



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:31 am GMT

PDB ID : 3J40
EMDB ID: : EMD-5678
Title : Validated Near-Atomic Resolution Structure of Bacteriophage Epsilon15 Derived from Cryo-EM and Modeling
Authors : Baker, M.L.; Hryc, C.F.; Zhang, Q.; Wu, W.; Jakana, J.; Haase-Pettingell, C.; Afonine, P.V.; Adams, P.D.; King, J.A.; Jiang, W.; Chiu, W.
Deposited on : 2013-05-30
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

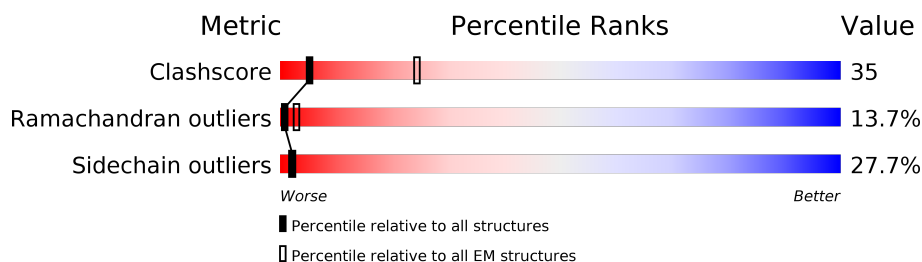
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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 | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | H | 111 | 25% 49% 23% . |
| 1 | I | 111 | 25% 42% 28% 5% |
| 1 | J | 111 | 25% 41% 29% 5% |
| 1 | K | 111 | 23% 52% 22% . |
| 1 | L | 111 | 23% 41% 28% 7% |
| 1 | M | 111 | 21% 46% 29% 5% |
| 1 | N | 111 | 27% 43% 26% . |
| 2 | A | 335 | 29% 50% 19% . |
| 2 | B | 335 | 38% 38% 22% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | C | 335 | <div><div></div><div>37%39%21%</div><div></div></div> |
| 2 | D | 335 | <div><div></div><div>28%49%20%</div><div></div></div> |
| 2 | E | 335 | <div><div></div><div>37%39%22%</div><div></div></div> |
| 2 | F | 335 | <div><div></div><div>37%42%19%</div><div></div></div> |
| 2 | G | 335 | <div><div></div><div>38%44%15%</div><div></div></div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24066 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 gp10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | N | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 521 | 143 | 181 | 5 | | |
| 1 | M | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 521 | 143 | 181 | 5 | | |
| 1 | H | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 521 | 143 | 181 | 5 | | |
| 1 | K | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 521 | 143 | 181 | 5 | | |
| 1 | I | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 521 | 143 | 181 | 5 | | |
| 1 | J | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 521 | 143 | 181 | 5 | | |
| 1 | L | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 521 | 143 | 181 | 5 | | |

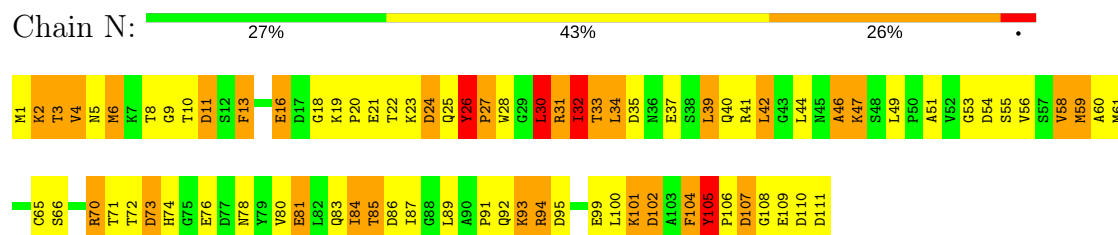
- Molecule 2 is a protein called gp7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | A | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2588 | 1620 | 453 | 502 | 13 | | |
| 2 | F | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2588 | 1620 | 453 | 502 | 13 | | |
| 2 | B | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2588 | 1620 | 453 | 502 | 13 | | |
| 2 | G | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2588 | 1620 | 453 | 502 | 13 | | |
| 2 | D | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2588 | 1620 | 453 | 502 | 13 | | |
| 2 | C | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2588 | 1620 | 453 | 502 | 13 | | |
| 2 | E | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2588 | 1620 | 453 | 502 | 13 | | |

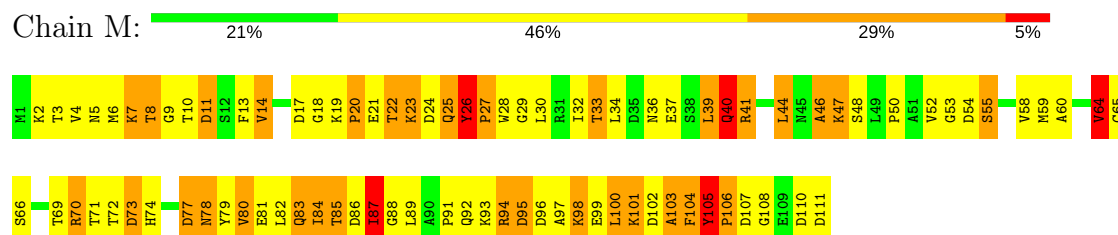
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

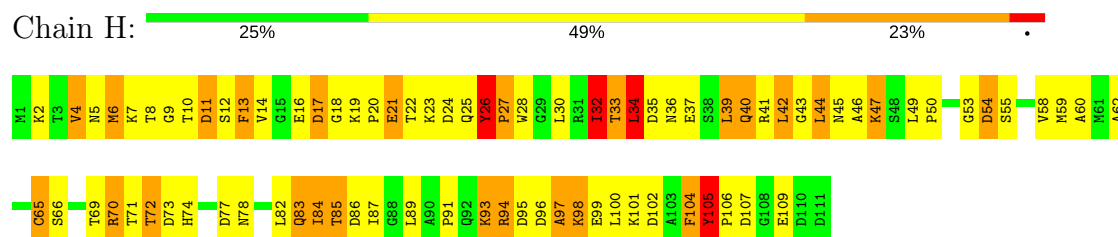
• Molecule 1: gp10



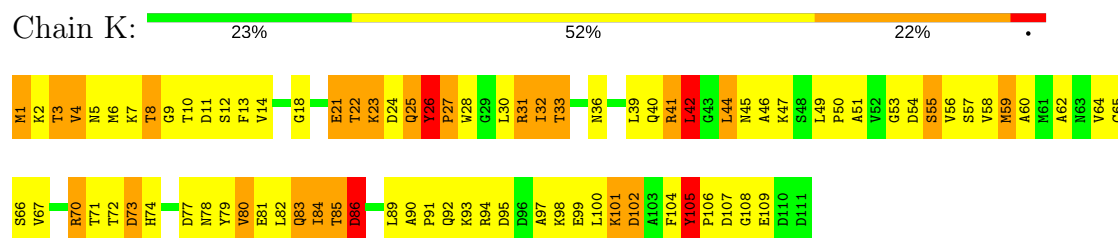
• Molecule 1: gp10



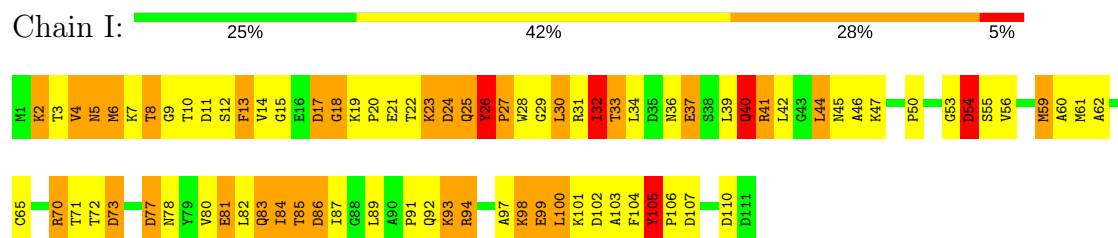
• Molecule 1: gp10



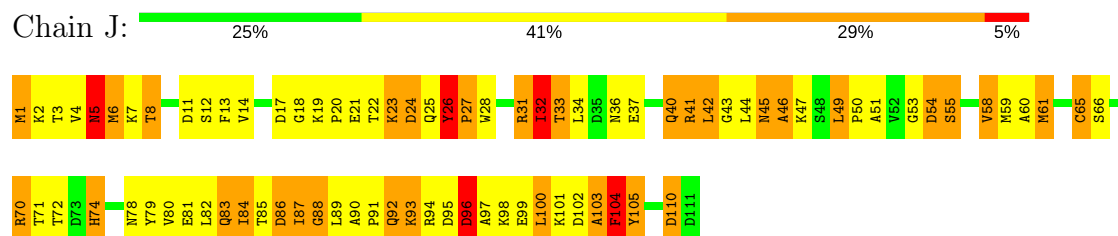
• Molecule 1: gp10



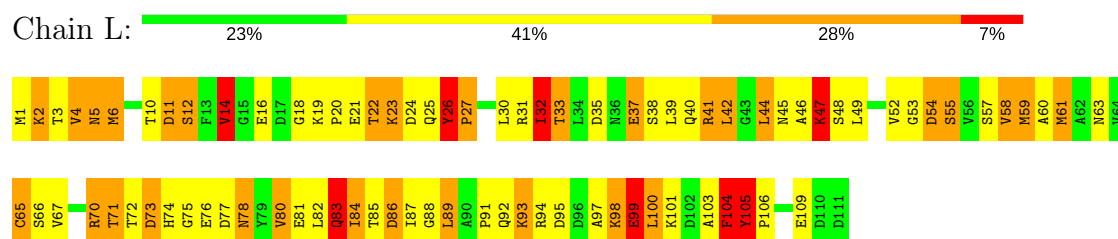
• Molecule 1: gp10



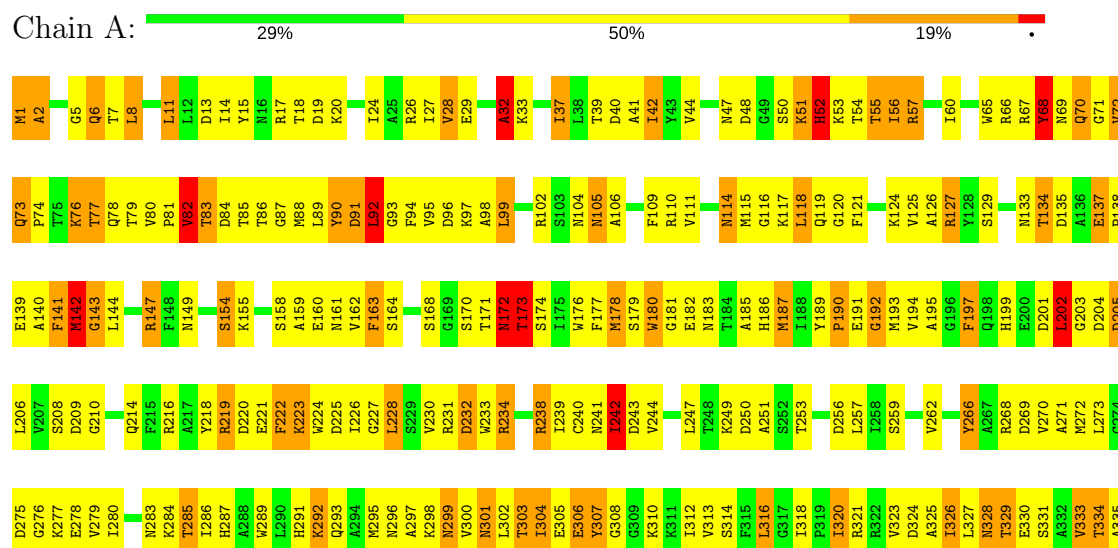
• Molecule 1: gp10



• Molecule 1: gp10

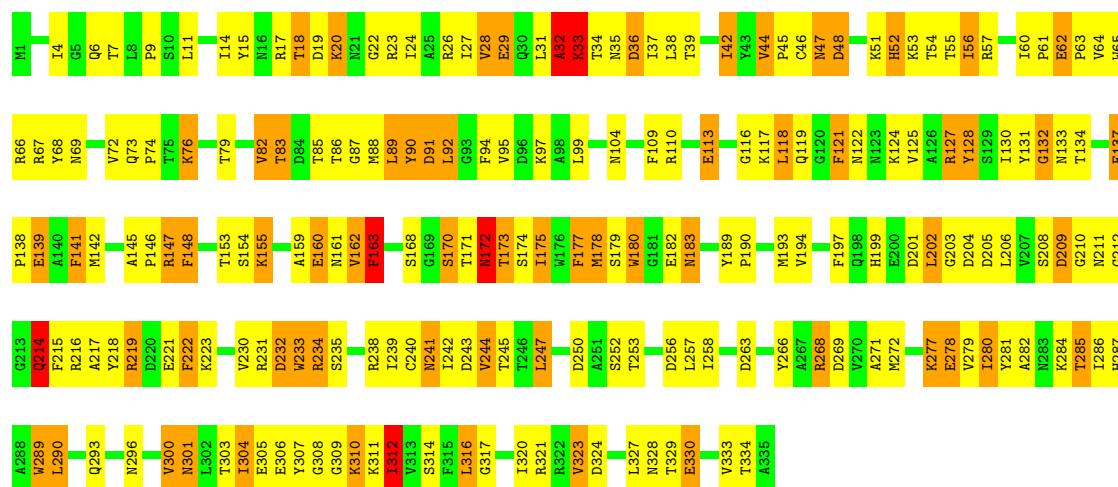


• Molecule 2: gp7



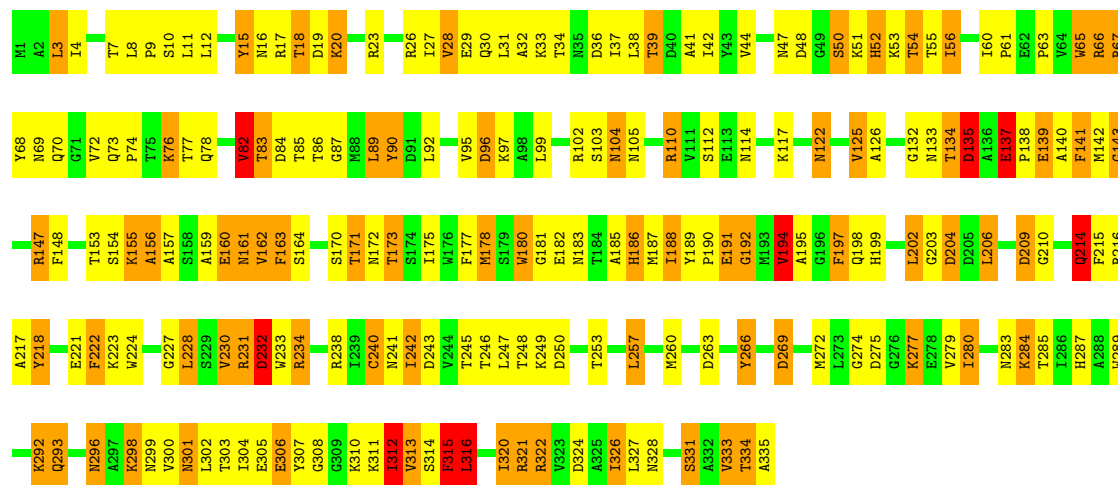
• Molecule 2: gp7





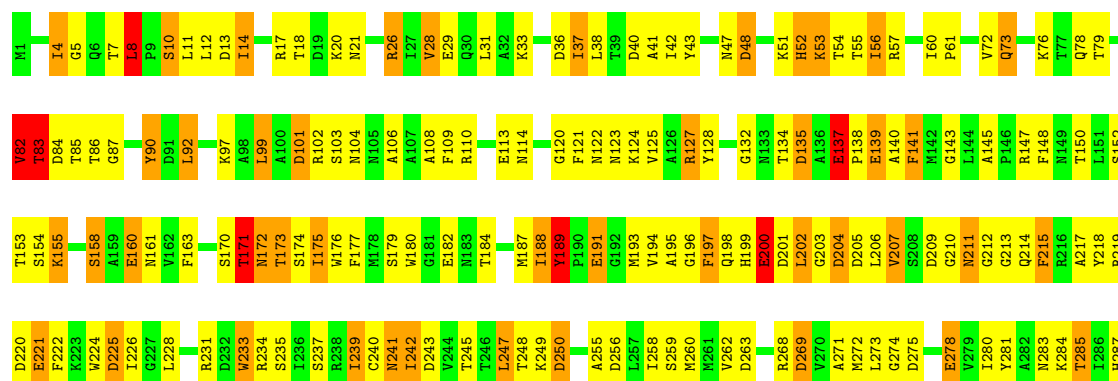
• Molecule 2: gp7

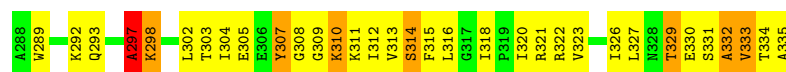
Chain B: 38% 38% 22%



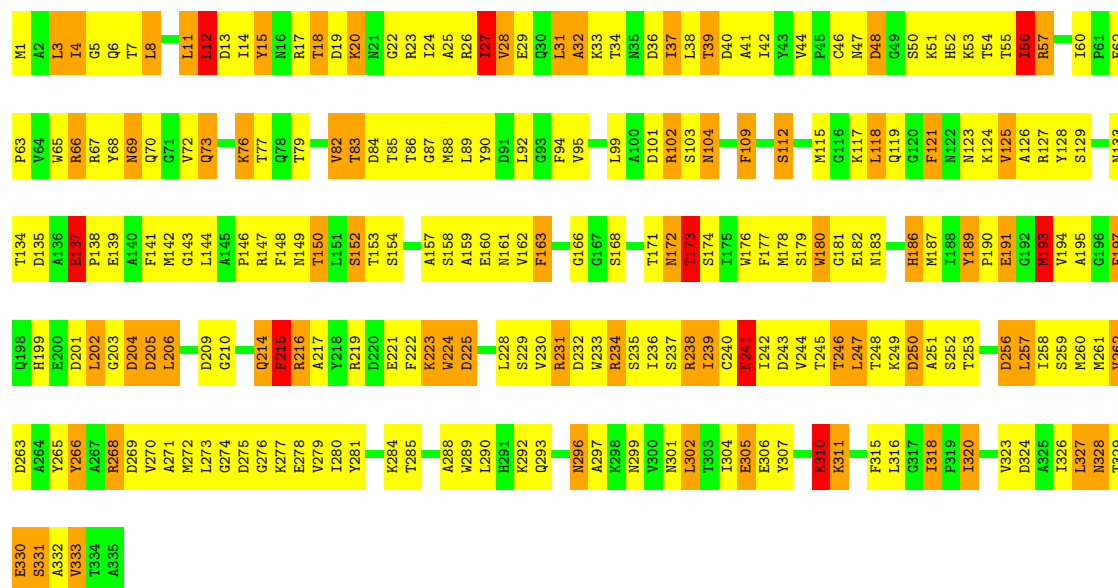
• Molecule 2: gp7

Chain G: 38% 44% 15%

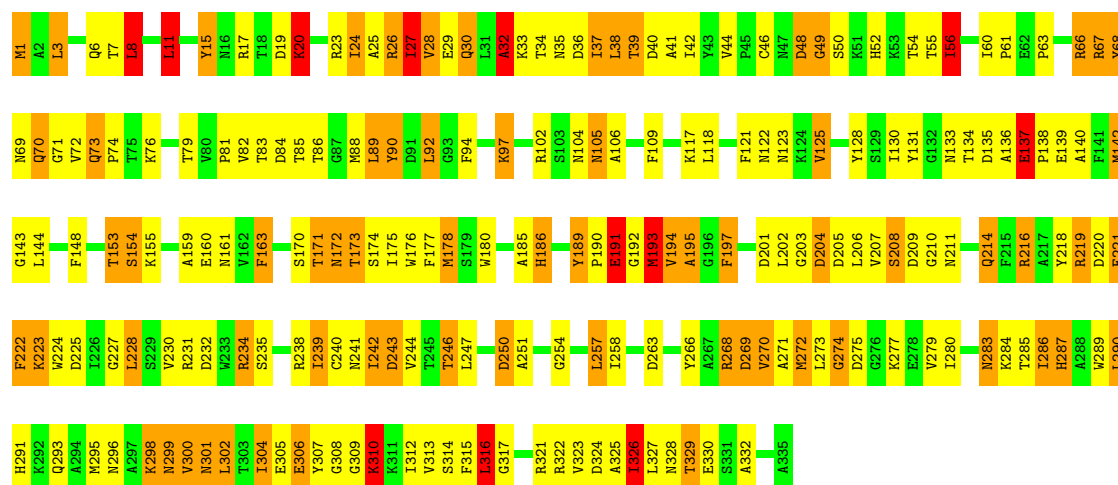




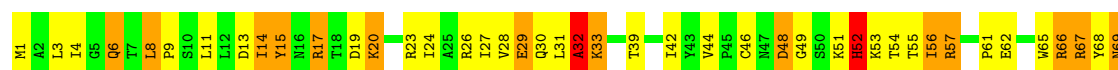
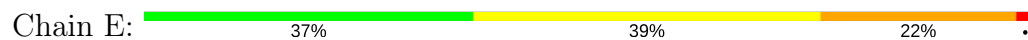
• Molecule 2: gp7



• Molecule 2: gp7



• Molecule 2: gp7



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| K284 | T285 | I286 | H287 | A288 | W289 | L290 | H291 | R292 | Q293 | N296 | A297 | K298 | N299 | V300 | N301 | L302 | T303 | I304 | E305 | E306 | Y307 | G308 | G309 | K310 | F315 | L316 | G317 | I318 | F319 | I320 | R321 | R322 | I326 | L327 | N328 | T329 | E330 | S331 | A332 | V333 | T334 | A335 | | | | | | | | | | | | | | | |
| R215 | R216 | A217 | T218 | R219 | F222 | K223 | W224 | D225 | L226 | G227 | L228 | S229 | V230 | R231 | D232 | W233 | R234 | S235 | I236 | S237 | R238 | I239 | C240 | R241 | I242 | D243 | T246 | L247 | T248 | K249 | D250 | A251 | S252 | T253 | D256 | L257 | L258 | S259 | M260 | D263 | A264 | D269 | V270 | A271 | M272 | L273 | G274 | D275 | G276 | K277 | E278 | V279 | I280 | | | | |
| T150 | L151 | S154 | K155 | A156 | A157 | S158 | A159 | E160 | N161 | V162 | F163 | S164 | G169 | S170 | T171 | N172 | T173 | S174 | I175 | W176 | F177 | M178 | S179 | W180 | G181 | N182 | N183 | T184 | A185 | H186 | M187 | I188 | Y189 | P190 | E191 | G192 | M193 | V194 | F197 | Q198 | H199 | E200 | D201 | L202 | G203 | D204 | D205 | L206 | V207 | P138 | S208 | D209 | G210 | N211 | G212 | G213 | Q214 |
| Q70 | G71 | W72 | Q73 | P74 | T77 | Q78 | T79 | V82 | T83 | H88 | L89 | Y90 | F94 | Y95 | D96 | K97 | A98 | L99 | A100 | D101 | R102 | S103 | N104 | N105 | A106 | E113 | K117 | L118 | Q119 | G120 | F121 | N122 | N123 | K124 | R127 | Y128 | S129 | I130 | Y131 | T134 | D135 | A136 | E137 | P138 | E139 | A140 | F141 | R147 | F148 | N149 | | | | | | | |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 14000 | Depositor |
| Resolution determination method | Gold Standard Definition (FSC at 0.143 cut-off) with two independent maps | Depositor |
| CTF correction method | per particle | Depositor |
| Microscope | JEOL 3200FSC | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 17 | Depositor |
| Minimum defocus (nm) | 400 | Depositor |
| Maximum defocus (nm) | 2700 | Depositor |
| Magnification | 53361 | Depositor |
| Image detector | Kodak SO163 film | 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 >2 | RMSZ | # Z >2 |
| 1 | H | 0.29 | 0/862 | 0.81 | 1/1166 (0.1%) |
| 1 | I | 0.31 | 0/862 | 0.79 | 0/1166 |
| 1 | J | 0.31 | 0/862 | 0.81 | 1/1166 (0.1%) |
| 1 | K | 0.31 | 0/862 | 0.81 | 1/1166 (0.1%) |
| 1 | L | 0.32 | 0/862 | 0.76 | 0/1166 |
| 1 | M | 0.31 | 0/862 | 0.80 | 0/1166 |
| 1 | N | 0.30 | 0/862 | 0.75 | 1/1166 (0.1%) |
| 2 | A | 0.31 | 0/2637 | 0.72 | 3/3573 (0.1%) |
| 2 | B | 0.31 | 0/2637 | 0.69 | 1/3573 (0.0%) |
| 2 | C | 0.30 | 0/2637 | 0.70 | 1/3573 (0.0%) |
| 2 | D | 0.31 | 0/2637 | 0.71 | 1/3573 (0.0%) |
| 2 | E | 0.31 | 0/2637 | 0.69 | 1/3573 (0.0%) |
| 2 | F | 0.31 | 0/2637 | 0.69 | 0/3573 |
| 2 | G | 0.30 | 0/2637 | 0.69 | 1/3573 (0.0%) |
| All | All | 0.31 | 0/24493 | 0.72 | 12/33173 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | H | 0 | 2 |
| 1 | I | 0 | 2 |
| 1 | J | 0 | 3 |
| 1 | K | 0 | 1 |
| 1 | L | 0 | 2 |
| 1 | M | 0 | 2 |
| 1 | N | 0 | 1 |
| 2 | A | 0 | 4 |
| 2 | B | 0 | 1 |
| 2 | C | 0 | 3 |
| 2 | D | 0 | 4 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | E | 0 | 4 |
| 2 | F | 0 | 5 |
| 2 | G | 0 | 5 |
| All | All | 0 | 39 |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | A | 92 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 2 | G | 99 | LEU | CA-CB-CG | 6.00 | 129.09 | 115.30 |
| 2 | A | 202 | LEU | CA-CB-CG | 5.63 | 128.25 | 115.30 |
| 2 | B | 316 | LEU | CA-CB-CG | 5.58 | 128.14 | 115.30 |
| 2 | D | 12 | LEU | CA-CB-CG | 5.55 | 128.06 | 115.30 |
| 1 | J | 104 | PHE | N-CA-C | 5.24 | 125.14 | 111.00 |
| 2 | C | 316 | LEU | CA-CB-CG | 5.23 | 127.33 | 115.30 |
| 2 | A | 316 | LEU | CA-CB-CG | 5.17 | 127.18 | 115.30 |
| 1 | K | 42 | LEU | CA-CB-CG | 5.17 | 127.18 | 115.30 |
| 1 | H | 34 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 2 | E | 316 | LEU | CA-CB-CG | 5.12 | 127.08 | 115.30 |
| 1 | N | 30 | LEU | CA-CB-CG | 5.09 | 127.02 | 115.30 |

There are no chirality outliers.

All (39) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | A | 137 | GLU | Peptide |
| 2 | A | 182 | GLU | Peptide |
| 2 | A | 241 | ASN | Peptide |
| 2 | A | 32 | ALA | Peptide |
| 2 | B | 137 | GLU | Peptide |
| 2 | C | 137 | GLU | Peptide |
| 2 | C | 195 | ALA | Peptide |
| 2 | C | 32 | ALA | Peptide |
| 2 | D | 137 | GLU | Peptide |
| 2 | D | 305 | GLU | Peptide |
| 2 | D | 31 | LEU | Peptide |
| 2 | D | 32 | ALA | Peptide |
| 2 | E | 137 | GLU | Peptide |
| 2 | E | 180 | TRP | Peptide |
| 2 | E | 31 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | E | 32 | ALA | Peptide |
| 2 | F | 137 | GLU | Peptide |
| 2 | F | 241 | ASN | Peptide |
| 2 | F | 31 | LEU | Peptide |
| 2 | F | 32 | ALA | Peptide |
| 2 | F | 48 | ASP | Peptide |
| 2 | G | 137 | GLU | Peptide |
| 2 | G | 171 | THR | Peptide |
| 2 | G | 189 | TYR | Peptide |
| 2 | G | 297 | ALA | Peptide |
| 2 | G | 82 | VAL | Peptide |
| 1 | H | 105 | TYR | Peptide |
| 1 | H | 34 | LEU | Peptide |
| 1 | I | 105 | TYR | Peptide |
| 1 | I | 34 | LEU | Peptide |
| 1 | J | 103 | ALA | Peptide |
| 1 | J | 45 | ASN | Peptide |
| 1 | J | 5 | ASN | Peptide |
| 1 | K | 105 | TYR | Peptide |
| 1 | L | 103 | ALA | Peptide |
| 1 | L | 83 | GLN | Peptide |
| 1 | M | 103 | ALA | Peptide |
| 1 | M | 77 | ASP | Peptide |
| 1 | N | 105 | TYR | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | H | 850 | 0 | 820 | 78 | 0 |
| 1 | I | 850 | 0 | 820 | 83 | 0 |
| 1 | J | 850 | 0 | 820 | 74 | 0 |
| 1 | K | 850 | 0 | 820 | 84 | 0 |
| 1 | L | 850 | 0 | 820 | 68 | 0 |
| 1 | M | 850 | 0 | 820 | 74 | 0 |
| 1 | N | 850 | 0 | 820 | 82 | 0 |
| 2 | A | 2588 | 0 | 2542 | 194 | 0 |
| 2 | B | 2588 | 0 | 2542 | 181 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | C | 2588 | 0 | 2542 | 169 | 0 |
| 2 | D | 2588 | 0 | 2542 | 211 | 0 |
| 2 | E | 2588 | 0 | 2542 | 180 | 0 |
| 2 | F | 2588 | 0 | 2542 | 195 | 0 |
| 2 | G | 2588 | 0 | 2542 | 146 | 0 |
| All | All | 24066 | 0 | 23534 | 1682 | 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 35.

