



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:35 AM GMT

PDB ID : 1V7N
Title : Human Thrombopoietin Functional Domain Complexed To Neutralizing Antibody TN1 Fab
Authors : Feese, M.D.; Tamada, T.; Kato, Y.; Maeda, Y.; Hirose, M.; Matsukura, Y.; Shigematsu, H.; Kato, T.; Miyazaki, H.; Kuroki, R.
Deposited on : 2003-12-18
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

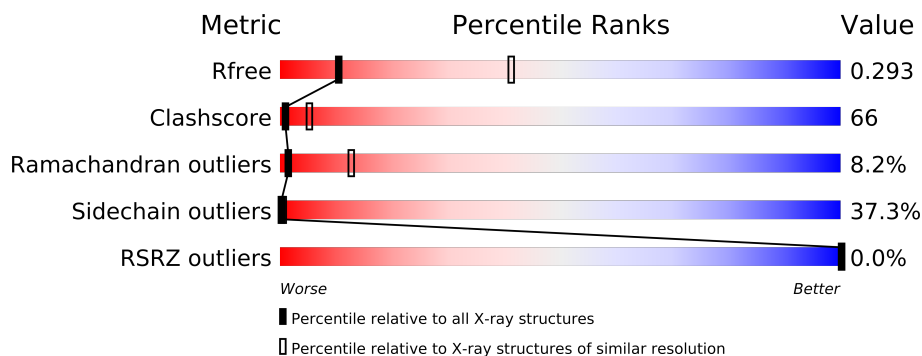
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1341 (3.40-3.20) |
| Clashscore | 79885 | 1696 (3.40-3.20) |
| Ramachandran outliers | 78287 | 1664 (3.40-3.20) |
| Sidechain outliers | 78261 | 1662 (3.40-3.20) |
| RSRZ outliers | 66119 | 1342 (3.40-3.20) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | L | 213 | |
| 1 | M | 213 | |
| 1 | N | 213 | |
| 1 | O | 213 | |
| 2 | H | 217 | |
| 2 | I | 217 | |
| 2 | J | 217 | |
| 2 | K | 217 | |
| 3 | V | 163 | |
| 3 | X | 163 | |
| 3 | Y | 163 | |
| 3 | Z | 163 | |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17466 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Monoclonal TN1 Fab Light Chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | L | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1638 | 1018 | 278 | 333 | 9 | | | |
| 1 | M | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1632 | 1015 | 277 | 332 | 8 | | | |
| 1 | N | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1632 | 1015 | 277 | 332 | 8 | | | |
| 1 | O | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1638 | 1018 | 278 | 333 | 9 | | | |

- Molecule 2 is a protein called Monoclonal TN1 Fab Heavy Chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | H | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1630 | 1030 | 271 | 321 | 8 | | | |
| 2 | I | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1630 | 1030 | 271 | 321 | 8 | | | |
| 2 | J | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1630 | 1030 | 271 | 321 | 8 | | | |
| 2 | K | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1630 | 1030 | 271 | 321 | 8 | | | |

- Molecule 3 is a protein called Thrombopoietin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | V | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1090 | 694 | 194 | 195 | 7 | | | |
| 3 | X | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1049 | 671 | 187 | 186 | 5 | | | |
| 3 | Y | 139 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1053 | 673 | 188 | 187 | 5 | | | |
| 3 | Z | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 669 | 187 | 184 | 5 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| V | 115 | ARG | GLN | ENGINEERED | UNP P40225 |
| X | 115 | ARG | GLN | ENGINEERED | UNP P40225 |
| Y | 115 | ARG | GLN | ENGINEERED | UNP P40225 |
| Z | 115 | ARG | GLN | ENGINEERED | UNP P40225 |

- Molecule 4 is water.

