THR:HA | 2:G:263:VAL:HG12 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:28:SER:O | 5:M:32:MET:HB2 | 2.15 | 0.46 |
| 1:A:542:GLU:HA | 1:A:646:THR:O | 2.15 | 0.46 |
| 1:A:562:PHE:CE1 | 1:A:641:LEU:HD21 | 2.50 | 0.46 |
| 1:A:611:TYR:CE1 | 1:A:616:PRO:HB2 | 2.51 | 0.46 |
| 1:B:653:GLN:OE1 | 1:B:658:LEU:HD22 | 2.15 | 0.46 |
| 1:D:536:LEU:HD21 | 1:D:630:LEU:O | 2.15 | 0.46 |
| 2:H:11:MET:HA | 2:H:14:LEU:HD12 | 1.97 | 0.46 |
| 2:G:203:LYS:HZ2 | 2:G:236:SER:C | 2.18 | 0.46 |
| 5:M:34:GLN:HA | 5:M:37:GLU:HB2 | 1.95 | 0.46 |
| 5:M:42:ALA:HA | 5:M:45:ARG:CZ | 2.44 | 0.46 |
| 1:A:111:PRO:HG3 | 1:A:321:GLY:O | 2.16 | 0.46 |
| 1:A:319:ASN:O | 1:A:320:SER:HB2 | 2.15 | 0.46 |
| 1:B:64:LEU:CA | 1:B:67:ARG:HH21 | 2.28 | 0.46 |
| 1:B:149:VAL:HG11 | 1:B:152:ILE:HD11 | 1.98 | 0.46 |
| 1:C:414:MET:CE | 1:C:414:MET:HA | 2.45 | 0.46 |
| 1:E:46:ILE:HD12 | 1:E:174:VAL:HG11 | 1.96 | 0.46 |
| 1:E:562:PHE:CD1 | 1:E:597:LEU:HG | 2.50 | 0.46 |
| 1:E:627:LEU:HG | 1:E:657:MET:HE1 | 1.97 | 0.46 |
| 2:I:200:TYR:HB2 | 3:K:47:ARG:HH12 | 1.79 | 0.46 |
| 2:J:63:ASN:O | 2:J:67:GLN:HG3 | 2.15 | 0.46 |
| 2:G:45:TYR:HB2 | 2:G:68:ALA:HB2 | 1.98 | 0.46 |
| 1:B:261:PRO:HB3 | 1:B:594:LYS:HZ2 | 1.78 | 0.46 |
| 1:C:45:TYR:CE2 | 1:C:70:ALA:HA | 2.50 | 0.46 |
| 1:C:355:LEU:O | 1:C:388:ARG:NH2 | 2.42 | 0.46 |
| 1:D:312:GLU:HG3 | 1:D:313:GLN:N | 2.31 | 0.46 |
| 1:D:542:GLU:OE2 | 1:D:649:LYS:HD2 | 2.16 | 0.46 |
| 1:D:571:ASP:O | 1:D:574:ILE:HG13 | 2.15 | 0.46 |
| 1:D:627:LEU:HA | 1:D:627:LEU:HD23 | 1.56 | 0.46 |
| 1:E:111:PRO:HB2 | 1:E:196:ILE:HD13 | 1.98 | 0.46 |
| 1:E:188:ALA:O | 1:E:189:GLU:C | 2.53 | 0.46 |
| 1:E:250:CYS:SG | 1:F:446:ARG:HD2 | 2.55 | 0.46 |
| 1:F:289:GLU:C | 1:F:291:LEU:H | 2.14 | 0.46 |
| 2:I:81:ALA:O | 2:I:85:PHE:HD1 | 1.99 | 0.46 |
| 4:L:210:ARG:HH21 | 5:M:31:ARG:HH21 | 1.63 | 0.46 |
| 1:B:249:GLY:N | 1:C:414:MET:HE1 | 2.30 | 0.46 |
| 1:B:628:VAL:HG13 | 1:C:571:ASP:OD1 | 2.16 | 0.46 |
| 1:C:240:PHE:HE2 | 1:D:456:HIS:HD1 | 1.62 | 0.46 |
| 1:C:536:LEU:CD1 | 1:C:640:LEU:HB3 | 2.46 | 0.46 |
| 1:C:568:CYS:HB2 | 1:C:602:VAL:HA | 1.97 | 0.46 |
| 2:I:21:VAL:HG23 | 2:I:38:ILE:HD13 | 1.96 | 0.46 |
| 2:G:98:GLN:C | 2:G:100:ALA:H | 2.19 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:252:LYS:O | 4:L:255:VAL:HG22 | 2.15 | 0.46 |
| 5:M:67:ILE:O | 5:M:71:MET:HG2 | 2.15 | 0.46 |
| 1:B:46:ILE:HD12 | 1:B:174:VAL:HG21 | 1.97 | 0.46 |
| 1:C:428:GLU:O | 1:C:431:VAL:HG12 | 2.15 | 0.46 |
| 1:E:510:TRP:CE3 | 1:E:511:GLY:HA3 | 2.50 | 0.46 |
| 1:F:325:ILE:HG13 | 1:F:369:VAL:HB | 1.96 | 0.46 |
| 1:F:503:ILE:HD11 | 1:F:554:ALA:HB3 | 1.98 | 0.46 |
| 2:G:118:THR:O | 2:G:122:LYS:HG2 | 2.15 | 0.46 |
| 4:L:212:LEU:HA | 4:L:215:MET:CE | 2.46 | 0.46 |
| 1:C:64:LEU:HA | 1:C:67:ARG:HH21 | 1.81 | 0.46 |
| 1:D:310:GLU:O | 1:D:313:GLN:CG | 2.64 | 0.46 |
| 1:D:407:LEU:O | 1:D:411:THR:HG23 | 2.16 | 0.46 |
| 1:D:519:ASP:O | 1:D:523:LEU:HG | 2.15 | 0.46 |
| 1:E:236:ALA:HA | 1:E:239:VAL:CG1 | 2.46 | 0.46 |
| 1:E:272:GLN:OE1 | 1:E:272:GLN:HA | 2.14 | 0.46 |
| 1:E:440:GLU:O | 1:E:444:LEU:HG | 2.16 | 0.46 |
| 2:J:203:LYS:HD3 | 2:J:236:SER:HB3 | 1.97 | 0.46 |
| 2:G:235:PHE:CD2 | 5:M:152:GLN:HA | 2.50 | 0.46 |
| 1:A:546:HIS:CE1 | 1:F:659:ASN:OD1 | 2.69 | 0.46 |
| 1:A:548:GLY:C | 1:A:550:THR:N | 2.65 | 0.46 |
| 1:B:76:GLN:HE21 | 1:B:78:ILE:CG2 | 2.29 | 0.46 |
| 1:B:249:GLY:HA3 | 1:C:414:MET:HE1 | 1.96 | 0.46 |
| 1:B:281:GLU:N | 1:B:282:PRO:HA | 2.31 | 0.46 |
| 1:C:106:ASN:HB3 | 1:C:143:LYS:HZ1 | 1.77 | 0.46 |
| 2:H:166:LEU:HD21 | 2:H:205:TYR:CE2 | 2.51 | 0.46 |
| 2:G:182:ILE:CG2 | 2:G:212:CYS:HB2 | 2.46 | 0.46 |
| 5:M:62:GLU:O | 5:M:66:HIS:HB2 | 2.16 | 0.46 |
| 1:A:398:PRO:HG3 | 1:A:436:PHE:C | 2.36 | 0.46 |
| 1:C:23:VAL:HG12 | 1:C:55:VAL:CG2 | 2.46 | 0.46 |
| 1:C:513:PRO:HA | 1:C:516:ARG:HG2 | 1.98 | 0.46 |
| 1:E:307:ALA:HA | 1:E:310:GLU:HG2 | 1.98 | 0.46 |
| 1:F:23:VAL:HG12 | 1:F:55:VAL:HG21 | 1.98 | 0.46 |
| 2:J:287:ILE:O | 2:J:291:GLU:HG3 | 2.15 | 0.46 |
| 2:G:79:HIS:O | 2:G:83:THR:HG23 | 2.15 | 0.46 |
| 2:G:203:LYS:HB3 | 2:G:240:GLU:HG3 | 1.98 | 0.46 |
| 4:L:210:ARG:NH2 | 5:M:31:ARG:HH21 | 2.13 | 0.46 |
| 1:A:23:VAL:HG12 | 1:A:55:VAL:HG21 | 1.98 | 0.46 |
| 1:A:242:PRO:O | 1:A:245:VAL:HG12 | 2.16 | 0.46 |
| 1:B:402:GLY:O | 1:B:406:ILE:HD12 | 2.15 | 0.46 |
| 1:B:523:LEU:HA | 1:B:526:GLN:HG2 | 1.98 | 0.46 |
| 1:C:540:LEU:HD22 | 1:C:661:PHE:CD2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:531:SER:HB3 | 1:E:534:THR:O | 2.16 | 0.46 |
| 2:H:95:ALA:CB | 2:H:97:PRO:HD2 | 2.46 | 0.46 |
| 3:K:29:ASN:HA | 4:L:198:ARG:NH1 | 2.30 | 0.46 |
| 5:M:184:LYS:HD2 | 5:M:184:LYS:N | 2.31 | 0.46 |
| 1:A:623:LEU:O | 1:A:626:LEU:HB3 | 2.16 | 0.45 |
| 1:A:713:LEU:CD2 | 1:A:732:LEU:HB3 | 2.41 | 0.45 |
| 1:B:24:VAL:HG23 | 1:B:51:THR:HG22 | 1.97 | 0.45 |
| 1:B:236:ALA:HA | 1:B:239:VAL:CG1 | 2.45 | 0.45 |
| 1:D:122:ILE:HD11 | 1:D:183:VAL:HG23 | 1.97 | 0.45 |
| 1:D:609:LEU:O | 1:D:610:ASP:OD1 | 2.34 | 0.45 |
| 1:F:517:VAL:HG21 | 1:F:667:VAL:HG22 | 1.98 | 0.45 |
| 2:H:159:SER:OG | 4:L:225:SER:HB2 | 2.15 | 0.45 |
| 2:I:200:TYR:O | 2:I:203:LYS:HE2 | 2.16 | 0.45 |
| 2:G:20:LYS:HG2 | 2:G:37:LYS:HB3 | 1.98 | 0.45 |
| 5:M:27:GLU:O | 5:M:31:ARG:HG3 | 2.16 | 0.45 |
| 1:A:91:CYS:O | 1:A:154:ALA:HA | 2.17 | 0.45 |
| 1:A:215:PHE:N | 1:A:231:PHE:CE2 | 2.84 | 0.45 |
| 1:B:627:LEU:CD2 | 1:B:657:MET:HG3 | 2.44 | 0.45 |
| 1:C:285:VAL:HA | 1:C:326:ILE:HG13 | 1.97 | 0.45 |
| 1:D:122:ILE:HD11 | 1:D:183:VAL:CG2 | 2.46 | 0.45 |
| 1:D:608:LEU:O | 1:D:622:VAL:HG11 | 2.16 | 0.45 |
| 1:E:519:ASP:O | 1:E:522:GLU:HB2 | 2.17 | 0.45 |
| 1:E:589:PHE:CE2 | 1:E:629:LEU:HD21 | 2.52 | 0.45 |
| 1:E:677:LEU:HD11 | 1:E:695:ALA:HA | 1.99 | 0.45 |
| 1:F:440:GLU:O | 1:F:444:LEU:HG | 2.16 | 0.45 |
| 1:F:545:PRO:CB | 1:F:546:HIS:HA | 2.44 | 0.45 |
| 1:F:707:ILE:O | 1:F:710:LEU:HB3 | 2.15 | 0.45 |
| 2:J:81:ALA:O | 2:J:85:PHE:HD1 | 1.98 | 0.45 |
| 1:B:121:PHE:CD2 | 1:B:183:VAL:HG21 | 2.52 | 0.45 |
| 1:B:423:ASP:HB2 | 1:B:479:ASP:N | 2.31 | 0.45 |
| 1:C:620:ASN:O | 1:C:624:GLN:HG2 | 2.15 | 0.45 |
| 1:F:242:PRO:HD2 | 1:F:243:GLU:N | 2.32 | 0.45 |
| 2:H:45:TYR:CE2 | 2:H:71:LEU:HD11 | 2.51 | 0.45 |
| 2:I:164:CYS:O | 2:I:168:VAL:HG23 | 2.16 | 0.45 |
| 2:I:214:PHE:H | 2:I:214:PHE:HD1 | 1.64 | 0.45 |
| 2:I:232:PHE:HB2 | 2:I:233:PRO:HD3 | 1.97 | 0.45 |
| 2:J:161:ALA:O | 2:J:165:LEU:HG | 2.16 | 0.45 |
| 2:J:195:SER:C | 2:J:197:LEU:H | 2.19 | 0.45 |
| 2:G:124:HIS:HE1 | 2:G:147:GLN:HB3 | 1.81 | 0.45 |
| 4:L:247:ALA:O | 4:L:251:THR:HG23 | 2.17 | 0.45 |
| 5:M:17:ARG:NE | 5:M:21:LEU:HD11 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:23:VAL:HG12 | 1:A:55:VAL:CG2 | 2.47 | 0.45 |
| 1:A:705:ILE:HD13 | 1:A:710:LEU:CD1 | 2.38 | 0.45 |
| 1:B:540:LEU:HD12 | 1:B:540:LEU:O | 2.16 | 0.45 |
| 1:C:128:GLN:O | 1:C:176:LEU:HD12 | 2.16 | 0.45 |
| 1:D:122:ILE:O | 1:D:126:ASN:HB3 | 2.16 | 0.45 |
| 1:D:533:ARG:HD2 | 1:E:505:ASN:ND2 | 2.32 | 0.45 |
| 1:D:564:PHE:HB3 | 1:D:598:SER:CB | 2.46 | 0.45 |
| 1:D:567:ILE:HG23 | 1:D:601:VAL:HB | 1.99 | 0.45 |
| 1:D:609:LEU:CD1 | 1:D:611:TYR:HB2 | 2.47 | 0.45 |
| 1:E:27:LYS:HD2 | 1:E:57:PRO:HG3 | 1.97 | 0.45 |
| 1:F:16:LEU:HD11 | 1:F:52:HIS:HD2 | 1.80 | 0.45 |
| 1:F:254:LYS:O | 1:F:368:LEU:HA | 2.16 | 0.45 |
| 3:K:56:ARG:HH21 | 5:M:174:GLN:CB | 2.30 | 0.45 |
| 5:M:176:ARG:HD3 | 5:M:180:ARG:NH1 | 2.31 | 0.45 |
| 1:A:258:LEU:O | 1:A:258:LEU:HD12 | 2.17 | 0.45 |
| 1:A:542:GLU:OE2 | 1:A:666:HIS:CD2 | 2.69 | 0.45 |
| 1:A:611:TYR:HA | 1:A:618:PHE:HB3 | 1.99 | 0.45 |
| 1:A:624:GLN:OE1 | 1:A:624:GLN:HA | 2.16 | 0.45 |
| 1:B:122:ILE:O | 1:B:126:ASN:HB3 | 2.17 | 0.45 |
| 1:C:121:PHE:HD2 | 1:C:183:VAL:HG21 | 1.81 | 0.45 |
| 1:D:36:ILE:HG23 | 1:D:36:ILE:O | 2.16 | 0.45 |
| 1:D:286:ASN:HB2 | 1:D:327:PHE:CD1 | 2.50 | 0.45 |
| 1:D:686:PHE:HB3 | 1:D:690:GLU:HG3 | 1.97 | 0.45 |
| 1:E:23:VAL:HG12 | 1:E:55:VAL:HG21 | 1.98 | 0.45 |
| 1:E:113:ASP:HA | 1:E:196:ILE:HG13 | 1.98 | 0.45 |
| 1:F:12:PRO:HG2 | 1:F:23:VAL:HG11 | 1.98 | 0.45 |
| 1:F:113:ASP:OD1 | 1:F:115:ASP:HB2 | 2.17 | 0.45 |
| 1:F:597:LEU:HA | 1:F:639:LYS:O | 2.17 | 0.45 |
| 1:F:618:PHE:HE1 | 1:F:620:ASN:HA | 1.82 | 0.45 |
| 2:I:63:ASN:O | 2:I:67:GLN:HG3 | 2.15 | 0.45 |
| 1:B:40:SER:CB | 1:B:41:PRO:CD | 2.94 | 0.45 |
| 1:B:125:PHE:HD2 | 1:B:130:PHE:HZ | 1.65 | 0.45 |
| 1:B:247:GLN:O | 1:C:414:MET:SD | 2.75 | 0.45 |
| 1:C:220:ILE:HD11 | 1:C:272:GLN:HG3 | 1.97 | 0.45 |
| 1:C:540:LEU:HD11 | 1:C:646:THR:HG22 | 1.99 | 0.45 |
| 1:D:326:ILE:HG22 | 1:D:370:ILE:CG1 | 2.47 | 0.45 |
| 1:E:45:TYR:CE2 | 1:E:70:ALA:HA | 2.52 | 0.45 |
| 1:E:101:PHE:CD2 | 1:E:107:ILE:HA | 2.51 | 0.45 |
| 1:E:436:PHE:HB3 | 1:E:440:GLU:CB | 2.47 | 0.45 |
| 1:E:507:ILE:HD13 | 1:E:507:ILE:HA | 1.75 | 0.45 |
| 1:E:527:GLN:HA | 1:F:719:GLN:HG3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:18:LEU:HA | 1:F:137:VAL:CG2 | 2.46 | 0.45 |
| 1:F:414:MET:SD | 1:F:449:GLN:NE2 | 2.88 | 0.45 |
| 1:F:705:ILE:HG12 | 1:F:706:GLY:O | 2.15 | 0.45 |
| 2:J:188:VAL:HG13 | 2:J:205:TYR:CD2 | 2.51 | 0.45 |
| 2:J:197:LEU:HD13 | 3:K:52:LYS:HE3 | 1.99 | 0.45 |
| 1:A:45:TYR:CE2 | 1:A:70:ALA:HA | 2.52 | 0.45 |
| 1:B:24:VAL:O | 1:B:51:THR:HA | 2.16 | 0.45 |
| 1:B:436:PHE:N | 1:B:436:PHE:CD1 | 2.84 | 0.45 |
| 1:B:536:LEU:HD12 | 1:B:640:LEU:O | 2.17 | 0.45 |
| 1:C:256:ILE:O | 1:C:370:ILE:HA | 2.17 | 0.45 |
| 1:D:303:ARG:HD3 | 1:D:353:GLN:CD | 2.37 | 0.45 |
| 1:D:710:LEU:HG | 1:D:714:ILE:HD11 | 1.99 | 0.45 |
| 1:E:586:LYS:NZ | 1:F:575:GLY:HA3 | 2.31 | 0.45 |
| 1:F:242:PRO:CD | 1:F:243:GLU:H | 2.28 | 0.45 |
| 1:F:327:PHE:CE2 | 1:F:369:VAL:HG21 | 2.52 | 0.45 |
| 1:F:605:ILE:O | 1:F:608:LEU:HG | 2.16 | 0.45 |
| 2:J:223:LEU:O | 2:J:227:LYS:HG3 | 2.16 | 0.45 |
| 1:A:69:TRP:CE2 | 1:A:134:GLN:HA | 2.52 | 0.45 |
| 1:A:489:LYS:N | 1:A:490:PRO:HD2 | 2.31 | 0.45 |
| 1:A:509:LYS:HG2 | 1:A:515:THR:OG1 | 2.17 | 0.45 |
| 1:B:218:MET:HA | 1:B:219:GLY:HA2 | 1.75 | 0.45 |
| 1:C:99:ILE:HG23 | 1:C:193:LEU:HD23 | 1.98 | 0.45 |
| 1:C:331:ASP:CA | 1:C:379:ILE:HD11 | 2.44 | 0.45 |
| 1:C:552:LEU:HD23 | 1:C:552:LEU:HA | 1.81 | 0.45 |
| 1:C:613:PRO:HD3 | 1:C:648:ARG:HH22 | 1.81 | 0.45 |
| 1:D:132:VAL:HG23 | 1:D:173:GLU:O | 2.17 | 0.45 |
| 1:E:86:ASP:O | 1:E:88:ALA:N | 2.49 | 0.45 |
| 1:F:119:ALA:O | 1:F:123:GLN:HB2 | 2.17 | 0.45 |
| 1:F:263:GLY:O | 1:F:398:PRO:HG3 | 2.17 | 0.45 |
| 1:F:449:GLN:O | 1:F:453:MET:HG2 | 2.17 | 0.45 |
| 1:F:552:LEU:O | 1:F:556:ILE:HG13 | 2.16 | 0.45 |
| 1:F:612:VAL:HG13 | 1:F:614:ILE:O | 2.16 | 0.45 |
| 2:J:72:HIS:O | 2:J:75:LEU:HB3 | 2.16 | 0.45 |
| 2:J:185:TYR:HA | 2:J:188:VAL:HG12 | 1.97 | 0.45 |
| 1:A:36:ILE:HG23 | 1:A:36:ILE:O | 2.15 | 0.45 |
| 1:A:122:ILE:O | 1:A:126:ASN:HB3 | 2.17 | 0.45 |
| 1:A:436:PHE:CD2 | 1:A:444:LEU:HD11 | 2.51 | 0.45 |
| 1:A:457:ILE:CD1 | 1:F:236:ALA:HB1 | 2.47 | 0.45 |
| 1:A:526:GLN:O | 1:A:530:ASN:HB2 | 2.16 | 0.45 |
| 1:B:348:ASP:O | 1:B:352:ASN:ND2 | 2.50 | 0.45 |
| 1:C:539:VAL:HG23 | 1:C:663:THR:HG23 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:589:PHE:CD2 | 1:D:629:LEU:HD13 | 2.52 | 0.45 |
| 1:E:299:GLU:HG3 | 1:E:349:THR:CB | 2.47 | 0.45 |
| 1:E:713:LEU:CD2 | 1:E:732:LEU:HD13 | 2.47 | 0.45 |
| 1:F:319:ASN:HB3 | 1:F:320:SER:HB2 | 1.97 | 0.45 |
| 2:H:176:GLU:O | 2:H:178:TYR:N | 2.47 | 0.45 |
| 3:K:82:ALA:O | 3:K:85:LYS:HB3 | 2.17 | 0.45 |
| 4:L:210:ARG:HG2 | 4:L:210:ARG:HH11 | 1.82 | 0.45 |
| 1:A:610:ASP:OD1 | 1:F:620:ASN:ND2 | 2.50 | 0.45 |
| 1:A:617:ARG:HG3 | 1:A:617:ARG:NH1 | 2.30 | 0.45 |
| 1:B:677:LEU:O | 1:B:681:GLU:HG3 | 2.17 | 0.45 |
| 1:C:511:GLY:C | 1:C:513:PRO:HD2 | 2.36 | 0.45 |
| 1:C:555:LYS:O | 1:C:559:GLU:HG2 | 2.17 | 0.45 |
| 1:D:303:ARG:HH11 | 1:D:357:LYS:CE | 2.30 | 0.45 |
| 1:D:670:ILE:HG12 | 1:D:705:ILE:O | 2.17 | 0.45 |
| 1:D:686:PHE:HB2 | 1:D:691:ARG:CG | 2.47 | 0.45 |
| 1:E:149:VAL:HG11 | 1:E:152:ILE:HD11 | 1.97 | 0.45 |
| 1:E:721:ASP:HB2 | 1:E:724:TYR:CD2 | 2.52 | 0.45 |
| 1:F:36:ILE:HG23 | 1:F:36:ILE:O | 2.17 | 0.45 |
| 2:H:53:LYS:HD2 | 2:I:117:PHE:CE2 | 2.51 | 0.45 |
| 2:H:78:LYS:HB3 | 2:H:110:ILE:HG23 | 1.98 | 0.45 |
| 2:H:116:ARG:NH1 | 2:H:116:ARG:HG3 | 2.32 | 0.45 |
| 2:H:203:LYS:HB2 | 2:H:203:LYS:HE3 | 1.52 | 0.45 |
| 2:I:236:SER:HA | 2:I:239:ARG:NH1 | 2.32 | 0.45 |
| 2:I:243:LEU:HD13 | 2:I:266:TYR:HB2 | 1.99 | 0.45 |
| 2:J:230:GLU:HG3 | 2:J:237:ASP:HB3 | 1.98 | 0.45 |
| 1:A:24:VAL:HG11 | 1:A:49:LEU:HD22 | 1.98 | 0.44 |
| 1:A:111:PRO:HG2 | 1:A:320:SER:HA | 1.99 | 0.44 |
| 1:A:270:ALA:HA | 1:A:273:ILE:HG22 | 1.98 | 0.44 |