All (1682) 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:L:89:LEU:HG | 1:L:91:PRO:HD3 | 1.48 | 0.94 |
| 2:D:101:ASP:HB2 | 2:D:104:ASN:HA | 1.52 | 0.91 |
| 2:G:200:GLU:HG2 | 2:G:219:ARG:H | 1.34 | 0.90 |
| 2:D:147:ARG:HH22 | 2:D:162:VAL:HG13 | 1.34 | 0.90 |
| 2:A:312:ILE:O | 2:A:314:SER:N | 2.06 | 0.89 |
| 2:E:90:TYR:HB2 | 2:E:223:LYS:HA | 1.55 | 0.88 |
| 2:A:234:ARG:HH12 | 2:B:33:LYS:HG3 | 1.38 | 0.88 |
| 2:E:299:ASN:OD1 | 2:E:301:ASN:ND2 | 2.08 | 0.87 |
| 2:F:172:ASN:HB3 | 2:F:243:ASP:HB3 | 1.57 | 0.86 |
| 2:G:187:MET:SD | 2:G:187:MET:N | 2.50 | 0.85 |
| 2:C:291:HIS:HB2 | 2:C:312:ILE:HD11 | 1.58 | 0.85 |
| 2:A:76:LYS:HE2 | 2:B:7:THR:HB | 1.56 | 0.85 |
| 2:F:132:GLY:H | 2:F:142:MET:HG3 | 1.41 | 0.84 |
| 2:A:301:ASN:HB2 | 2:F:300:VAL:HG23 | 1.57 | 0.84 |
| 2:A:307:TYR:HB2 | 2:A:308:GLY:HA2 | 1.61 | 0.83 |
| 2:C:1:MET:N | 2:C:1:MET:SD | 2.51 | 0.82 |
| 2:E:174:SER:HA | 2:E:241:ASN:HD21 | 1.45 | 0.82 |
| 1:N:58:VAL:HG22 | 1:N:59:MET:HG3 | 1.62 | 0.82 |
| 2:F:47:ASN:ND2 | 2:F:48:ASP:OD2 | 2.13 | 0.82 |
| 2:D:66:ARG:NH1 | 2:E:88:MET:SD | 2.53 | 0.81 |
| 2:G:145:ALA:HA | 2:G:333:VAL:HG12 | 1.63 | 0.81 |
| 2:B:92:LEU:HB3 | 2:B:221:GLU:HB2 | 1.61 | 0.80 |
| 2:F:307:TYR:HB2 | 2:F:308:GLY:HA2 | 1.61 | 0.80 |
| 1:M:18:GLY:HA3 | 1:M:91:PRO:HD2 | 1.62 | 0.80 |
| 2:E:95:VAL:HG23 | 2:E:218:TYR:HB3 | 1.64 | 0.80 |
| 2:G:241:ASN:HD22 | 2:G:242:ILE:HG13 | 1.47 | 0.80 |
| 2:D:173:THR:OG1 | 2:D:174:SER:N | 2.14 | 0.80 |
| 2:E:284:LYS:HA | 2:E:322:ARG:HH21 | 1.48 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:97:LYS:HZ2 | 2:F:216:ARG:HE | 1.28 | 0.79 |
| 2:C:329:THR:OG1 | 2:C:330:GLU:N | 2.15 | 0.79 |
| 1:N:89:LEU:HG | 1:N:91:PRO:HD3 | 1.65 | 0.79 |
| 1:J:45:ASN:HB3 | 1:J:96:ASP:HB3 | 1.65 | 0.78 |
| 1:I:89:LEU:HG | 1:I:91:PRO:HD3 | 1.64 | 0.78 |
| 2:G:307:TYR:O | 2:G:309:GLY:N | 2.16 | 0.78 |
| 2:D:234:ARG:HH12 | 2:E:32:ALA:HB1 | 1.48 | 0.77 |
| 2:B:70:GLN:HG2 | 1:J:3:THR:HG21 | 1.66 | 0.77 |
| 2:E:187:MET:SD | 2:E:187:MET:N | 2.55 | 0.77 |
| 2:C:209:ASP:N | 2:C:210:GLY:HA2 | 2.00 | 0.76 |
| 2:G:161:ASN:ND2 | 2:G:256:ASP:OD1 | 2.12 | 0.76 |
| 1:I:2:LYS:HE2 | 1:I:106:PRO:HG2 | 1.66 | 0.76 |
| 1:M:8:THR:HG22 | 1:M:9:GLY:HA2 | 1.66 | 0.76 |
| 2:F:14:ILE:O | 2:F:18:THR:OG1 | 2.02 | 0.76 |
| 2:G:90:TYR:HB2 | 2:G:222:PHE:O | 1.85 | 0.76 |
| 1:I:59:MET:HB2 | 1:I:60:ALA:HB2 | 1.68 | 0.76 |
| 1:I:92:GLN:HB3 | 1:I:93:LYS:HB3 | 1.68 | 0.76 |
| 2:E:252:SER:OG | 2:E:296:ASN:OD1 | 2.03 | 0.76 |
| 2:F:300:VAL:HG13 | 2:F:301:ASN:H | 1.51 | 0.76 |
| 2:A:209:ASP:N | 2:A:210:GLY:HA2 | 2.01 | 0.75 |
| 1:H:59:MET:HB2 | 1:H:60:ALA:HB2 | 1.67 | 0.75 |
| 2:B:209:ASP:N | 2:B:210:GLY:HA2 | 2.00 | 0.75 |
| 2:F:242:ILE:HB | 2:F:244:VAL:H | 1.51 | 0.75 |
| 2:A:141:PHE:O | 2:A:143:GLY:N | 2.19 | 0.75 |
| 1:J:20:PRO:HB3 | 1:J:21:GLU:HG3 | 1.68 | 0.75 |
| 1:K:1:MET:HB3 | 1:K:2:LYS:HE3 | 1.67 | 0.75 |
| 2:D:247:LEU:O | 2:D:289:TRP:NE1 | 2.18 | 0.74 |
| 2:C:173:THR:OG1 | 2:C:174:SER:N | 2.15 | 0.74 |
| 2:D:327:LEU:O | 2:D:328:ASN:ND2 | 2.20 | 0.74 |
| 2:E:296:ASN:O | 2:E:299:ASN:ND2 | 2.20 | 0.74 |
| 1:L:42:LEU:HD11 | 1:L:101:LYS:HG2 | 1.68 | 0.74 |
| 2:A:90:TYR:HB3 | 2:A:223:LYS:HA | 1.68 | 0.74 |
| 1:I:28:TRP:HA | 1:I:84:ILE:HG21 | 1.69 | 0.74 |
| 2:A:149:ASN:HB3 | 2:A:155:LYS:HB2 | 1.70 | 0.74 |
| 1:H:89:LEU:HG | 1:H:91:PRO:HD3 | 1.69 | 0.74 |
| 2:D:92:LEU:HB3 | 2:D:221:GLU:HG3 | 1.69 | 0.74 |
| 1:H:28:TRP:HA | 1:H:84:ILE:HG21 | 1.69 | 0.74 |
| 2:F:173:THR:OG1 | 2:F:174:SER:N | 2.21 | 0.74 |
| 1:M:8:THR:HG21 | 1:M:101:LYS:HB3 | 1.69 | 0.74 |
| 1:K:46:ALA:HB3 | 1:K:95:ASP:HB2 | 1.69 | 0.73 |
| 2:B:197:PHE:HE2 | 2:B:221:GLU:HB3 | 1.53 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:164:SER:HB3 | 2:E:331:SER:HB2 | 1.69 | 0.73 |
| 2:G:26:ARG:O | 2:G:26:ARG:NE | 2.21 | 0.73 |
| 2:A:297:ALA:O | 2:A:301:ASN:ND2 | 2.20 | 0.73 |
| 2:G:329:THR:OG1 | 2:G:330:GLU:N | 2.21 | 0.73 |
| 1:L:5:ASN:N | 1:L:5:ASN:OD1 | 2.22 | 0.73 |
| 2:A:17:ARG:HH11 | 2:F:57:ARG:HH21 | 1.37 | 0.73 |
| 2:B:155:LYS:O | 2:B:157:ALA:N | 2.22 | 0.73 |
| 2:B:32:ALA:HB1 | 2:B:33:LYS:HB2 | 1.71 | 0.73 |
| 2:A:244:VAL:HA | 2:A:247:LEU:HB3 | 1.70 | 0.73 |
| 2:A:326:ILE:HD13 | 2:A:327:LEU:H | 1.54 | 0.73 |
| 2:A:69:ASN:HB2 | 1:I:3:THR:HG21 | 1.69 | 0.73 |
| 1:K:9:GLY:HA2 | 1:K:101:LYS:HD2 | 1.70 | 0.73 |
| 2:A:291:HIS:HB2 | 2:A:312:ILE:HD11 | 1.71 | 0.72 |
| 2:D:17:ARG:NH1 | 2:D:112:SER:OG | 2.22 | 0.72 |
| 2:D:238:ARG:HH11 | 2:D:333:VAL:HG22 | 1.54 | 0.72 |
| 2:G:209:ASP:H | 2:G:211:ASN:H | 1.35 | 0.72 |
| 2:E:181:GLY:O | 2:E:231:ARG:NH2 | 2.22 | 0.72 |
| 2:B:160:GLU:HB2 | 2:B:240:CYS:H | 1.54 | 0.72 |
| 1:K:18:GLY:HA3 | 1:K:91:PRO:HD2 | 1.72 | 0.72 |
| 2:D:60:ILE:HD13 | 2:D:77:THR:HG23 | 1.71 | 0.72 |
| 1:N:24:ASP:OD1 | 1:N:24:ASP:N | 2.23 | 0.72 |
| 2:E:23:ARG:O | 2:E:26:ARG:NH2 | 2.23 | 0.72 |
| 2:F:95:VAL:HG22 | 2:F:218:TYR:HB2 | 1.71 | 0.71 |
| 1:N:22:THR:OG1 | 2:A:1:MET:O | 2.07 | 0.71 |
| 2:D:57:ARG:HB3 | 2:D:79:THR:HG22 | 1.72 | 0.71 |
| 1:L:94:ARG:NH2 | 1:L:95:ASP:O | 2.23 | 0.71 |
| 2:F:171:THR:O | 2:F:328:ASN:HA | 1.90 | 0.71 |
| 2:D:186:HIS:HD2 | 2:D:191:GLU:HA | 1.55 | 0.71 |
| 2:E:275:ASP:OD1 | 2:E:276:GLY:N | 2.22 | 0.71 |
| 2:F:160:GLU:HB2 | 2:F:240:CYS:H | 1.55 | 0.71 |
| 1:M:89:LEU:HG | 1:M:91:PRO:HD3 | 1.72 | 0.71 |
| 2:G:241:ASN:HB2 | 2:G:242:ILE:HG13 | 1.73 | 0.71 |
| 2:C:189:TYR:HB2 | 2:C:190:PRO:HD2 | 1.71 | 0.71 |
| 2:F:209:ASP:N | 2:F:210:GLY:HA2 | 2.06 | 0.71 |
| 2:F:72:VAL:HG12 | 2:F:73:GLN:HG2 | 1.72 | 0.70 |
| 2:G:175:ILE:HG12 | 2:G:239:ILE:HD11 | 1.73 | 0.70 |
| 2:D:202:LEU:HA | 2:D:216:ARG:HA | 1.71 | 0.70 |
| 2:D:252:SER:HA | 2:D:296:ASN:HB2 | 1.72 | 0.70 |
| 2:A:240:CYS:HB2 | 2:A:333:VAL:HG11 | 1.72 | 0.70 |
| 2:A:92:LEU:HD22 | 2:F:74:PRO:HB3 | 1.74 | 0.70 |
| 2:B:117:LYS:HD2 | 2:B:222:PHE:HE1 | 1.55 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:90:TYR:HB3 | 2:B:223:LYS:HA | 1.73 | 0.70 |
| 1:H:44:LEU:HB2 | 1:H:97:ALA:HB2 | 1.74 | 0.70 |
| 2:E:97:LYS:HE2 | 2:E:200:GLU:HB2 | 1.73 | 0.70 |
| 2:B:299:ASN:HA | 2:C:301:ASN:HD21 | 1.56 | 0.70 |
| 1:H:14:VAL:HA | 1:H:96:ASP:HA | 1.73 | 0.70 |
| 2:F:172:ASN:HB2 | 2:F:241:ASN:O | 1.91 | 0.70 |
| 2:A:187:MET:SD | 2:A:187:MET:N | 2.65 | 0.69 |
| 1:L:59:MET:HB2 | 1:L:60:ALA:HB2 | 1.74 | 0.69 |
| 2:A:127:ARG:O | 2:A:127:ARG:NH1 | 2.25 | 0.69 |
| 2:B:241:ASN:HB2 | 2:B:242:ILE:HG23 | 1.72 | 0.69 |
| 2:A:110:ARG:O | 2:A:114:ASN:ND2 | 2.25 | 0.69 |
| 2:D:245:THR:O | 2:D:248:THR:OG1 | 2.07 | 0.69 |
| 1:N:6:MET:HG2 | 2:A:1:MET:HB2 | 1.73 | 0.69 |
| 2:E:224:TRP:HD1 | 2:E:225:ASP:H | 1.39 | 0.69 |
| 2:D:63:PRO:HB2 | 2:E:89:LEU:HD11 | 1.74 | 0.69 |
| 2:D:248:THR:HA | 2:D:289:TRP:CZ2 | 2.28 | 0.69 |
| 1:I:42:LEU:HD13 | 1:I:101:LYS:HG3 | 1.75 | 0.69 |
| 1:N:18:GLY:H | 1:N:91:PRO:HD2 | 1.57 | 0.69 |
| 1:J:51:ALA:HB3 | 1:J:90:ALA:HB3 | 1.74 | 0.69 |
| 2:E:101:ASP:OD1 | 2:E:101:ASP:N | 2.26 | 0.69 |
| 1:J:41:ARG:HD2 | 1:J:41:ARG:H | 1.56 | 0.69 |
| 2:A:66:ARG:HD2 | 2:A:68:TYR:H | 1.58 | 0.69 |
| 1:L:52:VAL:HA | 1:L:88:GLY:HA3 | 1.74 | 0.69 |
| 1:N:92:GLN:HB3 | 1:N:93:LYS:HB3 | 1.73 | 0.69 |
| 2:E:241:ASN:HB2 | 2:E:242:ILE:HG23 | 1.75 | 0.68 |
| 1:N:30:LEU:O | 1:N:31:ARG:NE | 2.23 | 0.68 |
| 2:B:247:LEU:O | 2:B:289:TRP:NE1 | 2.24 | 0.68 |
| 2:B:187:MET:O | 2:B:189:TYR:N | 2.25 | 0.68 |
| 2:C:24:ILE:O | 2:C:26:ARG:NH2 | 2.27 | 0.68 |
| 2:E:182:GLU:HG3 | 2:E:231:ARG:HB3 | 1.74 | 0.68 |
| 1:K:21:GLU:OE2 | 1:K:23:LYS:NZ | 2.26 | 0.68 |
| 2:C:247:LEU:HB3 | 2:C:289:TRP:NE1 | 2.09 | 0.68 |
| 2:F:68:TYR:O | 2:F:69:ASN:ND2 | 2.26 | 0.68 |
| 2:G:271:ALA:HA | 2:G:273:LEU:H | 1.58 | 0.68 |
| 2:A:19:ASP:OD2 | 2:A:26:ARG:NH2 | 2.27 | 0.68 |
| 2:C:193:MET:O | 2:C:195:ALA:N | 2.26 | 0.68 |
| 1:J:46:ALA:HB3 | 1:J:96:ASP:HB2 | 1.74 | 0.68 |
| 2:A:68:TYR:HB2 | 1:I:2:LYS:HB2 | 1.76 | 0.68 |
| 1:N:10:THR:H | 1:N:11:ASP:HA | 1.59 | 0.68 |
| 2:C:315:PHE:HA | 2:C:316:LEU:HB3 | 1.75 | 0.68 |
| 2:F:171:THR:OG1 | 2:F:172:ASN:N | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:77:ASP:OD1 | 1:I:78:ASN:ND2 | 2.26 | 0.68 |
| 1:K:101:LYS:HE3 | 1:K:101:LYS:H | 1.59 | 0.68 |
| 2:A:158:SER:O | 2:A:160:GLU:N | 2.27 | 0.67 |
| 2:A:173:THR:OG1 | 2:A:174:SER:N | 2.26 | 0.67 |
| 2:B:289:TRP:O | 2:B:292:LYS:NZ | 2.27 | 0.67 |
| 1:K:101:LYS:HG2 | 1:K:102:ASP:H | 1.60 | 0.67 |
| 1:N:101:LYS:HD3 | 1:N:102:ASP:H | 1.58 | 0.67 |
| 1:I:2:LYS:NZ | 1:I:3:THR:O | 2.25 | 0.67 |
| 2:A:242:ILE:HG21 | 2:A:247:LEU:HD13 | 1.76 | 0.67 |
| 2:C:37:ILE:HG22 | 2:C:38:LEU:H | 1.59 | 0.67 |
| 2:G:195:ALA:HA | 2:G:197:PHE:H | 1.60 | 0.67 |
| 2:E:55:THR:O | 2:E:56:ILE:HG13 | 1.95 | 0.67 |
| 1:K:59:MET:HB2 | 1:K:60:ALA:HB2 | 1.77 | 0.67 |
| 2:D:252:SER:OG | 2:C:299:ASN:ND2 | 2.27 | 0.67 |
| 2:E:8:LEU:HD22 | 2:E:9:PRO:HD2 | 1.75 | 0.67 |
| 1:K:80:VAL:HG13 | 1:K:81:GLU:H | 1.60 | 0.67 |
| 2:B:173:THR:HG22 | 2:B:327:LEU:HA | 1.75 | 0.67 |
| 1:I:24:ASP:OD1 | 1:I:24:ASP:N | 2.28 | 0.66 |
| 2:A:17:ARG:HG3 | 2:F:79:THR:HG21 | 1.77 | 0.66 |
| 2:F:87:GLY:HA3 | 2:F:138:PRO:HG3 | 1.76 | 0.66 |
| 1:J:89:LEU:HG | 1:J:91:PRO:HD3 | 1.76 | 0.66 |
| 2:D:162:VAL:HG12 | 2:D:163:PHE:H | 1.60 | 0.66 |
| 2:F:124:LYS:O | 2:F:124:LYS:NZ | 2.28 | 0.66 |
| 1:N:65:CYS:SG | 1:N:66:SER:N | 2.69 | 0.66 |
| 2:A:178:MET:SD | 2:A:178:MET:N | 2.68 | 0.66 |
| 2:D:249:LYS:NZ | 2:D:253:THR:OG1 | 2.28 | 0.66 |
| 2:E:160:GLU:H | 2:E:239:ILE:HG22 | 1.60 | 0.66 |
| 2:F:271:ALA:HA | 2:F:272:MET:HB3 | 1.77 | 0.66 |
| 2:F:177:PHE:HB3 | 2:F:280:ILE:HA | 1.77 | 0.66 |
| 2:A:326:ILE:HG23 | 2:A:328:ASN:H | 1.61 | 0.66 |
| 2:B:12:LEU:O | 2:B:16:ASN:ND2 | 2.28 | 0.66 |
| 2:B:296:ASN:OD1 | 2:B:296:ASN:N | 2.28 | 0.66 |
| 1:M:21:GLU:HG3 | 1:M:22:THR:H | 1.61 | 0.66 |
| 2:C:283:ASN:HD21 | 2:C:286:ILE:HB | 1.60 | 0.66 |
| 2:G:187:MET:O | 2:G:189:TYR:N | 2.28 | 0.66 |
| 1:H:6:MET:H | 1:H:104:PHE:HE2 | 1.42 | 0.66 |
| 1:I:40:GLN:NE2 | 1:I:41:ARG:H | 1.93 | 0.66 |
| 2:B:172:ASN:HB2 | 2:B:242:ILE:N | 2.11 | 0.66 |
| 2:E:250:ASP:HA | 2:E:253:THR:HG22 | 1.77 | 0.66 |
| 2:B:315:PHE:HD1 | 2:B:316:LEU:HD13 | 1.61 | 0.66 |
| 2:D:90:TYR:OH | 2:C:66:ARG:NH2 | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:263:ASP:OD1 | 2:E:264:ALA:N | 2.29 | 0.66 |
| 2:F:90:TYR:OH | 2:E:66:ARG:NH2 | 2.29 | 0.66 |
| 2:F:9:PRO:HG3 | 2:F:95:VAL:HA | 1.78 | 0.66 |
| 2:F:258:ILE:HG21 | 2:F:290:LEU:HD23 | 1.78 | 0.66 |
| 1:N:59:MET:HB2 | 1:N:60:ALA:HB2 | 1.78 | 0.66 |
| 2:A:13:ASP:OD2 | 2:A:17:ARG:NH2 | 2.29 | 0.65 |
| 2:C:195:ALA:HB3 | 2:C:222:PHE:HA | 1.77 | 0.65 |
| 1:I:14:VAL:HA | 1:I:97:ALA:O | 1.95 | 0.65 |
| 2:A:1:MET:SD | 2:A:1:MET:N | 2.53 | 0.65 |
| 2:A:57:ARG:NH2 | 2:A:77:THR:OG1 | 2.28 | 0.65 |
| 2:B:284:LYS:O | 2:B:287:HIS:N | 2.30 | 0.65 |
| 2:C:258:ILE:HG12 | 2:C:290:LEU:HD23 | 1.78 | 0.65 |
| 2:G:110:ARG:O | 2:G:114:ASN:ND2 | 2.23 | 0.65 |
| 2:C:203:GLY:HA3 | 2:C:204:ASP:HB3 | 1.79 | 0.65 |
| 1:K:40:GLN:HG3 | 1:K:41:ARG:H | 1.61 | 0.65 |
| 2:A:271:ALA:HA | 2:A:272:MET:HB2 | 1.79 | 0.65 |
| 2:C:230:VAL:O | 2:C:232:ASP:N | 2.29 | 0.65 |
| 1:H:54:ASP:HB2 | 1:H:83:GLN:HB3 | 1.78 | 0.65 |
| 2:C:23:ARG:HD2 | 2:C:24:ILE:H | 1.62 | 0.65 |
| 2:D:288:ALA:HA | 2:C:266:TYR:HD1 | 1.60 | 0.65 |
| 1:J:8:THR:OG1 | 1:J:102:ASP:O | 2.11 | 0.65 |
| 2:A:171:THR:OG1 | 2:A:172:ASN:N | 2.28 | 0.65 |
| 2:C:283:ASN:HB3 | 2:C:325:ALA:HB3 | 1.79 | 0.65 |
| 2:G:214:GLN:HG3 | 2:G:215:PHE:H | 1.60 | 0.65 |
| 1:N:80:VAL:HG22 | 1:N:81:GLU:H | 1.62 | 0.65 |
| 1:H:7:LYS:HG3 | 2:F:67:ARG:HH12 | 1.62 | 0.65 |
| 1:I:44:LEU:HD13 | 1:I:45:ASN:H | 1.60 | 0.65 |
| 2:G:147:ARG:HB2 | 2:G:335:ALA:HA | 1.79 | 0.65 |
| 1:H:22:THR:O | 1:H:25:GLN:NE2 | 2.30 | 0.65 |
| 1:M:33:THR:OG1 | 2:G:53:LYS:NZ | 2.30 | 0.64 |
| 1:N:55:SER:OG | 1:N:56:VAL:N | 2.30 | 0.64 |
| 2:A:270:VAL:HG13 | 2:B:36:ASP:OD1 | 1.97 | 0.64 |
| 2:E:248:THR:HA | 2:E:289:TRP:CZ2 | 2.32 | 0.64 |
| 2:G:37:ILE:HG13 | 2:G:323:VAL:HG13 | 1.78 | 0.64 |
| 1:N:51:ALA:HA | 1:N:65:CYS:HA | 1.78 | 0.64 |
| 2:G:179:SER:HA | 2:G:278:GLU:HA | 1.80 | 0.64 |
| 1:L:22:THR:OG1 | 1:L:23:LYS:N | 2.31 | 0.64 |
| 1:M:59:MET:HB2 | 1:M:60:ALA:HB2 | 1.78 | 0.64 |
| 2:A:304:ILE:HG12 | 2:A:305:GLU:H | 1.63 | 0.64 |
| 2:D:203:GLY:HA2 | 2:D:204:ASP:CG | 2.18 | 0.64 |
| 2:A:70:GLN:HE22 | 1:I:3:THR:HB | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:E:96:ASP:OD1 | 2:E:99:LEU:N | 2.30 | 0.64 |
| 2:A:53:LYS:O | 2:A:83:THR:OG1 | 2.16 | 0.64 |
| 2:B:76:LYS:NZ | 2:C:6:GLN:O | 2.30 | 0.64 |
| 2:A:51:LYS:NZ | 2:A:83:THR:O | 2.31 | 0.64 |
| 2:D:215:PHE:HE2 | 2:D:217:ALA:HB2 | 1.63 | 0.64 |
| 2:E:274:GLY:O | 2:E:276:GLY:N | 2.31 | 0.64 |
| 2:G:4:ILE:HG22 | 2:G:5:GLY:H | 1.63 | 0.64 |
| 2:D:88:MET:SD | 2:C:66:ARG:NH1 | 2.70 | 0.63 |
| 2:E:177:PHE:CB | 2:E:280:ILE:HA | 2.29 | 0.63 |
| 2:A:142:MET:O | 2:A:144:LEU:N | 2.22 | 0.63 |
| 1:K:5:ASN:HD21 | 1:K:22:THR:HB | 1.62 | 0.63 |
| 2:D:17:ARG:HG3 | 2:C:79:THR:HG21 | 1.80 | 0.63 |
| 2:D:171:THR:HG1 | 2:D:244:VAL:H | 1.46 | 0.63 |
| 2:F:97:LYS:HB2 | 2:F:217:ALA:HA | 1.79 | 0.63 |
| 1:J:70:ARG:HE | 1:J:70:ARG:H | 1.46 | 0.63 |
| 2:E:326:ILE:HG13 | 2:E:328:ASN:H | 1.63 | 0.63 |
| 2:G:55:THR:OG1 | 2:G:56:ILE:N | 2.29 | 0.63 |
| 2:D:14:ILE:HG21 | 2:D:99:LEU:HD11 | 1.79 | 0.63 |
| 2:D:121:PHE:HE1 | 2:C:63:PRO:HB3 | 1.64 | 0.63 |
| 2:E:185:ALA:N | 2:E:227:GLY:O | 2.32 | 0.63 |
| 1:H:10:THR:HB | 1:H:101:LYS:HG3 | 1.80 | 0.63 |
| 1:M:29:GLY:H | 1:M:84:ILE:HG21 | 1.64 | 0.63 |
| 2:B:298:LYS:H | 2:B:298:LYS:HD2 | 1.63 | 0.63 |
| 2:C:154:SER:O | 2:C:154:SER:OG | 2.17 | 0.63 |
| 2:C:241:ASN:HB2 | 2:C:242:ILE:HA | 1.80 | 0.63 |
| 2:F:154:SER:OG | 2:F:155:LYS:N | 2.32 | 0.63 |
| 2:F:37:ILE:HD11 | 2:F:323:VAL:HA | 1.79 | 0.63 |
| 2:G:14:ILE:HG12 | 2:G:109:PHE:HZ | 1.62 | 0.63 |
| 2:G:92:LEU:HA | 2:G:221:GLU:HA | 1.80 | 0.63 |
| 2:B:198:GLN:HG2 | 2:B:199:HIS:H | 1.64 | 0.62 |
| 2:D:329:THR:OG1 | 2:D:330:GLU:N | 2.32 | 0.62 |
| 2:B:206:LEU:HD22 | 2:B:210:GLY:HA3 | 1.81 | 0.62 |
| 2:D:241:ASN:ND2 | 2:D:242:ILE:O | 2.32 | 0.62 |
| 2:F:278:GLU:OE1 | 2:F:279:VAL:N | 2.31 | 0.62 |
| 2:D:152:SER:OG | 2:D:153:THR:N | 2.33 | 0.62 |
| 2:D:278:GLU:N | 2:D:278:GLU:OE1 | 2.31 | 0.62 |
| 2:E:173:THR:O | 2:E:241:ASN:ND2 | 2.32 | 0.62 |
| 1:I:41:ARG:HG2 | 1:I:42:LEU:HD12 | 1.81 | 0.62 |
| 1:J:2:LYS:HZ3 | 1:J:5:ASN:H | 1.47 | 0.62 |
| 1:M:23:LYS:HA | 1:M:24:ASP:HB2 | 1.80 | 0.62 |
| 1:N:13:PHE:N | 1:N:16:GLU:OE1 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:11:LEU:HA | 2:E:14:ILE:HG22 | 1.82 | 0.62 |
| 2:F:133:ASN:ND2 | 2:F:139:GLU:O | 2.32 | 0.62 |
| 1:N:58:VAL:HG13 | 1:N:59:MET:H | 1.65 | 0.62 |
| 2:F:90:TYR:HB3 | 2:F:223:LYS:HA | 1.80 | 0.62 |
| 2:E:51:LYS:HB3 | 2:E:83:THR:HG21 | 1.81 | 0.62 |
| 2:G:52:HIS:HB3 | 2:G:83:THR:HG21 | 1.82 | 0.62 |
| 1:H:34:LEU:HD22 | 1:H:35:ASP:H | 1.65 | 0.62 |
| 1:N:13:PHE:H | 1:N:13:PHE:HD2 | 1.46 | 0.62 |
| 2:B:202:LEU:HB2 | 2:B:214:GLN:HA | 1.80 | 0.62 |
| 1:K:73:ASP:O | 1:K:74:HIS:ND1 | 2.32 | 0.62 |
| 1:N:46:ALA:HB1 | 1:N:47:LYS:HD3 | 1.81 | 0.61 |
| 2:A:133:ASN:O | 2:A:134:THR:OG1 | 2.17 | 0.61 |
| 2:F:116:GLY:HA3 | 2:E:57:ARG:HH21 | 1.64 | 0.61 |
| 2:G:171:THR:OG1 | 2:G:172:ASN:N | 2.34 | 0.61 |
| 2:F:285:THR:HG21 | 2:F:327:LEU:HD21 | 1.82 | 0.61 |
| 2:F:179:SER:H | 2:F:235:SER:HB3 | 1.64 | 0.61 |
| 2:F:92:LEU:HA | 2:F:221:GLU:HB2 | 1.81 | 0.61 |
| 1:K:2:LYS:HD3 | 2:C:67:ARG:HB2 | 1.82 | 0.61 |
| 2:A:65:TRP:CD1 | 2:B:89:LEU:HD12 | 2.35 | 0.61 |
| 2:C:7:THR:O | 2:C:8:LEU:HB2 | 2.00 | 0.61 |
| 2:G:101:ASP:HA | 2:G:104:ASN:HA | 1.81 | 0.61 |
| 2:A:55:THR:O | 2:A:56:ILE:HG13 | 2.01 | 0.61 |
| 2:E:161:ASN:ND2 | 2:E:256:ASP:OD2 | 2.34 | 0.61 |
| 2:F:284:LYS:O | 2:F:287:HIS:N | 2.28 | 0.61 |
| 2:G:209:ASP:HB3 | 2:G:213:GLY:H | 1.65 | 0.61 |
| 1:M:50:PRO:HG2 | 1:M:66:SER:HB3 | 1.82 | 0.61 |
| 2:A:96:ASP:HB3 | 2:A:99:LEU:HD23 | 1.82 | 0.61 |
| 2:D:82:VAL:HG13 | 2:D:83:THR:H | 1.65 | 0.61 |
| 1:J:54:ASP:HB2 | 1:J:83:GLN:HB3 | 1.82 | 0.61 |
| 1:M:47:LYS:H | 1:M:47:LYS:HD2 | 1.65 | 0.61 |
| 2:D:310:LYS:HB3 | 2:D:311:LYS:HD3 | 1.82 | 0.60 |
| 1:K:22:THR:OG1 | 1:K:25:GLN:OE1 | 2.17 | 0.60 |
| 2:C:241:ASN:HB2 | 2:C:242:ILE:HG23 | 1.83 | 0.60 |
| 2:F:44:VAL:HG21 | 2:F:183:ASN:HD22 | 1.64 | 0.60 |
| 1:H:65:CYS:SG | 1:H:66:SER:N | 2.74 | 0.60 |
| 1:J:2:LYS:NZ | 1:J:5:ASN:H | 1.99 | 0.60 |
| 2:A:52:HIS:HB3 | 2:A:83:THR:HG21 | 1.83 | 0.60 |
| 2:B:314:SER:O | 2:B:315:PHE:HB3 | 2.01 | 0.60 |
| 2:E:169:GLY:HA2 | 2:E:330:GLU:HB3 | 1.84 | 0.60 |
| 2:F:38:LEU:HD13 | 2:F:321:ARG:HH11 | 1.65 | 0.60 |
| 2:C:153:THR:O | 2:C:153:THR:OG1 | 2.19 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:5:ASN:N | 1:I:5:ASN:OD1 | 2.34 | 0.60 |
| 1:L:47:LYS:HB3 | 1:L:93:LYS:HE3 | 1.83 | 0.60 |
| 1:N:2:LYS:HD2 | 2:A:11:LEU:HD12 | 1.84 | 0.60 |
| 2:D:84:ASP:OD2 | 2:D:85:THR:N | 2.27 | 0.60 |
| 2:G:56:ILE:HG22 | 2:G:57:ARG:H | 1.66 | 0.60 |
| 1:J:26:TYR:O | 1:J:84:ILE:HG13 | 2.02 | 0.60 |
| 2:B:232:ASP:HB2 | 2:C:32:ALA:HB2 | 1.84 | 0.60 |
| 2:E:242:ILE:H | 2:E:243:ASP:HA | 1.66 | 0.60 |
| 2:F:33:LYS:HD2 | 2:E:56:ILE:HD13 | 1.83 | 0.60 |
| 2:D:183:ASN:O | 2:D:229:SER:OG | 2.17 | 0.60 |
| 2:D:209:ASP:N | 2:D:210:GLY:HA2 | 2.16 | 0.60 |
| 2:G:38:LEU:HG | 2:G:321:ARG:HD2 | 1.83 | 0.60 |
| 1:N:24:ASP:O | 2:A:5:GLY:HA2 | 2.01 | 0.60 |
| 2:B:192:GLY:HA2 | 2:B:224:TRP:NE1 | 2.16 | 0.60 |
| 2:C:37:ILE:HG23 | 2:C:323:VAL:HA | 1.84 | 0.60 |
| 2:F:97:LYS:HZ2 | 2:F:216:ARG:NE | 1.99 | 0.60 |
| 1:N:70:ARG:O | 1:N:70:ARG:NH1 | 2.32 | 0.60 |
| 2:A:203:GLY:HA2 | 2:A:204:ASP:CG | 2.22 | 0.60 |
| 2:G:220:ASP:OD2 | 2:G:221:GLU:N | 2.34 | 0.60 |
| 2:G:195:ALA:HB1 | 2:G:222:PHE:HA | 1.84 | 0.60 |
| 2:G:284:LYS:HD2 | 2:G:322:ARG:HH21 | 1.66 | 0.60 |
| 2:A:284:LYS:O | 2:A:287:HIS:N | 2.23 | 0.59 |
| 2:F:55:THR:O | 2:F:56:ILE:HG13 | 2.02 | 0.59 |