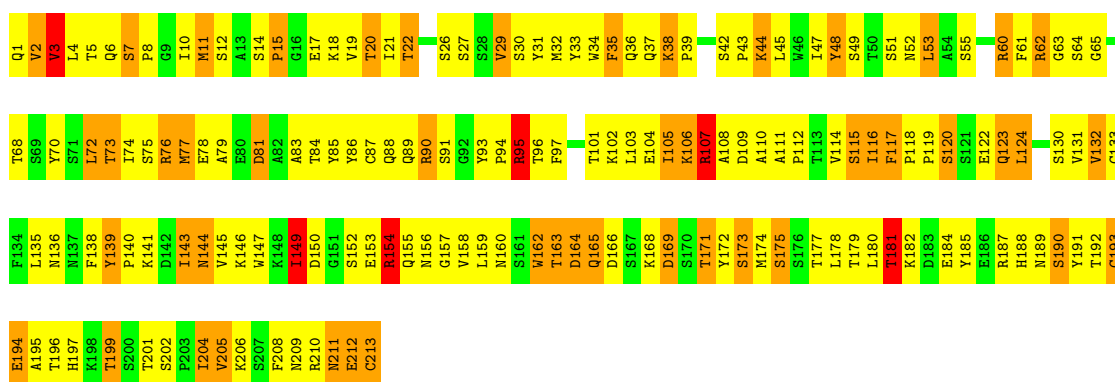
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4 | H | 17 | Total O 17 17 | 0 | 0 |
| 4 | I | 27 | Total O 27 27 | 0 | 0 |
| 4 | J | 13 | Total O 13 13 | 0 | 0 |
| 4 | K | 10 | Total O 10 10 | 0 | 0 |
| 4 | L | 20 | Total O 20 20 | 0 | 0 |
| 4 | M | 18 | Total O 18 18 | 0 | 0 |
| 4 | N | 19 | Total O 19 19 | 0 | 0 |
| 4 | O | 20 | Total O 20 20 | 0 | 0 |
| 4 | V | 7 | Total O 7 7 | 0 | 0 |
| 4 | X | 11 | Total O 11 11 | 0 | 0 |
| 4 | Y | 3 | Total O 3 3 | 0 | 0 |
| 4 | Z | 4 | Total O 4 4 | 0 | 0 |

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

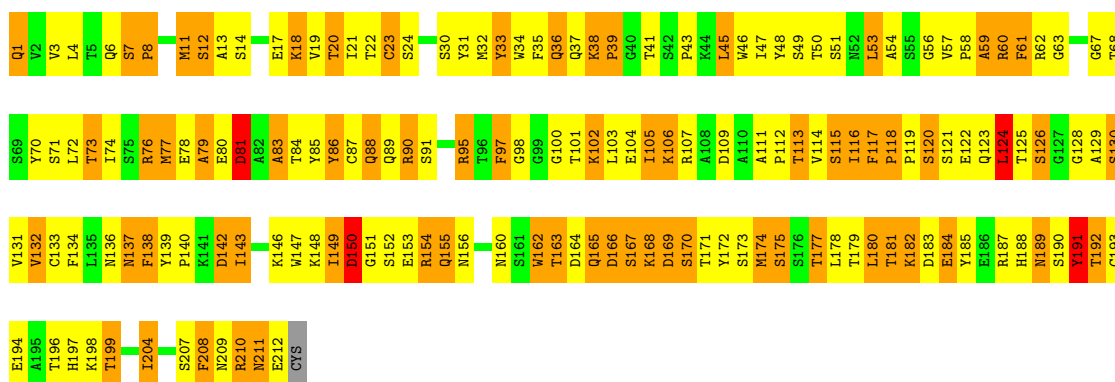
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain L:



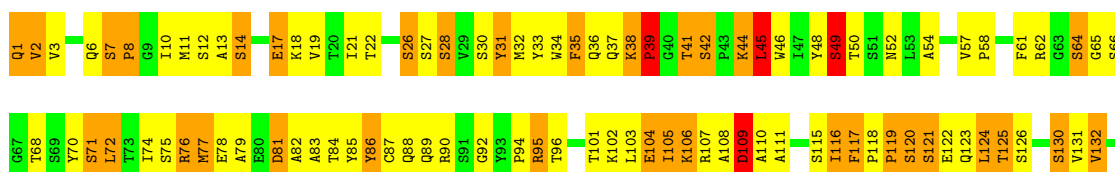
• Molecule 1: Monoclonal TN1 Fab Light Chain