| 1:A:502:TYR:N | 1:A:502:TYR:HD1 | 2.15 | 0.44 |
| 1:A:573:MET:HA | 1:A:576:PHE:CD2 | 2.53 | 0.44 |
| 1:A:636:GLN:HA | 1:A:637:GLY:HA2 | 1.47 | 0.44 |
| 1:A:721:ASP:O | 1:A:725:ARG:HG3 | 2.17 | 0.44 |
| 1:B:311:GLU:O | 1:B:314:ARG:HG2 | 2.17 | 0.44 |
| 1:D:227:PHE:O | 1:D:230:ILE:HG22 | 2.17 | 0.44 |
| 1:D:552:LEU:O | 1:D:556:ILE:HG13 | 2.18 | 0.44 |
| 1:D:628:VAL:O | 1:D:632:LYS:N | 2.51 | 0.44 |
| 1:E:101:PHE:HE1 | 1:E:193:LEU:HB2 | 1.82 | 0.44 |
| 1:E:325:ILE:HG13 | 1:E:369:VAL:HB | 1.98 | 0.44 |
| 1:E:377:ASP:OD1 | 1:E:378:LEU:N | 2.50 | 0.44 |
| 1:F:307:ALA:O | 1:F:310:GLU:HG2 | 2.17 | 0.44 |
| 1:F:428:GLU:O | 1:F:431:VAL:HG12 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:38:ILE:HD11 | 2:J:71:LEU:HB3 | 1.98 | 0.44 |
| 5:M:142:ARG:HG2 | 5:M:142:ARG:NH1 | 2.33 | 0.44 |
| 1:A:16:LEU:HD11 | 1:A:52:HIS:HD2 | 1.81 | 0.44 |
| 1:A:242:PRO:HD2 | 1:A:243:GLU:OE1 | 2.17 | 0.44 |
| 1:B:528:THR:HG21 | 1:B:641:LEU:HD13 | 2.00 | 0.44 |
| 1:C:547:SER:HB2 | 1:C:549:LYS:HG3 | 2.00 | 0.44 |
| 1:C:635:PRO:HB2 | 1:C:638:ARG:NH1 | 2.31 | 0.44 |
| 1:D:624:GLN:OE1 | 1:D:624:GLN:HA | 2.18 | 0.44 |
| 1:D:731:ALA:HA | 1:D:734:ARG:HH12 | 1.82 | 0.44 |
| 1:E:67:ARG:NH1 | 1:E:74:ILE:HD11 | 2.32 | 0.44 |
| 1:E:536:LEU:HD22 | 1:E:634:PRO:HD3 | 1.98 | 0.44 |
| 1:F:24:VAL:O | 1:F:51:THR:HA | 2.17 | 0.44 |
| 2:H:92:PHE:HB3 | 2:H:98:GLN:O | 2.16 | 0.44 |
| 2:I:166:LEU:HD21 | 2:I:205:TYR:CE2 | 2.52 | 0.44 |
| 2:I:243:LEU:HD22 | 2:I:266:TYR:CG | 2.51 | 0.44 |
| 2:J:20:LYS:NZ | 2:J:40:GLU:HG2 | 2.31 | 0.44 |
| 2:G:47:ARG:O | 2:G:50:ASN:HB3 | 2.17 | 0.44 |
| 2:G:283:ILE:O | 2:G:287:ILE:HG13 | 2.17 | 0.44 |
| 2:G:287:ILE:O | 2:G:291:GLU:HG3 | 2.17 | 0.44 |
| 3:K:43:VAL:HG13 | 4:L:215:MET:HE1 | 1.99 | 0.44 |
| 3:K:55:GLU:O | 3:K:59:LYS:HG3 | 2.18 | 0.44 |
| 1:A:410:HIS:NE2 | 1:A:442:GLU:HG2 | 2.32 | 0.44 |
| 1:B:246:GLU:HG3 | 1:C:417:HIS:CE1 | 2.53 | 0.44 |
| 1:C:544:PRO:HG2 | 1:C:669:ASN:CG | 2.37 | 0.44 |
| 1:D:510:TRP:NE1 | 1:D:514:VAL:HG21 | 2.33 | 0.44 |
| 1:E:563:PRO:HD2 | 1:E:597:LEU:O | 2.18 | 0.44 |
| 1:E:691:ARG:HA | 1:E:694:ILE:HD12 | 1.99 | 0.44 |
| 1:F:272:GLN:OE1 | 1:F:272:GLN:HA | 2.17 | 0.44 |
| 2:H:101:ILE:O | 2:H:105:MET:HG3 | 2.18 | 0.44 |
| 2:J:21:VAL:O | 2:J:21:VAL:HG22 | 2.18 | 0.44 |
| 2:J:182:ILE:CG2 | 2:J:212:CYS:HB2 | 2.47 | 0.44 |
| 1:A:502:TYR:N | 1:A:502:TYR:CD1 | 2.84 | 0.44 |
| 1:B:16:LEU:HD11 | 1:B:52:HIS:HD2 | 1.82 | 0.44 |
| 1:B:101:PHE:CD2 | 1:B:107:ILE:HA | 2.52 | 0.44 |
| 1:B:546:HIS:O | 1:B:547:SER:OG | 2.27 | 0.44 |
| 1:C:499:TYR:HB3 | 1:C:558:GLU:OE2 | 2.18 | 0.44 |
| 1:E:36:ILE:HG23 | 1:E:36:ILE:O | 2.17 | 0.44 |
| 1:E:69:TRP:NE1 | 1:E:134:GLN:HA | 2.33 | 0.44 |
| 1:E:254:LYS:O | 1:E:368:LEU:HA | 2.17 | 0.44 |
| 1:E:507:ILE:O | 1:E:507:ILE:HG22 | 2.17 | 0.44 |
| 1:F:525:VAL:HG11 | 1:F:560:SER:CB | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:588:ILE:O | 1:F:591:ASP:HB2 | 2.18 | 0.44 |
| 2:I:276:LEU:O | 2:I:280:LEU:HG | 2.18 | 0.44 |
| 2:J:243:LEU:O | 2:J:247:LEU:HG | 2.18 | 0.44 |
| 2:G:32:PHE:HD1 | 2:G:32:PHE:H | 1.65 | 0.44 |
| 1:B:569:SER:OG | 1:B:571:ASP:OD2 | 2.34 | 0.44 |
| 1:C:104:LYS:HA | 1:C:107:ILE:HD11 | 1.98 | 0.44 |
| 1:C:606:GLU:HB2 | 1:C:648:ARG:HD2 | 1.99 | 0.44 |
| 1:E:65:PRO:HG2 | 1:E:137:VAL:HG13 | 2.00 | 0.44 |
| 1:E:114:THR:CG2 | 1:E:195:LEU:HB3 | 2.47 | 0.44 |
| 1:E:327:PHE:CE2 | 1:E:369:VAL:HG21 | 2.52 | 0.44 |
| 1:E:539:VAL:HG13 | 1:E:643:ILE:HA | 2.00 | 0.44 |
| 1:E:586:LYS:NZ | 1:F:574:ILE:HG23 | 2.33 | 0.44 |
| 1:F:560:SER:HB2 | 1:F:562:PHE:CD1 | 2.52 | 0.44 |
| 2:H:75:LEU:O | 2:H:76:GLN:HB3 | 2.17 | 0.44 |
| 2:G:225:VAL:HG23 | 2:G:241:CYS:HB2 | 1.99 | 0.44 |
| 3:K:79:THR:O | 3:K:83:LYS:HG3 | 2.18 | 0.44 |
| 1:A:254:LYS:O | 1:A:368:LEU:HA | 2.17 | 0.44 |
| 1:D:527:GLN:HE22 | 1:E:716:MET:CA | 2.31 | 0.44 |
| 1:D:626:LEU:O | 1:D:630:LEU:HG | 2.17 | 0.44 |
| 1:D:632:LYS:HZ3 | 1:E:571:ASP:HB3 | 1.82 | 0.44 |
| 1:F:261:PRO:O | 1:F:264:CYS:HB2 | 2.18 | 0.44 |
| 1:F:324:ILE:HG12 | 1:F:368:LEU:HD11 | 2.00 | 0.44 |
| 1:F:436:PHE:CD2 | 1:F:444:LEU:HD11 | 2.53 | 0.44 |
| 2:G:81:ALA:O | 2:G:85:PHE:HD1 | 2.01 | 0.44 |
| 5:M:152:GLN:O | 5:M:156:ILE:HG13 | 2.18 | 0.44 |
| 1:A:611:TYR:HD1 | 1:A:618:PHE:HB3 | 1.82 | 0.44 |
| 1:C:76:GLN:HE21 | 1:C:78:ILE:CG2 | 2.30 | 0.44 |
| 1:C:688:ASP:HA | 1:C:691:ARG:NH1 | 2.32 | 0.44 |
| 1:C:721:ASP:HB2 | 1:C:724:TYR:CD1 | 2.52 | 0.44 |
| 1:F:218:MET:HA | 1:F:219:GLY:HA2 | 1.74 | 0.44 |
| 2:I:180:LYS:O | 2:I:184:ILE:HG13 | 2.18 | 0.44 |
| 2:J:216:ILE:HG12 | 2:J:220:ASN:HB2 | 1.98 | 0.44 |
| 2:G:75:LEU:O | 2:G:76:GLN:HB3 | 2.18 | 0.44 |
| 1:B:246:GLU:HA | 1:C:413:ARG:HH12 | 1.83 | 0.44 |
| 1:B:254:LYS:O | 1:B:368:LEU:HA | 2.18 | 0.44 |
| 1:B:353:GLN:HA | 1:C:288:PRO:CG | 2.47 | 0.44 |
| 1:B:609:LEU:HA | 1:B:609:LEU:HD23 | 1.60 | 0.44 |
| 1:C:149:VAL:HG11 | 1:C:152:ILE:HD11 | 1.99 | 0.44 |
| 1:C:257:LEU:HG | 1:C:371:GLY:O | 2.18 | 0.44 |
| 1:D:388:ARG:O | 1:D:389:LEU:HD23 | 2.18 | 0.44 |
| 1:D:627:LEU:CD2 | 1:D:657:MET:HG3 | 2.43 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:524:LEU:HD11 | 1:E:663:THR:HG21 | 1.99 | 0.44 |
| 1:F:69:TRP:CE2 | 1:F:134:GLN:HA | 2.53 | 0.44 |
| 1:F:315:ARG:HG3 | 1:F:316:LEU:HD12 | 2.00 | 0.44 |
| 2:H:169:ALA:HB2 | 2:H:184:ILE:HB | 2.00 | 0.44 |
| 2:G:167:LYS:HE2 | 2:G:171:TYR:HE2 | 1.83 | 0.44 |
| 1:D:25:SER:HB3 | 1:D:28:ASP:OD2 | 2.18 | 0.44 |
| 1:D:89:LYS:HB3 | 1:D:89:LYS:HZ3 | 1.83 | 0.44 |
| 1:D:236:ALA:HB1 | 1:E:453:MET:HG3 | 2.00 | 0.44 |
| 1:D:709:LYS:HA | 1:D:709:LYS:HD2 | 1.81 | 0.44 |
| 1:E:436:PHE:N | 1:E:436:PHE:CD1 | 2.86 | 0.44 |
| 1:E:641:LEU:HD12 | 1:E:641:LEU:O | 2.18 | 0.44 |
| 1:E:654:GLU:HG2 | 1:F:614:ILE:HD11 | 1.99 | 0.44 |
| 1:F:257:LEU:HB2 | 1:F:389:LEU:HD13 | 1.99 | 0.44 |
| 2:J:101:ILE:HB | 2:J:131:TYR:OH | 2.18 | 0.44 |
| 4:L:213:HIS:NE2 | 5:M:38:GLU:OE1 | 2.51 | 0.44 |
| 1:C:320:SER:O | 1:C:320:SER:OG | 2.31 | 0.43 |
| 1:C:528:THR:O | 1:C:639:LYS:HD3 | 2.18 | 0.43 |
| 1:C:582:CYS:SG | 1:C:621:LEU:HG | 2.58 | 0.43 |
| 1:C:671:ALA:HA | 1:C:703:VAL:O | 2.17 | 0.43 |
| 1:C:677:LEU:O | 1:C:681:GLU:OE1 | 2.36 | 0.43 |
| 1:F:240:PHE:HA | 1:F:241:PRO:HD3 | 1.75 | 0.43 |
| 1:F:307:ALA:HA | 1:F:310:GLU:HG2 | 1.99 | 0.43 |
| 2:H:38:ILE:CD1 | 2:H:71:LEU:HB3 | 2.47 | 0.43 |
| 2:H:167:LYS:HE2 | 2:H:171:TYR:CE2 | 2.53 | 0.43 |
| 2:H:200:TYR:CE2 | 5:M:38:GLU:HG2 | 2.53 | 0.43 |
| 2:I:203:LYS:HB2 | 2:I:203:LYS:HE3 | 1.74 | 0.43 |
| 2:J:108:ILE:HD12 | 2:J:127:ILE:HD12 | 1.99 | 0.43 |
| 2:J:247:LEU:HD22 | 2:J:259:TYR:CD1 | 2.52 | 0.43 |
| 4:L:216:PHE:CZ | 5:M:39:SER:HB2 | 2.53 | 0.43 |
| 1:A:355:LEU:HD22 | 1:A:388:ARG:NH1 | 2.33 | 0.43 |
| 1:A:624:GLN:HG3 | 1:B:610:ASP:CG | 2.38 | 0.43 |
| 1:B:531:SER:CB | 1:B:639:LYS:HD3 | 2.47 | 0.43 |
| 1:D:99:ILE:HD11 | 1:D:145:PHE:CD2 | 2.53 | 0.43 |
| 1:E:246:GLU:HG2 | 1:E:247:GLN:N | 2.33 | 0.43 |
| 1:E:696:GLN:OE1 | 1:E:696:GLN:HA | 2.18 | 0.43 |
| 1:F:122:ILE:O | 1:F:126:ASN:HB3 | 2.19 | 0.43 |
| 1:F:436:PHE:N | 1:F:436:PHE:CD1 | 2.85 | 0.43 |
| 1:F:589:PHE:O | 1:F:593:TYR:CD1 | 2.71 | 0.43 |
| 2:H:225:VAL:HG23 | 2:H:241:CYS:HB2 | 1.99 | 0.43 |
| 2:I:188:VAL:HG13 | 2:I:205:TYR:HD2 | 1.82 | 0.43 |
| 2:J:112:THR:HG23 | 2:J:117:PHE:CE1 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:204:ASP:OD2 | 2:G:208:LYS:HE2 | 2.18 | 0.43 |
| 1:A:609:LEU:HD23 | 1:A:609:LEU:HA | 1.78 | 0.43 |
| 1:A:713:LEU:HD23 | 1:A:713:LEU:HA | 1.74 | 0.43 |
| 1:B:257:LEU:HB2 | 1:B:389:LEU:HD13 | 2.00 | 0.43 |
| 1:B:508:ILE:HD13 | 1:B:683:LEU:HD21 | 2.00 | 0.43 |
| 1:B:669:ASN:OD1 | 1:B:706:GLY:HA2 | 2.17 | 0.43 |
| 1:D:149:VAL:HG11 | 1:D:152:ILE:HD11 | 2.00 | 0.43 |
| 1:D:543:GLY:O | 1:D:647:SER:HA | 2.18 | 0.43 |
| 1:E:91:CYS:O | 1:E:154:ALA:HA | 2.18 | 0.43 |
| 1:E:726:VAL:O | 1:E:730:LEU:HG | 2.19 | 0.43 |
| 2:H:58:TRP:HB3 | 2:H:95:ALA:HB2 | 2.00 | 0.43 |
| 2:J:178:TYR:OH | 2:J:282:ARG:HG2 | 2.18 | 0.43 |
| 2:J:256:VAL:HG21 | 2:J:288:GLN:CG | 2.48 | 0.43 |
| 2:G:83:THR:HB | 4:L:235:TYR:OH | 2.18 | 0.43 |
| 2:G:98:GLN:H | 2:G:98:GLN:CD | 2.22 | 0.43 |
| 2:G:247:LEU:HB3 | 2:G:259:TYR:HE1 | 1.84 | 0.43 |
| 5:M:63:GLY:O | 5:M:67:ILE:HG13 | 2.17 | 0.43 |
| 1:A:24:VAL:O | 1:A:51:THR:HA | 2.19 | 0.43 |
| 1:A:219:GLY:O | 1:A:220:ILE:HG13 | 2.18 | 0.43 |
| 1:A:242:PRO:O | 1:A:246:GLU:OE1 | 2.36 | 0.43 |
| 1:B:440:GLU:O | 1:B:444:LEU:HG | 2.19 | 0.43 |
| 1:C:48:THR:HG21 | 1:C:128:GLN:HG2 | 2.00 | 0.43 |
| 1:C:289:GLU:C | 1:C:291:LEU:H | 2.16 | 0.43 |
| 1:C:318:ALA:C | 1:C:319:ASN:HD22 | 2.21 | 0.43 |
| 1:C:511:GLY:CA | 1:C:513:PRO:HD2 | 2.48 | 0.43 |
| 1:C:569:SER:HB3 | 1:C:572:LYS:HG2 | 2.00 | 0.43 |
| 1:D:9:ALA:HA | 1:D:74:ILE:HG23 | 2.00 | 0.43 |
| 1:E:299:GLU:HG3 | 1:E:349:THR:OG1 | 2.19 | 0.43 |
| 1:E:628:VAL:HB | 1:F:574:ILE:HD12 | 2.00 | 0.43 |
| 1:E:705:ILE:CD1 | 1:E:713:LEU:HD12 | 2.49 | 0.43 |
| 2:I:161:ALA:O | 2:I:165:LEU:HG | 2.18 | 0.43 |
| 2:I:176:GLU:O | 2:I:178:TYR:N | 2.50 | 0.43 |
| 2:I:185:TYR:HA | 2:I:188:VAL:HG12 | 1.99 | 0.43 |
| 2:G:112:THR:HG23 | 2:G:117:PHE:CE1 | 2.53 | 0.43 |
| 3:K:56:ARG:HH21 | 5:M:174:GLN:HB3 | 1.83 | 0.43 |
| 1:A:235:PHE:N | 1:A:235:PHE:CD1 | 2.84 | 0.43 |
| 1:B:23:VAL:HG12 | 1:B:55:VAL:HG21 | 2.00 | 0.43 |
| 1:B:327:PHE:CE2 | 1:B:369:VAL:HG21 | 2.52 | 0.43 |
| 1:B:671:ALA:HA | 1:B:703:VAL:O | 2.18 | 0.43 |
| 1:C:39:THR:HG22 | 1:C:78:ILE:HG22 | 1.99 | 0.43 |
| 1:C:193:LEU:HG | 1:C:195:LEU:HG | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:408:HIS:O | 1:C:408:HIS:ND1 | 2.46 | 0.43 |
| 1:F:95:MET:HE3 | 1:F:97:ILE:HD11 | 1.99 | 0.43 |
| 2:H:186:GLU:O | 2:H:190:THR:HG23 | 2.19 | 0.43 |
| 2:I:112:THR:HG23 | 2:I:117:PHE:HE1 | 1.83 | 0.43 |
| 2:J:230:GLU:HG2 | 2:J:231:LEU:H | 1.81 | 0.43 |
| 5:M:188:ASN:O | 5:M:192:ILE:HG13 | 2.19 | 0.43 |
| 1:A:222:GLY:CA | 1:A:402:GLY:HA3 | 2.48 | 0.43 |
| 1:A:407:LEU:CD1 | 1:A:426:ILE:HG23 | 2.48 | 0.43 |
| 1:B:187:LYS:HZ3 | 1:B:315:ARG:NH1 | 2.17 | 0.43 |
| 1:B:651:VAL:CG1 | 1:B:655:MET:HE3 | 2.48 | 0.43 |
| 1:C:64:LEU:CA | 1:C:67:ARG:HH21 | 2.31 | 0.43 |
| 1:C:378:LEU:HD23 | 1:C:378:LEU:HA | 1.83 | 0.43 |
| 1:D:50:ARG:HG2 | 1:D:50:ARG:HH11 | 1.84 | 0.43 |
| 1:D:67:ARG:HH11 | 1:D:74:ILE:HD11 | 1.82 | 0.43 |
| 1:D:331:ASP:O | 1:D:332:ALA:HB3 | 2.19 | 0.43 |
| 1:D:566:LYS:HA | 1:D:566:LYS:HD3 | 1.81 | 0.43 |
| 1:E:717:SER:OG | 1:E:729:PHE:HB2 | 2.19 | 0.43 |
| 1:F:310:GLU:OE2 | 1:F:357:LYS:NZ | 2.50 | 0.43 |
| 1:F:589:PHE:N | 1:F:589:PHE:CD1 | 2.85 | 0.43 |
| 2:H:163:LYS:O | 2:H:167:LYS:HG2 | 2.19 | 0.43 |
| 2:I:134:GLU:O | 2:I:136:VAL:HG23 | 2.18 | 0.43 |
| 2:I:182:ILE:O | 2:I:186:GLU:HG2 | 2.17 | 0.43 |
| 2:J:59:SER:OG | 2:J:97:PRO:HD3 | 2.18 | 0.43 |
| 2:J:134:GLU:O | 2:J:136:VAL:HG23 | 2.19 | 0.43 |
| 2:G:256:VAL:HG21 | 2:G:288:GLN:CG | 2.48 | 0.43 |
| 1:B:507:ILE:HG13 | 1:B:555:LYS:HD3 | 2.00 | 0.43 |
| 1:C:99:ILE:HD11 | 1:C:145:PHE:CD2 | 2.53 | 0.43 |
| 1:E:311:GLU:O | 1:E:314:ARG:HG2 | 2.18 | 0.43 |
| 1:E:388:ARG:O | 1:E:389:LEU:HD23 | 2.18 | 0.43 |
| 1:E:627:LEU:HG | 1:E:657:MET:CE | 2.48 | 0.43 |
| 1:F:96:THR:HG22 | 1:F:150:LYS:HB2 | 2.00 | 0.43 |
| 1:F:555:LYS:HD3 | 1:F:559:GLU:HG2 | 2.01 | 0.43 |
| 2:H:162:ASN:HD22 | 2:H:188:VAL:HG23 | 1.84 | 0.43 |
| 2:G:78:LYS:HB2 | 2:G:114:MET:HE2 | 2.01 | 0.43 |
| 5:M:32:MET:O | 5:M:36:VAL:HG22 | 2.18 | 0.43 |
| 1:B:240:PHE:HA | 1:B:241:PRO:HD3 | 1.75 | 0.43 |
| 1:B:242:PRO:HD2 | 1:B:243:GLU:N | 2.33 | 0.43 |
| 1:C:297:GLU:O | 1:C:301:ASN:N | 2.39 | 0.43 |
| 1:E:585:MET:HG3 | 1:E:589:PHE:CE2 | 2.53 | 0.43 |
| 1:F:73:SER:O | 1:F:76:GLN:HG2 | 2.18 | 0.43 |
| 2:H:21:VAL:O | 2:H:21:VAL:HG13 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:118:THR:O | 2:H:122:LYS:HG2 | 2.18 | 0.43 |
| 2:H:239:ARG:NH2 | 4:L:213:HIS:CE1 | 2.87 | 0.43 |
| 2:H:275:TRP:CE3 | 2:H:276:LEU:HD23 | 2.54 | 0.43 |
| 2:I:201:SER:N | 3:K:47:ARG:HH12 | 2.16 | 0.43 |
| 5:M:23:ASP:O | 5:M:26:LEU:HB3 | 2.18 | 0.43 |
| 1:A:106:ASN:HB3 | 1:A:143:LYS:NZ | 2.34 | 0.43 |
| 1:B:8:ALA:HB3 | 1:B:73:SER:O | 2.19 | 0.43 |
| 1:B:95:MET:HE2 | 1:B:97:ILE:HD11 | 2.01 | 0.43 |
| 1:B:121:PHE:HD2 | 1:B:183:VAL:HG21 | 1.84 | 0.43 |
| 1:B:259:TYR:CD2 | 1:B:376:PRO:HD3 | 2.54 | 0.43 |
| 1:D:7:GLN:O | 1:D:59:SER:HB2 | 2.19 | 0.43 |
| 1:D:541:LEU:HD12 | 1:D:541:LEU:O | 2.19 | 0.43 |
| 1:E:241:PRO:HA | 1:E:242:PRO:HA | 1.62 | 0.43 |
| 1:E:628:VAL:HB | 1:F:574:ILE:CD1 | 2.48 | 0.43 |
| 1:F:536:LEU:HD11 | 1:F:633:ALA:HA | 2.00 | 0.43 |