| 1:K:53:GLY:O | 1:K:86:ASP:HA | 2.02 | 0.59 |
| 1:K:70:ARG:O | 1:K:71:THR:OG1 | 2.18 | 0.59 |
| 1:K:89:LEU:HG | 1:K:91:PRO:HD3 | 1.84 | 0.59 |
| 1:M:80:VAL:HG13 | 1:M:81:GLU:H | 1.64 | 0.59 |
| 2:D:193:MET:H | 2:D:224:TRP:HE3 | 1.50 | 0.59 |
| 1:H:27:PRO:HA | 1:H:84:ILE:HG13 | 1.83 | 0.59 |
| 1:H:83:GLN:OE1 | 1:H:84:ILE:N | 2.35 | 0.59 |
| 2:B:312:ILE:HD12 | 2:B:313:VAL:H | 1.66 | 0.59 |
| 2:C:301:ASN:OD1 | 2:C:302:LEU:N | 2.35 | 0.59 |
| 2:D:103:SER:OG | 2:D:104:ASN:N | 2.35 | 0.59 |
| 2:G:271:ALA:HA | 2:G:273:LEU:N | 2.16 | 0.59 |
| 1:N:26:TYR:O | 1:N:84:ILE:HG13 | 2.03 | 0.59 |
| 2:D:142:MET:O | 2:D:144:LEU:N | 2.35 | 0.59 |
| 2:D:15:TYR:O | 2:D:18:THR:OG1 | 2.14 | 0.59 |
| 2:D:19:ASP:OD2 | 2:D:23:ARG:N | 2.30 | 0.59 |
| 2:A:284:LYS:O | 2:A:286:ILE:N | 2.35 | 0.59 |
| 2:C:195:ALA:HB2 | 2:C:223:LYS:HG2 | 1.83 | 0.59 |
| 1:K:89:LEU:HD23 | 1:K:89:LEU:H | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:13:PHE:N | 1:N:13:PHE:CD2 | 2.69 | 0.59 |
| 2:A:197:PHE:CE2 | 2:A:221:GLU:HG3 | 2.37 | 0.59 |
| 2:A:60:ILE:HD13 | 2:A:77:THR:HB | 1.85 | 0.59 |
| 1:I:2:LYS:HG2 | 1:I:3:THR:O | 2.03 | 0.59 |
| 2:A:65:TRP:HA | 2:B:89:LEU:HB3 | 1.85 | 0.59 |
| 2:D:230:VAL:O | 2:D:232:ASP:N | 2.30 | 0.59 |
| 2:E:301:ASN:CG | 2:E:302:LEU:H | 2.06 | 0.59 |
| 2:F:250:ASP:OD1 | 2:F:257:LEU:HA | 2.03 | 0.59 |
| 1:L:24:ASP:N | 1:L:24:ASP:OD1 | 2.35 | 0.59 |
| 2:A:91:ASP:N | 2:A:91:ASP:OD2 | 2.36 | 0.59 |
| 2:D:241:ASN:OD1 | 2:D:241:ASN:N | 2.36 | 0.59 |
| 1:K:40:GLN:OE1 | 1:K:41:ARG:NH2 | 2.36 | 0.59 |
| 2:A:177:PHE:CB | 2:A:280:ILE:HA | 2.33 | 0.58 |
| 2:C:195:ALA:HB3 | 2:C:223:LYS:H | 1.67 | 0.58 |
| 2:D:7:THR:HG21 | 2:C:74:PRO:C | 2.23 | 0.58 |
| 2:G:160:GLU:N | 2:G:239:ILE:HG22 | 2.17 | 0.58 |
| 1:J:93:LYS:HD2 | 1:J:94:ARG:H | 1.68 | 0.58 |
| 2:A:42:ILE:HD11 | 2:A:183:ASN:HB3 | 1.84 | 0.58 |
| 2:A:278:GLU:OE2 | 2:A:279:VAL:N | 2.36 | 0.58 |
| 2:D:315:PHE:CD1 | 2:D:316:LEU:HB2 | 2.38 | 0.58 |
| 2:E:204:ASP:N | 2:E:204:ASP:OD1 | 2.35 | 0.58 |
| 1:M:83:GLN:OE1 | 1:M:84:ILE:N | 2.33 | 0.58 |
| 1:N:32:ILE:O | 1:N:33:THR:OG1 | 2.20 | 0.58 |
| 2:G:209:ASP:N | 2:G:210:GLY:HA2 | 2.18 | 0.58 |
| 2:B:198:GLN:N | 2:B:198:GLN:OE1 | 2.35 | 0.58 |
| 2:F:209:ASP:H | 2:F:211:ASN:H | 1.50 | 0.58 |
| 1:H:47:LYS:H | 1:H:47:LYS:HD3 | 1.67 | 0.58 |
| 1:L:40:GLN:CD | 1:L:41:ARG:H | 2.06 | 0.58 |
| 2:A:89:LEU:HB3 | 2:F:65:TRP:CD1 | 2.39 | 0.58 |
| 2:B:274:GLY:H | 2:B:275:ASP:HB3 | 1.67 | 0.58 |
| 2:F:199:HIS:HB2 | 2:F:219:ARG:HD2 | 1.85 | 0.58 |
| 2:G:86:THR:OG1 | 2:G:87:GLY:N | 2.37 | 0.58 |
| 1:M:10:THR:HG23 | 1:M:20:PRO:HB2 | 1.86 | 0.58 |
| 2:A:70:GLN:H | 2:A:70:GLN:NE2 | 2.02 | 0.58 |
| 2:C:170:SER:O | 2:C:172:ASN:N | 2.34 | 0.58 |
| 2:F:280:ILE:HG12 | 2:F:320:ILE:HG22 | 1.84 | 0.58 |
| 1:L:19:LYS:HG3 | 1:L:20:PRO:HD3 | 1.84 | 0.58 |
| 1:M:40:GLN:O | 1:M:73:ASP:HA | 2.02 | 0.58 |
| 2:E:19:ASP:OD2 | 2:E:26:ARG:NH2 | 2.36 | 0.58 |
| 2:F:203:GLY:HA2 | 2:F:204:ASP:HB2 | 1.84 | 0.58 |
| 2:F:82:VAL:HG13 | 2:F:83:THR:H | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:298:LYS:HD2 | 2:G:298:LYS:N | 2.19 | 0.58 |
| 1:K:41:ARG:HH11 | 1:K:100:LEU:HD13 | 1.69 | 0.58 |
| 2:D:176:TRP:CZ2 | 2:D:238:ARG:HD3 | 2.38 | 0.58 |
| 1:N:10:THR:N | 1:N:11:ASP:HA | 2.18 | 0.58 |
| 2:B:164:SER:HB2 | 2:B:331:SER:HB2 | 1.84 | 0.58 |
| 2:D:230:VAL:C | 2:D:232:ASP:H | 2.07 | 0.58 |
| 2:F:287:HIS:CE1 | 2:F:312:ILE:HD11 | 2.38 | 0.58 |
| 2:G:297:ALA:HB1 | 2:G:298:LYS:HD2 | 1.86 | 0.58 |
| 1:H:40:GLN:HE22 | 1:H:41:ARG:NE | 2.02 | 0.58 |
| 2:B:52:HIS:N | 2:B:83:THR:OG1 | 2.37 | 0.57 |
| 2:C:272:MET:SD | 2:C:273:LEU:N | 2.78 | 0.57 |
| 2:F:91:ASP:N | 2:F:221:GLU:OE2 | 2.37 | 0.57 |
| 1:H:17:ASP:OD1 | 1:H:18:GLY:N | 2.37 | 0.57 |
| 2:B:299:ASN:OD1 | 2:B:301:ASN:ND2 | 2.37 | 0.57 |
| 2:B:50:SER:OG | 2:B:51:LYS:N | 2.37 | 0.57 |
| 2:E:158:SER:HA | 2:E:238:ARG:O | 2.04 | 0.57 |
| 1:I:80:VAL:HG13 | 1:I:81:GLU:H | 1.69 | 0.57 |
| 2:C:133:ASN:HB2 | 2:C:140:ALA:HA | 1.85 | 0.57 |
| 2:C:185:ALA:N | 2:C:227:GLY:O | 2.33 | 0.57 |
| 2:E:177:PHE:O | 2:E:237:SER:OG | 2.17 | 0.57 |
| 2:F:243:ASP:O | 2:F:245:THR:N | 2.35 | 0.57 |
| 2:F:304:ILE:HG23 | 2:F:305:GLU:H | 1.67 | 0.57 |
| 1:K:5:ASN:OD1 | 1:K:6:MET:HB2 | 2.04 | 0.57 |
| 2:D:69:ASN:ND2 | 1:L:3:THR:O | 2.37 | 0.57 |
| 2:E:271:ALA:HA | 2:E:272:MET:HB3 | 1.85 | 0.57 |
| 2:G:271:ALA:CA | 2:G:273:LEU:H | 2.16 | 0.57 |
| 1:H:40:GLN:HE22 | 1:H:41:ARG:HE | 1.52 | 0.57 |
| 1:J:5:ASN:CG | 1:J:6:MET:H | 2.07 | 0.57 |
| 1:N:18:GLY:N | 1:N:91:PRO:HD2 | 2.19 | 0.57 |
| 2:A:202:LEU:HA | 2:A:216:ARG:HA | 1.85 | 0.57 |
| 2:A:72:VAL:HG13 | 2:A:73:GLN:H | 1.68 | 0.57 |
| 2:B:162:VAL:HG12 | 2:B:163:PHE:H | 1.67 | 0.57 |
| 2:B:206:LEU:H | 2:B:206:LEU:HD13 | 1.70 | 0.57 |
| 2:A:37:ILE:HD13 | 2:A:126:ALA:HB2 | 1.87 | 0.57 |
| 1:J:41:ARG:HD2 | 1:J:41:ARG:N | 2.19 | 0.57 |
| 2:A:247:LEU:O | 2:A:289:TRP:NE1 | 2.37 | 0.57 |
| 2:B:10:SER:O | 2:B:12:LEU:N | 2.37 | 0.57 |
| 2:D:11:LEU:HA | 2:D:14:ILE:HG22 | 1.87 | 0.57 |
| 1:K:5:ASN:ND2 | 1:K:22:THR:HB | 2.20 | 0.57 |
| 1:N:76:GLU:HA | 1:M:80:VAL:HG11 | 1.87 | 0.57 |
| 2:A:106:ALA:O | 2:A:110:ARG:HG2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:55:THR:O | 2:B:56:ILE:HG13 | 2.05 | 0.57 |
| 2:C:142:MET:O | 2:C:144:LEU:N | 2.37 | 0.57 |
| 2:E:298:LYS:NZ | 2:E:298:LYS:O | 2.31 | 0.57 |
| 2:F:183:ASN:OD1 | 2:F:183:ASN:N | 2.22 | 0.57 |
| 1:J:1:MET:N | 1:J:1:MET:SD | 2.77 | 0.57 |
| 2:D:121:PHE:CE1 | 2:C:63:PRO:HB3 | 2.39 | 0.57 |
| 2:E:177:PHE:HB3 | 2:E:280:ILE:HA | 1.86 | 0.57 |
| 2:F:241:ASN:HB2 | 2:F:242:ILE:HG12 | 1.85 | 0.57 |
| 1:H:32:ILE:O | 1:H:33:THR:OG1 | 2.18 | 0.57 |
| 1:J:41:ARG:HD3 | 1:J:42:LEU:HG | 1.86 | 0.57 |
| 2:A:185:ALA:N | 2:A:227:GLY:O | 2.36 | 0.56 |
| 2:D:36:ASP:HB2 | 2:C:270:VAL:O | 2.05 | 0.56 |
| 2:D:55:THR:O | 2:D:56:ILE:HG13 | 2.04 | 0.56 |
| 1:L:98:LYS:O | 1:L:99:GLU:HB2 | 2.04 | 0.56 |
| 2:B:221:GLU:OE1 | 2:B:222:PHE:N | 2.35 | 0.56 |
| 2:F:130:ILE:HG23 | 2:F:131:TYR:CD1 | 2.40 | 0.56 |
| 1:H:45:ASN:ND2 | 1:H:95:ASP:OD1 | 2.37 | 0.56 |
| 1:I:46:ALA:HB2 | 1:I:70:ARG:HB3 | 1.86 | 0.56 |
| 1:N:25:GLN:N | 1:N:25:GLN:OE1 | 2.35 | 0.56 |
| 2:B:292:LYS:HZ3 | 2:B:293:GLN:HB3 | 1.69 | 0.56 |
| 2:C:26:ARG:HE | 2:C:26:ARG:N | 2.02 | 0.56 |
| 1:J:78:ASN:ND2 | 1:J:79:TYR:H | 2.03 | 0.56 |
| 1:M:44:LEU:HB2 | 1:M:97:ALA:HB2 | 1.86 | 0.56 |
| 2:G:206:LEU:HG | 2:G:207:VAL:H | 1.68 | 0.56 |
| 1:M:25:GLN:NE2 | 1:M:86:ASP:O | 2.38 | 0.56 |
| 2:D:186:HIS:CD2 | 2:D:191:GLU:HA | 2.38 | 0.56 |
| 1:J:70:ARG:NE | 1:J:70:ARG:H | 2.03 | 0.56 |
| 1:K:2:LYS:HG3 | 1:K:3:THR:O | 2.04 | 0.56 |
| 2:A:177:PHE:HB2 | 2:A:280:ILE:HA | 1.88 | 0.56 |
| 2:F:235:SER:HA | 2:F:268:ARG:NH2 | 2.20 | 0.56 |
| 1:I:22:THR:HG21 | 1:I:87:ILE:HG23 | 1.88 | 0.56 |
| 1:M:40:GLN:HG3 | 1:M:101:LYS:C | 2.26 | 0.56 |
| 1:N:41:ARG:HG3 | 1:N:42:LEU:H | 1.71 | 0.56 |
| 2:D:41:ALA:HB1 | 2:D:180:TRP:HE1 | 1.70 | 0.56 |
| 1:L:27:PRO:HA | 1:L:84:ILE:HG23 | 1.86 | 0.56 |
| 1:M:99:GLU:HG2 | 1:M:101:LYS:NZ | 2.19 | 0.56 |
| 1:N:84:ILE:O | 1:N:85:THR:OG1 | 2.23 | 0.56 |
| 2:A:231:ARG:HE | 2:B:31:LEU:HD11 | 1.70 | 0.56 |
| 2:C:186:HIS:ND1 | 2:C:186:HIS:O | 2.39 | 0.56 |
| 2:C:177:PHE:HB2 | 2:C:279:VAL:O | 2.05 | 0.56 |
| 2:F:85:THR:OG1 | 2:F:86:THR:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:83:THR:OG1 | 2:G:84:ASP:N | 2.36 | 0.56 |
| 2:A:104:ASN:OD1 | 2:A:105:ASN:N | 2.39 | 0.56 |
| 2:B:17:ARG:O | 2:B:26:ARG:NH1 | 2.39 | 0.56 |
| 2:B:234:ARG:NH1 | 2:C:32:ALA:HA | 2.20 | 0.56 |
| 2:F:201:ASP:OD1 | 2:F:219:ARG:NH2 | 2.31 | 0.56 |
| 2:G:315:PHE:CD1 | 2:G:316:LEU:HB3 | 2.40 | 0.56 |
| 1:L:89:LEU:HD22 | 1:L:104:PHE:CZ | 2.41 | 0.56 |
| 1:N:28:TRP:CA | 1:N:84:ILE:HG21 | 2.35 | 0.56 |
| 2:C:284:LYS:O | 2:C:287:HIS:N | 2.25 | 0.56 |
| 2:D:172:ASN:N | 2:D:172:ASN:OD1 | 2.39 | 0.56 |
| 2:D:189:TYR:HD1 | 2:D:189:TYR:H | 1.51 | 0.56 |
| 1:J:65:CYS:SG | 1:J:66:SER:N | 2.78 | 0.56 |
| 1:J:78:ASN:HD22 | 1:J:79:TYR:H | 1.53 | 0.56 |
| 1:L:60:ALA:N | 1:L:61:MET:SD | 2.73 | 0.56 |
| 2:A:160:GLU:HB3 | 2:A:333:VAL:HB | 1.88 | 0.56 |
| 2:A:160:GLU:HB3 | 2:A:334:THR:H | 1.71 | 0.56 |
| 2:B:171:THR:HB | 2:B:328:ASN:ND2 | 2.21 | 0.56 |
| 2:C:137:GLU:OE1 | 1:J:1:MET:N | 2.35 | 0.56 |
| 2:D:17:ARG:HH11 | 2:D:112:SER:HG | 1.53 | 0.56 |
| 2:G:187:MET:C | 2:G:189:TYR:H | 2.09 | 0.56 |
| 2:C:89:LEU:HD21 | 2:C:125:VAL:HG23 | 1.88 | 0.55 |
| 2:E:187:MET:HE3 | 2:E:225:ASP:HB2 | 1.86 | 0.55 |
| 1:H:40:GLN:HB2 | 1:H:101:LYS:O | 2.06 | 0.55 |
| 1:J:22:THR:HB | 1:J:87:ILE:HG23 | 1.88 | 0.55 |
| 2:B:245:THR:O | 2:B:248:THR:OG1 | 2.15 | 0.55 |
| 2:B:42:ILE:HG21 | 2:B:181:GLY:H | 1.71 | 0.55 |
| 1:I:12:SER:HB3 | 1:I:100:LEU:HB2 | 1.88 | 0.55 |
| 2:D:67:ARG:O | 1:L:2:LYS:HB3 | 2.07 | 0.55 |
| 1:N:34:LEU:O | 1:N:78:ASN:ND2 | 2.39 | 0.55 |
| 2:A:147:ARG:HB2 | 2:A:333:VAL:O | 2.06 | 0.55 |
| 2:A:228:LEU:HD13 | 2:A:228:LEU:H | 1.72 | 0.55 |
| 2:A:230:VAL:O | 2:A:232:ASP:N | 2.28 | 0.55 |
| 1:M:3:THR:HG22 | 2:E:69:ASN:HD21 | 1.71 | 0.55 |
| 1:N:70:ARG:O | 1:N:71:THR:OG1 | 2.25 | 0.55 |
| 2:A:176:TRP:CZ2 | 2:A:238:ARG:HD3 | 2.41 | 0.55 |
| 1:K:13:PHE:HD2 | 1:K:14:VAL:H | 1.54 | 0.55 |
| 1:N:110:ASP:OD2 | 1:N:111:ASP:N | 2.40 | 0.55 |
| 2:A:70:GLN:HG2 | 2:A:71:GLY:N | 2.22 | 0.55 |
| 2:D:157:ALA:HB2 | 2:D:236:ILE:HG13 | 1.86 | 0.55 |
| 2:D:157:ALA:O | 2:D:238:ARG:N | 2.37 | 0.55 |
| 1:H:41:ARG:HG3 | 1:H:42:LEU:H | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:21:GLU:O | 1:K:23:LYS:NZ | 2.31 | 0.55 |
| 2:G:10:SER:O | 2:G:12:LEU:N | 2.36 | 0.55 |
| 2:G:110:ARG:HH22 | 2:G:198:GLN:HB3 | 1.72 | 0.55 |
| 1:K:55:SER:OG | 1:K:56:VAL:N | 2.37 | 0.55 |
| 2:A:133:ASN:HB2 | 2:A:140:ALA:HA | 1.89 | 0.55 |
| 2:A:249:LYS:O | 2:A:253:THR:OG1 | 2.18 | 0.55 |
| 2:F:171:THR:C | 2:F:172:ASN:HD22 | 2.10 | 0.55 |
| 1:H:18:GLY:O | 1:H:91:PRO:HD2 | 2.06 | 0.55 |
| 1:M:46:ALA:HB1 | 1:M:47:LYS:HD2 | 1.89 | 0.55 |
| 2:A:115:MET:HA | 2:A:118:LEU:HD23 | 1.89 | 0.55 |
| 2:A:8:LEU:HD12 | 2:A:94:PHE:HB2 | 1.89 | 0.55 |
| 2:C:299:ASN:OD1 | 2:C:300:VAL:N | 2.36 | 0.55 |
| 2:E:17:ARG:NH1 | 2:E:113:GLU:OE1 | 2.27 | 0.55 |
| 2:G:84:ASP:OD1 | 2:G:85:THR:N | 2.29 | 0.55 |
| 2:D:302:LEU:HA | 2:C:302:LEU:HD21 | 1.89 | 0.55 |
| 2:E:293:GLN:NE2 | 2:E:293:GLN:O | 2.36 | 0.55 |
| 2:F:279:VAL:HG13 | 2:F:281:TYR:HE2 | 1.72 | 0.55 |
| 2:F:296:ASN:OD1 | 2:F:296:ASN:N | 2.38 | 0.55 |
| 1:H:6:MET:HG2 | 1:H:7:LYS:N | 2.20 | 0.55 |
| 1:L:22:THR:OG1 | 1:L:25:GLN:OE1 | 2.22 | 0.55 |
| 2:B:32:ALA:HB1 | 2:B:33:LYS:CB | 2.36 | 0.54 |
| 2:D:221:GLU:HG2 | 2:D:222:PHE:H | 1.72 | 0.54 |
| 2:D:48:ASP:HB3 | 2:E:20:LYS:NZ | 2.22 | 0.54 |
| 2:D:63:PRO:HB2 | 2:E:89:LEU:CD1 | 2.37 | 0.54 |
| 2:F:52:HIS:N | 2:F:83:THR:OG1 | 2.40 | 0.54 |
| 2:G:172:ASN:HB3 | 2:G:241:ASN:O | 2.06 | 0.54 |
| 2:B:17:ARG:NH2 | 2:B:112:SER:OG | 2.38 | 0.54 |
| 2:B:203:GLY:HA2 | 2:B:204:ASP:CG | 2.28 | 0.54 |
| 2:F:88:MET:SD | 2:E:66:ARG:NH1 | 2.81 | 0.54 |
| 1:K:21:GLU:O | 1:K:23:LYS:HG3 | 2.06 | 0.54 |
| 2:B:132:GLY:HA3 | 2:B:140:ALA:HA | 1.87 | 0.54 |
| 2:B:178:MET:N | 2:B:178:MET:SD | 2.80 | 0.54 |
| 2:D:296:ASN:OD1 | 2:D:296:ASN:N | 2.40 | 0.54 |
| 2:E:224:TRP:HD1 | 2:E:225:ASP:N | 2.06 | 0.54 |
| 2:F:202:LEU:HB3 | 2:F:215:PHE:H | 1.72 | 0.54 |
| 1:H:105:TYR:HB3 | 1:H:106:PRO:CD | 2.37 | 0.54 |
| 1:I:105:TYR:HB2 | 1:I:106:PRO:HD3 | 1.88 | 0.54 |
| 1:K:78:ASN:CG | 1:K:79:TYR:H | 2.11 | 0.54 |
| 2:B:147:ARG:NE | 2:B:333:VAL:O | 2.36 | 0.54 |
| 2:F:76:LYS:H | 2:F:76:LYS:HE2 | 1.73 | 0.54 |
| 1:H:8:THR:OG1 | 1:H:9:GLY:HA2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:42:ILE:HG23 | 2:A:180:TRP:HD1 | 1.73 | 0.54 |
| 2:A:86:THR:OG1 | 2:A:226:ILE:O | 2.18 | 0.54 |
| 2:C:33:LYS:O | 2:C:34:THR:OG1 | 2.25 | 0.54 |
| 1:K:3:THR:HG23 | 2:C:69:ASN:HB2 | 1.90 | 0.54 |
| 2:D:37:ILE:HG21 | 2:D:126:ALA:HB1 | 1.90 | 0.54 |
| 2:A:181:GLY:O | 2:A:231:ARG:NH2 | 2.41 | 0.54 |
| 2:F:284:LYS:O | 2:F:286:ILE:N | 2.41 | 0.54 |
| 2:G:298:LYS:HD2 | 2:G:298:LYS:H | 1.72 | 0.54 |
| 2:D:247:LEU:HD21 | 2:D:256:ASP:O | 2.07 | 0.54 |
| 2:D:37:ILE:HG23 | 2:D:324:ASP:HB3 | 1.90 | 0.54 |
| 2:G:86:THR:HG21 | 2:G:187:MET:SD | 2.48 | 0.54 |
| 2:G:87:GLY:HA3 | 2:G:138:PRO:HB3 | 1.90 | 0.54 |
| 1:I:83:GLN:OE1 | 1:I:84:ILE:N | 2.41 | 0.54 |
| 2:A:155:LYS:O | 2:A:158:SER:OG | 2.25 | 0.54 |
| 2:E:233:TRP:O | 2:E:234:ARG:HB2 | 2.08 | 0.54 |
| 2:G:173:THR:HG22 | 2:G:327:LEU:HA | 1.89 | 0.54 |
| 2:G:86:THR:OG1 | 2:G:226:ILE:O | 2.16 | 0.54 |
| 1:K:46:ALA:HA | 1:K:70:ARG:HH12 | 1.73 | 0.54 |
| 1:M:69:THR:HA | 1:M:70:ARG:NH2 | 2.22 | 0.54 |
| 2:B:284:LYS:HG3 | 2:B:322:ARG:HH21 | 1.73 | 0.54 |
| 2:D:177:PHE:HB2 | 2:D:279:VAL:O | 2.08 | 0.54 |
| 2:G:56:ILE:HD11 | 2:G:82:VAL:HG21 | 1.90 | 0.54 |
| 1:I:54:ASP:HB2 | 1:I:83:GLN:HB3 | 1.90 | 0.54 |
| 2:E:316:LEU:H | 2:E:318:ILE:HG12 | 1.73 | 0.54 |
| 2:G:37:ILE:HG13 | 2:G:323:VAL:HA | 1.90 | 0.54 |
| 1:I:8:THR:OG1 | 1:I:102:ASP:O | 2.20 | 0.54 |
| 1:K:70:ARG:H | 1:K:70:ARG:NE | 2.05 | 0.54 |
| 2:A:224:TRP:HD1 | 2:A:225:ASP:N | 2.06 | 0.53 |
| 2:C:160:GLU:HB2 | 2:C:240:CYS:H | 1.74 | 0.53 |
| 2:G:195:ALA:CB | 2:G:222:PHE:HA | 2.37 | 0.53 |
| 1:L:37:GLU:HG3 | 1:L:105:TYR:HA | 1.90 | 0.53 |
| 1:M:27:PRO:HA | 1:M:84:ILE:HG13 | 1.90 | 0.53 |
| 2:D:65:TRP:HA | 2:E:89:LEU:HB2 | 1.91 | 0.53 |
| 2:F:333:VAL:HG13 | 2:F:334:THR:H | 1.73 | 0.53 |
| 1:K:3:THR:HG21 | 2:C:70:GLN:HB2 | 1.90 | 0.53 |
| 2:F:180:TRP:CE3 | 2:F:180:TRP:HA | 2.44 | 0.53 |
| 2:C:214:GLN:CD | 2:C:214:GLN:H | 2.11 | 0.53 |
| 2:D:275:ASP:OD1 | 2:D:276:GLY:N | 2.41 | 0.53 |
| 2:D:3:LEU:O | 2:D:6:GLN:N | 2.41 | 0.53 |
| 2:E:228:LEU:H | 2:E:228:LEU:HD13 | 1.73 | 0.53 |
| 2:F:118:LEU:O | 2:F:122:ASN:ND2 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:202:LEU:HA | 2:F:215:PHE:O | 2.09 | 0.53 |
| 2:F:243:ASP:C | 2:F:245:THR:H | 2.11 | 0.53 |
| 1:J:60:ALA:N | 1:J:61:MET:SD | 2.82 | 0.53 |
| 2:D:33:LYS:O | 2:D:34:THR:OG1 | 2.23 | 0.53 |
| 2:E:147:ARG:H | 2:E:147:ARG:NE | 2.07 | 0.53 |
| 2:E:258:ILE:HG12 | 2:E:290:LEU:HD23 | 1.90 | 0.53 |
| 2:F:177:PHE:N | 2:F:177:PHE:HD2 | 2.06 | 0.53 |
| 2:F:42:ILE:HD11 | 2:F:183:ASN:HA | 1.89 | 0.53 |
| 2:A:70:GLN:NE2 | 1:I:3:THR:HB | 2.23 | 0.53 |
| 1:K:2:LYS:HE2 | 2:C:68:TYR:H | 1.73 | 0.53 |
| 2:A:179:SER:HB3 | 2:A:278:GLU:HG2 | 1.90 | 0.53 |
| 2:D:249:LYS:HZ2 | 2:D:250:ASP:H | 1.57 | 0.53 |
| 2:D:3:LEU:HB3 | 2:D:6:GLN:HA | 1.90 | 0.53 |
| 2:E:177:PHE:HB2 | 2:E:280:ILE:HA | 1.90 | 0.53 |
| 2:F:289:TRP:HA | 2:F:289:TRP:CE3 | 2.43 | 0.53 |
| 2:F:52:HIS:ND1 | 2:F:52:HIS:O | 2.38 | 0.53 |
| 2:G:214:GLN:HG3 | 2:G:215:PHE:N | 2.24 | 0.53 |
| 1:I:26:TYR:CE2 | 1:I:84:ILE:HD11 | 2.43 | 0.53 |
| 1:L:99:GLU:O | 1:L:100:LEU:HB2 | 2.08 | 0.53 |
| 1:N:73:ASP:O | 1:N:74:HIS:ND1 | 2.42 | 0.53 |
| 2:A:205:ASP:N | 2:A:205:ASP:OD2 | 2.41 | 0.53 |
| 1:K:1:MET:HB3 | 1:K:2:LYS:HB2 | 1.91 | 0.53 |
| 2:F:116:GLY:HA3 | 2:E:57:ARG:NH2 | 2.24 | 0.53 |
| 2:F:214:GLN:O | 2:F:214:GLN:NE2 | 2.42 | 0.53 |
| 2:F:278:GLU:CD | 2:F:279:VAL:H | 2.12 | 0.53 |
| 2:G:154:SER:OG | 2:G:155:LYS:N | 2.39 | 0.53 |
| 1:H:36:ASN:HB3 | 1:H:78:ASN:HA | 1.91 | 0.53 |
| 1:I:70:ARG:O | 1:I:71:THR:OG1 | 2.27 | 0.53 |
| 1:L:71:THR:HB | 1:L:74:HIS:HE1 | 1.74 | 0.53 |
| 1:L:47:LYS:HD3 | 1:L:93:LYS:NZ | 2.23 | 0.53 |
| 2:B:292:LYS:HZ2 | 2:B:292:LYS:HB3 | 1.74 | 0.53 |
| 2:D:288:ALA:HA | 2:C:266:TYR:CD1 | 2.42 | 0.53 |
| 1:J:89:LEU:HB3 | 1:J:104:PHE:CZ | 2.44 | 0.53 |
| 2:A:266:TYR:HE2 | 2:B:287:HIS:HD1 | 1.58 | 0.52 |
| 2:C:172:ASN:HB3 | 2:C:243:ASP:HA | 1.91 | 0.52 |
| 2:E:134:THR:O | 1:L:41:ARG:NE | 2.29 | 0.52 |
| 2:F:177:PHE:CD2 | 2:F:177:PHE:N | 2.76 | 0.52 |
| 1:H:7:LYS:HD2 | 2:F:67:ARG:HH22 | 1.74 | 0.52 |
| 2:B:20:LYS:HA | 2:B:20:LYS:HE2 | 1.91 | 0.52 |
| 2:F:130:ILE:HG23 | 2:F:131:TYR:HD1 | 1.72 | 0.52 |
| 1:L:20:PRO:HB3 | 1:L:21:GLU:HG3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:149:ASN:OD1 | 2:D:150:THR:N | 2.37 | 0.52 |
| 2:D:47:ASN:HB2 | 2:E:20:LYS:HE2 | 1.92 | 0.52 |
| 2:E:210:GLY:O | 2:E:211:ASN:HB2 | 2.08 | 0.52 |
| 1:I:105:TYR:HB2 | 1:I:106:PRO:CD | 2.39 | 0.52 |
| 1:I:17:ASP:O | 1:I:19:LYS:N | 2.28 | 0.52 |
| 1:I:39:LEU:O | 1:I:103:ALA:N | 2.43 | 0.52 |
| 1:I:84:ILE:O | 1:I:85:THR:OG1 | 2.27 | 0.52 |
| 2:B:177:PHE:HB3 | 2:B:280:ILE:HA | 1.90 | 0.52 |
| 2:C:135:ASP:O | 2:C:137:GLU:N | 2.42 | 0.52 |
| 2:D:34:THR:HG21 | 2:D:119:GLN:HG2 | 1.90 | 0.52 |
| 2:D:260:MET:HA | 2:D:263:ASP:HB3 | 1.91 | 0.52 |
| 2:F:90:TYR:CE1 | 2:E:66:ARG:HG3 | 2.45 | 0.52 |
| 2:D:248:THR:HA | 2:D:289:TRP:HZ2 | 1.74 | 0.52 |
| 2:D:280:ILE:HD13 | 2:D:320:ILE:HB | 1.92 | 0.52 |
| 2:F:170:SER:HB3 | 2:F:171:THR:HG22 | 1.92 | 0.52 |
| 2:F:20:LYS:HD2 | 2:E:53:LYS:HE3 | 1.91 | 0.52 |
| 2:F:205:ASP:HB2 | 2:F:210:GLY:H | 1.74 | 0.52 |
| 2:A:102:ARG:NH1 | 2:G:225:ASP:OD2 | 2.42 | 0.52 |
| 1:H:23:LYS:HG3 | 1:H:24:ASP:HA | 1.91 | 0.52 |
| 1:M:39:LEU:HD22 | 1:M:40:GLN:HA | 1.91 | 0.52 |
| 2:A:303:THR:HG22 | 2:F:300:VAL:HG22 | 1.92 | 0.52 |
| 2:B:164:SER:HA | 2:B:170:SER:HB2 | 1.92 | 0.52 |
| 2:C:105:ASN:O | 2:C:105:ASN:ND2 | 2.43 | 0.52 |
| 2:D:157:ALA:HA | 2:D:237:SER:HA | 1.91 | 0.52 |
| 2:F:307:TYR:CB | 2:F:308:GLY:HA2 | 2.34 | 0.52 |
| 2:B:185:ALA:N | 2:B:227:GLY:O | 2.43 | 0.52 |
| 2:D:189:TYR:CG | 2:D:190:PRO:HD3 | 2.45 | 0.52 |
| 2:F:89:LEU:HD12 | 2:E:65:TRP:CZ3 | 2.45 | 0.52 |
| 2:F:205:ASP:CB | 2:F:210:GLY:H | 2.23 | 0.52 |
| 2:A:120:GLY:HA3 | 2:F:60:ILE:HG13 | 1.91 | 0.52 |
| 2:G:173:THR:OG1 | 2:G:174:SER:N | 2.40 | 0.52 |
| 1:I:19:LYS:NZ | 1:I:87:ILE:HG21 | 2.24 | 0.52 |
| 2:B:65:TRP:HB3 | 2:C:88:MET:O | 2.10 | 0.52 |
| 2:F:241:ASN:HB2 | 2:F:242:ILE:CD1 | 2.40 | 0.52 |
| 2:F:242:ILE:HB | 2:F:244:VAL:N | 2.22 | 0.52 |
| 2:F:289:TRP:HA | 2:F:289:TRP:HE3 | 1.74 | 0.52 |
| 2:C:66:ARG:HG3 | 2:C:71:GLY:HA2 | 1.91 | 0.52 |