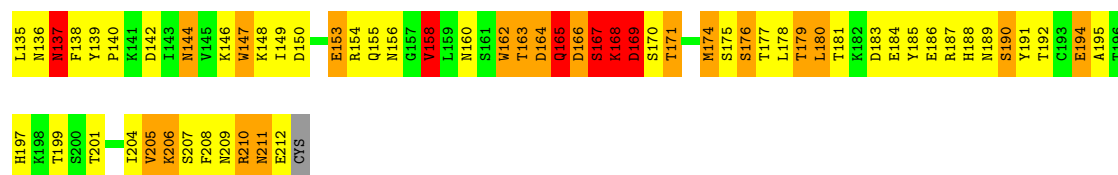
Chain M:



• Molecule 1: Monoclonal TN1 Fab Light Chain

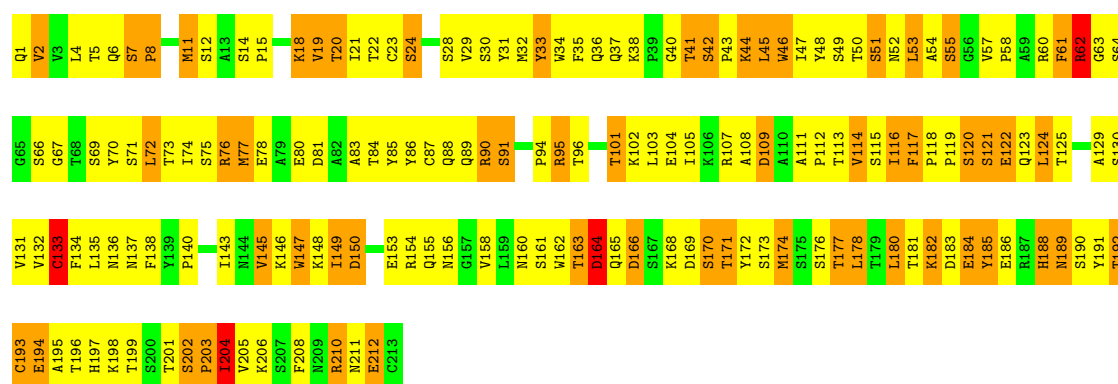
Chain N:





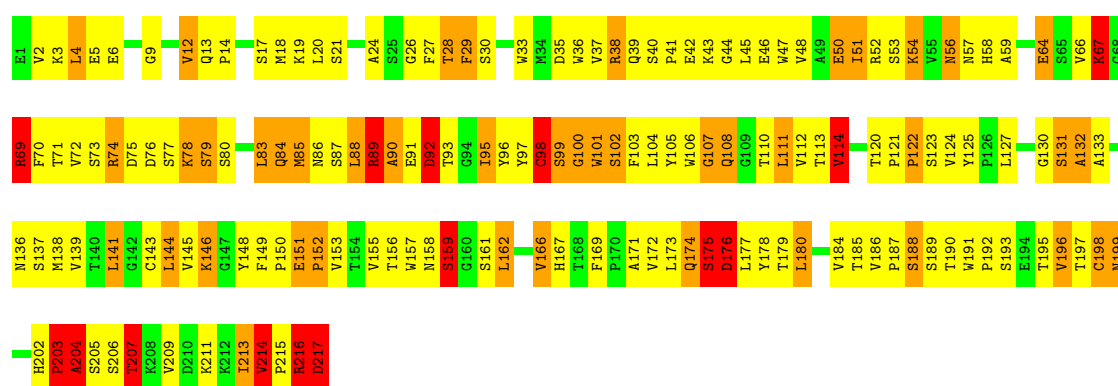
• Molecule 1: Monoclonal TN1 Fab Light Chain