| 1:F:690:GLU:O | 1:F:694:ILE:HG13 | 2.19 | 0.43 |
| 2:I:200:TYR:C | 3:K:47:ARG:NH1 | 2.72 | 0.43 |
| 2:J:186:GLU:O | 2:J:190:THR:HG23 | 2.18 | 0.43 |
| 2:G:261:GLU:O | 2:G:265:GLU:HG3 | 2.18 | 0.43 |
| 1:A:437:SER:OG | 1:A:440:GLU:HG2 | 2.19 | 0.43 |
| 1:A:632:LYS:HE3 | 1:A:633:ALA:O | 2.19 | 0.43 |
| 1:A:686:PHE:CE2 | 1:A:714:ILE:HG23 | 2.54 | 0.43 |
| 1:A:690:GLU:HB3 | 1:A:726:VAL:HG22 | 2.01 | 0.43 |
| 1:B:576:PHE:HB2 | 1:B:581:LYS:CG | 2.49 | 0.43 |
| 1:B:707:ILE:O | 1:B:711:LEU:HG | 2.19 | 0.43 |
| 1:C:284:VAL:HB | 1:C:325:ILE:HA | 2.01 | 0.43 |
| 1:D:356:SER:OG | 1:E:288:PRO:HB3 | 2.18 | 0.43 |
| 1:D:539:VAL:CG1 | 1:D:643:ILE:HG13 | 2.49 | 0.43 |
| 1:D:562:PHE:CD2 | 1:D:597:LEU:HG | 2.54 | 0.43 |
| 1:E:676:LEU:O | 1:E:680:LEU:HG | 2.19 | 0.43 |
| 2:J:244:MET:O | 2:J:248:LEU:HG | 2.19 | 0.43 |
| 3:K:77:PHE:CE1 | 5:M:78:LEU:HD11 | 2.52 | 0.43 |
| 1:A:575:GLY:HA3 | 1:F:586:LYS:CE | 2.49 | 0.42 |
| 1:A:653:GLN:HB2 | 1:A:658:LEU:HD23 | 2.01 | 0.42 |
| 1:B:324:ILE:HG12 | 1:B:368:LEU:HD11 | 2.01 | 0.42 |
| 1:C:218:MET:HA | 1:C:219:GLY:HA2 | 1.82 | 0.42 |
| 1:C:258:LEU:HD12 | 1:C:258:LEU:O | 2.19 | 0.42 |
| 1:C:540:LEU:HD22 | 1:C:661:PHE:CE2 | 2.54 | 0.42 |
| 1:C:542:GLU:HG2 | 1:C:666:HIS:HA | 2.01 | 0.42 |
| 1:C:603:ASP:HA | 1:C:645:THR:OG1 | 2.19 | 0.42 |
| 1:D:63:SER:C | 1:D:67:ARG:HE | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:586:LYS:O | 1:E:589:PHE:HB2 | 2.19 | 0.42 |
| 1:F:311:GLU:O | 1:F:314:ARG:HG2 | 2.18 | 0.42 |
| 2:H:277:THR:O | 2:H:281:LEU:HD13 | 2.19 | 0.42 |
| 2:I:40:GLU:O | 2:I:44:ILE:HG13 | 2.19 | 0.42 |
| 2:J:21:VAL:HG21 | 2:J:71:LEU:HD22 | 2.01 | 0.42 |
| 2:J:243:LEU:HD22 | 2:J:266:TYR:CG | 2.54 | 0.42 |
| 2:J:289:GLY:O | 2:J:293:ASP:HB2 | 2.19 | 0.42 |
| 1:A:64:LEU:O | 1:A:68:LYS:HG3 | 2.19 | 0.42 |
| 1:A:115:ASP:CG | 1:A:242:PRO:HG3 | 2.40 | 0.42 |
| 1:B:407:LEU:O | 1:B:411:THR:OG1 | 2.28 | 0.42 |
| 1:B:536:LEU:HD22 | 1:B:632:LYS:O | 2.19 | 0.42 |
| 1:B:541:LEU:HA | 1:B:665:ILE:O | 2.19 | 0.42 |
| 1:B:612:VAL:HG13 | 1:B:614:ILE:O | 2.19 | 0.42 |
| 1:C:385:ARG:HA | 1:C:386:PRO:HD3 | 1.92 | 0.42 |
| 1:D:331:ASP:CA | 1:D:379:ILE:HD11 | 2.48 | 0.42 |
| 1:D:406:ILE:HD12 | 1:D:406:ILE:HG23 | 1.68 | 0.42 |
| 1:E:265:GLY:O | 1:E:268:LEU:HG | 2.19 | 0.42 |
| 1:E:648:ARG:NE | 1:E:651:VAL:HG13 | 2.34 | 0.42 |
| 1:F:677:LEU:O | 1:F:681:GLU:HG3 | 2.19 | 0.42 |
| 2:H:10:ALA:HB1 | 2:H:52:PHE:CZ | 2.53 | 0.42 |
| 2:I:159:SER:OG | 3:K:55:GLU:HG2 | 2.18 | 0.42 |
| 2:J:142:ILE:HG23 | 2:J:168:VAL:HG13 | 2.01 | 0.42 |
| 2:J:179:GLN:O | 2:J:182:ILE:HG12 | 2.19 | 0.42 |
| 2:G:18:GLU:HA | 2:G:21:VAL:HG12 | 2.01 | 0.42 |
| 5:M:178:ILE:HG22 | 5:M:182:MET:HE2 | 2.00 | 0.42 |
| 1:A:52:HIS:C | 1:A:54:SER:H | 2.23 | 0.42 |
| 1:A:108:ASP:OD2 | 1:A:315:ARG:NH1 | 2.43 | 0.42 |
| 1:A:503:ILE:O | 1:A:505:ASN:N | 2.40 | 0.42 |
| 1:B:397:LEU:CD1 | 1:B:596:GLN:HG3 | 2.50 | 0.42 |
| 1:C:186:GLU:HG3 | 1:C:186:GLU:O | 2.18 | 0.42 |
| 1:D:74:ILE:HG13 | 2:J:218:MET:CE | 2.49 | 0.42 |
| 1:D:268:LEU:HA | 1:D:271:ARG:CD | 2.49 | 0.42 |
| 1:D:510:TRP:CB | 1:D:679:ALA:HB2 | 2.48 | 0.42 |
| 1:E:299:GLU:HG3 | 1:E:349:THR:HB | 2.01 | 0.42 |
| 1:F:114:THR:CG2 | 1:F:200:LYS:HG2 | 2.49 | 0.42 |
| 1:F:525:VAL:HG11 | 1:F:560:SER:HA | 2.01 | 0.42 |
| 1:F:526:GLN:O | 1:F:530:ASN:HB2 | 2.19 | 0.42 |
| 1:F:552:LEU:HD12 | 1:F:667:VAL:HG21 | 2.01 | 0.42 |
| 1:F:686:PHE:HB3 | 1:F:690:GLU:HB2 | 2.00 | 0.42 |
| 2:I:58:TRP:HB3 | 2:I:95:ALA:CB | 2.49 | 0.42 |
| 2:I:203:LYS:NZ | 2:I:236:SER:HB3 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:256:ILE:HG22 | 1:C:391:VAL:CG1 | 2.49 | 0.42 |
| 1:C:510:TRP:CZ3 | 1:C:670:ILE:HG12 | 2.54 | 0.42 |
| 1:D:573:MET:SD | 1:D:608:LEU:HD22 | 2.59 | 0.42 |
| 1:E:46:ILE:HG21 | 1:E:85:PHE:CZ | 2.54 | 0.42 |
| 1:E:527:GLN:HA | 1:F:719:GLN:CD | 2.39 | 0.42 |
| 1:F:232:ARG:O | 1:F:236:ALA:HB3 | 2.18 | 0.42 |
| 1:F:270:ALA:HA | 1:F:273:ILE:HG22 | 2.01 | 0.42 |
| 2:I:119:ILE:HD12 | 2:I:122:LYS:HG3 | 2.01 | 0.42 |
| 2:I:179:GLN:HG3 | 2:I:180:LYS:N | 2.35 | 0.42 |
| 2:J:66:CYS:SG | 2:J:92:PHE:HE2 | 2.43 | 0.42 |
| 2:G:39:GLU:HB2 | 2:G:75:LEU:HD11 | 2.01 | 0.42 |
| 1:A:110:ASN:HD22 | 1:A:321:GLY:HA2 | 1.83 | 0.42 |
| 1:D:498:ASP:O | 1:D:501:SER:HB3 | 2.18 | 0.42 |
| 1:E:406:ILE:O | 1:E:409:ILE:HG22 | 2.20 | 0.42 |
| 1:F:230:ILE:HD11 | 1:F:391:VAL:HG11 | 2.00 | 0.42 |
| 2:H:247:LEU:HD22 | 2:H:259:TYR:CD1 | 2.54 | 0.42 |
| 2:I:45:TYR:HE2 | 2:I:71:LEU:HD11 | 1.85 | 0.42 |
| 5:M:17:ARG:HE | 5:M:21:LEU:HD11 | 1.83 | 0.42 |
| 1:A:65:PRO:HG2 | 1:A:137:VAL:HG13 | 2.01 | 0.42 |
| 1:B:309:ALA:HB1 | 1:B:367:ILE:HG21 | 2.01 | 0.42 |
| 1:B:593:TYR:OH | 1:B:632:LYS:HG2 | 2.19 | 0.42 |
| 1:C:23:VAL:HG12 | 1:C:55:VAL:HG21 | 2.00 | 0.42 |
| 1:C:519:ASP:O | 1:C:523:LEU:HG | 2.19 | 0.42 |
| 1:D:690:GLU:O | 1:D:694:ILE:HG13 | 2.19 | 0.42 |
| 1:F:143:LYS:HB3 | 1:F:145:PHE:HE1 | 1.84 | 0.42 |
| 1:F:557:ALA:HB2 | 1:F:601:VAL:HG21 | 2.02 | 0.42 |
| 1:F:602:VAL:O | 1:F:644:GLY:HA2 | 2.20 | 0.42 |
| 1:F:615:GLY:HA3 | 1:F:616:PRO:C | 2.39 | 0.42 |
| 1:F:678:GLU:O | 1:F:682:LEU:HG | 2.20 | 0.42 |
| 2:H:182:ILE:CG2 | 2:H:212:CYS:HB2 | 2.50 | 0.42 |
| 2:I:203:LYS:HB3 | 2:I:240:GLU:HG3 | 2.00 | 0.42 |
| 2:J:21:VAL:HG23 | 2:J:38:ILE:CD1 | 2.50 | 0.42 |
| 4:L:211:GLU:O | 4:L:214:ASP:HB2 | 2.19 | 0.42 |
| 1:A:52:HIS:HA | 1:A:53:PRO:HD3 | 1.91 | 0.42 |
| 1:A:624:GLN:CG | 1:B:610:ASP:OD2 | 2.66 | 0.42 |
| 1:A:686:PHE:O | 1:A:691:ARG:NH2 | 2.53 | 0.42 |
| 1:B:507:ILE:CG1 | 1:B:555:LYS:HD3 | 2.50 | 0.42 |
| 1:B:541:LEU:HD12 | 1:B:541:LEU:O | 2.20 | 0.42 |
| 1:B:555:LYS:O | 1:B:559:GLU:HG2 | 2.20 | 0.42 |
| 1:C:101:PHE:CE1 | 1:C:193:LEU:HD13 | 2.54 | 0.42 |
| 1:C:121:PHE:CD2 | 1:C:183:VAL:HG21 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:632:LYS:HG3 | 1:D:571:ASP:CG | 2.40 | 0.42 |
| 1:C:686:PHE:HB3 | 1:C:690:GLU:OE2 | 2.20 | 0.42 |
| 1:D:114:THR:HG21 | 1:D:200:LYS:CG | 2.49 | 0.42 |
| 1:F:377:ASP:OD1 | 1:F:378:LEU:N | 2.52 | 0.42 |
| 1:F:694:ILE:O | 1:F:698:VAL:HG22 | 2.20 | 0.42 |
| 2:J:98:GLN:C | 2:J:100:ALA:H | 2.23 | 0.42 |
| 2:G:208:LYS:HG2 | 2:G:275:TRP:CZ3 | 2.55 | 0.42 |
| 2:G:245:LYS:HB2 | 2:G:245:LYS:NZ | 2.35 | 0.42 |
| 3:K:46:MET:HG3 | 4:L:216:PHE:CE1 | 2.55 | 0.42 |
| 1:A:262:PRO:CG | 1:A:374:ASN:OD1 | 2.66 | 0.42 |
| 1:A:299:GLU:OE1 | 1:A:303:ARG:NH2 | 2.51 | 0.42 |
| 1:A:316:LEU:O | 1:A:320:SER:HB2 | 2.20 | 0.42 |
| 1:B:286:ASN:OD1 | 1:B:327:PHE:HD1 | 2.03 | 0.42 |
| 1:B:397:LEU:HD23 | 1:B:398:PRO:HD2 | 2.01 | 0.42 |
| 1:B:502:TYR:CE2 | 1:B:567:ILE:HD13 | 2.55 | 0.42 |
| 1:B:539:VAL:HA | 1:B:663:THR:O | 2.19 | 0.42 |
| 1:C:325:ILE:O | 1:C:369:VAL:HA | 2.19 | 0.42 |
| 1:D:313:GLN:HG3 | 1:D:314:ARG:N | 2.34 | 0.42 |
| 1:D:511:GLY:CA | 1:D:675:GLN:HE21 | 2.33 | 0.42 |
| 1:E:11:CYS:HA | 1:E:12:PRO:HD3 | 1.97 | 0.42 |
| 1:E:534:THR:HG21 | 1:F:712:MET:HA | 2.01 | 0.42 |
| 1:E:669:ASN:CG | 1:E:706:GLY:HA2 | 2.40 | 0.42 |
| 1:F:297:GLU:O | 1:F:300:ALA:HB3 | 2.19 | 0.42 |
| 2:H:198:LEU:C | 2:H:200:TYR:N | 2.73 | 0.42 |
| 2:I:15:ALA:O | 2:I:19:ARG:HG3 | 2.19 | 0.42 |
| 2:I:277:THR:O | 2:I:281:LEU:HD13 | 2.20 | 0.42 |
| 2:J:98:GLN:NE2 | 2:J:98:GLN:H | 2.18 | 0.42 |
| 2:J:260:THR:HG21 | 2:J:284:LYS:HE3 | 2.01 | 0.42 |
| 2:G:38:ILE:CD1 | 2:G:71:LEU:HB3 | 2.50 | 0.42 |
| 5:M:78:LEU:CD1 | 5:M:195:ALA:HB1 | 2.50 | 0.42 |
| 1:A:231:PHE:CE2 | 1:A:235:PHE:HD2 | 2.38 | 0.42 |
| 1:A:319:ASN:O | 1:A:320:SER:CB | 2.67 | 0.42 |
| 1:A:718:LEU:O | 1:A:725:ARG:NE | 2.52 | 0.42 |
| 1:B:246:GLU:HG2 | 1:B:247:GLN:N | 2.35 | 0.42 |
| 1:C:35:VAL:HG11 | 1:C:49:LEU:HD11 | 2.02 | 0.42 |
| 1:D:268:LEU:O | 1:D:271:ARG:HG2 | 2.20 | 0.42 |
| 1:E:240:PHE:HD2 | 1:E:244:ILE:CG2 | 2.26 | 0.42 |
| 1:E:713:LEU:HD23 | 1:E:713:LEU:HA | 1.79 | 0.42 |
| 1:F:582:CYS:SG | 1:F:586:LYS:HE3 | 2.60 | 0.42 |
| 2:H:101:ILE:HB | 2:H:131:TYR:OH | 2.20 | 0.42 |
| 2:H:203:LYS:HD3 | 2:H:236:SER:CB | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:195:SER:C | 2:G:197:LEU:H | 2.23 | 0.42 |
| 1:A:261:PRO:HD2 | 1:A:395:ILE:O | 2.20 | 0.42 |
| 1:B:631:LYS:NZ | 1:C:604:ASP:OD2 | 2.35 | 0.42 |
| 1:C:38:ARG:HH11 | 1:C:38:ARG:HG2 | 1.84 | 0.42 |
| 1:C:38:ARG:HG3 | 1:C:44:LYS:HE2 | 2.01 | 0.42 |
| 1:C:291:LEU:HA | 1:C:298:SER:CB | 2.50 | 0.42 |
| 1:D:23:VAL:HG12 | 1:D:55:VAL:CG2 | 2.50 | 0.42 |
| 1:D:659:ASN:OD1 | 1:E:546:HIS:HE1 | 2.03 | 0.42 |
| 1:E:268:LEU:HD12 | 1:E:269:LEU:N | 2.35 | 0.42 |
| 1:E:307:ALA:O | 1:E:310:GLU:HG2 | 2.20 | 0.42 |
| 1:F:242:PRO:O | 1:F:245:VAL:HG12 | 2.20 | 0.42 |
| 2:H:246:LYS:NZ | 2:H:258:SER:HB3 | 2.35 | 0.42 |
| 2:I:69:ALA:HB1 | 2:I:85:PHE:CD1 | 2.55 | 0.42 |
| 2:I:184:ILE:O | 2:I:188:VAL:HG12 | 2.20 | 0.42 |
| 2:J:72:HIS:CE1 | 2:J:77:SER:HB2 | 2.55 | 0.42 |
| 2:J:282:ARG:O | 2:J:286:THR:HG23 | 2.19 | 0.42 |
| 2:G:45:TYR:HE2 | 2:G:71:LEU:HD11 | 1.84 | 0.42 |
| 3:K:42:VAL:HG21 | 5:M:157:ILE:HG23 | 2.02 | 0.42 |
| 1:A:706:GLY:O | 1:A:710:LEU:N | 2.50 | 0.41 |
| 1:B:24:VAL:HG11 | 1:B:49:LEU:HD22 | 2.02 | 0.41 |
| 1:B:512:ASP:N | 1:B:513:PRO:CD | 2.83 | 0.41 |
| 1:C:95:MET:CG | 1:C:152:ILE:HG12 | 2.49 | 0.41 |
| 1:C:355:LEU:HA | 1:C:388:ARG:NE | 2.34 | 0.41 |
| 1:C:590:ASP:HA | 1:C:593:TYR:HD2 | 1.80 | 0.41 |
| 1:D:96:THR:HA | 1:D:184:ALA:O | 2.20 | 0.41 |
| 1:D:231:PHE:HA | 1:D:235:PHE:CD2 | 2.55 | 0.41 |
| 1:D:319:ASN:HA | 1:D:320:SER:HA | 1.81 | 0.41 |
| 1:D:327:PHE:HB2 | 1:D:330:ILE:CG2 | 2.50 | 0.41 |
| 1:D:510:TRP:HZ2 | 1:D:668:PRO:O | 2.03 | 0.41 |
| 1:E:512:ASP:N | 1:E:513:PRO:CD | 2.82 | 0.41 |
| 1:F:24:VAL:HA | 1:F:55:VAL:HG11 | 2.02 | 0.41 |
| 1:F:605:ILE:N | 1:F:606:GLU:OE1 | 2.53 | 0.41 |
| 1:F:658:LEU:HA | 1:F:661:PHE:HD2 | 1.84 | 0.41 |
| 2:I:213:HIS:C | 2:I:215:CYS:H | 2.23 | 0.41 |
| 2:I:243:LEU:HD22 | 2:I:266:TYR:CD2 | 2.55 | 0.41 |
| 2:I:287:ILE:O | 2:I:291:GLU:HG3 | 2.20 | 0.41 |
| 2:J:53:LYS:HG3 | 2:J:58:TRP:CZ3 | 2.55 | 0.41 |
| 2:G:92:PHE:HD1 | 2:G:97:PRO:HG2 | 1.84 | 0.41 |
| 2:G:108:ILE:HD12 | 2:G:127:ILE:HD12 | 2.02 | 0.41 |
| 3:K:53:VAL:HG13 | 3:K:54:LEU:N | 2.35 | 0.41 |
| 1:A:7:GLN:H | 1:A:59:SER:HA | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:98:GLU:HB3 | 1:A:148:LEU:HB3 | 2.01 | 0.41 |
| 1:A:220:ILE:HG22 | 1:A:221:GLY:N | 2.33 | 0.41 |
| 1:A:322:LEU:HD13 | 1:A:366:ASN:O | 2.19 | 0.41 |
| 1:A:356:SER:CB | 1:B:288:PRO:HD3 | 2.50 | 0.41 |
| 1:A:517:VAL:HG13 | 1:A:665:ILE:CG2 | 2.50 | 0.41 |
| 1:B:69:TRP:CE2 | 1:B:134:GLN:HA | 2.54 | 0.41 |
| 1:B:388:ARG:O | 1:B:389:LEU:HD23 | 2.20 | 0.41 |
| 1:B:406:ILE:O | 1:B:409:ILE:HG22 | 2.19 | 0.41 |
| 1:B:513:PRO:O | 1:B:517:VAL:HG23 | 2.20 | 0.41 |
| 1:C:197:GLY:C | 1:C:198:LYS:HD2 | 2.40 | 0.41 |
| 1:C:503:ILE:O | 1:C:503:ILE:HG22 | 2.19 | 0.41 |
| 1:D:608:LEU:C | 1:D:622:VAL:HG11 | 2.41 | 0.41 |
| 1:F:236:ALA:HA | 1:F:239:VAL:CG1 | 2.49 | 0.41 |
| 1:F:629:LEU:O | 1:F:632:LYS:HB3 | 2.20 | 0.41 |
| 2:H:228:TYR:CE2 | 2:H:230:GLU:HB2 | 2.54 | 0.41 |
| 2:J:188:VAL:HG22 | 2:J:205:TYR:HE2 | 1.86 | 0.41 |
| 4:L:213:HIS:HD2 | 5:M:35:LEU:HA | 1.85 | 0.41 |
| 1:A:357:LYS:HA | 1:A:357:LYS:HE3 | 2.01 | 0.41 |
| 1:B:503:ILE:HG22 | 1:B:506:GLY:H | 1.85 | 0.41 |
| 1:C:386:PRO:HA | 1:C:390:GLU:CA | 2.37 | 0.41 |
| 1:C:696:GLN:O | 1:C:696:GLN:NE2 | 2.53 | 0.41 |
| 1:D:46:ILE:HD12 | 1:D:174:VAL:HG21 | 2.02 | 0.41 |
| 1:D:582:CYS:O | 1:D:586:LYS:HG3 | 2.19 | 0.41 |
| 1:E:259:TYR:HA | 1:E:373:THR:O | 2.20 | 0.41 |
| 1:F:502:TYR:CD2 | 1:F:503:ILE:HG13 | 2.55 | 0.41 |
| 1:F:502:TYR:HD2 | 1:F:503:ILE:HG13 | 1.85 | 0.41 |
| 2:J:91:ALA:O | 2:J:95:ALA:HB2 | 2.21 | 0.41 |
| 2:J:155:GLU:C | 2:J:157:SER:H | 2.23 | 0.41 |
| 2:J:268:SER:HA | 2:G:233:PRO:HG3 | 2.03 | 0.41 |
| 5:M:17:ARG:O | 5:M:21:LEU:HG | 2.20 | 0.41 |
| 1:B:38:ARG:HG3 | 1:B:44:LYS:HE3 | 2.03 | 0.41 |
| 1:B:523:LEU:O | 1:B:526:GLN:HG2 | 2.21 | 0.41 |
| 1:C:237:SER:OG | 1:C:252:HIS:ND1 | 2.45 | 0.41 |
| 1:C:526:GLN:OE1 | 1:C:530:ASN:ND2 | 2.54 | 0.41 |
| 1:C:676:LEU:HD12 | 1:C:705:ILE:CG2 | 2.44 | 0.41 |
| 1:D:271:ARG:HG2 | 1:D:272:GLN:N | 2.34 | 0.41 |
| 1:D:436:PHE:CE2 | 1:D:444:LEU:HD12 | 2.49 | 0.41 |
| 1:E:242:PRO:HD2 | 1:E:243:GLU:N | 2.34 | 0.41 |
| 1:E:250:CYS:SG | 1:F:446:ARG:HB2 | 2.60 | 0.41 |
| 1:E:451:THR:O | 1:E:454:ASN:HB3 | 2.20 | 0.41 |
| 1:E:697:GLN:O | 1:E:701:LYS:HD2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:18:LEU:HD23 | 1:F:137:VAL:HG21 | 2.02 | 0.41 |
| 1:F:388:ARG:O | 1:F:389:LEU:HD23 | 2.19 | 0.41 |