| 2:G:250:ASP:OD1 | 2:G:250:ASP:N | 2.43 | 0.52 |
| 1:I:2:LYS:HE3 | 1:I:2:LYS:H | 1.75 | 0.52 |
| 2:C:302:LEU:C | 2:C:304:ILE:H | 2.12 | 0.52 |
| 1:K:54:ASP:OD2 | 1:K:62:ALA:HB3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:36:ASN:HB3 | 1:K:79:TYR:HE2 | 1.75 | 0.51 |
| 2:D:66:ARG:CZ | 2:D:68:TYR:HA | 2.40 | 0.51 |
| 2:B:9:PRO:HG3 | 2:B:95:VAL:HG12 | 1.92 | 0.51 |
| 2:C:284:LYS:O | 2:C:286:ILE:N | 2.44 | 0.51 |
| 2:D:142:MET:C | 2:D:144:LEU:H | 2.13 | 0.51 |
| 2:D:14:ILE:HD13 | 2:D:109:PHE:CE2 | 2.45 | 0.51 |
| 2:F:175:ILE:HG13 | 2:F:239:ILE:HD13 | 1.93 | 0.51 |
| 2:G:248:THR:HA | 2:G:289:TRP:HZ2 | 1.74 | 0.51 |
| 2:G:78:GLN:OE1 | 2:G:78:GLN:N | 2.42 | 0.51 |
| 1:H:96:ASP:OD2 | 1:H:97:ALA:N | 2.43 | 0.51 |
| 1:I:44:LEU:HG | 1:I:98:LYS:O | 2.10 | 0.51 |
| 1:N:35:ASP:HA | 1:N:78:ASN:OD1 | 2.11 | 0.51 |
| 2:B:97:LYS:H | 2:B:217:ALA:HA | 1.75 | 0.51 |
| 2:E:173:THR:HB | 2:E:327:LEU:HD12 | 1.93 | 0.51 |
| 1:I:22:THR:HA | 1:I:25:GLN:HE22 | 1.75 | 0.51 |
| 1:J:28:TRP:CA | 1:J:84:ILE:HG21 | 2.40 | 0.51 |
| 1:K:100:LEU:HB3 | 1:K:101:LYS:HE3 | 1.92 | 0.51 |
| 2:A:328:ASN:O | 2:A:328:ASN:ND2 | 2.43 | 0.51 |
| 2:A:83:THR:HG22 | 2:A:84:ASP:H | 1.74 | 0.51 |
| 2:B:247:LEU:HD22 | 2:B:289:TRP:CD1 | 2.44 | 0.51 |
| 2:B:277:LYS:HZ3 | 2:B:277:LYS:HB2 | 1.76 | 0.51 |
| 2:E:192:GLY:HA2 | 2:E:224:TRP:NE1 | 2.26 | 0.51 |
| 1:M:3:THR:N | 2:E:67:ARG:HG2 | 2.26 | 0.51 |
| 1:J:17:ASP:OD1 | 1:J:18:GLY:N | 2.44 | 0.51 |
| 2:A:275:ASP:OD2 | 2:A:276:GLY:N | 2.44 | 0.51 |
| 2:A:70:GLN:H | 2:A:70:GLN:HE21 | 1.59 | 0.51 |
| 2:D:41:ALA:CB | 2:D:180:TRP:HE1 | 2.24 | 0.51 |
| 2:D:7:THR:HG21 | 2:C:74:PRO:HB2 | 1.92 | 0.51 |
| 1:H:34:LEU:O | 1:H:78:ASN:ND2 | 2.44 | 0.51 |
| 1:I:18:GLY:HA3 | 1:I:91:PRO:HG2 | 1.92 | 0.51 |
| 1:L:44:LEU:N | 1:L:100:LEU:HD11 | 2.25 | 0.51 |
| 1:M:98:LYS:C | 1:M:100:LEU:H | 2.14 | 0.51 |
| 1:M:8:THR:HG21 | 1:M:101:LYS:CB | 2.39 | 0.51 |
| 1:N:34:LEU:HD22 | 1:N:35:ASP:H | 1.76 | 0.51 |
| 2:E:90:TYR:CB | 2:E:223:LYS:HA | 2.36 | 0.51 |
| 2:E:246:THR:HA | 2:E:249:LYS:HD3 | 1.92 | 0.51 |
| 2:E:94:PHE:CD1 | 2:E:219:ARG:HB3 | 2.45 | 0.51 |
| 2:F:208:SER:N | 2:F:209:ASP:HA | 2.26 | 0.51 |
| 2:F:36:ASP:OD2 | 2:F:36:ASP:N | 2.44 | 0.51 |
| 1:H:7:LYS:CD | 2:F:67:ARG:HH22 | 2.23 | 0.51 |
| 1:N:105:TYR:CD1 | 2:A:11:LEU:HD11 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:333:VAL:O | 2:A:335:ALA:N | 2.44 | 0.51 |
| 2:D:296:ASN:HB3 | 2:C:299:ASN:ND2 | 2.26 | 0.51 |
| 2:D:199:HIS:O | 2:D:219:ARG:HB2 | 2.11 | 0.51 |
| 2:E:326:ILE:HG13 | 2:E:327:LEU:H | 1.76 | 0.51 |
| 2:G:209:ASP:H | 2:G:210:GLY:HA2 | 1.75 | 0.51 |
| 2:D:137:GLU:OE1 | 1:K:1:MET:N | 2.44 | 0.51 |
| 2:A:86:THR:OG1 | 2:A:87:GLY:N | 2.43 | 0.50 |
| 2:C:305:GLU:HG3 | 2:C:306:GLU:CD | 2.31 | 0.50 |
| 2:E:241:ASN:HD22 | 2:E:241:ASN:N | 2.09 | 0.50 |
| 2:E:300:VAL:HG13 | 2:E:301:ASN:H | 1.74 | 0.50 |
| 2:E:97:LYS:HG3 | 2:E:216:ARG:HB2 | 1.91 | 0.50 |
| 2:F:241:ASN:HB2 | 2:F:242:ILE:CG1 | 2.41 | 0.50 |
| 2:F:60:ILE:N | 2:F:61:PRO:HD3 | 2.26 | 0.50 |
| 1:K:31:ARG:HH21 | 1:K:31:ARG:C | 2.14 | 0.50 |
| 1:N:6:MET:HA | 2:A:2:ALA:HB2 | 1.93 | 0.50 |
| 2:B:60:ILE:HD11 | 2:C:117:LYS:HG2 | 1.91 | 0.50 |
| 2:F:209:ASP:H | 2:F:210:GLY:HA2 | 1.74 | 0.50 |
| 2:G:195:ALA:HA | 2:G:197:PHE:N | 2.26 | 0.50 |
| 2:G:209:ASP:H | 2:G:211:ASN:N | 2.06 | 0.50 |
| 2:G:298:LYS:HA | 2:G:298:LYS:NZ | 2.26 | 0.50 |
| 1:H:19:LYS:NZ | 1:H:87:ILE:HG21 | 2.25 | 0.50 |
| 2:A:160:GLU:CB | 2:A:334:THR:H | 2.25 | 0.50 |
| 2:A:41:ALA:CB | 2:A:180:TRP:HE1 | 2.24 | 0.50 |
| 2:A:314:SER:OG | 2:B:306:GLU:OE1 | 2.28 | 0.50 |
| 2:B:16:ASN:O | 2:B:18:THR:OG1 | 2.28 | 0.50 |
| 2:B:19:ASP:OD1 | 2:B:23:ARG:N | 2.37 | 0.50 |
| 2:C:243:ASP:O | 2:C:246:THR:HG22 | 2.11 | 0.50 |
| 1:H:6:MET:N | 1:H:104:PHE:HE2 | 2.09 | 0.50 |
| 1:I:102:ASP:OD1 | 1:I:103:ALA:N | 2.44 | 0.50 |
| 1:K:104:PHE:O | 1:K:105:TYR:HB2 | 2.10 | 0.50 |
| 2:A:178:MET:HG2 | 2:A:180:TRP:HZ3 | 1.75 | 0.50 |
| 2:A:93:GLY:O | 2:A:219:ARG:HB2 | 2.12 | 0.50 |
| 2:C:189:TYR:HB2 | 2:C:190:PRO:CD | 2.41 | 0.50 |
| 2:C:25:ALA:C | 2:C:26:ARG:HE | 2.14 | 0.50 |
| 2:D:154:SER:HB2 | 2:D:158:SER:OG | 2.10 | 0.50 |
| 2:E:224:TRP:CD1 | 2:E:225:ASP:N | 2.79 | 0.50 |
| 2:A:53:LYS:O | 2:A:82:VAL:HG13 | 2.10 | 0.50 |
| 2:G:209:ASP:HB2 | 2:G:212:GLY:H | 1.76 | 0.50 |
| 1:H:25:GLN:HB2 | 1:H:85:THR:O | 2.11 | 0.50 |
| 1:J:14:VAL:HG22 | 1:J:98:LYS:HA | 1.94 | 0.50 |
| 2:C:19:ASP:O | 2:C:20:LYS:HB3 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:320:ILE:O | 2:F:321:ARG:HD3 | 2.11 | 0.50 |
| 1:J:89:LEU:HD23 | 1:J:89:LEU:H | 1.77 | 0.50 |
| 1:K:28:TRP:N | 1:K:84:ILE:HG12 | 2.25 | 0.50 |
| 1:K:6:MET:HG3 | 1:K:22:THR:HG22 | 1.94 | 0.50 |
| 2:A:70:GLN:HG2 | 2:A:71:GLY:H | 1.76 | 0.50 |
| 2:B:67:ARG:O | 1:J:3:THR:HG22 | 2.12 | 0.50 |
| 2:D:94:PHE:CD1 | 2:D:219:ARG:HA | 2.46 | 0.50 |
| 2:D:299:ASN:HB2 | 2:E:303:THR:HG22 | 1.94 | 0.50 |
| 2:G:283:ASN:OD1 | 2:G:284:LYS:N | 2.40 | 0.50 |
| 1:N:2:LYS:HD3 | 1:N:3:THR:O | 2.12 | 0.50 |
| 2:A:242:ILE:HG12 | 2:A:243:ASP:HA | 1.94 | 0.50 |
| 2:A:86:THR:HG21 | 2:A:187:MET:SD | 2.52 | 0.50 |
| 2:B:163:PHE:CG | 2:B:164:SER:N | 2.80 | 0.50 |
| 2:G:235:SER:O | 2:G:268:ARG:HG3 | 2.12 | 0.50 |
| 1:H:69:THR:HB | 1:H:70:ARG:NH2 | 2.27 | 0.50 |
| 1:I:6:MET:HG2 | 1:I:104:PHE:CD2 | 2.47 | 0.50 |
| 1:J:36:ASN:OD1 | 1:J:37:GLU:N | 2.43 | 0.50 |
| 1:K:105:TYR:HB3 | 1:K:106:PRO:HD3 | 1.94 | 0.50 |
| 1:M:110:ASP:OD2 | 1:M:111:ASP:N | 2.38 | 0.50 |
| 1:N:25:GLN:NE2 | 1:N:86:ASP:O | 2.45 | 0.50 |
| 2:B:110:ARG:O | 2:B:114:ASN:HB2 | 2.12 | 0.49 |
| 2:B:171:THR:HB | 2:B:328:ASN:HD22 | 1.78 | 0.49 |
| 2:D:256:ASP:OD1 | 2:D:256:ASP:N | 2.45 | 0.49 |
| 1:H:10:THR:H | 1:H:11:ASP:HA | 1.75 | 0.49 |
| 1:I:70:ARG:O | 1:I:70:ARG:NE | 2.44 | 0.49 |
| 2:B:249:LYS:HA | 2:B:253:THR:HG21 | 1.94 | 0.49 |
| 2:B:307:TYR:HB2 | 2:B:308:GLY:HA2 | 1.93 | 0.49 |
| 2:A:72:VAL:HG21 | 2:B:92:LEU:HG | 1.93 | 0.49 |
| 2:C:178:MET:HA | 2:C:235:SER:O | 2.12 | 0.49 |
| 1:K:7:LYS:HG2 | 2:C:67:ARG:HH12 | 1.76 | 0.49 |
| 2:F:247:LEU:HD22 | 2:F:250:ASP:OD1 | 2.11 | 0.49 |
| 2:G:182:GLU:OE1 | 2:G:231:ARG:HB3 | 2.12 | 0.49 |
| 2:G:303:THR:OG1 | 2:G:304:ILE:N | 2.46 | 0.49 |
| 1:H:2:LYS:HG3 | 2:F:68:TYR:HB2 | 1.95 | 0.49 |
| 1:H:33:THR:HG22 | 1:H:34:LEU:HB3 | 1.95 | 0.49 |
| 1:L:23:LYS:HD2 | 1:L:24:ASP:HB3 | 1.93 | 0.49 |
| 2:A:53:LYS:O | 2:A:54:THR:OG1 | 2.27 | 0.49 |
| 2:B:242:ILE:HG22 | 2:B:246:THR:HB | 1.92 | 0.49 |
| 2:B:37:ILE:HD11 | 2:B:324:ASP:HB3 | 1.93 | 0.49 |
| 2:D:147:ARG:NH2 | 2:D:162:VAL:HG13 | 2.16 | 0.49 |
| 2:F:18:THR:HG22 | 2:F:19:ASP:H | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:54:ASP:HB3 | 1:M:86:ASP:H | 1.77 | 0.49 |
| 2:A:230:VAL:C | 2:A:232:ASP:H | 2.15 | 0.49 |
| 2:B:186:HIS:CD2 | 2:B:191:GLU:HG3 | 2.47 | 0.49 |
| 2:C:254:GLY:HA2 | 2:C:257:LEU:HD11 | 1.93 | 0.49 |
| 2:D:250:ASP:O | 2:D:293:GLN:HG3 | 2.12 | 0.49 |
| 2:E:172:ASN:HB2 | 2:E:241:ASN:O | 2.12 | 0.49 |
| 2:E:315:PHE:HA | 2:E:316:LEU:HB3 | 1.94 | 0.49 |
| 2:G:13:ASP:O | 2:G:17:ARG:N | 2.45 | 0.49 |
| 2:G:180:TRP:C | 2:G:182:GLU:H | 2.16 | 0.49 |
| 2:G:241:ASN:ND2 | 2:G:242:ILE:HG13 | 2.22 | 0.49 |
| 1:L:5:ASN:OD1 | 1:L:106:PRO:HG3 | 2.12 | 0.49 |
| 1:M:88:GLY:HA2 | 1:M:89:LEU:C | 2.33 | 0.49 |
| 1:N:71:THR:HB | 1:N:74:HIS:HE1 | 1.76 | 0.49 |
| 2:A:97:LYS:HE2 | 2:A:218:TYR:HB2 | 1.94 | 0.49 |
| 2:B:189:TYR:HB2 | 2:B:190:PRO:HD2 | 1.95 | 0.49 |
| 2:F:242:ILE:HB | 2:F:243:ASP:HA | 1.93 | 0.49 |
| 2:G:195:ALA:N | 2:G:196:GLY:HA3 | 2.27 | 0.49 |
| 1:H:91:PRO:HG3 | 1:H:101:LYS:NZ | 2.27 | 0.49 |
| 1:I:20:PRO:HB3 | 1:I:21:GLU:HG3 | 1.95 | 0.49 |
| 2:D:69:ASN:ND2 | 1:L:3:THR:OG1 | 2.46 | 0.49 |
| 1:L:47:LYS:HG2 | 1:L:70:ARG:HH21 | 1.77 | 0.49 |
| 1:M:28:TRP:HA | 1:M:84:ILE:HG21 | 1.94 | 0.49 |
| 1:N:105:TYR:HB3 | 1:N:106:PRO:CD | 2.42 | 0.49 |
| 1:N:71:THR:HB | 1:N:74:HIS:CE1 | 2.48 | 0.49 |
| 2:A:323:VAL:HG22 | 2:A:324:ASP:H | 1.78 | 0.49 |
| 2:C:27:ILE:O | 2:C:27:ILE:HG12 | 2.12 | 0.49 |
| 2:D:176:TRP:HZ2 | 2:D:238:ARG:HH21 | 1.61 | 0.49 |
| 2:E:279:VAL:HG12 | 2:E:280:ILE:H | 1.78 | 0.49 |
| 2:E:296:ASN:HD22 | 2:E:296:ASN:N | 2.11 | 0.49 |
| 2:F:89:LEU:HD23 | 2:F:121:PHE:CE2 | 2.47 | 0.49 |
| 1:J:5:ASN:ND2 | 1:J:6:MET:H | 2.09 | 0.49 |
| 1:J:83:GLN:OE1 | 1:J:84:ILE:N | 2.44 | 0.49 |
| 2:A:92:LEU:HB3 | 2:A:221:GLU:CB | 2.43 | 0.49 |
| 2:B:37:ILE:HD13 | 2:B:126:ALA:HB3 | 1.94 | 0.49 |
| 2:B:54:THR:HA | 2:C:27:ILE:HD11 | 1.94 | 0.49 |
| 2:E:163:PHE:CG | 2:E:164:SER:N | 2.80 | 0.49 |
| 2:E:186:HIS:O | 2:E:186:HIS:ND1 | 2.46 | 0.49 |
| 2:E:206:LEU:N | 2:E:210:GLY:HA2 | 2.28 | 0.49 |
| 2:E:291:HIS:NE2 | 2:E:309:GLY:HA3 | 2.27 | 0.49 |
| 1:J:41:ARG:HD3 | 1:J:42:LEU:H | 1.78 | 0.49 |
| 2:B:172:ASN:HB2 | 2:B:242:ILE:H | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:214:GLN:O | 2:E:215:PHE:HB3 | 2.13 | 0.49 |
| 2:E:94:PHE:HD1 | 2:E:219:ARG:HB3 | 1.78 | 0.49 |
| 1:I:10:THR:HB | 1:I:11:ASP:HA | 1.94 | 0.49 |
| 1:I:92:GLN:HB3 | 1:I:93:LYS:CB | 2.39 | 0.49 |
| 1:L:48:SER:HA | 1:L:92:GLN:O | 2.13 | 0.49 |
| 1:M:40:GLN:OE1 | 1:M:41:ARG:NH1 | 2.46 | 0.49 |
| 2:B:54:THR:HG22 | 2:B:55:THR:H | 1.77 | 0.49 |
| 2:D:258:ILE:O | 2:D:260:MET:N | 2.45 | 0.49 |
| 1:H:5:ASN:OD1 | 1:H:6:MET:N | 2.45 | 0.49 |
| 1:K:51:ALA:HB3 | 1:K:90:ALA:HB3 | 1.95 | 0.49 |
| 2:D:233:TRP:O | 2:D:234:ARG:HB2 | 2.13 | 0.49 |
| 2:D:42:ILE:HG12 | 2:D:180:TRP:CD1 | 2.48 | 0.49 |
| 2:E:174:SER:HA | 2:E:241:ASN:ND2 | 2.20 | 0.49 |
| 2:F:11:LEU:HA | 2:F:14:ILE:HG22 | 1.95 | 0.49 |
| 1:I:6:MET:H | 1:I:105:TYR:HE1 | 1.61 | 0.49 |
| 2:A:42:ILE:HG23 | 2:A:180:TRP:CD1 | 2.49 | 0.48 |
| 2:E:287:HIS:CE1 | 2:E:320:ILE:HD12 | 2.47 | 0.48 |
| 1:H:5:ASN:HB3 | 1:H:104:PHE:CE2 | 2.48 | 0.48 |
| 1:I:6:MET:HG3 | 1:I:7:LYS:N | 2.27 | 0.48 |
| 1:J:94:ARG:C | 1:J:96:ASP:H | 2.16 | 0.48 |
| 1:K:24:ASP:OD2 | 1:K:25:GLN:N | 2.45 | 0.48 |
| 2:A:299:ASN:O | 2:A:301:ASN:ND2 | 2.45 | 0.48 |
| 2:B:177:PHE:CB | 2:B:280:ILE:HA | 2.44 | 0.48 |
| 2:F:95:VAL:O | 2:F:217:ALA:HB1 | 2.13 | 0.48 |
| 2:G:191:GLU:OE2 | 2:G:191:GLU:N | 2.44 | 0.48 |
| 2:G:285:THR:HG21 | 2:G:327:LEU:HD13 | 1.95 | 0.48 |
| 1:H:47:LYS:HE3 | 1:H:94:ARG:HB3 | 1.95 | 0.48 |
| 1:M:40:GLN:NE2 | 1:M:101:LYS:HB2 | 2.28 | 0.48 |
| 2:A:240:CYS:HB2 | 2:A:333:VAL:CG1 | 2.42 | 0.48 |
| 2:B:246:THR:HA | 2:B:249:LYS:HD2 | 1.95 | 0.48 |
| 2:C:247:LEU:HD13 | 2:C:289:TRP:CD1 | 2.49 | 0.48 |
| 2:D:249:LYS:NZ | 2:D:250:ASP:H | 2.11 | 0.48 |
| 2:E:171:THR:HG23 | 2:E:243:ASP:HB2 | 1.96 | 0.48 |
| 1:K:10:THR:HB | 1:K:101:LYS:HB2 | 1.95 | 0.48 |
| 1:K:101:LYS:H | 1:K:101:LYS:CE | 2.25 | 0.48 |
| 2:A:283:ASN:HB3 | 2:A:325:ALA:HB3 | 1.96 | 0.48 |
| 2:B:147:ARG:HG3 | 2:B:334:THR:HA | 1.95 | 0.48 |
| 2:D:20:LYS:HZ2 | 2:C:48:ASP:HB3 | 1.79 | 0.48 |
| 2:D:72:VAL:O | 2:D:73:GLN:HB2 | 2.12 | 0.48 |
| 2:E:11:LEU:O | 2:E:15:TYR:HB2 | 2.13 | 0.48 |
| 2:E:67:ARG:HH21 | 2:E:67:ARG:HB2 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:40:ASP:CG | 2:G:41:ALA:H | 2.16 | 0.48 |
| 1:H:54:ASP:OD1 | 1:H:54:ASP:N | 2.46 | 0.48 |
| 1:L:6:MET:HE1 | 1:L:10:THR:HA | 1.95 | 0.48 |
| 2:A:177:PHE:HB3 | 2:A:280:ILE:HA | 1.95 | 0.48 |
| 2:B:250:ASP:O | 2:B:293:GLN:HB2 | 2.13 | 0.48 |
| 2:C:160:GLU:HG2 | 2:C:161:ASN:O | 2.14 | 0.48 |
| 2:C:94:PHE:CD1 | 2:C:219:ARG:HB3 | 2.48 | 0.48 |
| 2:F:90:TYR:HE1 | 2:E:66:ARG:HG3 | 1.79 | 0.48 |
| 2:B:69:ASN:HB2 | 1:J:3:THR:HG23 | 1.95 | 0.48 |
| 2:A:154:SER:OG | 2:A:155:LYS:N | 2.46 | 0.48 |
| 2:B:230:VAL:HG23 | 2:B:231:ARG:H | 1.78 | 0.48 |
| 2:C:224:TRP:HD1 | 2:C:225:ASP:H | 1.62 | 0.48 |
| 2:D:86:THR:OG1 | 2:D:87:GLY:N | 2.46 | 0.48 |
| 2:F:215:PHE:CE2 | 2:F:217:ALA:HB2 | 2.49 | 0.48 |
| 2:F:86:THR:OG1 | 2:F:87:GLY:N | 2.46 | 0.48 |
| 1:N:20:PRO:HB3 | 1:N:21:GLU:HG3 | 1.95 | 0.48 |
| 2:A:208:SER:N | 2:A:209:ASP:HA | 2.27 | 0.48 |
| 2:D:65:TRP:CZ2 | 2:E:128:TYR:HD1 | 2.31 | 0.48 |
| 2:E:46:CYS:SG | 2:E:185:ALA:HB1 | 2.53 | 0.48 |
| 2:A:272:MET:HE1 | 2:B:33:LYS:HA | 1.95 | 0.48 |
| 2:A:300:VAL:HB | 2:B:303:THR:OG1 | 2.13 | 0.48 |
| 2:B:326:ILE:HG23 | 2:B:328:ASN:H | 1.77 | 0.48 |
| 2:C:186:HIS:HD2 | 2:C:191:GLU:HA | 1.79 | 0.48 |
| 2:C:26:ARG:O | 2:C:28:VAL:N | 2.46 | 0.48 |
| 2:C:50:SER:O | 2:C:52:HIS:N | 2.42 | 0.48 |
| 2:F:241:ASN:HB2 | 2:F:242:ILE:HD13 | 1.95 | 0.48 |
| 2:A:307:TYR:CB | 2:A:308:GLY:HA2 | 2.34 | 0.48 |
| 2:E:154:SER:OG | 2:E:155:LYS:N | 2.45 | 0.48 |
| 2:F:189:TYR:HB2 | 2:F:190:PRO:HD2 | 1.96 | 0.48 |
| 2:F:242:ILE:HD12 | 2:F:247:LEU:CD2 | 2.43 | 0.48 |
| 2:F:33:LYS:HE2 | 2:E:233:TRP:HE1 | 1.79 | 0.48 |
| 2:G:241:ASN:CB | 2:G:242:ILE:HG13 | 2.44 | 0.48 |
| 1:H:49:LEU:O | 1:H:91:PRO:HA | 2.13 | 0.48 |
| 1:I:54:ASP:HB2 | 1:I:55:SER:H | 1.51 | 0.48 |
| 1:K:102:ASP:OD1 | 1:K:102:ASP:N | 2.47 | 0.48 |
| 1:N:94:ARG:HG3 | 1:N:95:ASP:H | 1.79 | 0.48 |
| 2:A:90:TYR:CB | 2:A:223:LYS:HA | 2.42 | 0.48 |
| 2:A:271:ALA:HB3 | 2:A:273:LEU:HG | 1.95 | 0.48 |
| 2:A:94:PHE:HE1 | 2:A:219:ARG:HG3 | 1.78 | 0.48 |
| 2:B:177:PHE:HB2 | 2:B:279:VAL:O | 2.14 | 0.48 |
| 2:C:55:THR:HA | 2:C:81:PRO:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:72:VAL:HG12 | 2:G:73:GLN:HG2 | 1.96 | 0.48 |
| 1:L:23:LYS:HA | 1:L:24:ASP:HA | 1.53 | 0.48 |
| 1:M:36:ASN:CG | 1:M:37:GLU:H | 2.16 | 0.48 |
| 2:A:125:VAL:O | 2:A:129:SER:OG | 2.26 | 0.47 |
| 2:D:215:PHE:HD2 | 2:D:215:PHE:C | 2.18 | 0.47 |
| 2:D:23:ARG:HG2 | 2:D:24:ILE:H | 1.79 | 0.47 |
| 2:D:3:LEU:HD12 | 2:D:4:ILE:HG22 | 1.95 | 0.47 |
| 2:F:287:HIS:NE2 | 2:F:320:ILE:HD13 | 2.29 | 0.47 |
| 1:K:23:LYS:HA | 1:K:24:ASP:HA | 1.44 | 0.47 |
| 2:A:91:ASP:O | 2:A:221:GLU:HB2 | 2.14 | 0.47 |
| 2:B:95:VAL:HG22 | 2:B:218:TYR:HB2 | 1.94 | 0.47 |
| 2:B:66:ARG:HG3 | 2:B:70:GLN:HB2 | 1.97 | 0.47 |
| 2:D:174:SER:HA | 2:D:242:ILE:HD11 | 1.95 | 0.47 |
| 1:H:47:LYS:HG3 | 1:H:93:LYS:HE3 | 1.95 | 0.47 |
| 1:I:6:MET:HG3 | 1:I:8:THR:H | 1.79 | 0.47 |
| 2:D:42:ILE:HD11 | 2:D:181:GLY:H | 1.78 | 0.47 |
| 1:J:88:GLY:HA2 | 1:J:89:LEU:HA | 1.59 | 0.47 |
| 2:A:50:SER:OG | 2:A:51:LYS:N | 2.46 | 0.47 |
| 2:B:160:GLU:HB2 | 2:B:240:CYS:N | 2.25 | 0.47 |
| 2:B:242:ILE:HB | 2:B:243:ASP:O | 2.14 | 0.47 |
| 2:D:37:ILE:HG23 | 2:D:324:ASP:H | 1.79 | 0.47 |
| 2:E:48:ASP:O | 2:E:188:ILE:HD11 | 2.14 | 0.47 |
| 2:E:39:THR:O | 2:E:39:THR:OG1 | 2.31 | 0.47 |
| 2:F:305:GLU:HA | 2:F:306:GLU:HA | 1.49 | 0.47 |
| 1:H:41:ARG:HG3 | 1:H:42:LEU:HG | 1.96 | 0.47 |
| 1:J:5:ASN:HD21 | 1:J:105:TYR:HE1 | 1.60 | 0.47 |
| 1:N:40:GLN:HB2 | 1:N:101:LYS:O | 2.15 | 0.47 |
| 2:B:246:THR:HA | 2:B:249:LYS:HB2 | 1.97 | 0.47 |
| 2:E:69:ASN:OD1 | 2:E:70:GLN:N | 2.48 | 0.47 |
| 2:G:280:ILE:HD13 | 2:G:320:ILE:HG12 | 1.95 | 0.47 |
| 2:A:271:ALA:HB1 | 2:A:273:LEU:N | 2.29 | 0.47 |
| 2:C:160:GLU:HB2 | 2:C:239:ILE:HA | 1.96 | 0.47 |
| 2:C:92:LEU:H | 2:C:92:LEU:HD13 | 1.78 | 0.47 |
| 2:G:242:ILE:H | 2:G:243:ASP:HA | 1.78 | 0.47 |
| 1:L:70:ARG:O | 1:L:71:THR:OG1 | 2.26 | 0.47 |
| 2:B:38:LEU:HD22 | 2:B:321:ARG:HG3 | 1.97 | 0.47 |
| 2:D:250:ASP:HA | 2:D:253:THR:OG1 | 2.15 | 0.47 |
| 2:F:282:ALA:O | 2:F:323:VAL:N | 2.34 | 0.47 |
| 2:G:122:ASN:HA | 2:G:125:VAL:HG12 | 1.97 | 0.47 |
| 2:G:7:THR:O | 2:G:8:LEU:HB2 | 2.14 | 0.47 |
| 1:H:26:TYR:CE2 | 1:H:84:ILE:HD11 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:5:ASN:HB3 | 1:K:104:PHE:O | 2.15 | 0.47 |
| 1:K:41:ARG:HG2 | 1:K:42:LEU:HD22 | 1.97 | 0.47 |
| 1:M:5:ASN:HD21 | 1:M:104:PHE:HE1 | 1.61 | 0.47 |
| 1:N:54:ASP:HB3 | 1:N:86:ASP:H | 1.80 | 0.47 |
| 2:A:195:ALA:CB | 2:A:222:PHE:HA | 2.44 | 0.47 |
| 2:B:66:ARG:HG3 | 2:B:70:GLN:H | 1.79 | 0.47 |
| 2:C:191:GLU:OE1 | 2:C:192:GLY:N | 2.42 | 0.47 |
| 2:C:92:LEU:HB3 | 2:C:221:GLU:HB3 | 1.97 | 0.47 |
| 2:C:176:TRP:CZ2 | 2:C:238:ARG:HD3 | 2.50 | 0.47 |
| 2:D:90:TYR:CZ | 2:C:66:ARG:HD3 | 2.50 | 0.47 |
| 2:G:20:LYS:O | 2:G:20:LYS:HG3 | 2.15 | 0.47 |
| 2:C:84:ASP:HA | 1:J:110:ASP:HA | 1.96 | 0.47 |
| 1:J:32:ILE:O | 1:J:33:THR:OG1 | 2.26 | 0.47 |
| 1:K:21:GLU:O | 1:K:23:LYS:N | 2.40 | 0.47 |
| 1:M:36:ASN:OD1 | 1:M:37:GLU:N | 2.45 | 0.47 |
| 1:M:36:ASN:H | 1:M:78:ASN:HD21 | 1.61 | 0.47 |
| 1:M:7:LYS:HZ3 | 1:M:8:THR:H | 1.63 | 0.47 |
| 1:N:42:LEU:O | 1:N:99:GLU:HG3 | 2.15 | 0.47 |
| 2:B:172:ASN:HA | 2:B:243:ASP:HB2 | 1.96 | 0.47 |
| 2:C:172:ASN:O | 2:C:328:ASN:HA | 2.15 | 0.47 |
| 2:E:4:ILE:C | 2:E:6:GLN:H | 2.18 | 0.47 |
| 1:H:7:LYS:HG2 | 1:H:8:THR:N | 2.29 | 0.47 |
| 1:L:89:LEU:HD13 | 1:L:104:PHE:HE2 | 1.80 | 0.47 |
| 1:M:84:ILE:O | 1:M:85:THR:OG1 | 2.24 | 0.47 |
| 2:B:180:TRP:HA | 2:B:180:TRP:CE3 | 2.50 | 0.47 |
| 2:C:11:LEU:HD23 | 2:C:102:ARG:HH12 | 1.80 | 0.47 |
| 2:D:23:ARG:HB3 | 2:D:25:ALA:O | 2.15 | 0.47 |
| 2:E:66:ARG:HE | 2:E:68:TYR:H | 1.61 | 0.47 |
| 2:F:177:PHE:HB3 | 2:F:280:ILE:HB | 1.97 | 0.47 |
| 2:F:178:MET:HG2 | 2:F:178:MET:O | 2.14 | 0.47 |
| 1:I:44:LEU:HD21 | 1:I:97:ALA:HA | 1.97 | 0.47 |
| 1:N:23:LYS:HA | 1:N:24:ASP:HA | 1.57 | 0.47 |
| 2:A:51:LYS:O | 2:A:52:HIS:HB2 | 2.15 | 0.47 |
| 2:A:74:PRO:HA | 2:B:92:LEU:O | 2.15 | 0.47 |
| 2:D:234:ARG:O | 2:D:268:ARG:HG3 | 2.14 | 0.47 |
| 2:D:277:LYS:HA | 2:D:277:LYS:HD3 | 1.79 | 0.47 |
| 2:A:89:LEU:HB3 | 2:F:65:TRP:HD1 | 1.78 | 0.47 |
| 1:J:41:ARG:CD | 1:J:42:LEU:H | 2.28 | 0.47 |
| 2:E:184:THR:HA | 2:E:228:LEU:HA | 1.96 | 0.46 |
| 2:E:172:ASN:ND2 | 2:E:241:ASN:O | 2.40 | 0.46 |
| 2:F:124:LYS:HZ3 | 2:F:127:ARG:HB3 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:331:SER:O | 2:G:333:VAL:N | 2.49 | 0.46 |
| 1:I:28:TRP:C | 1:I:84:ILE:HG12 | 2.35 | 0.46 |
| 1:I:54:ASP:N | 1:I:54:ASP:OD1 | 2.48 | 0.46 |
| 1:J:28:TRP:HA | 1:J:84:ILE:HG21 | 1.97 | 0.46 |
| 1:N:94:ARG:HD2 | 1:N:94:ARG:HA | 1.60 | 0.46 |
| 2:A:92:LEU:HB3 | 2:A:221:GLU:HB3 | 1.98 | 0.46 |
| 2:B:122:ASN:O | 2:B:125:VAL:HG12 | 2.15 | 0.46 |
| 2:C:90:TYR:CB | 2:C:223:LYS:HA | 2.45 | 0.46 |
| 2:D:92:LEU:HA | 2:D:221:GLU:HA | 1.97 | 0.46 |
| 2:F:271:ALA:HB1 | 2:F:272:MET:C | 2.35 | 0.46 |