Chain O:



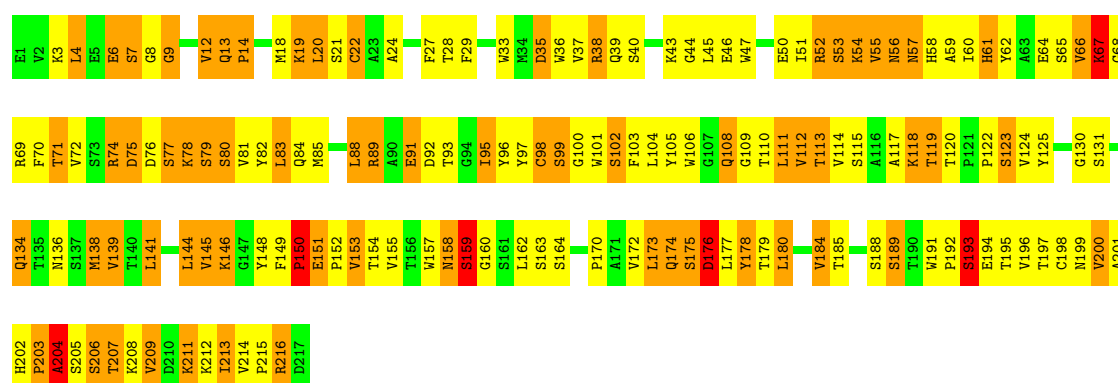
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain H:



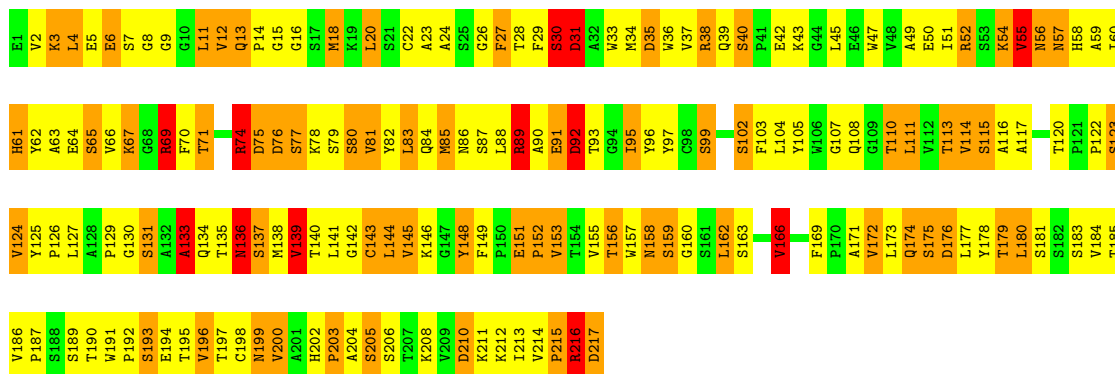
• Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain I:



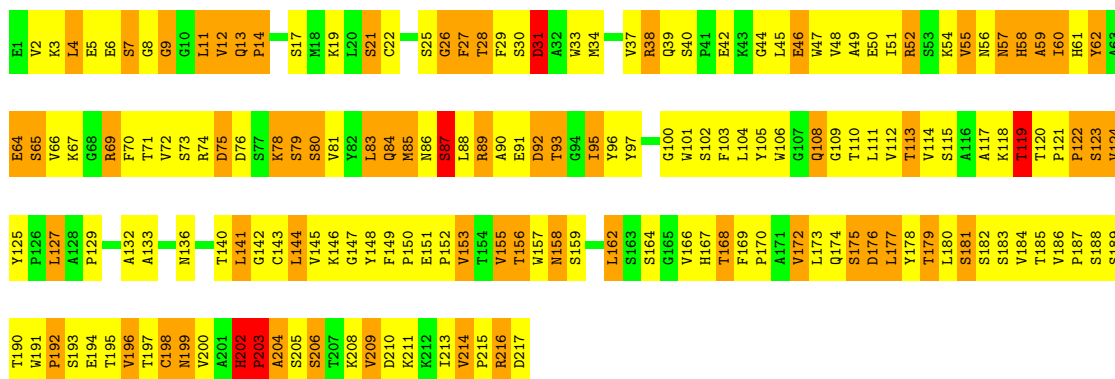
- Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain J:



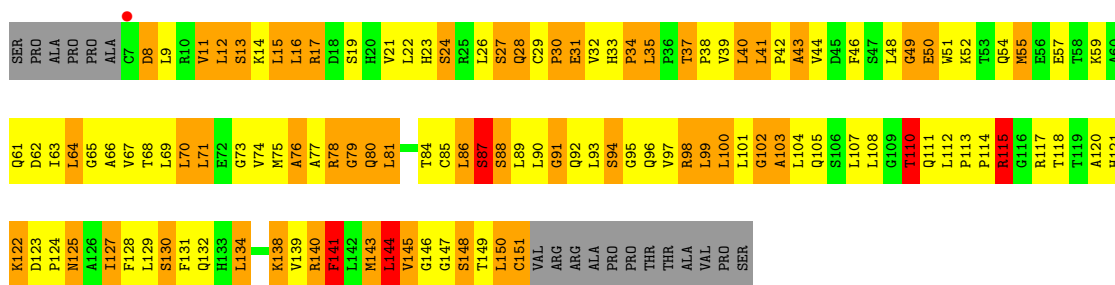
- Molecule 2: Monoclonal TN1 Fab Heavy Chain

Chain K:



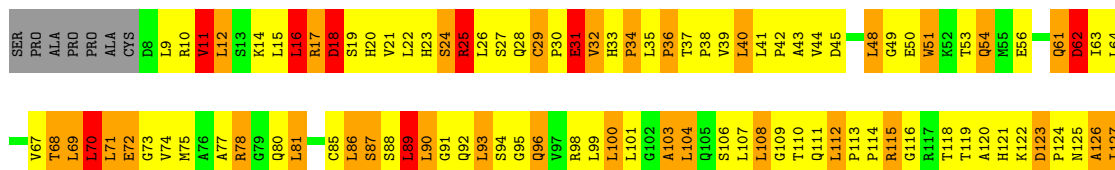
- Molecule 3: Thrombopoietin

Chain V:



- Molecule 3: Thrombopoietin

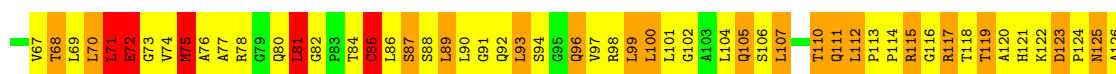
Chain X:





• Molecule 3: Thrombopoietin

Chain Y:



• Molecule 3: Thrombopoietin

Chain Z:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 133.04Å 46.58Å 191.36Å 90.00° 90.28° 90.00° | Depositor |
| Resolution (Å) | 57.63 – 3.30 57.63 – 3.30 | Depositor EDS |
| % Data completeness (in resolution range) | 98.5 (57.63-3.30) 98.4 (57.63-3.30) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.10 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.57 (at 3.33Å) | Xtriage |
| Refinement program | REFMAC 5.1.19 | Depositor |
| R, R_{free} | 0.167 , 0.305 0.163 , 0.293 | Depositor DCC |
| R_{free} test set | 1801 reflections (5.29%) | DCC |
| Wilson B-factor (Å ²) | 43.0 | Xtriage |
| Anisotropy | 0.719 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 34.0 | EDS |
| Estimated twinning fraction | 0.055 for h,-k,-l | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$ | Xtriage |
| Outliers | 0 of 35816 reflections | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 17466 | wwPDB-VP |
| Average B, all atoms (Å ²) | 29.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | L | 1.31 | 7/1676 (0.4%) | 1.35 | 11/2274 (0.5%) |
| 1 | M | 1.33 | 3/1670 (0.2%) | 1.42 | 13/2266 (0.6%) |
| 1 | N | 1.28 | 3/1670 (0.2%) | 1.39 | 12/2266 (0.5%) |
| 1 | O | 1.26 | 4/1676 (0.2%) | 1.39 | 11/2274 (0.5%) |
| 2 | H | 1.37 | 10/1674 (0.6%) | 1.40 | 17/2289 (0.7%) |
| 2 | I | 1.23 | 3/1674 (0.2%) | 1.39 | 9/2289 (0.4%) |
| 2 | J | 1.25 | 1/1674 (0.1%) | 1.45 | 20/2289 (0.9%) |
| 2 | K | 1.21 | 2/1674 (0.1%) | 1.40 | 14/2289 (0.6%) |
| 3 | V | 1.23 | 3/1109 (0.3%) | 1.38 | 5/1506 (0.3%) |
| 3 | X | 1.14 | 1/1068 (0.1%) | 1.37 | 13/1451 (0.9%) |
| 3 | Y | 1.24 | 2/1072 (0.2%) | 1.48 | 15/1456 (1.0%) |
| 3 | Z | 1.13 | 2/1064 (0.2%) | 1.26 | 6/1445 (0.4%) |
| All | All | 1.26 | 41/17701 (0.2%) | 1.39 | 146/24094 (0.6%) |

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 | M | 0 | 2 |
| 1 | N | 0 | 2 |
| 2 | H | 0 | 2 |
| 2 | I | 0 | 5 |
| 2 | J | 0 | 3 |
| 2 | K | 0 | 2 |
| 3 | X | 0 | 1 |
| 3 | Y | 0 | 1 |
| 3 | Z | 0 | 2 |
| All | All | 0 | 20 |