| 2:H:200:TYR:O | 4:L:217:MET:CE | 2.68 | 0.41 |
| 2:J:101:ILE:O | 2:J:105:MET:HG3 | 2.20 | 0.41 |
| 2:G:281:LEU:O | 2:G:285:LYS:HG3 | 2.20 | 0.41 |
| 1:A:380:ASP:OD1 | 1:A:381:GLU:N | 2.54 | 0.41 |
| 1:B:232:ARG:O | 1:B:236:ALA:HB3 | 2.20 | 0.41 |
| 1:C:621:LEU:HD11 | 1:D:575:GLY:HA2 | 2.01 | 0.41 |
| 1:D:543:GLY:N | 1:D:549:LYS:HD3 | 2.30 | 0.41 |
| 1:D:669:ASN:OD1 | 1:D:669:ASN:N | 2.46 | 0.41 |
| 1:E:686:PHE:O | 1:E:691:ARG:NH1 | 2.53 | 0.41 |
| 1:E:721:ASP:HB2 | 1:E:724:TYR:HD2 | 1.85 | 0.41 |
| 1:F:46:ILE:HD12 | 1:F:174:VAL:HG21 | 2.02 | 0.41 |
| 1:F:319:ASN:HA | 1:F:320:SER:HA | 1.91 | 0.41 |
| 1:F:545:PRO:HB3 | 1:F:546:HIS:HA | 2.02 | 0.41 |
| 2:I:119:ILE:HD11 | 2:I:123:HIS:HE1 | 1.85 | 0.41 |
| 2:I:182:ILE:HG22 | 2:I:212:CYS:HB2 | 2.01 | 0.41 |
| 2:J:184:ILE:O | 2:J:188:VAL:HG12 | 2.21 | 0.41 |
| 2:J:277:THR:O | 2:J:281:LEU:HD13 | 2.20 | 0.41 |
| 1:B:95:MET:CG | 1:B:152:ILE:HG12 | 2.50 | 0.41 |
| 1:B:326:ILE:HG22 | 1:B:370:ILE:CG1 | 2.49 | 0.41 |
| 1:C:517:VAL:HG13 | 1:C:665:ILE:HG21 | 2.01 | 0.41 |
| 1:C:690:GLU:HB2 | 1:C:726:VAL:CG2 | 2.43 | 0.41 |
| 1:C:709:LYS:HD2 | 1:C:709:LYS:HA | 1.82 | 0.41 |
| 1:C:711:LEU:N | 1:C:711:LEU:HD23 | 2.36 | 0.41 |
| 1:D:313:GLN:O | 1:D:317:GLY:CA | 2.68 | 0.41 |
| 1:E:40:SER:HB2 | 1:E:41:PRO:HD2 | 2.02 | 0.41 |
| 1:E:618:PHE:CD1 | 1:E:618:PHE:C | 2.93 | 0.41 |
| 1:F:64:LEU:HA | 1:F:67:ARG:HH21 | 1.84 | 0.41 |
| 1:F:242:PRO:CD | 1:F:243:GLU:N | 2.83 | 0.41 |
| 2:H:134:GLU:O | 2:H:136:VAL:HG23 | 2.20 | 0.41 |
| 2:H:237:ASP:C | 2:H:239:ARG:H | 2.23 | 0.41 |
| 2:J:201:SER:HB2 | 5:M:165:LEU:CD1 | 2.43 | 0.41 |
| 2:G:277:THR:O | 2:G:281:LEU:HD13 | 2.21 | 0.41 |
| 3:K:79:THR:HG22 | 3:K:83:LYS:HE3 | 2.02 | 0.41 |
| 1:A:517:VAL:HG13 | 1:A:665:ILE:HG21 | 2.02 | 0.41 |
| 1:A:620:ASN:O | 1:A:624:GLN:HG2 | 2.21 | 0.41 |
| 1:A:652:LEU:HA | 1:A:655:MET:SD | 2.60 | 0.41 |
| 1:A:673:GLY:O | 1:A:676:LEU:HB3 | 2.20 | 0.41 |
| 1:B:347:HIS:O | 1:B:350:VAL:HG22 | 2.20 | 0.41 |
| 1:B:690:GLU:O | 1:B:694:ILE:HG13 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:87:LYS:HA | 1:C:91:CYS:SG | 2.61 | 0.41 |
| 1:C:102:LEU:HD22 | 1:C:137:VAL:HG12 | 2.02 | 0.41 |
| 1:C:560:SER:HB2 | 1:C:562:PHE:CZ | 2.56 | 0.41 |
| 1:D:92:ILE:HG21 | 1:D:95:MET:HB2 | 2.02 | 0.41 |
| 1:E:324:ILE:HG12 | 1:E:368:LEU:HD11 | 2.02 | 0.41 |
| 1:E:598:SER:O | 1:E:640:LEU:HA | 2.20 | 0.41 |
| 1:F:601:VAL:HG22 | 1:F:643:ILE:HD12 | 2.03 | 0.41 |
| 2:H:156:GLU:O | 2:H:158:ASN:N | 2.53 | 0.41 |
| 2:H:175:LEU:O | 2:H:176:GLU:HB3 | 2.20 | 0.41 |
| 2:J:208:LYS:HG2 | 2:J:275:TRP:CZ3 | 2.56 | 0.41 |
| 3:K:39:VAL:HG22 | 5:M:157:ILE:HD11 | 2.03 | 0.41 |
| 1:A:86:ASP:C | 1:A:88:ALA:H | 2.22 | 0.41 |
| 1:A:215:PHE:N | 1:A:231:PHE:CZ | 2.89 | 0.41 |
| 1:A:610:ASP:OD1 | 1:F:624:GLN:HG3 | 2.20 | 0.41 |
| 1:A:707:ILE:HA | 1:A:710:LEU:HB2 | 2.03 | 0.41 |
| 1:B:94:THR:HB | 1:B:153:GLU:HB2 | 2.02 | 0.41 |
| 1:B:313:GLN:O | 1:B:317:GLY:N | 2.53 | 0.41 |
| 1:B:423:ASP:CB | 1:B:479:ASP:N | 2.84 | 0.41 |
| 1:C:241:PRO:HA | 1:C:242:PRO:HA | 1.65 | 0.41 |
| 1:D:72:LEU:C | 2:J:218:MET:SD | 2.99 | 0.41 |
| 1:E:297:GLU:O | 1:E:300:ALA:HB3 | 2.21 | 0.41 |
| 1:E:643:ILE:N | 1:E:643:ILE:HD12 | 2.35 | 0.41 |
| 2:H:82:ALA:HB2 | 2:H:110:ILE:HG21 | 2.02 | 0.41 |
| 2:G:169:ALA:HB2 | 2:G:184:ILE:HB | 2.03 | 0.41 |
| 1:A:240:PHE:CG | 1:A:244:ILE:HD11 | 2.56 | 0.41 |
| 1:A:261:PRO:HB3 | 1:A:594:LYS:HD3 | 2.03 | 0.41 |
| 1:A:612:VAL:CG1 | 1:A:617:ARG:HB2 | 2.50 | 0.41 |
| 1:A:676:LEU:HD12 | 1:A:710:LEU:HD11 | 2.03 | 0.41 |
| 1:B:52:HIS:C | 1:B:54:SER:H | 2.24 | 0.41 |
| 1:B:406:ILE:HD12 | 1:B:406:ILE:H | 1.86 | 0.41 |
| 1:B:533:ARG:CG | 1:B:534:THR:H | 2.24 | 0.41 |
| 1:C:22:ALA:HB3 | 1:C:49:LEU:HD23 | 2.03 | 0.41 |
| 1:C:499:TYR:OH | 1:C:565:ILE:HB | 2.20 | 0.41 |
| 1:C:648:ARG:HD3 | 1:C:651:VAL:HG21 | 2.02 | 0.41 |
| 1:C:726:VAL:H | 1:C:726:VAL:HG23 | 1.64 | 0.41 |
| 1:D:249:GLY:HA3 | 1:E:413:ARG:NH1 | 2.36 | 0.41 |
| 1:D:258:LEU:HD12 | 1:D:258:LEU:O | 2.21 | 0.41 |
| 1:D:303:ARG:HH11 | 1:D:357:LYS:HE3 | 1.85 | 0.41 |
| 1:D:331:ASP:HA | 1:D:379:ILE:CD1 | 2.51 | 0.41 |
| 1:D:349:THR:HA | 1:D:352:ASN:HD22 | 1.85 | 0.41 |
| 1:D:618:PHE:CD2 | 1:D:655:MET:HE1 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:711:LEU:O | 1:D:715:GLU:HG2 | 2.21 | 0.41 |
| 1:E:35:VAL:HG13 | 1:E:49:LEU:HD11 | 2.02 | 0.41 |
| 1:E:231:PHE:O | 1:E:235:PHE:CD2 | 2.74 | 0.41 |
| 1:E:607:ARG:HD3 | 1:E:607:ARG:HA | 1.82 | 0.41 |
| 1:F:400:GLU:OE2 | 1:F:434:LYS:HA | 2.21 | 0.41 |
| 1:F:406:ILE:O | 1:F:409:ILE:HG22 | 2.20 | 0.41 |
| 1:F:510:TRP:HZ3 | 1:F:675:GLN:NE2 | 2.19 | 0.41 |
| 2:H:18:GLU:HA | 2:H:21:VAL:CG1 | 2.48 | 0.41 |
| 2:H:98:GLN:C | 2:H:100:ALA:H | 2.25 | 0.41 |
| 2:H:116:ARG:HG3 | 2:H:116:ARG:HH11 | 1.86 | 0.41 |
| 2:H:126:SER:O | 2:H:130:ILE:HG13 | 2.21 | 0.41 |
| 2:H:160:SER:O | 2:H:163:LYS:HB3 | 2.21 | 0.41 |
| 2:H:200:TYR:N | 2:H:200:TYR:CD1 | 2.89 | 0.41 |
| 2:I:39:GLU:HB2 | 2:I:75:LEU:CD1 | 2.50 | 0.41 |
| 2:I:162:ASN:HD22 | 2:I:162:ASN:H | 1.69 | 0.41 |
| 2:I:182:ILE:CG2 | 2:I:212:CYS:HB2 | 2.50 | 0.41 |
| 2:I:256:VAL:O | 2:I:256:VAL:HG22 | 2.21 | 0.41 |
| 2:J:10:ALA:O | 2:J:14:LEU:HG | 2.21 | 0.41 |
| 2:J:163:LYS:O | 2:J:167:LYS:HG2 | 2.20 | 0.41 |
| 2:J:167:LYS:HE2 | 2:J:171:TYR:CE2 | 2.55 | 0.41 |
| 2:J:256:VAL:HG22 | 2:J:256:VAL:O | 2.21 | 0.41 |
| 2:G:276:LEU:O | 2:G:280:LEU:HG | 2.20 | 0.41 |
| 3:K:48:VAL:HG12 | 3:K:52:LYS:NZ | 2.36 | 0.41 |
| 3:K:56:ARG:CD | 5:M:171:ILE:HG23 | 2.41 | 0.41 |
| 3:K:77:PHE:HZ | 5:M:74:ALA:HB1 | 1.85 | 0.41 |
| 4:L:194:GLU:O | 4:L:198:ARG:HB2 | 2.21 | 0.41 |
| 4:L:216:PHE:O | 4:L:219:MET:HB3 | 2.21 | 0.41 |
| 4:L:237:VAL:O | 4:L:241:VAL:HG23 | 2.21 | 0.41 |
| 1:B:184:ALA:HB1 | 1:B:200:LYS:O | 2.20 | 0.41 |
| 1:B:289:GLU:C | 1:B:291:LEU:N | 2.73 | 0.41 |
| 1:B:307:ALA:O | 1:B:310:GLU:HG2 | 2.20 | 0.41 |
| 1:B:377:ASP:OD1 | 1:B:378:LEU:N | 2.54 | 0.41 |
| 1:B:385:ARG:HH21 | 1:B:388:ARG:CZ | 2.34 | 0.41 |
| 1:D:24:VAL:HG11 | 1:D:49:LEU:HD22 | 2.02 | 0.41 |
| 1:D:527:GLN:HA | 1:E:719:GLN:HG3 | 2.02 | 0.41 |
| 1:D:570:PRO:O | 1:D:573:MET:HB3 | 2.21 | 0.41 |
| 1:E:92:ILE:HG13 | 1:E:176:LEU:N | 2.36 | 0.41 |
| 1:E:596:GLN:HA | 1:E:638:ARG:HA | 2.03 | 0.41 |
| 1:E:623:LEU:HD23 | 1:E:624:GLN:NE2 | 2.36 | 0.41 |
| 1:E:705:ILE:HD12 | 1:E:713:LEU:HD12 | 2.02 | 0.41 |
| 1:F:86:ASP:O | 1:F:88:ALA:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:101:PHE:CE1 | 1:F:193:LEU:HD13 | 2.55 | 0.41 |
| 1:F:264:CYS:SG | 1:F:395:ILE:CG2 | 3.06 | 0.41 |
| 1:F:542:GLU:N | 1:F:665:ILE:O | 2.52 | 0.41 |
| 2:H:179:GLN:HG3 | 2:H:180:LYS:N | 2.35 | 0.41 |
| 2:J:235:PHE:CG | 3:K:38:GLN:NE2 | 2.89 | 0.41 |
| 2:G:275:TRP:CE3 | 2:G:276:LEU:HD23 | 2.55 | 0.41 |
| 1:A:549:LYS:CB | 1:A:667:VAL:HG21 | 2.51 | 0.40 |
| 1:B:612:VAL:HG12 | 1:B:617:ARG:O | 2.21 | 0.40 |
| 1:C:16:LEU:HD11 | 1:C:52:HIS:HD2 | 1.86 | 0.40 |
| 1:C:189:GLU:O | 1:C:190:ASN:HB2 | 2.20 | 0.40 |
| 1:C:313:GLN:NE2 | 1:C:365:ASN:O | 2.52 | 0.40 |
| 1:C:379:ILE:HA | 1:C:379:ILE:HD13 | 1.71 | 0.40 |
| 1:C:691:ARG:HB2 | 1:C:691:ARG:NH1 | 2.35 | 0.40 |
| 1:D:186:GLU:HG3 | 1:D:186:GLU:O | 2.21 | 0.40 |
| 1:D:223:LEU:HD23 | 1:D:223:LEU:O | 2.21 | 0.40 |
| 1:D:377:ASP:OD1 | 1:D:378:LEU:N | 2.54 | 0.40 |
| 1:E:63:SER:O | 1:E:67:ARG:HG3 | 2.21 | 0.40 |
| 1:E:627:LEU:HD13 | 1:F:607:ARG:CZ | 2.51 | 0.40 |
| 1:E:640:LEU:HG | 1:E:642:ILE:CD1 | 2.51 | 0.40 |
| 1:F:50:ARG:HG2 | 1:F:50:ARG:HH11 | 1.86 | 0.40 |
| 1:F:97:ILE:HG21 | 1:F:147:LEU:HD22 | 2.04 | 0.40 |
| 1:F:436:PHE:HD2 | 1:F:444:LEU:HD11 | 1.86 | 0.40 |
| 1:F:658:LEU:HD12 | 1:F:658:LEU:O | 2.21 | 0.40 |
| 2:J:82:ALA:HB2 | 2:J:110:ILE:HG21 | 2.03 | 0.40 |
| 2:J:256:VAL:HG11 | 2:J:288:GLN:HG2 | 2.03 | 0.40 |
| 5:M:25:SER:O | 5:M:28:SER:HB3 | 2.22 | 0.40 |
| 1:A:63:SER:O | 1:A:67:ARG:HG3 | 2.21 | 0.40 |
| 1:C:52:HIS:HA | 1:C:53:PRO:HD3 | 1.93 | 0.40 |
| 1:C:388:ARG:HB2 | 1:C:388:ARG:CZ | 2.52 | 0.40 |
| 1:C:407:LEU:O | 1:C:411:THR:OG1 | 2.30 | 0.40 |
| 1:C:629:LEU:HA | 1:C:629:LEU:HD23 | 1.76 | 0.40 |
| 1:D:612:VAL:HG13 | 1:D:614:ILE:O | 2.21 | 0.40 |
| 1:F:577:SER:O | 1:F:581:LYS:HG3 | 2.22 | 0.40 |
| 1:F:609:LEU:HD23 | 1:F:609:LEU:HA | 1.80 | 0.40 |
| 2:H:147:GLN:HG2 | 2:H:151:TYR:CE2 | 2.57 | 0.40 |
| 2:H:256:VAL:HG22 | 2:H:256:VAL:O | 2.21 | 0.40 |
| 2:I:240:GLU:OE1 | 2:I:241:CYS:HB3 | 2.21 | 0.40 |
| 2:G:118:THR:HG22 | 2:G:155:GLU:HG3 | 2.03 | 0.40 |
| 5:M:30:ARG:NH2 | 5:M:145:GLU:OE2 | 2.54 | 0.40 |
| 1:A:38:ARG:HG2 | 1:A:38:ARG:HH11 | 1.85 | 0.40 |
| 1:A:377:ASP:OD2 | 1:A:378:LEU:HD23 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:566:LYS:HD3 | 1:A:566:LYS:HA | 1.68 | 0.40 |
| 1:B:249:GLY:CA | 1:C:414:MET:HE1 | 2.51 | 0.40 |
| 1:B:519:ASP:OD1 | 1:B:520:ASP:N | 2.55 | 0.40 |
| 1:C:25:SER:HB3 | 1:C:28:ASP:OD2 | 2.21 | 0.40 |
| 1:C:319:ASN:HA | 1:C:320:SER:HA | 1.87 | 0.40 |
| 1:C:324:ILE:HD12 | 1:C:324:ILE:N | 2.36 | 0.40 |
| 1:C:627:LEU:HA | 1:C:627:LEU:HD23 | 1.77 | 0.40 |
| 1:D:263:GLY:HA2 | 1:D:439:ALA:HB3 | 2.04 | 0.40 |
| 1:D:397:LEU:HD22 | 1:D:435:ASN:O | 2.22 | 0.40 |
| 1:D:511:GLY:HA3 | 1:D:675:GLN:HE21 | 1.85 | 0.40 |
| 1:E:490:PRO:HA | 1:E:491:ALA:CB | 2.36 | 0.40 |
| 1:F:241:PRO:HA | 1:F:242:PRO:HA | 1.53 | 0.40 |
| 2:H:287:ILE:O | 2:H:291:GLU:HG3 | 2.21 | 0.40 |
| 2:J:45:TYR:CB | 2:J:68:ALA:HB2 | 2.51 | 0.40 |
| 2:J:98:GLN:H | 2:J:98:GLN:CD | 2.25 | 0.40 |
| 3:K:56:ARG:HD2 | 5:M:171:ILE:CG2 | 2.41 | 0.40 |
| 5:M:158:GLY:O | 5:M:161:ARG:HB3 | 2.22 | 0.40 |
| 1:A:240:PHE:HA | 1:A:241:PRO:HD3 | 1.91 | 0.40 |
| 1:A:693:THR:O | 1:A:697:GLN:OE1 | 2.40 | 0.40 |
| 1:B:546:HIS:HB3 | 1:B:547:SER:H | 1.42 | 0.40 |
| 1:C:47:PHE:HZ | 1:C:70:ALA:HB2 | 1.86 | 0.40 |
| 1:C:510:TRP:O | 1:C:675:GLN:HG3 | 2.21 | 0.40 |
| 1:C:604:ASP:H | 1:C:645:THR:HG1 | 1.67 | 0.40 |
| 1:C:638:ARG:HH11 | 1:C:638:ARG:HG3 | 1.86 | 0.40 |
| 1:D:221:GLY:O | 1:D:406:ILE:HD11 | 2.21 | 0.40 |
| 1:D:407:LEU:HB2 | 1:D:426:ILE:HG23 | 2.02 | 0.40 |
| 1:D:573:MET:HA | 1:D:576:PHE:CD2 | 2.57 | 0.40 |
| 1:E:140:PHE:O | 1:E:141:ASN:HB2 | 2.21 | 0.40 |
| 2:H:198:LEU:HD21 | 4:L:224:GLU:OE1 | 2.21 | 0.40 |
| 2:H:201:SER:C | 2:H:203:LYS:H | 2.24 | 0.40 |
| 2:I:179:GLN:HB3 | 2:I:214:PHE:HB3 | 2.02 | 0.40 |
| 2:J:203:LYS:HD2 | 2:J:236:SER:O | 2.21 | 0.40 |
| 2:G:96:ASP:H | 2:G:97:PRO:HD2 | 1.86 | 0.40 |
| 4:L:191:ALA:HB3 | 4:L:194:GLU:HG2 | 2.03 | 0.40 |
| 1:A:231:PHE:CD1 | 1:A:235:PHE:CE2 | 3.01 | 0.40 |
| 1:A:300:ALA:O | 1:A:303:ARG:HG2 | 2.21 | 0.40 |
| 1:A:732:LEU:HD23 | 1:A:732:LEU:HA | 1.86 | 0.40 |
| 1:B:113:ASP:HA | 1:B:196:ILE:HG13 | 2.04 | 0.40 |
| 1:B:242:PRO:CD | 1:B:243:GLU:N | 2.85 | 0.40 |
| 1:B:531:SER:CA | 1:B:639:LYS:HD3 | 2.51 | 0.40 |
| 1:C:24:VAL:HG12 | 1:C:60:VAL:HG22 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:624:GLN:HA | 1:C:624:GLN:OE1 | 2.21 | 0.40 |
| 1:E:95:MET:CE | 1:E:97:ILE:HD11 | 2.51 | 0.40 |
| 1:E:441:LEU:O | 1:E:445:VAL:HG23 | 2.22 | 0.40 |
| 1:F:101:PHE:HD1 | 1:F:101:PHE:H | 1.68 | 0.40 |
| 2:H:237:ASP:C | 2:H:239:ARG:N | 2.75 | 0.40 |
| 2:J:38:ILE:CD1 | 2:J:71:LEU:HB3 | 2.52 | 0.40 |
| 2:J:175:LEU:HD23 | 2:J:177:GLN:NE2 | 2.36 | 0.40 |
| 2:G:101:ILE:HB | 2:G:131:TYR:OH | 2.20 | 0.40 |
| 2:G:219:LEU:HD12 | 2:G:223:LEU:HB2 | 2.04 | 0.40 |
| 2:G:266:TYR:C | 2:G:268:SER:N | 2.75 | 0.40 |
| 4:L:223:VAL:HG13 | 4:L:224:GLU:N | 2.36 | 0.40 |
| 5:M:56:GLN:HA | 5:M:59:ARG:NH2 | 2.35 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | A | 668/747 (89%) | 614 (92%) | 37 (6%) | 17 (2%) | 5 | 32 |
| 1 | B | 662/747 (89%) | 593 (90%) | 55 (8%) | 14 (2%) | 7 | 36 |
| 1 | C | 666/747 (89%) | 615 (92%) | 39 (6%) | 12 (2%) | 8 | 40 |
| 1 | D | 663/747 (89%) | 607 (92%) | 47 (7%) | 9 (1%) | 11 | 46 |
| 1 | E | 658/747 (88%) | 603 (92%) | 41 (6%) | 14 (2%) | 7 | 36 |
| 1 | F | 644/747 (86%) | 587 (91%) | 44 (7%) | 13 (2%) | 7 | 38 |
| 2 | G | 284/297 (96%) | 230 (81%) | 43 (15%) | 11 (4%) | 3 | 23 |
| 2 | H | 284/297 (96%) | 229 (81%) | 46 (16%) | 9 (3%) | 4 | 26 |
| 2 | I | 284/297 (96%) | 227 (80%) | 48 (17%) | 9 (3%) | 4 | 26 |
| 2 | J | 284/297 (96%) | 232 (82%) | 41 (14%) | 11 (4%) | 3 | 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3 | K | 59/63 (94%) | 56 (95%) | 2 (3%) | 1 (2%) | 9 | 42 |
| 4 | L | 64/67 (96%) | 56 (88%) | 8 (12%) | 0 | 100 | 100 |
| 5 | M | 127/188 (68%) | 124 (98%) | 3 (2%) | 0 | 100 | 100 |
| All | All | 5347/5988 (89%) | 4773 (89%) | 454 (8%) | 120 (2%) | 10 | 35 |