| 2:F:92:LEU:HD12 | 2:E:72:VAL:HG22 | 1.96 | 0.46 |
| 1:K:1:MET:N | 1:K:1:MET:SD | 2.88 | 0.46 |
| 1:L:66:SER:OG | 1:L:67:VAL:N | 2.47 | 0.46 |
| 1:M:44:LEU:HB2 | 1:M:97:ALA:CB | 2.45 | 0.46 |
| 2:F:286:ILE:HD13 | 2:F:286:ILE:HA | 1.85 | 0.46 |
| 2:G:28:VAL:HG13 | 2:G:29:GLU:HG3 | 1.97 | 0.46 |
| 1:H:36:ASN:OD1 | 1:H:37:GLU:N | 2.49 | 0.46 |
| 1:J:27:PRO:HA | 1:J:84:ILE:HG23 | 1.96 | 0.46 |
| 1:J:59:MET:HB2 | 1:J:60:ALA:HB2 | 1.97 | 0.46 |
| 1:L:35:ASP:HA | 1:L:78:ASN:OD1 | 2.14 | 0.46 |
| 2:A:79:THR:OG1 | 2:A:80:VAL:N | 2.45 | 0.46 |
| 2:C:307:TYR:HB2 | 2:C:308:GLY:HA3 | 1.96 | 0.46 |
| 2:D:215:PHE:CD2 | 2:D:215:PHE:C | 2.89 | 0.46 |
| 2:D:201:ASP:OD2 | 2:D:219:ARG:NH2 | 2.49 | 0.46 |
| 2:D:76:LYS:HZ1 | 2:E:6:GLN:C | 2.19 | 0.46 |
| 1:I:22:THR:OG1 | 1:I:25:GLN:NE2 | 2.49 | 0.46 |
| 1:J:20:PRO:HA | 1:J:21:GLU:HA | 1.45 | 0.46 |
| 1:M:40:GLN:CD | 1:M:101:LYS:HB2 | 2.36 | 0.46 |
| 1:M:64:VAL:HG23 | 1:M:65:CYS:H | 1.79 | 0.46 |
| 1:N:71:THR:HG22 | 1:N:72:THR:H | 1.80 | 0.46 |
| 2:A:88:MET:HG2 | 2:A:225:ASP:HB2 | 1.96 | 0.46 |
| 2:C:142:MET:C | 2:C:144:LEU:H | 2.19 | 0.46 |
| 1:K:8:THR:HB | 1:K:101:LYS:NZ | 2.31 | 0.46 |
| 1:L:14:VAL:C | 1:L:16:GLU:H | 2.19 | 0.46 |
| 1:L:80:VAL:HG13 | 1:L:81:GLU:H | 1.81 | 0.46 |
| 2:A:47:ASN:O | 2:A:52:HIS:HA | 2.16 | 0.46 |
| 2:C:209:ASP:N | 2:C:209:ASP:OD1 | 2.49 | 0.46 |
| 2:C:94:PHE:HD1 | 2:C:219:ARG:HB3 | 1.79 | 0.46 |
| 2:E:305:GLU:HA | 2:E:306:GLU:HA | 1.48 | 0.46 |
| 2:F:87:GLY:HA3 | 2:F:138:PRO:CG | 2.44 | 0.46 |
| 2:G:106:ALA:O | 2:G:110:ARG:HG2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:46:ALA:H | 1:H:70:ARG:HB3 | 1.79 | 0.46 |
| 1:J:23:LYS:HA | 1:J:24:ASP:HA | 1.43 | 0.46 |
| 1:K:26:TYR:CE2 | 1:K:84:ILE:HD11 | 2.50 | 0.46 |
| 1:L:63:ASN:HD21 | 1:L:65:CYS:HB3 | 1.80 | 0.46 |
| 2:C:208:SER:HA | 2:C:209:ASP:HA | 1.43 | 0.46 |
| 2:C:37:ILE:HD12 | 2:C:323:VAL:C | 2.36 | 0.46 |
| 2:F:160:GLU:HG2 | 2:F:161:ASN:N | 2.30 | 0.46 |
| 2:F:180:TRP:HB2 | 2:F:277:LYS:HE2 | 1.97 | 0.46 |
| 2:F:39:THR:O | 2:F:39:THR:OG1 | 2.28 | 0.46 |
| 2:G:203:GLY:HA2 | 2:G:204:ASP:HB2 | 1.96 | 0.46 |
| 1:I:23:LYS:HA | 1:I:24:ASP:HA | 1.51 | 0.46 |
| 1:I:92:GLN:OE1 | 1:I:93:LYS:HA | 2.16 | 0.46 |
| 1:J:80:VAL:HG13 | 1:J:81:GLU:H | 1.81 | 0.46 |
| 1:K:10:THR:H | 1:K:11:ASP:HA | 1.80 | 0.46 |
| 1:M:17:ASP:OD1 | 1:M:18:GLY:N | 2.49 | 0.46 |
| 2:A:57:ARG:HH22 | 2:B:17:ARG:NH1 | 2.14 | 0.46 |
| 2:B:192:GLY:O | 2:B:194:VAL:N | 2.49 | 0.46 |
| 2:B:197:PHE:CE2 | 2:B:221:GLU:HB3 | 2.41 | 0.46 |
| 2:D:112:SER:O | 2:D:115:MET:HG2 | 2.15 | 0.46 |
| 2:D:195:ALA:HB1 | 2:D:222:PHE:HD2 | 1.80 | 0.46 |
| 2:F:178:MET:HA | 2:F:235:SER:O | 2.15 | 0.46 |
| 2:G:28:VAL:HG22 | 2:G:29:GLU:HG3 | 1.97 | 0.46 |
| 2:G:90:TYR:HD2 | 2:G:90:TYR:O | 1.99 | 0.46 |
| 1:H:39:LEU:N | 1:H:102:ASP:OD2 | 2.49 | 0.46 |
| 1:I:4:VAL:HA | 1:I:5:ASN:HA | 1.55 | 0.46 |
| 1:M:11:ASP:C | 1:M:13:PHE:H | 2.19 | 0.46 |
| 2:D:166:GLY:O | 2:D:331:SER:OG | 2.30 | 0.46 |
| 2:G:26:ARG:NE | 2:G:28:VAL:HG23 | 2.30 | 0.46 |
| 1:H:11:ASP:OD1 | 1:H:101:LYS:HB2 | 2.16 | 0.46 |
| 1:H:26:TYR:HA | 1:H:27:PRO:HD3 | 1.77 | 0.46 |
| 1:I:94:ARG:HA | 1:I:94:ARG:HD3 | 1.52 | 0.46 |
| 1:N:9:GLY:HA2 | 1:N:101:LYS:HD2 | 1.97 | 0.46 |
| 2:B:154:SER:O | 2:B:233:TRP:HH2 | 1.98 | 0.46 |
| 2:B:85:THR:OG1 | 2:B:86:THR:N | 2.49 | 0.46 |
| 2:D:274:GLY:HA2 | 2:D:275:ASP:HA | 1.51 | 0.46 |
| 2:D:31:LEU:HB2 | 2:C:56:ILE:HG22 | 1.98 | 0.46 |
| 2:D:50:SER:OG | 2:D:51:LYS:N | 2.49 | 0.46 |
| 2:F:138:PRO:HA | 2:F:139:GLU:HA | 1.49 | 0.46 |
| 2:F:180:TRP:HE3 | 2:F:180:TRP:HA | 1.81 | 0.46 |
| 2:F:179:SER:HB2 | 2:F:278:GLU:HG2 | 1.98 | 0.46 |
| 2:G:141:PHE:O | 2:G:141:PHE:HD2 | 1.99 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:12:SER:OG | 1:L:12:SER:O | 2.32 | 0.46 |
| 1:M:48:SER:HA | 1:M:92:GLN:O | 2.16 | 0.46 |
| 1:N:9:GLY:HA3 | 1:N:11:ASP:OD1 | 2.15 | 0.46 |
| 1:N:21:GLU:N | 2:A:1:MET:SD | 2.90 | 0.45 |
| 2:D:102:ARG:O | 2:D:102:ARG:NE | 2.49 | 0.45 |
| 2:D:124:LYS:HD2 | 2:D:128:TYR:CD2 | 2.51 | 0.45 |
| 2:E:13:ASP:OD2 | 2:E:17:ARG:NH2 | 2.48 | 0.45 |
| 2:F:147:ARG:HB2 | 2:F:147:ARG:HH11 | 1.81 | 0.45 |
| 2:F:250:ASP:HA | 2:F:253:THR:OG1 | 2.16 | 0.45 |
| 2:A:39:THR:HA | 2:A:40:ASP:C | 2.36 | 0.45 |
| 2:B:60:ILE:HD11 | 2:C:117:LYS:NZ | 2.31 | 0.45 |
| 2:D:65:TRP:CH2 | 2:E:128:TYR:HD1 | 2.34 | 0.45 |
| 2:E:161:ASN:N | 2:E:240:CYS:O | 2.43 | 0.45 |
| 1:K:44:LEU:HB2 | 1:K:99:GLU:OE2 | 2.15 | 0.45 |
| 2:A:141:PHE:CD1 | 2:A:141:PHE:C | 2.89 | 0.45 |
| 2:G:187:MET:HB3 | 2:G:189:TYR:CE1 | 2.51 | 0.45 |
| 1:J:61:MET:N | 1:J:61:MET:SD | 2.88 | 0.45 |
| 2:B:67:ARG:NH1 | 1:J:7:LYS:HD2 | 2.31 | 0.45 |
| 1:K:25:GLN:HG3 | 1:K:85:THR:O | 2.17 | 0.45 |
| 1:L:46:ALA:HB2 | 1:L:70:ARG:HB3 | 1.98 | 0.45 |
| 1:M:19:LYS:N | 1:M:20:PRO:HD2 | 2.32 | 0.45 |
| 1:M:64:VAL:O | 1:M:65:CYS:HB2 | 2.16 | 0.45 |
| 2:C:192:GLY:O | 2:C:194:VAL:N | 2.46 | 0.45 |
| 2:E:203:GLY:N | 2:E:215:PHE:O | 2.49 | 0.45 |
| 2:G:242:ILE:HD12 | 2:G:243:ASP:HA | 1.98 | 0.45 |
| 2:G:305:GLU:O | 2:G:312:ILE:HA | 2.16 | 0.45 |
| 1:H:98:LYS:HG2 | 1:H:98:LYS:H | 1.58 | 0.45 |
| 1:K:71:THR:HB | 1:K:74:HIS:CE1 | 2.52 | 0.45 |
| 2:B:233:TRP:O | 2:B:233:TRP:CG | 2.69 | 0.45 |
| 2:C:159:ALA:HB1 | 2:C:263:ASP:OD2 | 2.15 | 0.45 |
| 2:C:163:PHE:HD2 | 2:C:243:ASP:H | 1.65 | 0.45 |
| 2:C:170:SER:O | 2:C:328:ASN:HB2 | 2.17 | 0.45 |
| 2:D:124:LYS:O | 2:D:127:ARG:HB2 | 2.16 | 0.45 |
| 2:D:160:GLU:HG3 | 2:D:240:CYS:HB3 | 1.98 | 0.45 |
| 2:D:27:ILE:HG12 | 2:D:27:ILE:O | 2.15 | 0.45 |
| 2:E:1:MET:O | 2:E:1:MET:HG3 | 2.17 | 0.45 |
| 2:G:260:MET:O | 2:G:263:ASP:HB3 | 2.17 | 0.45 |
| 1:I:53:GLY:O | 1:I:86:ASP:HA | 2.17 | 0.45 |
| 1:K:46:ALA:CA | 1:K:70:ARG:HH12 | 2.29 | 0.45 |
| 1:K:7:LYS:HD2 | 1:K:8:THR:H | 1.82 | 0.45 |
| 1:L:16:GLU:OE2 | 1:L:18:GLY:N | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:70:ARG:HE | 1:L:70:ARG:HB3 | 1.60 | 0.45 |
| 2:B:92:LEU:HB3 | 2:B:221:GLU:CB | 2.39 | 0.45 |
| 2:D:88:MET:HG2 | 2:D:225:ASP:OD1 | 2.17 | 0.45 |
| 2:E:205:ASP:HB2 | 2:E:210:GLY:CA | 2.47 | 0.45 |
| 2:E:53:LYS:O | 2:E:54:THR:OG1 | 2.25 | 0.45 |
| 1:H:50:PRO:HG2 | 1:H:66:SER:HB3 | 1.97 | 0.45 |
| 1:J:24:ASP:OD2 | 1:J:24:ASP:N | 2.50 | 0.45 |
| 1:L:38:SER:O | 1:L:75:GLY:HA2 | 2.17 | 0.45 |
| 1:M:53:GLY:O | 1:M:86:ASP:HA | 2.16 | 0.45 |
| 1:M:94:ARG:HE | 1:M:94:ARG:HA | 1.80 | 0.45 |
| 1:N:109:GLU:CD | 1:N:110:ASP:H | 2.20 | 0.45 |
| 2:A:117:LYS:HE2 | 2:A:222:PHE:HE1 | 1.81 | 0.45 |
| 2:B:299:ASN:O | 2:B:301:ASN:N | 2.50 | 0.45 |
| 2:D:189:TYR:N | 2:D:189:TYR:CD1 | 2.84 | 0.45 |
| 2:E:147:ARG:HB3 | 2:E:333:VAL:HG22 | 1.99 | 0.45 |
| 2:G:250:ASP:OD1 | 2:G:255:ALA:HB3 | 2.16 | 0.45 |
| 1:I:55:SER:OG | 1:I:56:VAL:N | 2.49 | 0.45 |
| 1:J:92:GLN:CD | 1:J:93:LYS:HB3 | 2.37 | 0.45 |
| 1:L:53:GLY:O | 1:L:86:ASP:HA | 2.17 | 0.45 |
| 2:B:60:ILE:HD11 | 2:C:117:LYS:HZ2 | 1.81 | 0.45 |
| 2:D:115:MET:HA | 2:D:118:LEU:HD23 | 1.98 | 0.45 |
| 2:F:37:ILE:HG23 | 2:F:38:LEU:O | 2.17 | 0.45 |
| 2:G:152:SER:OG | 2:G:153:THR:N | 2.49 | 0.45 |
| 1:J:49:LEU:O | 1:J:91:PRO:HA | 2.16 | 0.45 |
| 1:K:45:ASN:HB3 | 1:K:95:ASP:CG | 2.37 | 0.45 |
| 1:M:19:LYS:HE3 | 1:M:87:ILE:HG21 | 1.98 | 0.45 |
| 1:N:28:TRP:HA | 1:N:84:ILE:HG21 | 1.98 | 0.45 |
| 1:N:42:LEU:H | 1:N:42:LEU:HG | 1.61 | 0.45 |
| 2:B:160:GLU:HG2 | 2:B:161:ASN:O | 2.16 | 0.45 |
| 2:B:76:LYS:HD3 | 2:B:76:LYS:H | 1.82 | 0.45 |
| 2:C:176:TRP:CE2 | 2:C:238:ARG:HD3 | 2.52 | 0.45 |
| 2:C:35:ASN:OD1 | 2:C:123:ASN:ND2 | 2.50 | 0.45 |
| 2:D:247:LEU:HD22 | 2:D:247:LEU:HA | 1.76 | 0.45 |
| 2:D:62:GLU:N | 2:D:62:GLU:OE1 | 2.50 | 0.45 |
| 2:F:141:PHE:HZ | 2:F:178:MET:SD | 2.39 | 0.45 |
| 2:F:230:VAL:O | 2:F:232:ASP:N | 2.49 | 0.45 |
| 2:F:241:ASN:CB | 2:F:242:ILE:HG12 | 2.46 | 0.45 |
| 2:F:38:LEU:HA | 2:F:38:LEU:HD23 | 1.83 | 0.45 |
| 2:F:47:ASN:HA | 2:F:48:ASP:HA | 1.63 | 0.45 |
| 2:G:182:GLU:OE2 | 2:G:231:ARG:NH1 | 2.50 | 0.45 |
| 1:K:92:GLN:HB3 | 1:K:93:LYS:HB3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:47:LYS:HA | 1:M:70:ARG:NH2 | 2.32 | 0.45 |
| 2:A:201:ASP:HB3 | 2:A:202:LEU:H | 1.57 | 0.45 |
| 2:A:85:THR:OG1 | 2:A:86:THR:N | 2.49 | 0.45 |
| 2:B:17:ARG:O | 2:B:26:ARG:HD2 | 2.16 | 0.45 |
| 2:D:4:ILE:HG12 | 2:D:5:GLY:H | 1.81 | 0.45 |
| 2:E:238:ARG:HG2 | 2:E:239:ILE:N | 2.32 | 0.45 |
| 2:F:28:VAL:HA | 2:F:29:GLU:HA | 1.65 | 0.45 |
| 2:G:274:GLY:HA3 | 2:G:275:ASP:HA | 1.67 | 0.45 |
| 1:K:107:ASP:HA | 1:K:108:GLY:HA3 | 1.60 | 0.45 |
| 1:L:5:ASN:HB2 | 1:L:105:TYR:CZ | 2.52 | 0.45 |
| 1:L:94:ARG:HD2 | 1:L:94:ARG:HA | 1.75 | 0.45 |
| 1:M:27:PRO:HB3 | 1:M:85:THR:OG1 | 2.17 | 0.45 |
| 1:N:107:ASP:HA | 1:N:108:GLY:HA3 | 1.77 | 0.45 |
| 2:A:84:ASP:OD2 | 2:A:85:THR:HG22 | 2.17 | 0.44 |
| 2:C:121:PHE:HE1 | 2:C:224:TRP:HE3 | 1.64 | 0.44 |
| 2:C:171:THR:OG1 | 2:C:243:ASP:OD1 | 2.27 | 0.44 |
| 2:C:268:ARG:O | 2:C:269:ASP:HB3 | 2.17 | 0.44 |
| 2:D:179:SER:HB2 | 2:D:278:GLU:HG3 | 1.98 | 0.44 |
| 2:D:69:ASN:HB3 | 1:L:2:LYS:HG3 | 1.98 | 0.44 |
| 2:F:119:GLN:HA | 2:F:122:ASN:HD21 | 1.81 | 0.44 |
| 1:I:25:GLN:HG3 | 1:I:86:ASP:OD2 | 2.17 | 0.44 |
| 1:I:8:THR:OG1 | 1:I:9:GLY:HA2 | 2.17 | 0.44 |
| 1:J:53:GLY:O | 1:J:86:ASP:HA | 2.16 | 0.44 |
| 1:L:70:ARG:H | 1:L:70:ARG:NE | 2.15 | 0.44 |
| 1:M:54:ASP:O | 1:M:55:SER:HB2 | 2.17 | 0.44 |
| 2:A:41:ALA:HB1 | 2:A:180:TRP:HE1 | 1.82 | 0.44 |
| 2:A:66:ARG:HD2 | 2:A:68:TYR:N | 2.31 | 0.44 |
| 2:B:280:ILE:HG23 | 2:B:320:ILE:HA | 1.98 | 0.44 |
| 2:B:51:LYS:O | 2:B:52:HIS:HB2 | 2.17 | 0.44 |
| 2:C:326:ILE:HD13 | 2:C:327:LEU:H | 1.81 | 0.44 |
| 2:C:37:ILE:HD11 | 2:C:324:ASP:HB2 | 1.99 | 0.44 |
| 2:D:318:ILE:H | 2:D:318:ILE:HG13 | 1.45 | 0.44 |
| 2:F:110:ARG:HH12 | 2:F:218:TYR:HD1 | 1.65 | 0.44 |
| 1:H:40:GLN:NE2 | 1:H:41:ARG:HG2 | 2.32 | 0.44 |
| 1:I:20:PRO:HA | 1:I:21:GLU:HA | 1.57 | 0.44 |
| 1:I:32:ILE:O | 1:I:33:THR:OG1 | 2.27 | 0.44 |
| 1:I:93:LYS:HG3 | 1:I:94:ARG:H | 1.82 | 0.44 |
| 1:L:11:ASP:CG | 1:L:101:LYS:HD2 | 2.38 | 0.44 |
| 2:C:29:GLU:HB2 | 2:C:30:GLN:H | 1.57 | 0.44 |
| 2:D:205:ASP:OD2 | 2:D:214:GLN:N | 2.50 | 0.44 |
| 2:D:51:LYS:HB3 | 2:D:83:THR:HG21 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:147:ARG:NE | 2:E:148:PHE:HD2 | 2.14 | 0.44 |
| 2:E:8:LEU:HD23 | 2:E:94:PHE:HB2 | 1.99 | 0.44 |
| 2:F:113:GLU:OE1 | 2:E:77:THR:HG21 | 2.17 | 0.44 |
| 2:G:247:LEU:HD13 | 2:G:293:GLN:NE2 | 2.32 | 0.44 |
| 1:H:37:GLU:OE2 | 1:H:39:LEU:HG | 2.17 | 0.44 |
| 1:I:30:LEU:O | 1:I:31:ARG:NE | 2.50 | 0.44 |
| 1:K:40:GLN:HB2 | 1:K:102:ASP:HA | 1.98 | 0.44 |
| 1:L:105:TYR:HB2 | 1:L:106:PRO:CA | 2.48 | 0.44 |
| 2:B:274:GLY:HA3 | 2:B:275:ASP:HA | 1.88 | 0.44 |
| 2:B:63:PRO:HG3 | 2:C:121:PHE:CD2 | 2.53 | 0.44 |
| 2:C:326:ILE:HD13 | 2:C:328:ASN:H | 1.82 | 0.44 |
| 2:D:249:LYS:O | 2:D:251:ALA:N | 2.50 | 0.44 |
| 2:D:48:ASP:HB3 | 2:E:20:LYS:HZ3 | 1.82 | 0.44 |
| 1:J:94:ARG:HD2 | 1:J:94:ARG:HA | 1.59 | 0.44 |
| 2:A:163:PHE:CG | 2:A:164:SER:N | 2.85 | 0.44 |
| 2:A:266:TYR:HE1 | 2:B:311:LYS:HG2 | 1.83 | 0.44 |
| 2:B:141:PHE:C | 2:B:143:GLY:H | 2.21 | 0.44 |
| 2:B:74:PRO:HG3 | 2:C:94:PHE:CD2 | 2.53 | 0.44 |
| 2:D:33:LYS:HA | 2:C:234:ARG:HH22 | 1.82 | 0.44 |
| 2:G:193:MET:HA | 2:G:224:TRP:HE3 | 1.82 | 0.44 |
| 2:G:47:ASN:HA | 2:G:48:ASP:HA | 1.59 | 0.44 |
| 2:B:315:PHE:HA | 2:B:316:LEU:HA | 1.65 | 0.44 |
| 2:B:162:VAL:HG12 | 2:B:335:ALA:HB2 | 1.99 | 0.44 |
| 2:D:161:ASN:HB3 | 2:D:241:ASN:ND2 | 2.33 | 0.44 |
| 2:D:19:ASP:OD2 | 2:D:26:ARG:NH2 | 2.51 | 0.44 |
| 2:D:271:ALA:HA | 2:D:272:MET:HB3 | 1.99 | 0.44 |
| 1:H:53:GLY:O | 1:H:86:ASP:HA | 2.18 | 0.44 |
| 1:H:4:VAL:HA | 1:H:5:ASN:HA | 1.69 | 0.44 |
| 1:J:5:ASN:CG | 1:J:6:MET:N | 2.70 | 0.44 |
| 2:A:11:LEU:HA | 2:A:14:ILE:HG22 | 2.00 | 0.44 |
| 2:A:190:PRO:HB2 | 2:A:194:VAL:HG11 | 2.00 | 0.44 |
| 2:B:180:TRP:HE3 | 2:B:180:TRP:HA | 1.82 | 0.44 |
| 2:C:130:ILE:HG13 | 2:C:131:TYR:CD2 | 2.52 | 0.44 |
| 2:E:51:LYS:O | 2:E:52:HIS:HB2 | 2.18 | 0.44 |
| 2:F:128:TYR:CD1 | 2:E:65:TRP:HZ2 | 2.35 | 0.44 |
| 2:F:147:ARG:HG2 | 2:F:334:THR:HB | 1.99 | 0.44 |
| 2:F:170:SER:HA | 2:F:171:THR:HA | 1.83 | 0.44 |
| 1:H:13:PHE:H | 1:H:16:GLU:CG | 2.31 | 0.44 |
| 1:H:40:GLN:HE21 | 1:H:100:LEU:HB3 | 1.82 | 0.44 |
| 2:B:326:ILE:HD13 | 2:B:328:ASN:H | 1.83 | 0.44 |
| 2:C:283:ASN:HD21 | 2:C:286:ILE:H | 1.64 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:223:LYS:NZ | 2:D:223:LYS:HB3 | 2.32 | 0.44 |
| 2:E:316:LEU:HA | 2:E:317:GLY:HA2 | 1.66 | 0.44 |
| 2:F:202:LEU:HD13 | 2:F:214:GLN:HG2 | 2.00 | 0.44 |
| 2:G:259:SER:O | 2:G:262:VAL:HG12 | 2.18 | 0.44 |
| 2:G:280:ILE:HB | 2:G:320:ILE:HG12 | 1.98 | 0.44 |
| 1:J:40:GLN:HE22 | 1:J:41:ARG:NH2 | 2.15 | 0.44 |
| 1:K:70:ARG:O | 1:K:70:ARG:HG2 | 2.18 | 0.44 |
| 1:L:23:LYS:HD2 | 1:L:23:LYS:HA | 1.86 | 0.44 |
| 1:L:5:ASN:HB2 | 1:L:6:MET:H | 1.71 | 0.44 |
| 1:M:93:LYS:HG3 | 1:M:94:ARG:H | 1.83 | 0.44 |
| 2:B:305:GLU:HA | 2:B:306:GLU:HA | 1.66 | 0.44 |
| 2:B:280:ILE:HG12 | 2:B:320:ILE:HD13 | 2.00 | 0.44 |
| 2:C:206:LEU:HG | 2:C:207:VAL:H | 1.83 | 0.44 |
| 2:C:329:THR:HG1 | 2:C:330:GLU:H | 1.62 | 0.44 |
| 2:D:244:VAL:O | 2:D:248:THR:HG23 | 2.17 | 0.44 |
| 2:E:170:SER:HA | 2:E:171:THR:HA | 1.78 | 0.44 |
| 2:E:175:ILE:HG13 | 2:E:239:ILE:HG13 | 2.00 | 0.44 |
| 2:E:217:ALA:O | 2:E:218:TYR:HB2 | 2.16 | 0.44 |
| 2:G:150:THR:N | 2:G:152:SER:O | 2.51 | 0.44 |
| 1:J:89:LEU:HD11 | 1:J:102:ASP:OD2 | 2.18 | 0.44 |
| 1:K:4:VAL:HA | 1:K:5:ASN:HA | 1.69 | 0.44 |
| 1:L:4:VAL:HA | 1:L:5:ASN:HA | 1.73 | 0.44 |
| 2:A:251:ALA:HA | 2:A:292:LYS:NZ | 2.33 | 0.43 |
| 2:C:48:ASP:OD2 | 2:C:48:ASP:N | 2.29 | 0.43 |
| 2:D:242:ILE:N | 2:D:243:ASP:HA | 2.33 | 0.43 |
| 2:D:316:LEU:H | 2:D:318:ILE:HG13 | 1.82 | 0.43 |
| 2:E:182:GLU:HG3 | 2:E:231:ARG:HD3 | 1.99 | 0.43 |
| 2:E:97:LYS:HE3 | 2:E:218:TYR:N | 2.33 | 0.43 |
| 2:F:257:LEU:HD23 | 2:F:257:LEU:H | 1.82 | 0.43 |
| 1:L:54:ASP:HB2 | 1:L:83:GLN:HB3 | 1.99 | 0.43 |
| 2:A:161:ASN:HB3 | 2:A:240:CYS:HB3 | 2.00 | 0.43 |
| 2:A:170:SER:HA | 2:A:171:THR:HA | 1.67 | 0.43 |
| 2:A:28:VAL:HA | 2:A:29:GLU:HA | 1.66 | 0.43 |
| 2:C:84:ASP:OD2 | 2:C:85:THR:N | 2.46 | 0.43 |
| 2:D:230:VAL:C | 2:D:232:ASP:N | 2.71 | 0.43 |
| 2:E:149:ASN:O | 2:E:151:LEU:N | 2.47 | 0.43 |
| 2:E:273:LEU:HD23 | 2:E:273:LEU:H | 1.83 | 0.43 |
| 2:E:286:ILE:HD13 | 2:E:286:ILE:HA | 1.80 | 0.43 |
| 2:F:209:ASP:N | 2:F:210:GLY:CA | 2.79 | 0.43 |
| 2:G:124:LYS:O | 2:G:127:ARG:HB2 | 2.18 | 0.43 |
| 2:G:268:ARG:HG2 | 2:G:272:MET:HE1 | 1.98 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:43:GLY:HA2 | 1:J:100:LEU:HG | 1.99 | 0.43 |
| 1:M:27:PRO:HB3 | 1:M:85:THR:HG1 | 1.84 | 0.43 |
| 2:B:160:GLU:HG2 | 2:B:161:ASN:N | 2.33 | 0.43 |
| 2:C:291:HIS:NE2 | 2:C:309:GLY:HA3 | 2.33 | 0.43 |
| 2:E:134:THR:O | 2:E:134:THR:OG1 | 2.36 | 0.43 |
| 2:F:37:ILE:HD11 | 2:F:324:ASP:N | 2.33 | 0.43 |
| 2:G:97:LYS:HB2 | 2:G:217:ALA:O | 2.17 | 0.43 |
| 1:J:47:LYS:HE3 | 1:J:70:ARG:HH21 | 1.82 | 0.43 |
| 1:K:71:THR:HB | 1:K:74:HIS:HE1 | 1.83 | 0.43 |
| 1:M:98:LYS:HB3 | 1:M:98:LYS:HE3 | 1.77 | 0.43 |
| 2:B:170:SER:HA | 2:B:171:THR:OG1 | 2.18 | 0.43 |
| 2:C:203:GLY:HA3 | 2:C:204:ASP:CB | 2.47 | 0.43 |
| 2:C:39:THR:HA | 2:C:40:ASP:O | 2.19 | 0.43 |
| 2:C:85:THR:OG1 | 2:C:86:THR:N | 2.51 | 0.43 |
| 2:D:12:LEU:HD13 | 2:D:13:ASP:N | 2.33 | 0.43 |
| 2:D:182:GLU:OE2 | 2:D:231:ARG:NH1 | 2.51 | 0.43 |
| 2:D:4:ILE:HG12 | 2:D:5:GLY:N | 2.34 | 0.43 |
| 2:F:97:LYS:HE2 | 2:F:218:TYR:CD2 | 2.53 | 0.43 |
| 1:H:23:LYS:CG | 1:H:24:ASP:HA | 2.49 | 0.43 |
| 2:A:69:ASN:CB | 1:I:3:THR:HG21 | 2.41 | 0.43 |
| 1:L:1:MET:HA | 1:L:2:LYS:HA | 1.58 | 0.43 |
| 1:L:46:ALA:CB | 1:L:70:ARG:HB3 | 2.47 | 0.43 |
| 2:D:138:PRO:HA | 2:D:139:GLU:HA | 1.55 | 0.43 |
| 2:F:148:PHE:O | 2:F:154:SER:OG | 2.15 | 0.43 |
| 2:F:209:ASP:OD1 | 2:F:212:GLY:N | 2.51 | 0.43 |
| 1:H:93:LYS:HG3 | 1:H:94:ARG:H | 1.83 | 0.43 |
| 1:K:50:PRO:HA | 1:K:91:PRO:HA | 1.99 | 0.43 |
| 1:M:28:TRP:C | 1:M:84:ILE:HG12 | 2.38 | 0.43 |
| 1:N:53:GLY:O | 1:N:86:ASP:HA | 2.18 | 0.43 |
| 2:A:192:GLY:O | 2:A:194:VAL:N | 2.52 | 0.43 |
| 2:B:250:ASP:OD1 | 2:B:293:GLN:HG2 | 2.19 | 0.43 |
| 2:D:171:THR:HG21 | 2:D:245:THR:HG23 | 2.00 | 0.43 |
| 2:D:197:PHE:N | 2:D:197:PHE:CD2 | 2.87 | 0.43 |
| 2:D:22:GLY:HA3 | 2:D:23:ARG:HA | 1.48 | 0.43 |
| 2:D:301:ASN:CG | 2:C:300:VAL:HG23 | 2.39 | 0.43 |
| 2:E:246:THR:O | 2:E:249:LYS:HG2 | 2.18 | 0.43 |
| 2:G:250:ASP:HB2 | 2:G:293:GLN:NE2 | 2.34 | 0.43 |
| 1:J:94:ARG:HG3 | 1:J:95:ASP:H | 1.83 | 0.43 |
| 1:K:105:TYR:HB3 | 1:K:106:PRO:CD | 2.49 | 0.43 |
| 1:K:57:SER:HA | 1:K:85:THR:HG21 | 1.99 | 0.43 |
| 1:N:26:TYR:HA | 1:N:27:PRO:HD3 | 1.85 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:242:ILE:HB | 2:A:243:ASP:O | 2.19 | 0.43 |
| 2:B:28:VAL:HA | 2:B:29:GLU:HA | 1.77 | 0.43 |
| 2:D:178:MET:HG3 | 2:D:180:TRP:HZ3 | 1.84 | 0.43 |
| 2:F:180:TRP:C | 2:F:182:GLU:H | 2.22 | 0.43 |
| 2:G:240:CYS:HB3 | 2:G:334:THR:HA | 2.01 | 0.43 |
| 2:G:313:VAL:O | 2:G:314:SER:OG | 2.32 | 0.43 |
| 1:J:70:ARG:O | 1:J:71:THR:OG1 | 2.34 | 0.43 |
| 1:L:72:THR:HG22 | 1:L:73:ASP:OD1 | 2.18 | 0.43 |
| 1:M:47:LYS:HA | 1:M:70:ARG:HH21 | 1.82 | 0.43 |
| 2:A:95:VAL:HG22 | 2:A:218:TYR:O | 2.18 | 0.43 |
| 2:B:189:TYR:HB2 | 2:B:190:PRO:CD | 2.49 | 0.43 |
| 2:C:244:VAL:O | 2:C:247:LEU:HB2 | 2.19 | 0.43 |
| 2:E:157:ALA:HB1 | 2:E:236:ILE:HG23 | 2.01 | 0.43 |
| 2:E:189:TYR:HB2 | 2:E:190:PRO:CD | 2.49 | 0.43 |
| 2:E:95:VAL:HB | 2:E:96:ASP:H | 1.61 | 0.43 |
| 2:E:97:LYS:HE3 | 2:E:218:TYR:H | 1.84 | 0.43 |
| 2:G:309:GLY:HA2 | 2:G:310:LYS:O | 2.19 | 0.43 |
| 1:J:101:LYS:HD2 | 1:J:101:LYS:N | 2.33 | 0.43 |
| 1:L:55:SER:HA | 1:L:83:GLN:NE2 | 2.33 | 0.43 |
| 1:N:4:VAL:HA | 1:N:5:ASN:HA | 1.53 | 0.43 |
| 1:N:8:THR:HA | 1:N:9:GLY:HA2 | 1.78 | 0.43 |
| 2:A:155:LYS:HD2 | 2:A:155:LYS:HA | 1.89 | 0.43 |
| 2:A:280:ILE:HB | 2:A:320:ILE:HB | 2.00 | 0.43 |