All (41) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | L | 139 | TYR | CB-CG | -11.08 | 1.35 | 1.51 |
| 2 | H | 151 | GLU | CD-OE2 | 8.63 | 1.35 | 1.25 |
| 1 | L | 48 | TYR | CD2-CE2 | -7.57 | 1.27 | 1.39 |
| 2 | J | 143 | CYS | CB-SG | -7.46 | 1.69 | 1.82 |
| 2 | H | 98 | CYS | CB-SG | -7.02 | 1.70 | 1.82 |
| 1 | M | 59 | ALA | CA-CB | -6.58 | 1.38 | 1.52 |
| 1 | L | 139 | TYR | CD2-CE2 | -6.48 | 1.29 | 1.39 |
| 1 | L | 139 | TYR | CD1-CE1 | -6.15 | 1.30 | 1.39 |
| 2 | H | 97 | TYR | CD1-CE1 | -6.08 | 1.30 | 1.39 |
| 3 | Y | 75 | MET | SD-CE | 5.87 | 2.10 | 1.77 |
| 1 | O | 62 | ARG | CB-CG | -5.87 | 1.36 | 1.52 |
| 2 | K | 62 | TYR | CE1-CZ | -5.85 | 1.30 | 1.38 |
| 2 | I | 209 | VAL | CA-CB | 5.82 | 1.67 | 1.54 |
| 1 | O | 34 | TRP | CB-CG | -5.68 | 1.40 | 1.50 |
| 1 | N | 46 | TRP | CB-CG | -5.64 | 1.40 | 1.50 |
| 2 | H | 97 | TYR | CD2-CE2 | -5.63 | 1.30 | 1.39 |
| 2 | K | 168 | THR | CA-CB | -5.57 | 1.38 | 1.53 |
| 3 | Z | 45 | ASP | CB-CG | 5.55 | 1.63 | 1.51 |
| 2 | H | 143 | CYS | CB-SG | -5.55 | 1.72 | 1.81 |
| 1 | L | 62 | ARG | CG-CD | 5.53 | 1.65 | 1.51 |
| 1 | N | 147 | TRP | CB-CG | -5.49 | 1.40 | 1.50 |
| 1 | O | 11 | MET | SD-CE | 5.48 | 2.08 | 1.77 |
| 1 | L | 162 | TRP | CB-CG | -5.47 | 1.40 | 1.50 |
| 1 | M | 86 | TYR | CE1-CZ | -5.45 | 1.31 | 1.38 |
| 3 | V | 21 | VAL | CA-CB | -5.43 | 1.43 | 1.54 |
| 2 | H | 5 | GLU | CD-OE1 | 5.43 | 1.31 | 1.25 |
| 2 | H | 5 | GLU | CG-CD | 5.36 | 1.59 | 1.51 |
| 2 | H | 214 | VAL | CA-CB | -5.25 | 1.43 | 1.54 |
| 3 | X | 128 | PHE | CE2-CZ | 5.23 | 1.47 | 1.37 |
| 2 | H | 151 | GLU | CD-OE1 | 5.22 | 1.31 | 1.25 |
| 1 | N | 31 | TYR | CD2-CE2 | -5.21 | 1.31 | 1.39 |
| 3 | V | 110 | THR | CA-CB | -5.20 | 1.39 | 1.53 |
| 2 | H | 97 | TYR | CB-CG | -5.14 | 1.44 | 1.51 |
| 2 | I | 108 | GLN | CG-CD | 5.14 | 1.62 | 1.51 |
| 3 | Y | 72 | GLU | CD-OE1 | 5.14 | 1.31 | 1.25 |
| 3 | V | 141 | PHE | CB-CG | 5.13 | 1.60 | 1.51 |
| 1 | M | 184 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 2 | I | 54 | LYS | CD-CE | 5.07 | 1.64 | 1.51 |
| 1 | O | 147 | TRP | CB-CG | -5.04 | 1.41 | 1.50 |
| 1 | L | 48 | TYR | CD1-CE1 | -5.03 | 1.31 | 1.39 |
| 3 | Z | 136 | ARG | CG-CD | 5.02 | 1.64 | 1.51 |