All (120) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 223 | LEU |
| 1 | A | 293 | LYS |
| 1 | A | 294 | TYR |
| 1 | A | 318 | ALA |
| 1 | A | 320 | SER |
| 1 | A | 333 | ILE |
| 1 | A | 397 | LEU |
| 1 | A | 498 | ASP |
| 1 | A | 504 | MET |
| 1 | B | 12 | PRO |
| 1 | B | 283 | LYS |
| 1 | B | 297 | GLU |
| 1 | B | 318 | ALA |
| 1 | B | 439 | ALA |
| 1 | B | 489 | LYS |
| 1 | C | 297 | GLU |
| 1 | C | 318 | ALA |
| 1 | C | 497 | GLU |
| 1 | C | 498 | ASP |
| 1 | C | 578 | GLU |
| 1 | D | 188 | ALA |
| 1 | D | 283 | LYS |
| 1 | D | 318 | ALA |
| 1 | D | 489 | LYS |
| 1 | E | 283 | LYS |
| 1 | E | 297 | GLU |
| 1 | E | 318 | ALA |
| 1 | E | 439 | ALA |
| 1 | E | 489 | LYS |
| 1 | F | 200 | LYS |
| 1 | F | 283 | LYS |
| 1 | F | 297 | GLU |
| 1 | F | 318 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 439 | ALA |
| 2 | H | 58 | TRP |
| 2 | H | 79 | HIS |
| 2 | I | 219 | LEU |
| 2 | J | 58 | TRP |
| 2 | J | 76 | GLN |
| 2 | G | 58 | TRP |
| 2 | G | 176 | GLU |
| 1 | C | 293 | LYS |
| 1 | C | 610 | ASP |
| 1 | E | 12 | PRO |
| 1 | E | 88 | ALA |
| 1 | E | 507 | ILE |
| 1 | F | 87 | LYS |
| 2 | H | 76 | GLN |
| 2 | H | 202 | ALA |
| 2 | I | 79 | HIS |
| 2 | J | 156 | GLU |
| 2 | G | 76 | GLN |
| 2 | G | 79 | HIS |
| 2 | G | 218 | MET |
| 1 | A | 12 | PRO |
| 1 | A | 241 | PRO |
| 1 | A | 242 | PRO |
| 1 | A | 264 | CYS |
| 1 | B | 241 | PRO |
| 1 | B | 293 | LYS |
| 1 | B | 502 | TYR |
| 1 | C | 241 | PRO |
| 1 | D | 293 | LYS |
| 1 | E | 241 | PRO |
| 1 | E | 293 | LYS |
| 1 | F | 12 | PRO |
| 1 | F | 241 | PRO |
| 1 | F | 293 | LYS |
| 2 | H | 240 | GLU |
| 2 | H | 256 | VAL |
| 2 | I | 58 | TRP |
| 2 | J | 34 | GLY |
| 2 | J | 77 | SER |
| 2 | J | 79 | HIS |
| 2 | J | 267 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G | 240 | GLU |
| 3 | K | 35 | THR |
| 1 | B | 546 | HIS |
| 1 | C | 87 | LYS |
| 1 | D | 12 | PRO |
| 1 | E | 87 | LYS |
| 1 | E | 189 | GLU |
| 1 | F | 397 | LEU |
| 2 | H | 157 | SER |
| 2 | I | 158 | ASN |
| 2 | I | 218 | MET |
| 2 | I | 240 | GLU |
| 2 | I | 256 | VAL |
| 2 | G | 267 | ASP |
| 1 | A | 53 | PRO |
| 1 | A | 398 | PRO |
| 1 | A | 668 | PRO |
| 1 | B | 53 | PRO |
| 1 | B | 547 | SER |
| 1 | C | 53 | PRO |
| 1 | D | 241 | PRO |
| 2 | H | 77 | SER |
| 2 | J | 232 | PHE |
| 2 | G | 23 | ASN |
| 2 | G | 177 | GLN |
| 1 | A | 87 | LYS |
| 1 | B | 490 | PRO |
| 1 | C | 12 | PRO |
| 1 | E | 438 | GLY |
| 1 | E | 490 | PRO |
| 1 | F | 438 | GLY |
| 1 | F | 668 | PRO |
| 2 | H | 176 | GLU |
| 2 | I | 267 | ASP |
| 2 | J | 256 | VAL |
| 2 | G | 232 | PHE |
| 1 | B | 438 | GLY |
| 1 | D | 488 | ILE |
| 1 | F | 684 | GLY |
| 2 | J | 96 | ASP |
| 2 | G | 196 | PRO |
| 1 | C | 490 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I | 30 | GLY |
| 2 | J | 21 | VAL |
| 1 | D | 545 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1 | A | 511/638 (80%) | 509 (100%) | 2 (0%) | 91 | 94 |
| 1 | B | 512/638 (80%) | 508 (99%) | 4 (1%) | 81 | 89 |
| 1 | C | 513/638 (80%) | 512 (100%) | 1 (0%) | 93 | 96 |
| 1 | D | 506/638 (79%) | 505 (100%) | 1 (0%) | 93 | 96 |
| 1 | E | 511/638 (80%) | 508 (99%) | 3 (1%) | 86 | 92 |
| 1 | F | 505/638 (79%) | 501 (99%) | 4 (1%) | 81 | 89 |
| 2 | G | 234/244 (96%) | 234 (100%) | 0 | 100 | 100 |
| 2 | H | 233/244 (96%) | 233 (100%) | 0 | 100 | 100 |
| 2 | I | 234/244 (96%) | 233 (100%) | 1 (0%) | 91 | 94 |
| 2 | J | 235/244 (96%) | 234 (100%) | 1 (0%) | 91 | 94 |
| 3 | K | 49/54 (91%) | 49 (100%) | 0 | 100 | 100 |
| 4 | L | 56/61 (92%) | 56 (100%) | 0 | 100 | 100 |
| 5 | M | 114/161 (71%) | 114 (100%) | 0 | 100 | 100 |
| All | All | 4213/5080 (83%) | 4196 (100%) | 17 (0%) | 91 | 94 |