| 2:B:138:PRO:HA | 2:B:139:GLU:HA | 1.55 | 0.43 |
| 2:B:15:TYR:HA | 2:B:15:TYR:HD2 | 1.73 | 0.43 |
| 2:C:17:ARG:HD3 | 2:C:17:ARG:HA | 1.75 | 0.43 |
| 2:C:139:GLU:HG3 | 2:C:228:LEU:HD12 | 2.01 | 0.43 |
| 2:C:314:SER:HB3 | 2:C:315:PHE:H | 1.58 | 0.43 |
| 2:C:60:ILE:N | 2:C:61:PRO:HD3 | 2.33 | 0.43 |
| 2:D:7:THR:CG2 | 2:C:74:PRO:HB2 | 2.48 | 0.43 |
| 2:D:182:GLU:OE1 | 2:D:231:ARG:HB3 | 2.19 | 0.43 |
| 2:E:104:ASN:O | 2:E:106:ALA:N | 2.52 | 0.43 |
| 2:F:22:GLY:HA3 | 2:F:23:ARG:HA | 1.58 | 0.43 |
| 2:F:242:ILE:HD12 | 2:F:247:LEU:HD23 | 1.99 | 0.43 |
| 2:G:138:PRO:HA | 2:G:139:GLU:HA | 1.51 | 0.43 |
| 1:I:5:ASN:HB2 | 1:I:6:MET:H | 1.48 | 0.43 |
| 1:L:49:LEU:O | 1:L:91:PRO:HA | 2.19 | 0.43 |
| 1:L:73:ASP:O | 1:L:74:HIS:ND1 | 2.51 | 0.43 |
| 1:M:94:ARG:HG3 | 1:M:95:ASP:N | 2.34 | 0.43 |
| 2:B:172:ASN:HB2 | 2:B:241:ASN:C | 2.39 | 0.43 |
| 2:D:315:PHE:HA | 2:D:316:LEU:HA | 1.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:172:ASN:HB2 | 2:F:241:ASN:C | 2.39 | 0.43 |
| 2:F:241:ASN:CG | 2:F:242:ILE:HG12 | 2.40 | 0.43 |
| 2:F:285:THR:O | 2:F:289:TRP:HB2 | 2.19 | 0.43 |
| 2:G:158:SER:O | 2:G:158:SER:OG | 2.24 | 0.43 |
| 2:G:176:TRP:HB2 | 2:G:281:TYR:HB2 | 2.00 | 0.43 |
| 2:G:245:THR:O | 2:G:249:LYS:HD3 | 2.19 | 0.43 |
| 2:G:332:ALA:C | 2:G:334:THR:H | 2.22 | 0.43 |
| 1:H:42:LEU:HG | 1:H:42:LEU:H | 1.68 | 0.43 |
| 1:I:54:ASP:OD1 | 1:I:62:ALA:HB3 | 2.18 | 0.43 |
| 1:K:26:TYR:HA | 1:K:27:PRO:HD3 | 1.72 | 0.43 |
| 1:K:5:ASN:HD21 | 1:K:22:THR:CB | 2.31 | 0.43 |
| 1:M:26:TYR:HA | 1:M:27:PRO:HD3 | 1.74 | 0.43 |
| 1:N:37:GLU:O | 1:N:104:PHE:HB3 | 2.18 | 0.43 |
| 1:N:105:TYR:HB3 | 1:N:106:PRO:HD3 | 2.01 | 0.43 |
| 2:A:32:ALA:HA | 2:F:234:ARG:NH1 | 2.34 | 0.42 |
| 2:A:88:MET:SD | 2:F:66:ARG:NH2 | 2.92 | 0.42 |
| 2:B:66:ARG:HG2 | 2:B:68:TYR:H | 1.84 | 0.42 |
| 2:C:201:ASP:OD2 | 2:C:219:ARG:NH1 | 2.52 | 0.42 |
| 2:C:197:PHE:HE2 | 2:C:221:GLU:HG3 | 1.83 | 0.42 |
| 2:D:281:TYR:HD1 | 2:D:323:VAL:HB | 1.83 | 0.42 |
| 2:D:86:THR:HG1 | 2:D:87:GLY:H | 1.67 | 0.42 |
| 2:E:172:ASN:N | 2:E:172:ASN:OD1 | 2.51 | 0.42 |
| 2:F:36:ASP:OD1 | 2:E:270:VAL:HG23 | 2.18 | 0.42 |
| 1:H:71:THR:HG22 | 1:H:72:THR:H | 1.84 | 0.42 |
| 1:I:17:ASP:C | 1:I:19:LYS:H | 2.18 | 0.42 |
| 1:I:29:GLY:O | 1:I:30:LEU:HD13 | 2.18 | 0.42 |
| 1:K:26:TYR:O | 1:K:84:ILE:HG13 | 2.19 | 0.42 |
| 1:L:47:LYS:HG2 | 1:L:70:ARG:NH2 | 2.32 | 0.42 |
| 1:N:10:THR:HB | 1:N:101:LYS:HG2 | 2.01 | 0.42 |
| 2:A:170:SER:HB3 | 2:A:171:THR:HG22 | 2.00 | 0.42 |
| 2:A:68:TYR:HA | 2:A:68:TYR:HD2 | 1.53 | 0.42 |
| 2:A:76:LYS:N | 2:A:76:LYS:HE3 | 2.34 | 0.42 |
| 2:C:246:THR:O | 2:C:250:ASP:HB3 | 2.19 | 0.42 |
| 2:C:82:VAL:HG22 | 2:C:83:THR:H | 1.85 | 0.42 |
| 2:D:160:GLU:HB2 | 2:D:239:ILE:HG22 | 2.01 | 0.42 |
| 2:D:326:ILE:HD12 | 2:D:326:ILE:HA | 1.85 | 0.42 |
| 2:E:180:TRP:HB2 | 2:E:277:LYS:HG2 | 2.01 | 0.42 |
| 2:E:300:VAL:O | 2:E:302:LEU:HG | 2.18 | 0.42 |
| 2:F:90:TYR:HB2 | 2:F:221:GLU:OE2 | 2.18 | 0.42 |
| 1:H:28:TRP:C | 1:H:84:ILE:HG12 | 2.40 | 0.42 |
| 1:I:42:LEU:O | 1:I:100:LEU:HD23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:22:THR:HG21 | 1:K:104:PHE:CZ | 2.53 | 0.42 |
| 2:D:70:GLN:OE1 | 1:L:3:THR:HG21 | 2.19 | 0.42 |
| 1:N:28:TRP:N | 1:N:84:ILE:HG21 | 2.34 | 0.42 |
| 2:A:233:TRP:O | 2:A:233:TRP:CG | 2.72 | 0.42 |
| 2:A:7:THR:O | 2:A:8:LEU:HB2 | 2.19 | 0.42 |
| 2:D:20:LYS:NZ | 2:C:48:ASP:HB3 | 2.34 | 0.42 |
| 2:D:125:VAL:O | 2:D:129:SER:OG | 2.33 | 0.42 |
| 2:E:15:TYR:HA | 2:E:15:TYR:HD2 | 1.61 | 0.42 |
| 2:F:94:PHE:CD1 | 2:F:219:ARG:HB3 | 2.54 | 0.42 |
| 2:F:279:VAL:CG2 | 2:F:321:ARG:HG2 | 2.49 | 0.42 |
| 1:I:55:SER:H | 1:I:83:GLN:HB3 | 1.84 | 0.42 |
| 1:M:99:GLU:HG2 | 1:M:101:LYS:HZ1 | 1.83 | 0.42 |
| 2:B:117:LYS:HD2 | 2:B:222:PHE:CE1 | 2.44 | 0.42 |
| 2:B:155:LYS:HB3 | 2:B:156:ALA:H | 1.67 | 0.42 |
| 2:B:38:LEU:HB3 | 2:B:39:THR:H | 1.63 | 0.42 |
| 2:B:87:GLY:HA3 | 2:B:138:PRO:HB3 | 2.02 | 0.42 |
| 2:C:247:LEU:HB3 | 2:C:289:TRP:CE2 | 2.54 | 0.42 |
| 2:C:72:VAL:HG12 | 2:C:73:GLN:HB2 | 2.02 | 0.42 |
| 2:D:121:PHE:HA | 2:D:121:PHE:HD1 | 1.74 | 0.42 |
| 2:D:249:LYS:HB3 | 2:D:249:LYS:HE3 | 1.76 | 0.42 |
| 2:D:265:TYR:O | 2:D:268:ARG:NH2 | 2.52 | 0.42 |
| 2:E:29:GLU:HB3 | 2:E:30:GLN:H | 1.57 | 0.42 |
| 2:F:162:VAL:O | 2:F:163:PHE:HB2 | 2.19 | 0.42 |
| 2:F:94:PHE:CE2 | 2:E:74:PRO:HG3 | 2.54 | 0.42 |
| 1:J:96:ASP:O | 1:J:98:LYS:NZ | 2.36 | 0.42 |
| 1:N:93:LYS:HG2 | 1:N:94:ARG:H | 1.83 | 0.42 |
| 2:D:123:ASN:O | 2:D:127:ARG:HG3 | 2.20 | 0.42 |
| 2:D:94:PHE:HE1 | 2:D:219:ARG:HG2 | 1.84 | 0.42 |
| 2:G:155:LYS:HD2 | 2:G:155:LYS:HA | 1.69 | 0.42 |
| 2:G:240:CYS:CB | 2:G:334:THR:HA | 2.50 | 0.42 |
| 1:K:94:ARG:HD2 | 1:K:94:ARG:HA | 1.91 | 0.42 |
| 1:M:65:CYS:SG | 1:M:66:SER:N | 2.92 | 0.42 |
| 1:N:101:LYS:CD | 1:N:102:ASP:H | 2.28 | 0.42 |
| 2:A:199:HIS:HB3 | 2:A:219:ARG:NH1 | 2.35 | 0.42 |
| 2:C:172:ASN:HB3 | 2:C:242:ILE:H | 1.85 | 0.42 |
| 2:D:37:ILE:HG22 | 2:D:323:VAL:HG22 | 2.00 | 0.42 |
| 2:E:183:ASN:O | 2:E:229:SER:OG | 2.30 | 0.42 |
| 2:E:61:PRO:CB | 2:E:62:GLU:HB3 | 2.49 | 0.42 |
| 2:G:160:GLU:H | 2:G:239:ILE:HG22 | 1.84 | 0.42 |
| 1:H:12:SER:O | 1:H:98:LYS:HA | 2.20 | 0.42 |
| 1:I:104:PHE:HB3 | 1:I:105:TYR:H | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:83:GLN:O | 1:K:84:ILE:HB | 2.19 | 0.42 |
| 1:M:14:VAL:HG13 | 1:M:96:ASP:CB | 2.49 | 0.42 |
| 2:A:161:ASN:CG | 2:A:162:VAL:H | 2.22 | 0.42 |
| 2:A:250:ASP:HB2 | 2:A:293:GLN:NE2 | 2.34 | 0.42 |
| 2:B:102:ARG:HA | 2:B:103:SER:HA | 1.82 | 0.42 |
| 2:B:218:TYR:HA | 2:B:218:TYR:HD1 | 1.78 | 0.42 |
| 2:B:274:GLY:H | 2:B:275:ASP:CB | 2.32 | 0.42 |
| 2:A:266:TYR:HE2 | 2:B:287:HIS:ND1 | 2.16 | 0.42 |
| 2:C:195:ALA:CB | 2:C:222:PHE:HA | 2.48 | 0.42 |
| 2:C:298:LYS:HG3 | 2:C:298:LYS:H | 1.60 | 0.42 |
| 2:D:42:ILE:HG12 | 2:D:180:TRP:HD1 | 1.84 | 0.42 |
| 2:E:208:SER:N | 2:E:209:ASP:HA | 2.34 | 0.42 |
| 2:E:315:PHE:HD1 | 2:E:316:LEU:HB3 | 1.84 | 0.42 |
| 2:F:172:ASN:ND2 | 2:F:330:GLU:O | 2.52 | 0.42 |
| 2:G:173:THR:CG2 | 2:G:327:LEU:HA | 2.49 | 0.42 |
| 2:G:260:MET:SD | 2:G:260:MET:N | 2.91 | 0.42 |
| 1:H:6:MET:HB3 | 1:H:104:PHE:CZ | 2.54 | 0.42 |
| 1:H:20:PRO:HA | 1:H:21:GLU:HA | 1.80 | 0.42 |
| 1:H:94:ARG:HA | 1:H:94:ARG:HD2 | 1.71 | 0.42 |
| 1:N:6:MET:HB2 | 1:N:104:PHE:CZ | 2.54 | 0.42 |
| 1:N:19:LYS:HG3 | 1:N:87:ILE:HD12 | 2.01 | 0.42 |
| 2:B:292:LYS:HB3 | 2:B:292:LYS:NZ | 2.34 | 0.42 |
| 2:B:82:VAL:HB | 2:B:83:THR:H | 1.54 | 0.42 |
| 1:K:2:LYS:HE2 | 2:C:68:TYR:CG | 2.55 | 0.42 |
| 2:F:6:GLN:HG2 | 2:F:7:THR:N | 2.34 | 0.42 |
| 2:G:197:PHE:O | 2:G:197:PHE:HD2 | 2.03 | 0.42 |
| 2:A:124:LYS:HG2 | 2:F:63:PRO:HG2 | 2.01 | 0.42 |
| 2:B:51:LYS:HZ2 | 2:B:51:LYS:HB2 | 1.85 | 0.42 |
| 2:C:138:PRO:HA | 2:C:139:GLU:HA | 1.57 | 0.42 |
| 2:D:153:THR:O | 2:D:153:THR:OG1 | 2.37 | 0.42 |
| 2:D:209:ASP:N | 2:D:210:GLY:CA | 2.81 | 0.42 |
| 2:D:82:VAL:O | 2:D:83:THR:HG22 | 2.20 | 0.42 |
| 2:E:130:ILE:O | 2:E:131:TYR:HB2 | 2.20 | 0.42 |
| 1:I:13:PHE:HA | 1:I:13:PHE:HD2 | 1.72 | 0.42 |
| 1:K:49:LEU:O | 1:K:91:PRO:HA | 2.19 | 0.42 |
| 1:M:21:GLU:HG3 | 1:M:22:THR:N | 2.33 | 0.42 |
| 1:M:52:VAL:HG22 | 1:M:64:VAL:HG22 | 2.02 | 0.42 |
| 2:A:259:SER:O | 2:A:262:VAL:HG22 | 2.20 | 0.42 |
| 2:B:266:TYR:HA | 2:B:266:TYR:HD1 | 1.64 | 0.42 |
| 2:B:60:ILE:HD13 | 2:B:77:THR:HG23 | 2.02 | 0.42 |
| 2:C:97:LYS:HG2 | 2:C:216:ARG:HH12 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:102:ARG:HA | 2:D:103:SER:HA | 1.78 | 0.42 |
| 2:E:97:LYS:HZ2 | 2:E:216:ARG:HE | 1.67 | 0.42 |
| 2:F:32:ALA:CA | 2:E:234:ARG:HH12 | 2.33 | 0.42 |
| 2:E:53:LYS:HA | 2:E:53:LYS:HD3 | 1.82 | 0.42 |
| 2:F:92:LEU:HD13 | 2:E:74:PRO:HA | 2.01 | 0.42 |
| 2:F:124:LYS:NZ | 2:F:127:ARG:HB3 | 2.34 | 0.42 |
| 2:F:20:LYS:HB2 | 2:F:20:LYS:HE2 | 1.85 | 0.42 |
| 2:G:204:ASP:HA | 2:G:205:ASP:HB2 | 2.02 | 0.42 |
| 1:L:3:THR:HA | 1:L:5:ASN:O | 2.20 | 0.42 |
| 1:N:101:LYS:HE2 | 1:N:101:LYS:HB2 | 1.83 | 0.42 |
| 2:A:161:ASN:ND2 | 2:A:162:VAL:H | 2.18 | 0.41 |
| 2:A:94:PHE:CE1 | 2:A:219:ARG:HG3 | 2.54 | 0.41 |
| 2:A:305:GLU:HA | 2:A:306:GLU:HA | 1.75 | 0.41 |
| 2:B:260:MET:HE2 | 2:B:260:MET:HB2 | 1.94 | 0.41 |
| 2:B:234:ARG:NH1 | 2:B:272:MET:HB2 | 2.35 | 0.41 |
| 2:B:51:LYS:HA | 2:B:84:ASP:O | 2.20 | 0.41 |
| 2:C:15:TYR:HD2 | 2:C:15:TYR:HA | 1.57 | 0.41 |
| 2:C:274:GLY:HA3 | 2:C:275:ASP:HA | 1.62 | 0.41 |
| 2:F:300:VAL:HG13 | 2:F:301:ASN:N | 2.28 | 0.41 |
| 2:G:233:TRP:NE1 | 2:G:234:ARG:HG2 | 2.35 | 0.41 |
| 2:G:280:ILE:HD11 | 2:G:318:ILE:CG1 | 2.50 | 0.41 |
| 2:G:28:VAL:HA | 2:G:29:GLU:HA | 1.62 | 0.41 |
| 1:J:23:LYS:HD3 | 1:J:24:ASP:HA | 2.02 | 0.41 |
| 2:A:39:THR:OG1 | 2:A:39:THR:O | 2.39 | 0.41 |
| 2:A:80:VAL:HG22 | 2:A:81:PRO:O | 2.20 | 0.41 |
| 2:C:140:ALA:O | 2:C:228:LEU:HD11 | 2.19 | 0.41 |
| 2:D:53:LYS:O | 2:D:54:THR:OG1 | 2.33 | 0.41 |
| 2:E:177:PHE:HB2 | 2:E:279:VAL:O | 2.20 | 0.41 |
| 1:I:7:LYS:HE2 | 1:I:7:LYS:HB3 | 1.74 | 0.41 |
| 2:A:302:LEU:HD12 | 2:B:302:LEU:HB3 | 2.01 | 0.41 |
| 2:A:173:THR:HB | 2:A:326:ILE:O | 2.20 | 0.41 |
| 2:B:7:THR:O | 2:B:8:LEU:HB2 | 2.19 | 0.41 |
| 2:C:316:LEU:HA | 2:C:317:GLY:HA2 | 1.70 | 0.41 |
| 2:D:178:MET:HA | 2:D:235:SER:O | 2.20 | 0.41 |
| 2:E:205:ASP:C | 2:E:210:GLY:HA2 | 2.41 | 0.41 |
| 2:E:49:GLY:HA2 | 2:E:188:ILE:HD11 | 2.02 | 0.41 |
| 2:F:199:HIS:HB2 | 2:F:219:ARG:CD | 2.49 | 0.41 |
| 2:F:252:SER:OG | 2:F:296:ASN:HB2 | 2.21 | 0.41 |
| 2:F:272:MET:HG3 | 2:F:272:MET:O | 2.21 | 0.41 |
| 1:I:26:TYR:HA | 1:I:27:PRO:HD3 | 1.85 | 0.41 |
| 1:I:55:SER:O | 1:I:85:THR:OG1 | 2.32 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:8:THR:CG2 | 1:M:102:ASP:H | 2.33 | 0.41 |
| 1:N:47:LYS:HD3 | 1:N:47:LYS:H | 1.86 | 0.41 |
| 2:B:103:SER:OG | 2:B:104:ASN:N | 2.54 | 0.41 |
| 2:B:41:ALA:HA | 2:B:180:TRP:CD1 | 2.55 | 0.41 |
| 2:B:247:LEU:HD23 | 2:B:247:LEU:HA | 1.90 | 0.41 |
| 2:D:261:MET:HG3 | 2:D:262:VAL:HG13 | 2.02 | 0.41 |
| 2:D:28:VAL:HA | 2:D:29:GLU:HA | 1.79 | 0.41 |
| 2:F:233:TRP:CE3 | 2:F:234:ARG:HA | 2.56 | 0.41 |
| 2:F:309:GLY:O | 2:F:311:LYS:N | 2.53 | 0.41 |
| 2:G:202:LEU:H | 2:G:202:LEU:HD13 | 1.84 | 0.41 |
| 1:J:54:ASP:HB2 | 1:J:55:SER:H | 1.60 | 0.41 |
| 1:L:16:GLU:CD | 1:L:18:GLY:H | 2.24 | 0.41 |
| 2:A:32:ALA:HA | 2:F:234:ARG:HH12 | 1.85 | 0.41 |
| 2:B:147:ARG:CD | 2:B:147:ARG:H | 2.34 | 0.41 |
| 2:E:138:PRO:HA | 2:E:139:GLU:HA | 1.63 | 0.41 |
| 2:E:97:LYS:NZ | 2:E:201:ASP:O | 2.43 | 0.41 |
| 2:E:61:PRO:HB3 | 2:E:62:GLU:HB3 | 2.02 | 0.41 |
| 2:G:258:ILE:HA | 2:G:258:ILE:HD12 | 1.89 | 0.41 |
| 1:I:36:ASN:OD1 | 1:I:37:GLU:N | 2.53 | 0.41 |
| 1:L:26:TYR:HA | 1:L:27:PRO:HD3 | 1.79 | 0.41 |
| 2:D:266:TYR:HB3 | 2:E:288:ALA:CB | 2.50 | 0.41 |
| 1:J:71:THR:HG22 | 1:J:72:THR:H | 1.85 | 0.41 |
| 1:K:66:SER:OG | 1:K:67:VAL:N | 2.53 | 0.41 |
| 1:M:20:PRO:HA | 1:M:21:GLU:HA | 1.60 | 0.41 |
| 2:A:111:VAL:HA | 2:A:114:ASN:HD21 | 1.85 | 0.41 |
| 2:A:234:ARG:NH1 | 2:A:272:MET:HE1 | 2.36 | 0.41 |
| 2:A:329:THR:HG23 | 2:A:330:GLU:H | 1.86 | 0.41 |
| 2:B:202:LEU:HA | 2:B:215:PHE:O | 2.21 | 0.41 |
| 2:D:305:GLU:HG3 | 2:C:310:LYS:HE3 | 2.02 | 0.41 |
| 2:C:48:ASP:HB2 | 2:C:49:GLY:H | 1.59 | 0.41 |
| 2:D:38:LEU:O | 2:D:39:THR:OG1 | 2.32 | 0.41 |
| 2:E:173:THR:OG1 | 2:E:174:SER:N | 2.49 | 0.41 |
| 2:F:145:ALA:N | 2:F:146:PRO:HD2 | 2.35 | 0.41 |
| 2:F:66:ARG:HD3 | 2:F:68:TYR:HA | 2.03 | 0.41 |
| 1:H:54:ASP:OD1 | 1:H:62:ALA:HB3 | 2.21 | 0.41 |
| 1:I:6:MET:HG2 | 1:I:104:PHE:CG | 2.56 | 0.41 |
| 1:I:26:TYR:HE2 | 1:I:84:ILE:HD11 | 1.85 | 0.41 |
| 1:N:1:MET:HA | 1:N:2:LYS:HA | 1.61 | 0.41 |
| 2:A:266:TYR:OH | 2:B:311:LYS:HB3 | 2.20 | 0.41 |
| 2:B:134:THR:HB | 2:B:135:ASP:H | 1.70 | 0.41 |
| 2:B:137:GLU:HB3 | 2:B:138:PRO:CD | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:47:ASN:HA | 2:B:48:ASP:HA | 1.75 | 0.41 |
| 2:C:106:ALA:O | 2:C:109:PHE:HB3 | 2.21 | 0.41 |
| 2:D:311:LYS:HD3 | 2:D:311:LYS:H | 1.86 | 0.41 |
| 2:E:102:ARG:HG2 | 2:E:102:ARG:O | 2.21 | 0.41 |
| 2:E:225:ASP:N | 2:E:225:ASP:OD2 | 2.51 | 0.41 |
| 2:E:285:THR:HG21 | 2:E:327:LEU:HD13 | 2.02 | 0.41 |
| 1:H:43:GLY:HA2 | 1:H:99:GLU:OE1 | 2.20 | 0.41 |
| 1:I:105:TYR:N | 1:I:105:TYR:CD1 | 2.84 | 0.41 |
| 1:M:29:GLY:N | 1:M:84:ILE:HG12 | 2.34 | 0.41 |
| 1:N:37:GLU:OE2 | 1:N:39:LEU:HD23 | 2.21 | 0.41 |
| 1:N:54:ASP:O | 1:N:61:MET:HB2 | 2.21 | 0.41 |
| 2:D:206:LEU:HA | 2:D:206:LEU:HD22 | 1.89 | 0.41 |
| 2:D:3:LEU:O | 2:D:6:GLN:HG3 | 2.21 | 0.41 |
| 2:E:138:PRO:HB2 | 2:E:139:GLU:CD | 2.41 | 0.41 |
| 2:E:309:GLY:O | 2:E:310:LYS:HG2 | 2.21 | 0.41 |
| 2:E:66:ARG:NE | 2:E:68:TYR:H | 2.18 | 0.41 |
| 2:G:280:ILE:HD11 | 2:G:318:ILE:HD12 | 2.03 | 0.41 |
| 1:H:84:ILE:O | 1:H:85:THR:OG1 | 2.34 | 0.41 |
| 1:H:94:ARG:HG3 | 1:H:95:ASP:H | 1.86 | 0.41 |
| 1:J:71:THR:HB | 1:J:74:HIS:CE1 | 2.56 | 0.41 |
| 1:N:10:THR:CB | 1:N:101:LYS:HG2 | 2.51 | 0.41 |
| 2:A:300:VAL:HA | 2:B:301:ASN:O | 2.20 | 0.41 |
| 2:C:271:ALA:HB1 | 2:C:273:LEU:N | 2.36 | 0.41 |
| 2:C:295:MET:HG3 | 2:C:296:ASN:OD1 | 2.21 | 0.41 |
| 2:D:146:PRO:CG | 2:D:152:SER:HB3 | 2.51 | 0.41 |
| 2:D:60:ILE:HD11 | 2:E:117:LYS:HE2 | 2.03 | 0.41 |
| 2:E:120:GLY:O | 2:E:123:ASN:HB3 | 2.21 | 0.41 |
| 2:E:26:ARG:O | 2:E:29:GLU:HA | 2.21 | 0.41 |
| 2:F:32:ALA:HA | 2:E:234:ARG:HH12 | 1.86 | 0.41 |
| 1:H:104:PHE:O | 1:H:105:TYR:HB2 | 2.21 | 0.41 |
| 1:H:97:ALA:HB1 | 1:H:99:GLU:OE1 | 2.20 | 0.41 |
| 1:I:31:ARG:HA | 1:I:31:ARG:CZ | 2.50 | 0.41 |
| 1:M:70:ARG:H | 1:M:70:ARG:HG2 | 1.63 | 0.41 |
| 2:D:39:THR:HA | 2:D:40:ASP:O | 2.21 | 0.41 |
| 2:E:242:ILE:HB | 2:E:243:ASP:O | 2.20 | 0.41 |
| 2:E:326:ILE:HG23 | 2:E:327:LEU:H | 1.85 | 0.41 |
| 2:G:113:GLU:N | 2:G:113:GLU:OE1 | 2.53 | 0.41 |
| 2:G:120:GLY:O | 2:G:123:ASN:HB3 | 2.21 | 0.41 |
| 2:G:135:ASP:C | 2:G:137:GLU:H | 2.25 | 0.41 |
| 2:G:60:ILE:N | 2:G:61:PRO:HD3 | 2.36 | 0.41 |
| 2:B:241:ASN:ND2 | 2:B:242:ILE:HD13 | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:B:301:ASN:HB2 | 2:C:304:ILE:O | 2.20 | 0.40 |
| 2:C:270:VAL:HG13 | 2:C:271:ALA:HA | 2.03 | 0.40 |
| 2:C:27:ILE:H | 2:C:27:ILE:HD13 | 1.85 | 0.40 |
| 2:C:55:THR:O | 2:C:56:ILE:HG12 | 2.21 | 0.40 |
| 2:D:280:ILE:HD11 | 2:D:318:ILE:CD1 | 2.51 | 0.40 |
| 2:F:97:LYS:NZ | 2:F:216:ARG:HE | 2.08 | 0.40 |
| 2:G:102:ARG:HA | 2:G:103:SER:HA | 1.77 | 0.40 |
| 2:G:272:MET:O | 2:G:275:ASP:HB3 | 2.21 | 0.40 |
| 1:I:40:GLN:HE22 | 1:I:42:LEU:HD12 | 1.87 | 0.40 |
| 1:J:31:ARG:CZ | 1:J:31:ARG:HB3 | 2.50 | 0.40 |
| 1:K:18:GLY:CA | 1:K:91:PRO:HD2 | 2.48 | 0.40 |
| 1:L:45:ASN:HB2 | 1:L:97:ALA:HA | 2.02 | 0.40 |
| 1:M:105:TYR:HD1 | 1:M:106:PRO:HD3 | 1.86 | 0.40 |
| 1:M:25:GLN:HB3 | 1:M:105:TYR:OH | 2.22 | 0.40 |
| 1:N:49:LEU:O | 1:N:91:PRO:HA | 2.20 | 0.40 |
| 2:B:73:GLN:H | 2:B:73:GLN:HG2 | 1.56 | 0.40 |
| 2:D:246:THR:HG1 | 2:D:246:THR:H | 1.49 | 0.40 |
| 2:D:29:GLU:N | 2:D:29:GLU:OE1 | 2.54 | 0.40 |
| 2:F:293:GLN:O | 2:F:293:GLN:NE2 | 2.53 | 0.40 |
| 2:F:316:LEU:HA | 2:F:317:GLY:HA2 | 1.71 | 0.40 |
| 1:J:40:GLN:NE2 | 1:J:101:LYS:HB2 | 2.36 | 0.40 |
| 1:M:87:ILE:HG12 | 1:M:87:ILE:H | 1.60 | 0.40 |
| 1:N:49:LEU:HB2 | 1:N:66:SER:O | 2.21 | 0.40 |
| 2:B:247:LEU:HB3 | 2:B:289:TRP:CE2 | 2.57 | 0.40 |
| 2:B:30:GLN:OE1 | 2:B:30:GLN:N | 2.54 | 0.40 |
| 2:B:96:ASP:O | 2:B:99:LEU:N | 2.54 | 0.40 |
| 2:D:172:ASN:HB3 | 2:D:241:ASN:O | 2.21 | 0.40 |
| 2:D:19:ASP:OD1 | 2:D:26:ARG:HA | 2.21 | 0.40 |
| 2:G:43:TYR:HD2 | 2:G:184:THR:OG1 | 2.03 | 0.40 |
| 2:G:97:LYS:H | 2:G:217:ALA:HA | 1.86 | 0.40 |
| 1:J:26:TYR:HA | 1:J:27:PRO:HD3 | 1.86 | 0.40 |
| 1:J:40:GLN:HG3 | 1:J:101:LYS:C | 2.41 | 0.40 |
| 1:J:47:LYS:HE3 | 1:J:70:ARG:NH2 | 2.36 | 0.40 |
| 1:L:32:ILE:O | 1:L:33:THR:OG1 | 2.32 | 0.40 |
| 1:N:34:LEU:HD22 | 1:N:35:ASP:N | 2.36 | 0.40 |
| 2:A:116:GLY:O | 2:A:119:GLN:HG2 | 2.22 | 0.40 |
| 2:B:42:ILE:HG22 | 2:B:180:TRP:HB3 | 2.04 | 0.40 |
| 2:D:160:GLU:N | 2:D:160:GLU:OE1 | 2.55 | 0.40 |
| 2:D:39:THR:HA | 2:D:40:ASP:C | 2.42 | 0.40 |
| 2:F:61:PRO:CB | 2:F:62:GLU:HB3 | 2.51 | 0.40 |
| 2:G:109:PHE:O | 2:G:113:GLU:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:G:132:GLY:O | 2:G:140:ALA:HA | 2.21 | 0.40 |
| 2:G:268:ARG:HG2 | 2:G:269:ASP:H | 1.86 | 0.40 |
| 2:G:305:GLU:HG3 | 2:G:307:TYR:H | 1.85 | 0.40 |
| 1:I:59:MET:HA | 1:I:60:ALA:HA | 1.90 | 0.40 |
| 1:J:89:LEU:HG | 1:J:91:PRO:CD | 2.47 | 0.40 |
| 1:N:2:LYS:NZ | 2:A:11:LEU:HB3 | 2.37 | 0.40 |
| 2:A:96:ASP:OD2 | 2:A:98:ALA:HB3 | 2.22 | 0.40 |
| 2:D:301:ASN:OD1 | 2:C:300:VAL:HG23 | 2.21 | 0.40 |
| 2:E:124:LYS:HA | 2:E:124:LYS:HD3 | 1.89 | 0.40 |
| 2:F:221:GLU:CD | 2:F:222:PHE:H | 2.24 | 0.40 |
| 1:H:47:LYS:H | 1:H:47:LYS:CD | 2.32 | 0.40 |
| 1:K:31:ARG:HH22 | 1:K:33:THR:H | 1.69 | 0.40 |
| 1:K:32:ILE:O | 1:K:33:THR:OG1 | 2.31 | 0.40 |
| 1:M:107:ASP:OD2 | 1:M:108:GLY:N | 2.54 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 1 | H | 109/111 (98%) | 56 (51%) | 38 (35%) | 15 (14%) | 0 | 6 |
| 1 | I | 109/111 (98%) | 54 (50%) | 34 (31%) | 21 (19%) | 0 | 3 |
| 1 | J | 109/111 (98%) | 54 (50%) | 33 (30%) | 22 (20%) | 0 | 2 |
| 1 | K | 109/111 (98%) | 63 (58%) | 27 (25%) | 19 (17%) | 0 | 3 |
| 1 | L | 109/111 (98%) | 54 (50%) | 31 (28%) | 24 (22%) | 0 | 2 |
| 1 | M | 109/111 (98%) | 49 (45%) | 34 (31%) | 26 (24%) | 0 | 1 |
| 1 | N | 109/111 (98%) | 60 (55%) | 34 (31%) | 15 (14%) | 0 | 6 |
| 2 | A | 333/335 (99%) | 211 (63%) | 82 (25%) | 40 (12%) | 0 | 8 |
| 2 | B | 333/335 (99%) | 207 (62%) | 85 (26%) | 41 (12%) | 0 | 7 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 2 | C | 333/335 (99%) | 205 (62%) | 80 (24%) | 48 (14%) | 0 | 5 |
| 2 | D | 333/335 (99%) | 200 (60%) | 92 (28%) | 41 (12%) | 0 | 7 |
| 2 | E | 333/335 (99%) | 215 (65%) | 79 (24%) | 39 (12%) | 0 | 8 |
| 2 | F | 333/335 (99%) | 199 (60%) | 93 (28%) | 41 (12%) | 0 | 7 |
| 2 | G | 333/335 (99%) | 215 (65%) | 87 (26%) | 31 (9%) | 1 | 15 |
| All | All | 3094/3122 (99%) | 1842 (60%) | 829 (27%) | 423 (14%) | 1 | 6 |