All (17) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 305 | LEU |
| 1 | A | 322 | LEU |
| 1 | B | 305 | LEU |
| 1 | B | 322 | LEU |
| 1 | B | 325 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 327 | PHE |
| 1 | C | 676 | LEU |
| 1 | D | 305 | LEU |
| 1 | E | 305 | LEU |
| 1 | E | 322 | LEU |
| 1 | E | 327 | PHE |
| 1 | F | 305 | LEU |
| 1 | F | 322 | LEU |
| 1 | F | 519 | ASP |
| 1 | F | 536 | LEU |
| 2 | I | 28 | PHE |
| 2 | J | 183 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 110 | ASN |
| 1 | A | 194 | ASN |
| 1 | A | 319 | ASN |
| 1 | A | 353 | GLN |
| 1 | A | 685 | ASN |
| 1 | B | 128 | GLN |
| 1 | B | 313 | GLN |
| 1 | B | 352 | ASN |
| 1 | B | 526 | GLN |
| 1 | B | 561 | ASN |
| 1 | B | 620 | ASN |
| 1 | C | 20 | ASN |
| 1 | C | 194 | ASN |
| 1 | C | 319 | ASN |
| 1 | C | 659 | ASN |
| 1 | C | 675 | GLN |
| 1 | D | 106 | ASN |
| 1 | D | 128 | GLN |
| 1 | D | 313 | GLN |
| 1 | D | 352 | ASN |
| 1 | D | 353 | GLN |
| 1 | D | 527 | GLN |
| 1 | D | 659 | ASN |
| 1 | D | 675 | GLN |
| 1 | E | 43 | HIS |
| 1 | E | 527 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 546 | HIS |
| 1 | E | 666 | HIS |
| 1 | F | 252 | HIS |
| 2 | H | 72 | HIS |
| 2 | H | 162 | ASN |
| 2 | I | 72 | HIS |
| 2 | J | 50 | ASN |
| 2 | J | 98 | GLN |
| 2 | J | 162 | ASN |
| 2 | G | 50 | ASN |
| 2 | G | 72 | HIS |
| 3 | K | 38 | GLN |
| 4 | L | 226 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

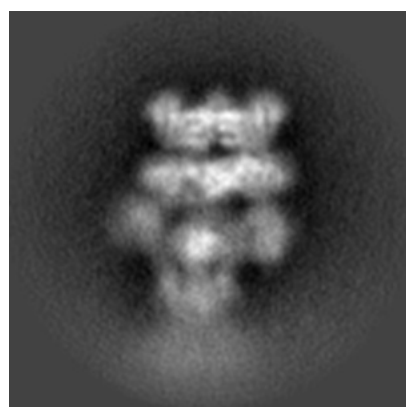
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6209. These allow visual inspection of the internal detail of the map and identification of artifacts.

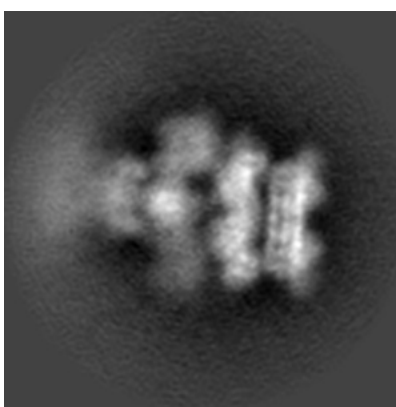
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

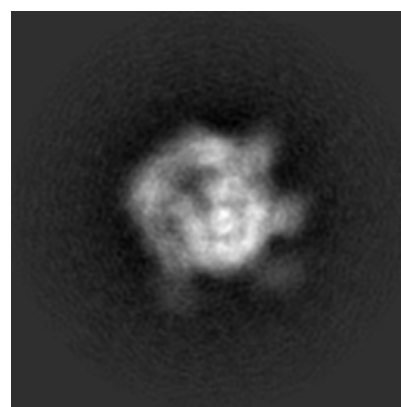
6.1.1 Primary map



X



Y

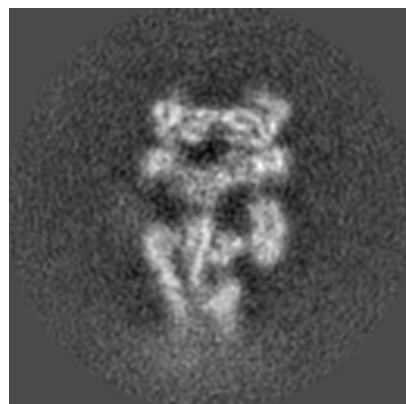


Z

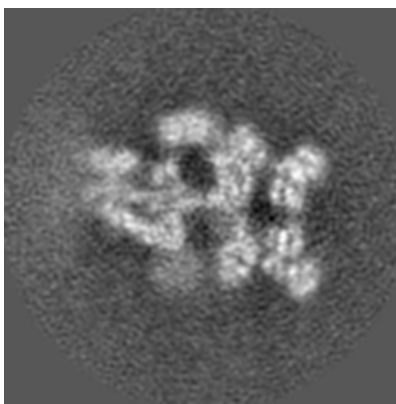
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

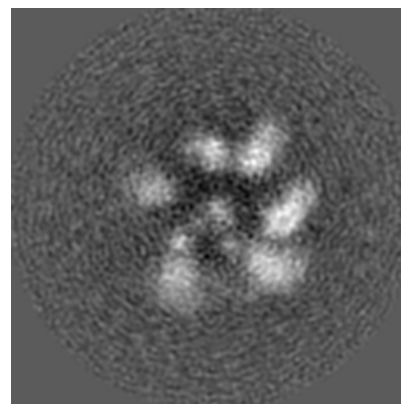
6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

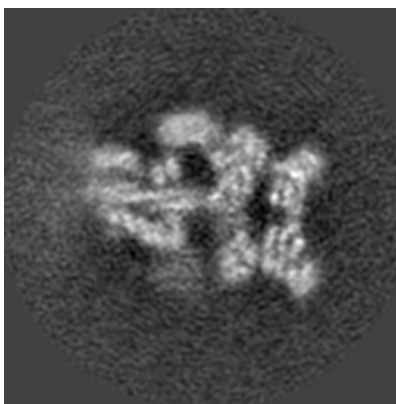
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

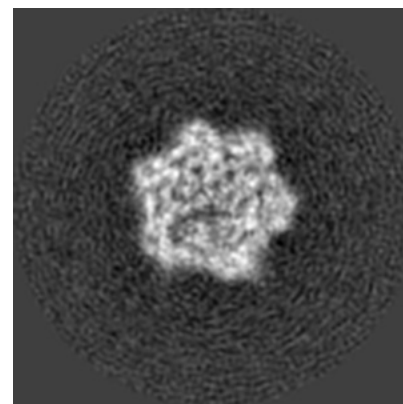
6.3.1 Primary map



X Index: 67



Y Index: 63

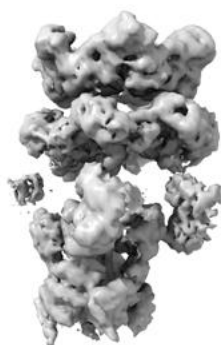


Z Index: 76

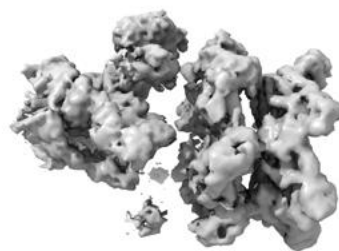
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

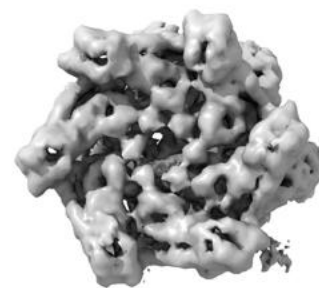
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