All (423) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 27 | PRO |
| 1 | N | 83 | GLN |
| 1 | N | 105 | TYR |
| 1 | M | 23 | LYS |
| 1 | M | 27 | PRO |
| 1 | M | 55 | SER |
| 1 | M | 73 | ASP |
| 1 | M | 83 | GLN |
| 1 | M | 84 | ILE |
| 1 | M | 103 | ALA |
| 2 | A | 28 | VAL |
| 2 | A | 32 | ALA |
| 2 | A | 52 | HIS |
| 2 | A | 56 | ILE |
| 2 | A | 134 | THR |
| 2 | A | 137 | GLU |
| 2 | A | 142 | MET |
| 2 | A | 143 | GLY |
| 2 | A | 154 | SER |
| 2 | A | 172 | ASN |
| 2 | A | 206 | LEU |
| 2 | A | 242 | ILE |
| 2 | A | 269 | ASP |
| 2 | A | 285 | THR |
| 2 | A | 301 | ASN |
| 2 | A | 313 | VAL |
| 2 | A | 331 | SER |
| 2 | A | 334 | THR |
| 1 | H | 27 | PRO |
| 1 | H | 84 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 105 | TYR |
| 2 | F | 4 | ILE |
| 2 | F | 27 | ILE |
| 2 | F | 28 | VAL |
| 2 | F | 33 | LYS |
| 2 | F | 56 | ILE |
| 2 | F | 137 | GLU |
| 2 | F | 148 | PHE |
| 2 | F | 172 | ASN |
| 2 | F | 234 | ARG |
| 2 | F | 244 | VAL |
| 2 | F | 269 | ASP |
| 2 | F | 285 | THR |
| 2 | F | 300 | VAL |
| 2 | F | 301 | ASN |
| 2 | F | 304 | ILE |
| 2 | F | 310 | LYS |
| 2 | B | 3 | LEU |
| 2 | B | 11 | LEU |
| 2 | B | 28 | VAL |
| 2 | B | 52 | HIS |
| 2 | B | 56 | ILE |
| 2 | B | 137 | GLU |
| 2 | B | 156 | ALA |
| 2 | B | 188 | ILE |
| 2 | B | 195 | ALA |
| 2 | B | 257 | LEU |
| 2 | B | 315 | PHE |
| 2 | B | 331 | SER |
| 2 | B | 333 | VAL |
| 2 | G | 4 | ILE |
| 2 | G | 8 | LEU |
| 2 | G | 56 | ILE |
| 2 | G | 137 | GLU |
| 2 | G | 155 | LYS |
| 2 | G | 172 | ASN |
| 2 | G | 308 | GLY |
| 2 | G | 326 | ILE |
| 2 | D | 4 | ILE |
| 2 | D | 8 | LEU |
| 2 | D | 28 | VAL |
| 2 | D | 52 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 56 | ILE |
| 2 | D | 82 | VAL |
| 2 | D | 133 | ASN |
| 2 | D | 137 | GLU |
| 2 | D | 163 | PHE |
| 2 | D | 214 | GLN |
| 2 | D | 215 | PHE |
| 2 | D | 216 | ARG |
| 2 | D | 234 | ARG |
| 2 | D | 250 | ASP |
| 2 | D | 302 | LEU |
| 1 | K | 22 | THR |
| 1 | K | 26 | TYR |
| 1 | K | 55 | SER |
| 1 | K | 83 | GLN |
| 1 | K | 86 | ASP |
| 2 | C | 20 | LYS |
| 2 | C | 28 | VAL |
| 2 | C | 32 | ALA |
| 2 | C | 37 | ILE |
| 2 | C | 56 | ILE |
| 2 | C | 137 | GLU |
| 2 | C | 171 | THR |
| 2 | C | 191 | GLU |
| 2 | C | 194 | VAL |
| 2 | C | 269 | ASP |
| 2 | C | 285 | THR |
| 2 | E | 28 | VAL |
| 2 | E | 32 | ALA |
| 2 | E | 52 | HIS |
| 2 | E | 56 | ILE |
| 2 | E | 83 | THR |
| 2 | E | 104 | ASN |
| 2 | E | 131 | TYR |
| 2 | E | 137 | GLU |
| 2 | E | 154 | SER |
| 2 | E | 163 | PHE |
| 2 | E | 215 | PHE |
| 2 | E | 275 | ASP |
| 2 | E | 327 | LEU |
| 1 | I | 26 | TYR |
| 1 | I | 84 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 105 | TYR |
| 1 | J | 27 | PRO |
| 1 | J | 46 | ALA |
| 1 | J | 84 | ILE |
| 1 | J | 97 | ALA |
| 1 | J | 103 | ALA |
| 1 | L | 12 | SER |
| 1 | L | 22 | THR |
| 1 | L | 84 | ILE |
| 1 | L | 99 | GLU |
| 1 | L | 104 | PHE |
| 1 | L | 105 | TYR |
| 1 | N | 4 | VAL |
| 1 | N | 32 | ILE |
| 1 | N | 84 | ILE |
| 1 | N | 85 | THR |
| 1 | N | 100 | LEU |
| 1 | M | 14 | VAL |
| 1 | M | 85 | THR |
| 2 | A | 2 | ALA |
| 2 | A | 27 | ILE |
| 2 | A | 159 | ALA |
| 2 | A | 234 | ARG |
| 2 | A | 303 | THR |
| 1 | H | 33 | THR |
| 1 | H | 55 | SER |
| 1 | H | 83 | GLN |
| 1 | H | 85 | THR |
| 2 | F | 24 | ILE |
| 2 | F | 32 | ALA |
| 2 | F | 132 | GLY |
| 2 | F | 163 | PHE |
| 2 | F | 197 | PHE |
| 2 | F | 231 | ARG |
| 2 | F | 303 | THR |
| 2 | F | 330 | GLU |
| 2 | B | 163 | PHE |
| 2 | B | 192 | GLY |
| 2 | B | 194 | VAL |
| 2 | B | 228 | LEU |
| 2 | B | 234 | ARG |
| 2 | B | 269 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 284 | LYS |
| 2 | B | 300 | VAL |
| 2 | B | 312 | ILE |
| 2 | G | 21 | ASN |
| 2 | G | 53 | LYS |
| 2 | G | 171 | THR |
| 2 | G | 188 | ILE |
| 2 | G | 200 | GLU |
| 2 | G | 241 | ASN |
| 2 | G | 297 | ALA |
| 2 | G | 332 | ALA |
| 2 | D | 32 | ALA |
| 2 | D | 104 | ASN |
| 2 | D | 143 | GLY |
| 2 | D | 159 | ALA |
| 2 | D | 194 | VAL |
| 2 | D | 204 | ASP |
| 2 | D | 259 | SER |
| 2 | D | 269 | ASP |
| 2 | D | 284 | LYS |
| 2 | D | 328 | ASN |
| 2 | D | 332 | ALA |
| 1 | K | 42 | LEU |
| 2 | C | 3 | LEU |
| 2 | C | 27 | ILE |
| 2 | C | 136 | ALA |
| 2 | C | 143 | GLY |
| 2 | C | 163 | PHE |
| 2 | C | 208 | SER |
| 2 | C | 211 | ASN |
| 2 | C | 251 | ALA |
| 2 | C | 304 | ILE |
| 2 | C | 310 | LYS |
| 2 | C | 326 | ILE |
| 2 | C | 332 | ALA |
| 2 | E | 17 | ARG |
| 2 | E | 27 | ILE |
| 2 | E | 33 | LYS |
| 2 | E | 77 | THR |
| 2 | E | 82 | VAL |
| 2 | E | 95 | VAL |
| 2 | E | 234 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 269 | ASP |
| 2 | E | 276 | GLY |
| 1 | I | 6 | MET |
| 1 | I | 18 | GLY |
| 1 | I | 23 | LYS |
| 1 | I | 32 | ILE |
| 1 | I | 83 | GLN |
| 1 | I | 85 | THR |
| 1 | J | 4 | VAL |
| 1 | J | 23 | LYS |
| 1 | J | 33 | THR |
| 1 | J | 55 | SER |
| 1 | J | 83 | GLN |
| 1 | J | 86 | ASP |
| 1 | J | 88 | GLY |
| 1 | J | 96 | ASP |
| 1 | L | 23 | LYS |
| 1 | L | 55 | SER |
| 1 | L | 85 | THR |
| 1 | N | 33 | THR |
| 1 | N | 107 | ASP |
| 1 | M | 33 | THR |
| 1 | M | 104 | PHE |
| 2 | A | 6 | GLN |
| 2 | A | 18 | THR |
| 2 | A | 82 | VAL |
| 2 | A | 105 | ASN |
| 2 | A | 163 | PHE |
| 2 | A | 173 | THR |
| 2 | A | 193 | MET |
| 2 | A | 214 | GLN |
| 1 | H | 4 | VAL |
| 1 | H | 77 | ASP |
| 2 | F | 45 | PRO |
| 2 | F | 52 | HIS |
| 2 | F | 54 | THR |
| 2 | F | 83 | THR |
| 2 | F | 155 | LYS |
| 2 | F | 193 | MET |
| 2 | F | 206 | LEU |
| 2 | F | 214 | GLN |
| 2 | B | 104 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 135 | ASP |
| 2 | B | 141 | PHE |
| 2 | B | 142 | MET |
| 2 | B | 301 | ASN |
| 2 | B | 304 | ILE |
| 2 | G | 52 | HIS |
| 2 | G | 83 | THR |
| 2 | G | 108 | ALA |
| 2 | G | 194 | VAL |
| 2 | G | 201 | ASP |
| 2 | G | 221 | GLU |
| 2 | G | 269 | ASP |
| 2 | G | 307 | TYR |
| 2 | D | 20 | LYS |
| 2 | D | 172 | ASN |
| 2 | D | 173 | THR |
| 2 | D | 193 | MET |
| 2 | D | 231 | ARG |
| 2 | D | 257 | LEU |
| 2 | D | 297 | ALA |
| 2 | D | 310 | LYS |
| 2 | D | 330 | GLU |
| 1 | K | 4 | VAL |
| 1 | K | 27 | PRO |
| 1 | K | 33 | THR |
| 1 | K | 73 | ASP |
| 1 | K | 97 | ALA |
| 2 | C | 38 | LEU |
| 2 | C | 49 | GLY |
| 2 | C | 104 | ASN |
| 2 | C | 257 | LEU |
| 2 | C | 274 | GLY |
| 2 | C | 302 | LEU |
| 2 | E | 3 | LEU |
| 2 | E | 69 | ASN |
| 2 | E | 141 | PHE |
| 2 | E | 326 | ILE |
| 1 | I | 27 | PRO |
| 1 | I | 99 | GLU |
| 1 | J | 12 | SER |
| 1 | J | 54 | ASP |
| 1 | J | 85 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 92 | GLN |
| 1 | L | 33 | THR |
| 1 | L | 100 | LEU |
| 1 | N | 46 | ALA |
| 1 | N | 58 | VAL |
| 1 | M | 20 | PRO |
| 1 | M | 41 | ARG |
| 1 | M | 46 | ALA |
| 1 | M | 95 | ASP |
| 1 | M | 106 | PRO |
| 2 | A | 33 | LYS |
| 2 | A | 68 | TYR |
| 1 | H | 32 | ILE |
| 2 | F | 46 | CYS |
| 2 | F | 47 | ASN |
| 2 | F | 159 | ALA |
| 2 | F | 170 | SER |
| 2 | B | 50 | SER |
| 2 | B | 53 | LYS |
| 2 | B | 82 | VAL |
| 2 | B | 134 | THR |
| 2 | B | 232 | ASP |
| 2 | G | 73 | GLN |
| 2 | G | 333 | VAL |
| 2 | D | 73 | GLN |
| 2 | D | 141 | PHE |
| 2 | D | 304 | ILE |
| 1 | K | 105 | TYR |
| 2 | C | 39 | THR |
| 2 | C | 68 | TYR |
| 2 | C | 73 | GLN |
| 2 | C | 105 | ASN |
| 2 | C | 231 | ARG |
| 2 | C | 287 | HIS |
| 2 | C | 301 | ASN |
| 2 | E | 8 | LEU |
| 2 | E | 24 | ILE |
| 2 | E | 73 | GLN |
| 2 | E | 155 | LYS |
| 2 | E | 274 | GLY |
| 2 | E | 304 | ILE |
| 2 | E | 331 | SER |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 73 | ASP |
| 1 | I | 77 | ASP |
| 1 | I | 86 | ASP |
| 1 | I | 107 | ASP |
| 1 | L | 44 | LEU |
| 1 | L | 47 | LYS |
| 1 | L | 73 | ASP |
| 1 | L | 83 | GLN |
| 1 | N | 73 | ASP |
| 1 | N | 102 | ASP |
| 1 | M | 4 | VAL |
| 1 | M | 40 | GLN |
| 1 | M | 77 | ASP |
| 2 | A | 138 | PRO |
| 1 | H | 73 | ASP |
| 1 | H | 97 | ALA |
| 2 | F | 82 | VAL |
| 2 | B | 39 | THR |
| 2 | B | 61 | PRO |
| 2 | B | 231 | ARG |
| 2 | B | 313 | VAL |
| 2 | G | 199 | HIS |
| 2 | G | 314 | SER |
| 2 | D | 39 | THR |
| 2 | D | 241 | ASN |
| 1 | K | 12 | SER |
| 1 | K | 84 | ILE |
| 1 | K | 102 | ASP |
| 2 | C | 70 | GLN |
| 2 | C | 154 | SER |
| 2 | C | 193 | MET |
| 2 | C | 204 | ASP |
| 2 | C | 234 | ARG |
| 2 | C | 272 | MET |
| 2 | E | 210 | GLY |
| 2 | E | 211 | ASN |
| 2 | E | 241 | ASN |
| 2 | E | 315 | PHE |
| 1 | I | 4 | VAL |
| 1 | I | 33 | THR |
| 1 | I | 54 | ASP |
| 1 | L | 26 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 27 | PRO |
| 1 | L | 54 | ASP |
| 1 | L | 77 | ASP |
| 1 | H | 17 | ASP |
| 1 | H | 26 | TYR |
| 2 | F | 53 | LYS |
| 2 | B | 27 | ILE |
| 2 | B | 159 | ALA |
| 2 | B | 214 | GLN |
| 1 | K | 77 | ASP |
| 2 | C | 11 | LEU |
| 2 | C | 41 | ALA |
| 2 | C | 299 | ASN |
| 1 | I | 40 | GLN |
| 1 | L | 4 | VAL |
| 1 | L | 14 | VAL |
| 1 | L | 86 | ASP |
| 1 | M | 32 | ILE |
| 1 | M | 80 | VAL |
| 1 | M | 105 | TYR |
| 2 | A | 72 | VAL |
| 2 | A | 304 | ILE |
| 2 | A | 318 | ILE |
| 2 | F | 194 | VAL |
| 1 | L | 32 | ILE |
| 1 | M | 26 | TYR |
| 2 | A | 73 | GLN |
| 2 | A | 192 | GLY |
| 1 | H | 58 | VAL |
| 2 | B | 143 | GLY |
| 2 | G | 82 | VAL |
| 2 | G | 207 | VAL |
| 1 | K | 58 | VAL |
| 1 | K | 80 | VAL |
| 2 | C | 8 | LEU |
| 1 | I | 15 | GLY |
| 1 | J | 26 | TYR |
| 1 | J | 32 | ILE |
| 1 | M | 64 | VAL |
| 2 | F | 162 | VAL |
| 2 | G | 143 | GLY |
| 2 | D | 27 | ILE |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 24 | ILE |
| 2 | E | 188 | ILE |
| 1 | J | 58 | VAL |
| 1 | J | 87 | ILE |
| 1 | L | 58 | VAL |
| 1 | N | 26 | TYR |
| 1 | M | 87 | ILE |
| 2 | A | 190 | PRO |
| 2 | F | 312 | ILE |
| 1 | K | 64 | VAL |
| 2 | C | 313 | VAL |
| 2 | E | 213 | GLY |
| 1 | M | 58 | VAL |
| 1 | I | 50 | PRO |
| 1 | J | 50 | 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 | H | 95/95 (100%) | 70 (74%) | 25 (26%) | 0 | 5 |
| 1 | I | 95/95 (100%) | 64 (67%) | 31 (33%) | 0 | 2 |
| 1 | J | 95/95 (100%) | 64 (67%) | 31 (33%) | 0 | 2 |
| 1 | K | 95/95 (100%) | 70 (74%) | 25 (26%) | 0 | 5 |
| 1 | L | 95/95 (100%) | 62 (65%) | 33 (35%) | 0 | 1 |
| 1 | M | 95/95 (100%) | 67 (70%) | 28 (30%) | 0 | 3 |
| 1 | N | 95/95 (100%) | 72 (76%) | 23 (24%) | 1 | 6 |
| 2 | A | 274/274 (100%) | 195 (71%) | 79 (29%) | 0 | 3 |
| 2 | B | 274/274 (100%) | 193 (70%) | 81 (30%) | 0 | 3 |
| 2 | C | 274/274 (100%) | 199 (73%) | 75 (27%) | 0 | 4 |
| 2 | D | 274/274 (100%) | 200 (73%) | 74 (27%) | 0 | 4 |
| 2 | E | 274/274 (100%) | 198 (72%) | 76 (28%) | 0 | 4 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|-------------|---|
| 2 | F | 274/274 (100%) | 205 (75%) | 69 (25%) | 0 | 6 |
| 2 | G | 274/274 (100%) | 209 (76%) | 65 (24%) | 1 | 6 |
| All | All | 2583/2583 (100%) | 1868 (72%) | 715 (28%) | 2 | 4 |