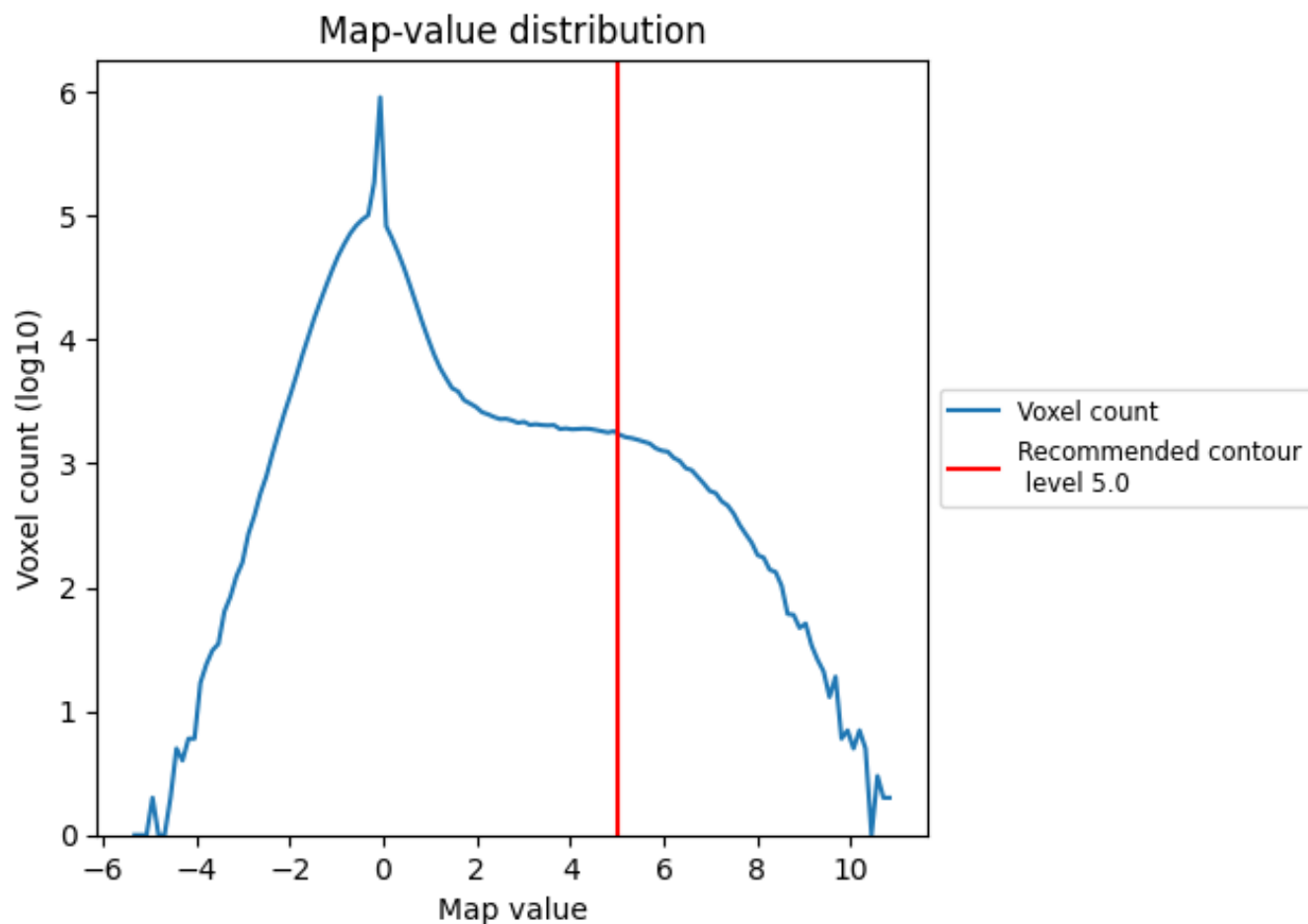
6.5 Mask visualisation

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

7 Map analysis [i](#)

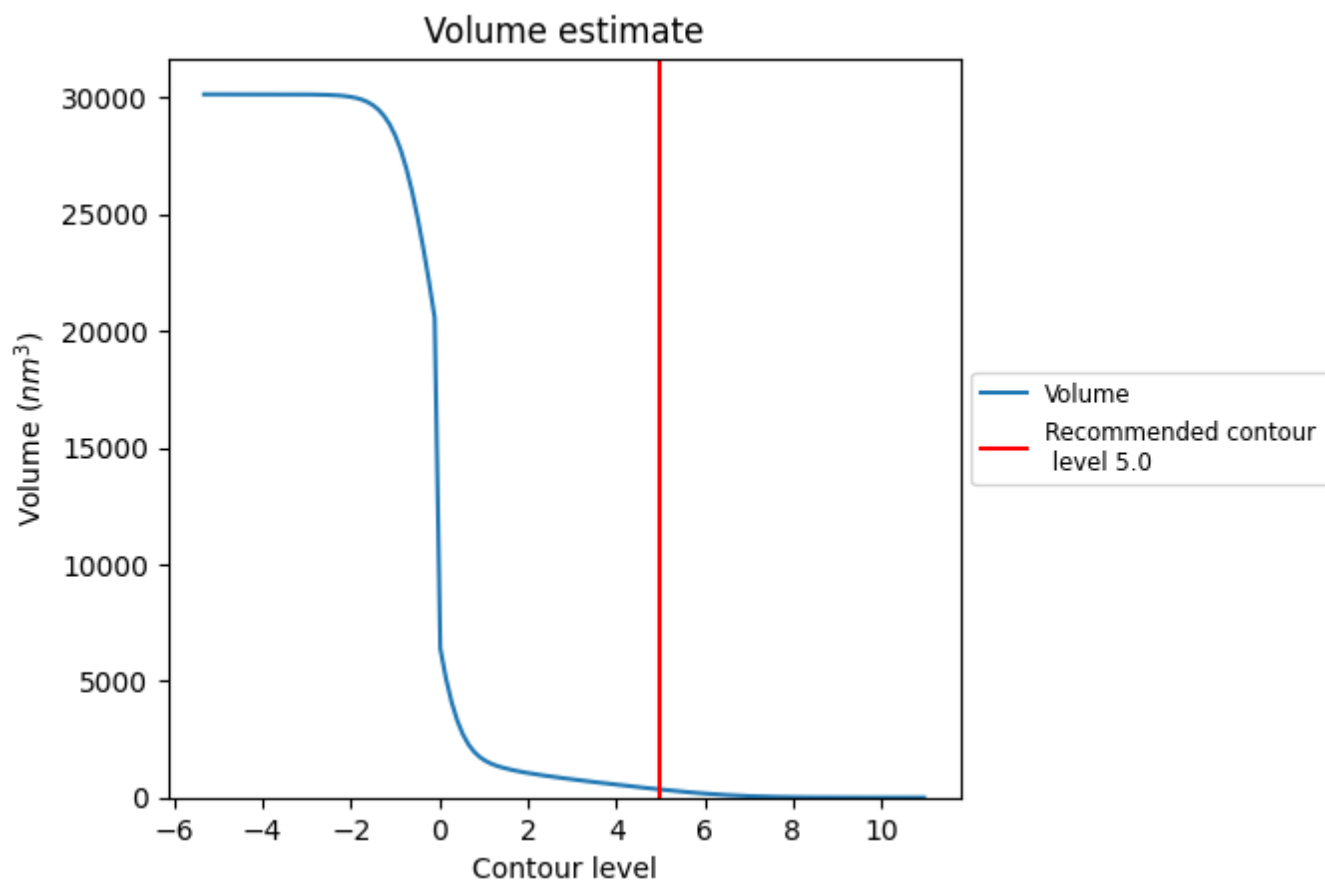
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

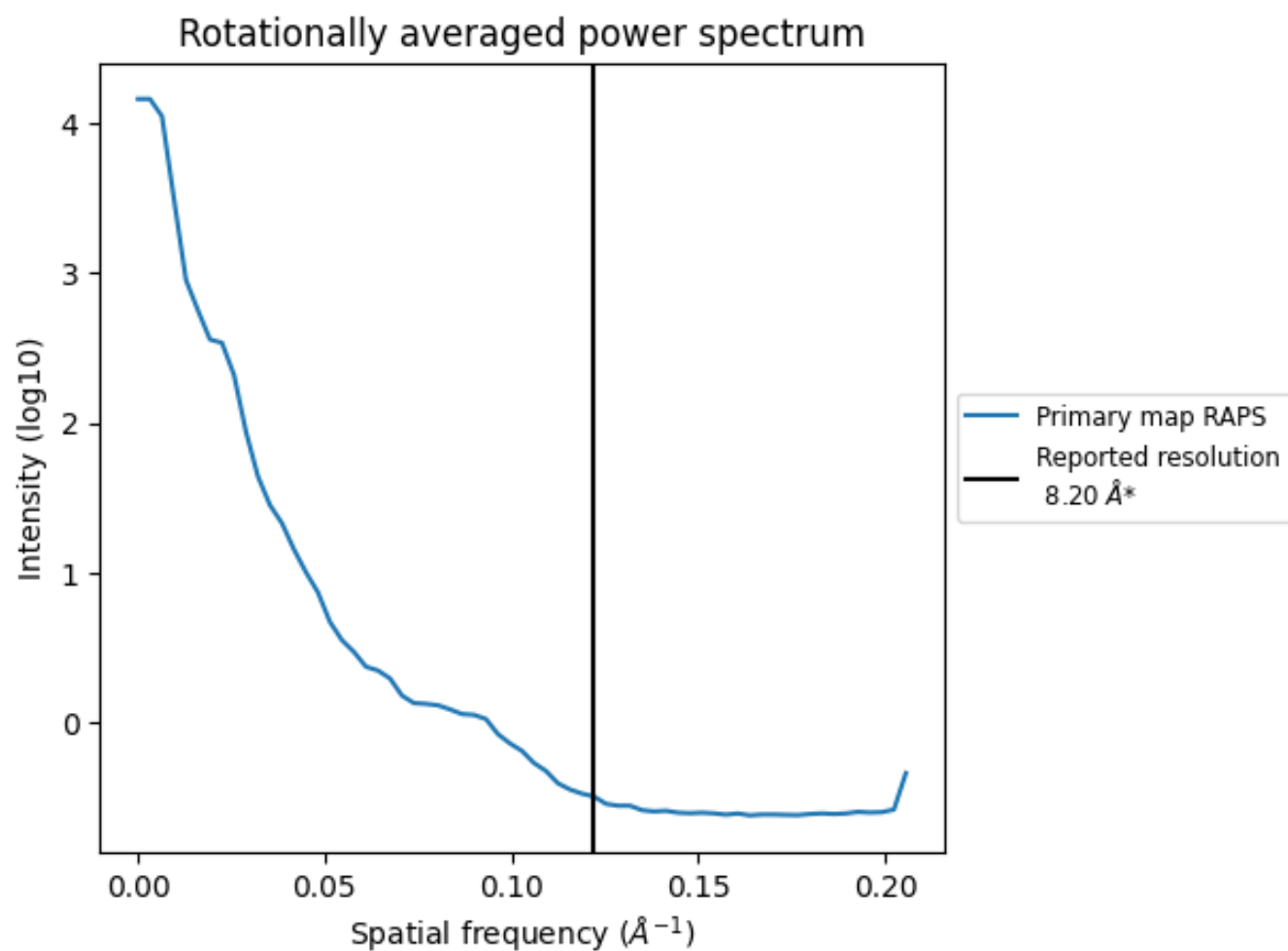
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 346 nm³; this corresponds to an approximate mass of 313 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 0.122 Å⁻¹

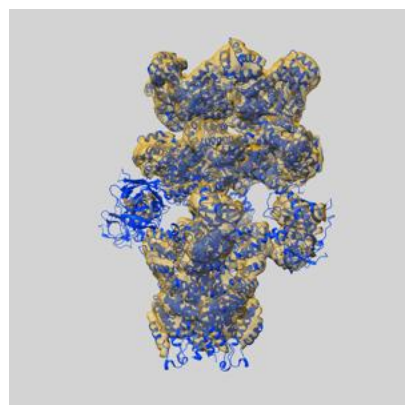
8 Fourier-Shell correlation

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

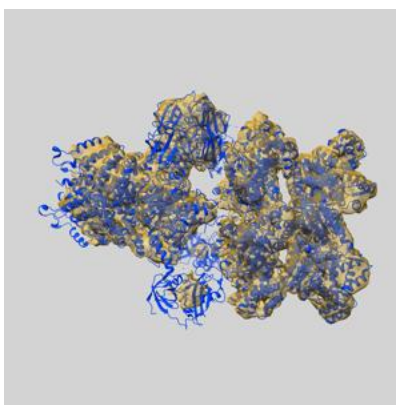
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6209 and PDB model 3J99. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

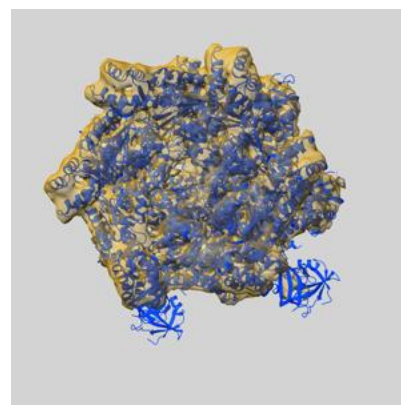
9.1 Map-model overlay [i](#)



X



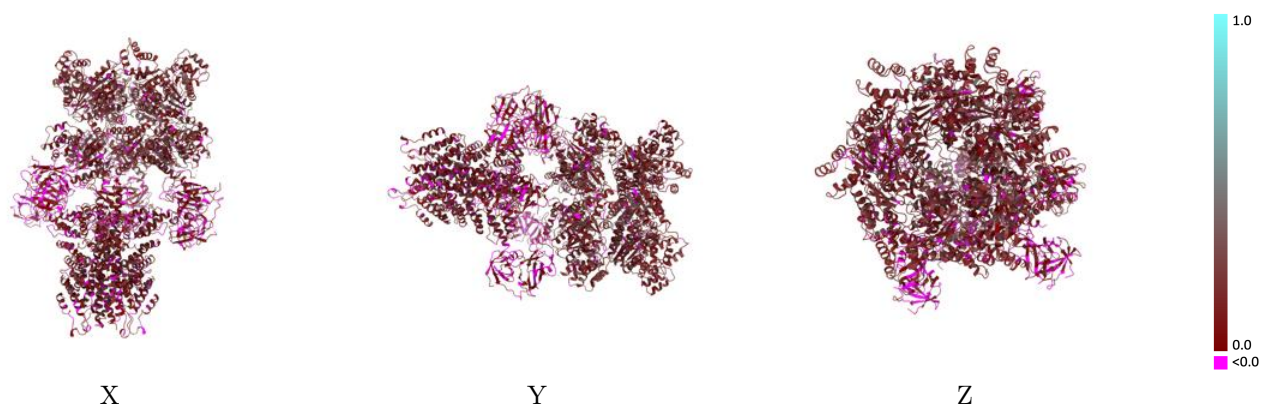
Y



Z

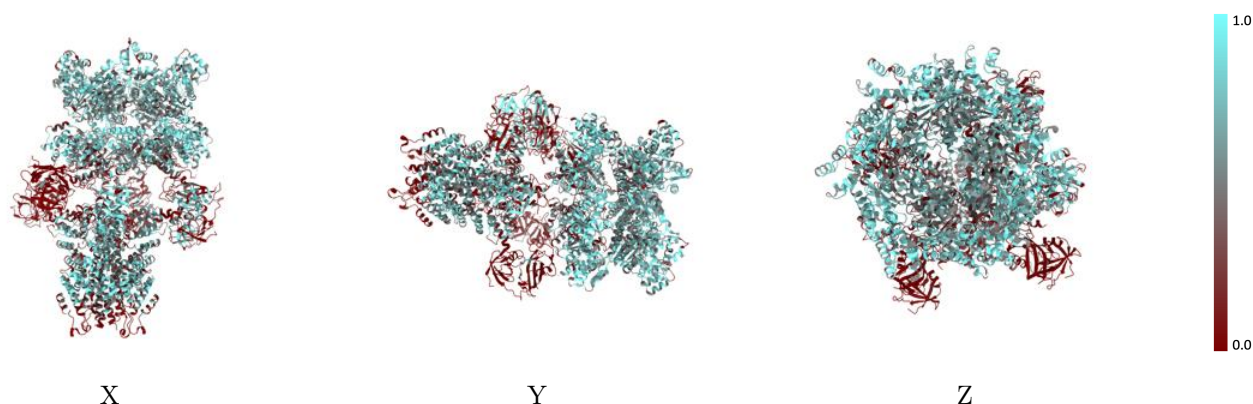
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



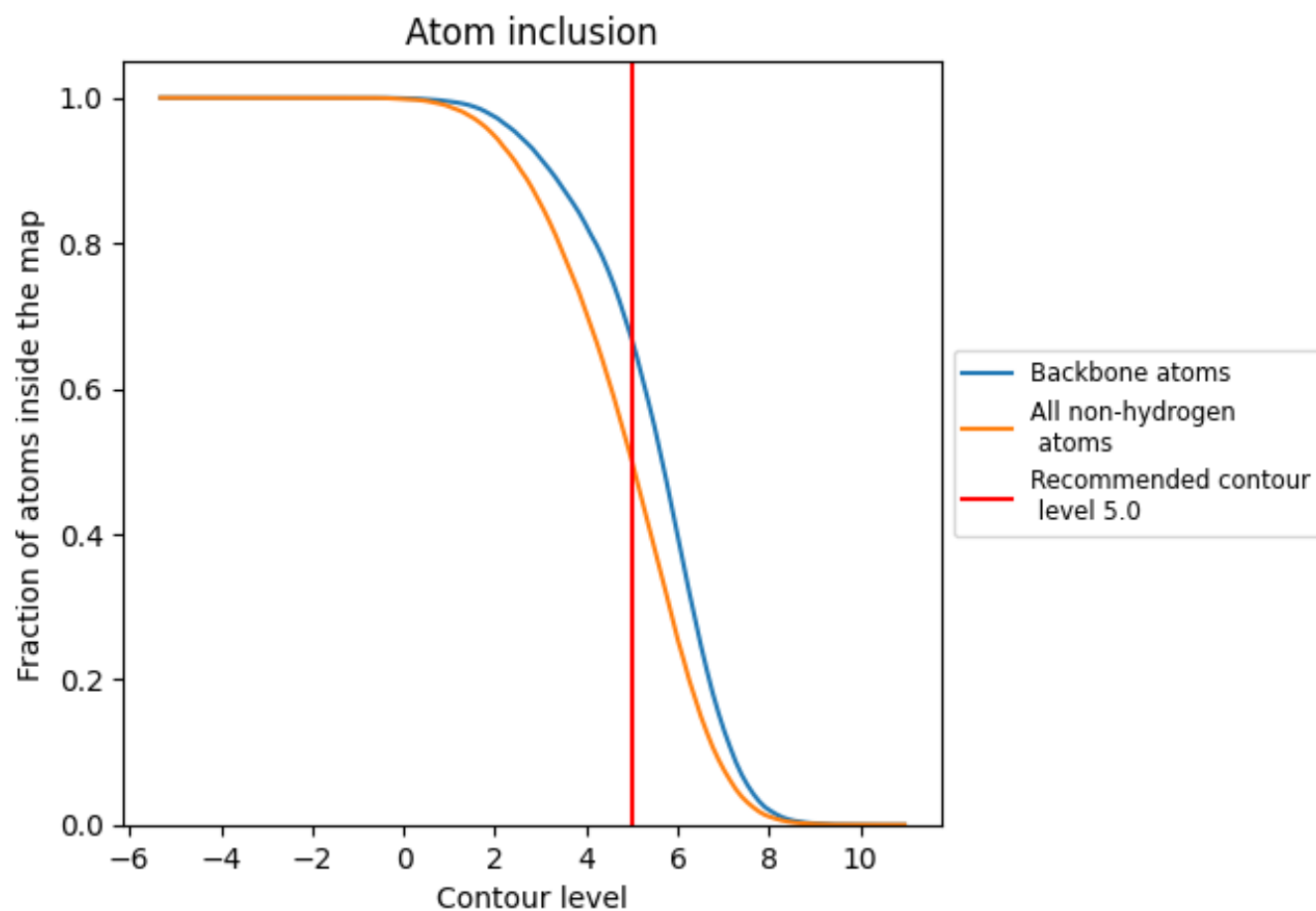
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.0).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 50% 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 (5.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.4998 |  0.1330 |
| A |  0.4581 |  0.1250 |
| B |  0.5978 |  0.1550 |
| C |  0.5120 |  0.1420 |
| D |  0.6027 |  0.1590 |
| E |  0.4493 |  0.1270 |
| F |  0.4060 |  0.1150 |
| G |  0.4304 |  0.1110 |
| H |  0.4874 |  0.1190 |
| I |  0.5264 |  0.1270 |
| J |  0.5353 |  0.1230 |
| K |  0.4872 |  0.1240 |
| L |  0.4873 |  0.1580 |
| M |  0.4186 |  0.1200 |