All (715) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 2 | LYS |
| 1 | N | 3 | THR |
| 1 | N | 6 | MET |
| 1 | N | 11 | ASP |
| 1 | N | 13 | PHE |
| 1 | N | 16 | GLU |
| 1 | N | 24 | ASP |
| 1 | N | 26 | TYR |
| 1 | N | 30 | LEU |
| 1 | N | 31 | ARG |
| 1 | N | 32 | ILE |
| 1 | N | 34 | LEU |
| 1 | N | 39 | LEU |
| 1 | N | 42 | LEU |
| 1 | N | 44 | LEU |
| 1 | N | 47 | LYS |
| 1 | N | 59 | MET |
| 1 | N | 70 | ARG |
| 1 | N | 81 | GLU |
| 1 | N | 93 | LYS |
| 1 | N | 94 | ARG |
| 1 | N | 101 | LYS |
| 1 | N | 104 | PHE |
| 1 | M | 2 | LYS |
| 1 | M | 6 | MET |
| 1 | M | 7 | LYS |
| 1 | M | 8 | THR |
| 1 | M | 11 | ASP |
| 1 | M | 22 | THR |
| 1 | M | 25 | GLN |
| 1 | M | 26 | TYR |
| 1 | M | 30 | LEU |
| 1 | M | 34 | LEU |
| 1 | M | 39 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 40 | GLN |
| 1 | M | 44 | LEU |
| 1 | M | 47 | LYS |
| 1 | M | 64 | VAL |
| 1 | M | 70 | ARG |
| 1 | M | 71 | THR |
| 1 | M | 72 | THR |
| 1 | M | 74 | HIS |
| 1 | M | 78 | ASN |
| 1 | M | 79 | TYR |
| 1 | M | 82 | LEU |
| 1 | M | 87 | ILE |
| 1 | M | 94 | ARG |
| 1 | M | 98 | LYS |
| 1 | M | 100 | LEU |
| 1 | M | 101 | LYS |
| 1 | M | 105 | TYR |
| 2 | A | 1 | MET |
| 2 | A | 6 | GLN |
| 2 | A | 8 | LEU |
| 2 | A | 11 | LEU |
| 2 | A | 15 | TYR |
| 2 | A | 20 | LYS |
| 2 | A | 24 | ILE |
| 2 | A | 37 | ILE |
| 2 | A | 42 | ILE |
| 2 | A | 44 | VAL |
| 2 | A | 48 | ASP |
| 2 | A | 51 | LYS |
| 2 | A | 52 | HIS |
| 2 | A | 55 | THR |
| 2 | A | 57 | ARG |
| 2 | A | 67 | ARG |
| 2 | A | 68 | TYR |
| 2 | A | 70 | GLN |
| 2 | A | 76 | LYS |
| 2 | A | 77 | THR |
| 2 | A | 78 | GLN |
| 2 | A | 82 | VAL |
| 2 | A | 83 | THR |
| 2 | A | 90 | TYR |
| 2 | A | 91 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 92 | LEU |
| 2 | A | 99 | LEU |
| 2 | A | 109 | PHE |
| 2 | A | 114 | ASN |
| 2 | A | 118 | LEU |
| 2 | A | 121 | PHE |
| 2 | A | 127 | ARG |
| 2 | A | 135 | ASP |
| 2 | A | 139 | GLU |
| 2 | A | 141 | PHE |
| 2 | A | 142 | MET |
| 2 | A | 147 | ARG |
| 2 | A | 168 | SER |
| 2 | A | 172 | ASN |
| 2 | A | 173 | THR |
| 2 | A | 178 | MET |
| 2 | A | 180 | TRP |
| 2 | A | 186 | HIS |
| 2 | A | 187 | MET |
| 2 | A | 189 | TYR |
| 2 | A | 191 | GLU |
| 2 | A | 197 | PHE |
| 2 | A | 202 | LEU |
| 2 | A | 205 | ASP |
| 2 | A | 219 | ARG |
| 2 | A | 220 | ASP |
| 2 | A | 222 | PHE |
| 2 | A | 223 | LYS |
| 2 | A | 228 | LEU |
| 2 | A | 232 | ASP |
| 2 | A | 238 | ARG |
| 2 | A | 239 | ILE |
| 2 | A | 242 | ILE |
| 2 | A | 256 | ASP |
| 2 | A | 257 | LEU |
| 2 | A | 266 | TYR |
| 2 | A | 268 | ARG |
| 2 | A | 277 | LYS |
| 2 | A | 285 | THR |
| 2 | A | 292 | LYS |
| 2 | A | 295 | MET |
| 2 | A | 296 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 298 | LYS |
| 2 | A | 299 | ASN |
| 2 | A | 306 | GLU |
| 2 | A | 307 | TYR |
| 2 | A | 310 | LYS |
| 2 | A | 316 | LEU |
| 2 | A | 320 | ILE |
| 2 | A | 321 | ARG |
| 2 | A | 326 | ILE |
| 2 | A | 328 | ASN |
| 2 | A | 329 | THR |
| 2 | A | 333 | VAL |
| 1 | H | 6 | MET |
| 1 | H | 11 | ASP |
| 1 | H | 13 | PHE |
| 1 | H | 21 | GLU |
| 1 | H | 26 | TYR |
| 1 | H | 30 | LEU |
| 1 | H | 32 | ILE |
| 1 | H | 34 | LEU |
| 1 | H | 39 | LEU |
| 1 | H | 40 | GLN |
| 1 | H | 42 | LEU |
| 1 | H | 44 | LEU |
| 1 | H | 47 | LYS |
| 1 | H | 54 | ASP |
| 1 | H | 65 | CYS |
| 1 | H | 70 | ARG |
| 1 | H | 72 | THR |
| 1 | H | 74 | HIS |
| 1 | H | 82 | LEU |
| 1 | H | 93 | LYS |
| 1 | H | 94 | ARG |
| 1 | H | 98 | LYS |
| 1 | H | 104 | PHE |
| 1 | H | 107 | ASP |
| 1 | H | 109 | GLU |
| 2 | F | 15 | TYR |
| 2 | F | 17 | ARG |
| 2 | F | 18 | THR |
| 2 | F | 20 | LYS |
| 2 | F | 26 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 29 | GLU |
| 2 | F | 33 | LYS |
| 2 | F | 34 | THR |
| 2 | F | 35 | ASN |
| 2 | F | 36 | ASP |
| 2 | F | 42 | ILE |
| 2 | F | 44 | VAL |
| 2 | F | 51 | LYS |
| 2 | F | 62 | GLU |
| 2 | F | 64 | VAL |
| 2 | F | 76 | LYS |
| 2 | F | 89 | LEU |
| 2 | F | 90 | TYR |
| 2 | F | 91 | ASP |
| 2 | F | 92 | LEU |
| 2 | F | 99 | LEU |
| 2 | F | 104 | ASN |
| 2 | F | 109 | PHE |
| 2 | F | 113 | GLU |
| 2 | F | 117 | LYS |
| 2 | F | 118 | LEU |
| 2 | F | 121 | PHE |
| 2 | F | 125 | VAL |
| 2 | F | 127 | ARG |
| 2 | F | 128 | TYR |
| 2 | F | 134 | THR |
| 2 | F | 139 | GLU |
| 2 | F | 141 | PHE |
| 2 | F | 147 | ARG |
| 2 | F | 153 | THR |
| 2 | F | 160 | GLU |
| 2 | F | 163 | PHE |
| 2 | F | 168 | SER |
| 2 | F | 172 | ASN |
| 2 | F | 173 | THR |
| 2 | F | 175 | ILE |
| 2 | F | 177 | PHE |
| 2 | F | 178 | MET |
| 2 | F | 180 | TRP |
| 2 | F | 183 | ASN |
| 2 | F | 202 | LEU |
| 2 | F | 209 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 214 | GLN |
| 2 | F | 219 | ARG |
| 2 | F | 222 | PHE |
| 2 | F | 232 | ASP |
| 2 | F | 233 | TRP |
| 2 | F | 238 | ARG |
| 2 | F | 247 | LEU |
| 2 | F | 256 | ASP |
| 2 | F | 263 | ASP |
| 2 | F | 266 | TYR |
| 2 | F | 268 | ARG |
| 2 | F | 277 | LYS |
| 2 | F | 278 | GLU |
| 2 | F | 280 | ILE |
| 2 | F | 289 | TRP |
| 2 | F | 290 | LEU |
| 2 | F | 310 | LYS |
| 2 | F | 312 | ILE |
| 2 | F | 314 | SER |
| 2 | F | 316 | LEU |
| 2 | F | 323 | VAL |
| 2 | F | 329 | THR |
| 2 | B | 3 | LEU |
| 2 | B | 4 | ILE |
| 2 | B | 15 | TYR |
| 2 | B | 18 | THR |
| 2 | B | 20 | LYS |
| 2 | B | 34 | THR |
| 2 | B | 44 | VAL |
| 2 | B | 54 | THR |
| 2 | B | 65 | TRP |
| 2 | B | 66 | ARG |
| 2 | B | 67 | ARG |
| 2 | B | 72 | VAL |
| 2 | B | 76 | LYS |
| 2 | B | 78 | GLN |
| 2 | B | 82 | VAL |
| 2 | B | 83 | THR |
| 2 | B | 89 | LEU |
| 2 | B | 90 | TYR |
| 2 | B | 96 | ASP |
| 2 | B | 105 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 110 | ARG |
| 2 | B | 122 | ASN |
| 2 | B | 125 | VAL |
| 2 | B | 133 | ASN |
| 2 | B | 135 | ASP |
| 2 | B | 139 | GLU |
| 2 | B | 147 | ARG |
| 2 | B | 148 | PHE |
| 2 | B | 153 | THR |
| 2 | B | 155 | LYS |
| 2 | B | 160 | GLU |
| 2 | B | 161 | ASN |
| 2 | B | 162 | VAL |
| 2 | B | 171 | THR |
| 2 | B | 173 | THR |
| 2 | B | 175 | ILE |
| 2 | B | 178 | MET |
| 2 | B | 180 | TRP |
| 2 | B | 182 | GLU |
| 2 | B | 183 | ASN |
| 2 | B | 186 | HIS |
| 2 | B | 188 | ILE |
| 2 | B | 191 | GLU |
| 2 | B | 194 | VAL |
| 2 | B | 197 | PHE |
| 2 | B | 202 | LEU |
| 2 | B | 204 | ASP |
| 2 | B | 206 | LEU |
| 2 | B | 209 | ASP |
| 2 | B | 214 | GLN |
| 2 | B | 216 | ARG |
| 2 | B | 218 | TYR |
| 2 | B | 222 | PHE |
| 2 | B | 228 | LEU |
| 2 | B | 230 | VAL |
| 2 | B | 232 | ASP |
| 2 | B | 238 | ARG |
| 2 | B | 240 | CYS |
| 2 | B | 242 | ILE |
| 2 | B | 257 | LEU |
| 2 | B | 263 | ASP |
| 2 | B | 266 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 269 | ASP |
| 2 | B | 277 | LYS |
| 2 | B | 280 | ILE |
| 2 | B | 283 | ASN |
| 2 | B | 285 | THR |
| 2 | B | 292 | LYS |
| 2 | B | 293 | GLN |
| 2 | B | 296 | ASN |
| 2 | B | 298 | LYS |
| 2 | B | 306 | GLU |
| 2 | B | 310 | LYS |
| 2 | B | 312 | ILE |
| 2 | B | 315 | PHE |
| 2 | B | 316 | LEU |
| 2 | B | 320 | ILE |
| 2 | B | 321 | ARG |
| 2 | B | 322 | ARG |
| 2 | B | 326 | ILE |
| 2 | B | 334 | THR |
| 2 | G | 8 | LEU |
| 2 | G | 10 | SER |
| 2 | G | 11 | LEU |
| 2 | G | 14 | ILE |
| 2 | G | 18 | THR |
| 2 | G | 26 | ARG |
| 2 | G | 28 | VAL |
| 2 | G | 31 | LEU |
| 2 | G | 33 | LYS |
| 2 | G | 36 | ASP |
| 2 | G | 37 | ILE |
| 2 | G | 42 | ILE |
| 2 | G | 48 | ASP |
| 2 | G | 51 | LYS |
| 2 | G | 54 | THR |
| 2 | G | 76 | LYS |
| 2 | G | 79 | THR |
| 2 | G | 83 | THR |
| 2 | G | 90 | TYR |
| 2 | G | 92 | LEU |
| 2 | G | 99 | LEU |
| 2 | G | 101 | ASP |
| 2 | G | 121 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G | 127 | ARG |
| 2 | G | 128 | TYR |
| 2 | G | 134 | THR |
| 2 | G | 135 | ASP |
| 2 | G | 139 | GLU |
| 2 | G | 141 | PHE |
| 2 | G | 148 | PHE |
| 2 | G | 158 | SER |
| 2 | G | 160 | GLU |
| 2 | G | 163 | PHE |
| 2 | G | 170 | SER |
| 2 | G | 171 | THR |
| 2 | G | 173 | THR |
| 2 | G | 175 | ILE |
| 2 | G | 177 | PHE |
| 2 | G | 188 | ILE |
| 2 | G | 189 | TYR |
| 2 | G | 191 | GLU |
| 2 | G | 197 | PHE |
| 2 | G | 200 | GLU |
| 2 | G | 202 | LEU |
| 2 | G | 204 | ASP |
| 2 | G | 211 | ASN |
| 2 | G | 215 | PHE |
| 2 | G | 218 | TYR |
| 2 | G | 225 | ASP |
| 2 | G | 228 | LEU |
| 2 | G | 233 | TRP |
| 2 | G | 237 | SER |
| 2 | G | 239 | ILE |
| 2 | G | 242 | ILE |
| 2 | G | 247 | LEU |
| 2 | G | 250 | ASP |
| 2 | G | 278 | GLU |
| 2 | G | 285 | THR |
| 2 | G | 287 | HIS |
| 2 | G | 292 | LYS |
| 2 | G | 298 | LYS |
| 2 | G | 302 | LEU |
| 2 | G | 310 | LYS |
| 2 | G | 311 | LYS |
| 2 | G | 329 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 1 | MET |
| 2 | D | 3 | LEU |
| 2 | D | 8 | LEU |
| 2 | D | 11 | LEU |
| 2 | D | 12 | LEU |
| 2 | D | 15 | TYR |
| 2 | D | 18 | THR |
| 2 | D | 27 | ILE |
| 2 | D | 37 | ILE |
| 2 | D | 44 | VAL |
| 2 | D | 46 | CYS |
| 2 | D | 48 | ASP |
| 2 | D | 56 | ILE |
| 2 | D | 57 | ARG |
| 2 | D | 66 | ARG |
| 2 | D | 69 | ASN |
| 2 | D | 76 | LYS |
| 2 | D | 83 | THR |
| 2 | D | 89 | LEU |
| 2 | D | 95 | VAL |
| 2 | D | 102 | ARG |
| 2 | D | 109 | PHE |
| 2 | D | 112 | SER |
| 2 | D | 117 | LYS |
| 2 | D | 118 | LEU |
| 2 | D | 121 | PHE |
| 2 | D | 125 | VAL |
| 2 | D | 134 | THR |
| 2 | D | 135 | ASP |
| 2 | D | 148 | PHE |
| 2 | D | 150 | THR |
| 2 | D | 152 | SER |
| 2 | D | 168 | SER |
| 2 | D | 173 | THR |
| 2 | D | 180 | TRP |
| 2 | D | 186 | HIS |
| 2 | D | 187 | MET |
| 2 | D | 189 | TYR |
| 2 | D | 191 | GLU |
| 2 | D | 193 | MET |
| 2 | D | 197 | PHE |
| 2 | D | 202 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 205 | ASP |
| 2 | D | 206 | LEU |
| 2 | D | 215 | PHE |
| 2 | D | 223 | LYS |
| 2 | D | 224 | TRP |
| 2 | D | 225 | ASP |
| 2 | D | 228 | LEU |
| 2 | D | 238 | ARG |
| 2 | D | 239 | ILE |
| 2 | D | 241 | ASN |
| 2 | D | 246 | THR |
| 2 | D | 247 | LEU |
| 2 | D | 256 | ASP |
| 2 | D | 257 | LEU |
| 2 | D | 262 | VAL |
| 2 | D | 266 | TYR |
| 2 | D | 268 | ARG |
| 2 | D | 270 | VAL |
| 2 | D | 273 | LEU |
| 2 | D | 285 | THR |
| 2 | D | 290 | LEU |
| 2 | D | 292 | LYS |
| 2 | D | 296 | ASN |
| 2 | D | 306 | GLU |
| 2 | D | 307 | TYR |
| 2 | D | 310 | LYS |
| 2 | D | 311 | LYS |
| 2 | D | 318 | ILE |
| 2 | D | 320 | ILE |
| 2 | D | 327 | LEU |
| 2 | D | 331 | SER |
| 2 | D | 333 | VAL |
| 1 | K | 1 | MET |
| 1 | K | 3 | THR |
| 1 | K | 8 | THR |
| 1 | K | 21 | GLU |
| 1 | K | 23 | LYS |
| 1 | K | 25 | GLN |
| 1 | K | 26 | TYR |
| 1 | K | 30 | LEU |
| 1 | K | 31 | ARG |
| 1 | K | 32 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 39 | LEU |
| 1 | K | 41 | ARG |
| 1 | K | 44 | LEU |
| 1 | K | 47 | LYS |
| 1 | K | 59 | MET |
| 1 | K | 65 | CYS |
| 1 | K | 70 | ARG |
| 1 | K | 72 | THR |
| 1 | K | 82 | LEU |
| 1 | K | 85 | THR |
| 1 | K | 86 | ASP |
| 1 | K | 98 | LYS |
| 1 | K | 101 | LYS |
| 1 | K | 105 | TYR |
| 1 | K | 109 | GLU |
| 2 | C | 1 | MET |
| 2 | C | 3 | LEU |
| 2 | C | 8 | LEU |
| 2 | C | 11 | LEU |
| 2 | C | 15 | TYR |
| 2 | C | 20 | LYS |
| 2 | C | 26 | ARG |
| 2 | C | 27 | ILE |
| 2 | C | 30 | GLN |
| 2 | C | 36 | ASP |
| 2 | C | 42 | ILE |
| 2 | C | 44 | VAL |
| 2 | C | 46 | CYS |
| 2 | C | 48 | ASP |
| 2 | C | 54 | THR |
| 2 | C | 56 | ILE |
| 2 | C | 66 | ARG |
| 2 | C | 67 | ARG |
| 2 | C | 76 | LYS |
| 2 | C | 89 | LEU |
| 2 | C | 90 | TYR |
| 2 | C | 92 | LEU |
| 2 | C | 97 | LYS |
| 2 | C | 118 | LEU |
| 2 | C | 122 | ASN |
| 2 | C | 125 | VAL |
| 2 | C | 128 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 134 | THR |
| 2 | C | 142 | MET |
| 2 | C | 148 | PHE |
| 2 | C | 153 | THR |
| 2 | C | 155 | LYS |
| 2 | C | 172 | ASN |
| 2 | C | 173 | THR |
| 2 | C | 175 | ILE |
| 2 | C | 178 | MET |
| 2 | C | 180 | TRP |
| 2 | C | 186 | HIS |
| 2 | C | 189 | TYR |
| 2 | C | 191 | GLU |
| 2 | C | 193 | MET |
| 2 | C | 197 | PHE |
| 2 | C | 202 | LEU |
| 2 | C | 205 | ASP |
| 2 | C | 214 | GLN |
| 2 | C | 216 | ARG |
| 2 | C | 218 | TYR |
| 2 | C | 219 | ARG |
| 2 | C | 220 | ASP |
| 2 | C | 221 | GLU |
| 2 | C | 222 | PHE |
| 2 | C | 223 | LYS |
| 2 | C | 228 | LEU |
| 2 | C | 239 | ILE |
| 2 | C | 242 | ILE |
| 2 | C | 243 | ASP |
| 2 | C | 246 | THR |
| 2 | C | 250 | ASP |
| 2 | C | 268 | ARG |
| 2 | C | 270 | VAL |
| 2 | C | 277 | LYS |
| 2 | C | 280 | ILE |
| 2 | C | 283 | ASN |
| 2 | C | 286 | ILE |
| 2 | C | 290 | LEU |
| 2 | C | 293 | GLN |
| 2 | C | 298 | LYS |
| 2 | C | 300 | VAL |
| 2 | C | 306 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 310 | LYS |
| 2 | C | 316 | LEU |
| 2 | C | 321 | ARG |
| 2 | C | 322 | ARG |
| 2 | C | 326 | ILE |
| 2 | C | 329 | THR |
| 2 | E | 6 | GLN |
| 2 | E | 14 | ILE |
| 2 | E | 15 | TYR |
| 2 | E | 20 | LYS |
| 2 | E | 29 | GLU |
| 2 | E | 33 | LYS |
| 2 | E | 42 | ILE |
| 2 | E | 44 | VAL |
| 2 | E | 48 | ASP |
| 2 | E | 52 | HIS |
| 2 | E | 57 | ARG |
| 2 | E | 66 | ARG |
| 2 | E | 67 | ARG |
| 2 | E | 79 | THR |
| 2 | E | 89 | LEU |
| 2 | E | 90 | TYR |
| 2 | E | 95 | VAL |
| 2 | E | 101 | ASP |
| 2 | E | 102 | ARG |
| 2 | E | 113 | GLU |
| 2 | E | 118 | LEU |
| 2 | E | 121 | PHE |
| 2 | E | 124 | LYS |
| 2 | E | 127 | ARG |
| 2 | E | 128 | TYR |
| 2 | E | 134 | THR |
| 2 | E | 135 | ASP |
| 2 | E | 139 | GLU |
| 2 | E | 141 | PHE |
| 2 | E | 147 | ARG |
| 2 | E | 150 | THR |
| 2 | E | 151 | LEU |
| 2 | E | 162 | VAL |
| 2 | E | 171 | THR |
| 2 | E | 175 | ILE |
| 2 | E | 176 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 179 | SER |
| 2 | E | 182 | GLU |
| 2 | E | 186 | HIS |
| 2 | E | 187 | MET |
| 2 | E | 188 | ILE |
| 2 | E | 189 | TYR |
| 2 | E | 194 | VAL |
| 2 | E | 197 | PHE |
| 2 | E | 198 | GLN |
| 2 | E | 204 | ASP |
| 2 | E | 207 | VAL |
| 2 | E | 215 | PHE |
| 2 | E | 216 | ARG |
| 2 | E | 218 | TYR |
| 2 | E | 219 | ARG |
| 2 | E | 222 | PHE |
| 2 | E | 225 | ASP |
| 2 | E | 228 | LEU |
| 2 | E | 236 | ILE |
| 2 | E | 238 | ARG |
| 2 | E | 241 | ASN |
| 2 | E | 242 | ILE |
| 2 | E | 250 | ASP |
| 2 | E | 260 | MET |
| 2 | E | 270 | VAL |
| 2 | E | 273 | LEU |
| 2 | E | 277 | LYS |
| 2 | E | 280 | ILE |
| 2 | E | 284 | LYS |
| 2 | E | 285 | THR |
| 2 | E | 293 | GLN |
| 2 | E | 296 | ASN |
| 2 | E | 298 | LYS |
| 2 | E | 303 | THR |
| 2 | E | 306 | GLU |
| 2 | E | 307 | TYR |
| 2 | E | 316 | LEU |
| 2 | E | 320 | ILE |
| 2 | E | 322 | ARG |
| 2 | E | 329 | THR |
| 1 | I | 2 | LYS |
| 1 | I | 5 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 8 | THR |
| 1 | I | 13 | PHE |
| 1 | I | 17 | ASP |
| 1 | I | 24 | ASP |
| 1 | I | 25 | GLN |
| 1 | I | 26 | TYR |
| 1 | I | 30 | LEU |
| 1 | I | 32 | ILE |
| 1 | I | 37 | GLU |
| 1 | I | 40 | GLN |
| 1 | I | 41 | ARG |
| 1 | I | 44 | LEU |
| 1 | I | 47 | LYS |
| 1 | I | 54 | ASP |
| 1 | I | 59 | MET |
| 1 | I | 61 | MET |
| 1 | I | 65 | CYS |
| 1 | I | 70 | ARG |
| 1 | I | 72 | THR |
| 1 | I | 73 | ASP |
| 1 | I | 81 | GLU |
| 1 | I | 82 | LEU |
| 1 | I | 93 | LYS |
| 1 | I | 94 | ARG |
| 1 | I | 98 | LYS |
| 1 | I | 99 | GLU |
| 1 | I | 100 | LEU |
| 1 | I | 105 | TYR |
| 1 | I | 110 | ASP |
| 1 | J | 1 | MET |
| 1 | J | 5 | ASN |
| 1 | J | 6 | MET |
| 1 | J | 8 | THR |
| 1 | J | 11 | ASP |
| 1 | J | 13 | PHE |
| 1 | J | 19 | LYS |
| 1 | J | 24 | ASP |
| 1 | J | 25 | GLN |
| 1 | J | 26 | TYR |
| 1 | J | 31 | ARG |
| 1 | J | 32 | ILE |
| 1 | J | 34 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 40 | GLN |
| 1 | J | 41 | ARG |
| 1 | J | 42 | LEU |
| 1 | J | 44 | LEU |
| 1 | J | 49 | LEU |
| 1 | J | 58 | VAL |
| 1 | J | 61 | MET |
| 1 | J | 65 | CYS |
| 1 | J | 70 | ARG |
| 1 | J | 74 | HIS |
| 1 | J | 82 | LEU |
| 1 | J | 93 | LYS |
| 1 | J | 96 | ASP |
| 1 | J | 99 | GLU |
| 1 | J | 100 | LEU |
| 1 | J | 104 | PHE |
| 1 | J | 105 | TYR |
| 1 | J | 110 | ASP |
| 1 | L | 2 | LYS |
| 1 | L | 5 | ASN |
| 1 | L | 6 | MET |
| 1 | L | 11 | ASP |
| 1 | L | 14 | VAL |
| 1 | L | 26 | TYR |
| 1 | L | 30 | LEU |
| 1 | L | 31 | ARG |
| 1 | L | 32 | ILE |
| 1 | L | 37 | GLU |
| 1 | L | 39 | LEU |
| 1 | L | 41 | ARG |
| 1 | L | 42 | LEU |
| 1 | L | 47 | LYS |
| 1 | L | 57 | SER |
| 1 | L | 58 | VAL |
| 1 | L | 59 | MET |
| 1 | L | 61 | MET |
| 1 | L | 65 | CYS |
| 1 | L | 70 | ARG |
| 1 | L | 71 | THR |
| 1 | L | 76 | GLU |
| 1 | L | 78 | ASN |
| 1 | L | 80 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 82 | LEU |
| 1 | L | 87 | ILE |
| 1 | L | 89 | LEU |
| 1 | L | 93 | LYS |
| 1 | L | 98 | LYS |
| 1 | L | 99 | GLU |
| 1 | L | 104 | PHE |
| 1 | L | 105 | TYR |
| 1 | L | 109 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 70 | GLN |
| 2 | A | 105 | ASN |
| 2 | A | 114 | ASN |
| 2 | A | 119 | GLN |
| 1 | H | 40 | GLN |
| 1 | H | 45 | ASN |
| 1 | H | 78 | ASN |
| 2 | F | 47 | ASN |
| 2 | F | 69 | ASN |
| 2 | F | 122 | ASN |
| 2 | F | 172 | ASN |
| 2 | F | 214 | GLN |
| 2 | B | 293 | GLN |
| 2 | B | 301 | ASN |
| 2 | B | 328 | ASN |
| 2 | G | 293 | GLN |
| 2 | D | 69 | ASN |
| 2 | D | 122 | ASN |
| 1 | K | 5 | ASN |
| 2 | C | 123 | ASN |
| 2 | C | 199 | HIS |
| 2 | C | 214 | GLN |
| 2 | E | 16 | ASN |
| 2 | E | 241 | ASN |
| 1 | I | 25 | GLN |
| 1 | I | 40 | GLN |
| 1 | J | 78 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.