All (146) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | O | 53 | LEU | CA-CB-CG | -11.11 | 89.75 | 115.30 |
| 1 | M | 169 | ASP | CB-CG-OD2 | 10.62 | 127.85 | 118.30 |
| 3 | X | 140 | ARG | NE-CZ-NH1 | 10.01 | 125.30 | 120.30 |
| 1 | N | 109 | ASP | CB-CG-OD2 | 9.86 | 127.17 | 118.30 |
| 1 | N | 81 | ASP | CB-CG-OD2 | 9.80 | 127.12 | 118.30 |
| 3 | X | 45 | ASP | CB-CG-OD2 | 9.74 | 127.07 | 118.30 |
| 2 | H | 144 | LEU | CA-CB-CG | -9.38 | 93.72 | 115.30 |
| 2 | I | 83 | LEU | CA-CB-CG | -9.36 | 93.77 | 115.30 |
| 1 | N | 8 | PRO | N-CD-CG | -8.67 | 90.19 | 103.20 |
| 2 | H | 143 | CYS | CA-CB-SG | -8.58 | 98.55 | 114.00 |
| 1 | M | 81 | ASP | CB-CG-OD1 | -8.52 | 110.63 | 118.30 |
| 3 | Y | 136 | ARG | NE-CZ-NH1 | 8.50 | 124.55 | 120.30 |
| 2 | H | 176 | ASP | CB-CG-OD2 | 8.46 | 125.92 | 118.30 |
| 2 | I | 203 | PRO | N-CD-CG | -8.40 | 90.59 | 103.20 |
| 2 | H | 216 | ARG | NE-CZ-NH1 | 8.25 | 124.43 | 120.30 |
| 2 | K | 175 | SER | N-CA-CB | -8.22 | 98.17 | 110.50 |
| 3 | V | 64 | LEU | CB-CG-CD2 | -8.15 | 97.15 | 111.00 |
| 1 | N | 166 | ASP | CB-CG-OD2 | 8.07 | 125.56 | 118.30 |
| 1 | M | 142 | ASP | CB-CG-OD2 | 8.06 | 125.56 | 118.30 |
| 3 | Y | 71 | LEU | CA-CB-CG | -8.06 | 96.76 | 115.30 |
| 2 | J | 89 | ARG | NE-CZ-NH2 | -8.02 | 116.29 | 120.30 |
| 3 | Y | 71 | LEU | CB-CG-CD1 | -7.99 | 97.42 | 111.00 |
| 1 | L | 95 | ARG | NE-CZ-NH1 | -7.94 | 116.33 | 120.30 |
| 1 | M | 60 | ARG | NE-CZ-NH1 | -7.91 | 116.35 | 120.30 |
| 2 | K | 203 | PRO | N-CD-CG | -7.84 | 91.44 | 103.20 |
| 1 | L | 205 | VAL | CB-CA-C | -7.76 | 96.66 | 111.40 |
| 1 | N | 142 | ASP | CB-CG-OD2 | 7.75 | 125.27 | 118.30 |
| 2 | I | 176 | ASP | CB-CG-OD2 | 7.64 | 125.17 | 118.30 |
| 2 | J | 76 | ASP | CB-CG-OD2 | 7.61 | 125.15 | 118.30 |
| 1 | N | 109 | ASP | CB-CG-OD1 | -7.47 | 111.57 | 118.30 |
| 3 | V | 114 | PRO | N-CD-CG | -7.45 | 92.03 | 103.20 |
| 1 | M | 81 | ASP | CB-CG-OD2 | 7.40 | 124.96 | 118.30 |
| 1 | O | 164 | ASP | CB-CG-OD2 | 7.36 | 124.92 | 118.30 |
| 2 | H | 162 | LEU | CB-CG-CD1 | -7.34 | 98.51 | 111.00 |
| 1 | L | 81 | ASP | CB-CG-OD2 | 7.23 | 124.81 | 118.30 |
| 3 | Y | 136 | ARG | NE-CZ-NH2 | -7.12 | 116.74 | 120.30 |
| 1 | O | 109 | ASP | CB-CG-OD2 | 7.03 | 124.63 | 118.30 |
| 2 | J | 31 | ASP | CB-CG-OD2 | 6.96 | 124.56 | 118.30 |
| 3 | X | 108 | LEU | CA-CB-CG | -6.95 | 99.32 | 115.30 |
| 3 | Y | 30 | PRO | N-CD-CG | -6.90 | 92.85 | 103.20 |
| 2 | K | 202 | HIS | N-CA-C | -6.88 | 92.41 | 111.00 |
| 2 | K | 192 | PRO | N-CD-CG | -6.86 | 92.91 | 103.20 |
| 1 | L | 95 | ARG | NE-CZ-NH2 | 6.85 | 123.73 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | N | 150 | ASP | CB-CG-OD2 | 6.85 | 124.46 | 118.30 |
| 2 | J | 145 | VAL | N-CA-C | -6.80 | 92.62 | 111.00 |
| 2 | I | 35 | ASP | CB-CG-OD2 | 6.75 | 124.37 | 118.30 |
| 3 | X | 104 | LEU | CB-CG-CD2 | -6.75 | 99.53 | 111.00 |
| 3 | Y | 18 | ASP | CB-CG-OD2 | 6.73 | 124.36 | 118.30 |
| 2 | K | 76 | ASP | CB-CG-OD2 | 6.66 | 124.30 | 118.30 |
| 2 | J | 176 | ASP | CB-CG-OD2 | 6.60 | 124.24 | 118.30 |
| 2 | H | 122 | PRO | N-CD-CG | -6.49 | 93.47 | 103.20 |
| 3 | X | 29 | CYS | CA-CB-SG | 6.45 | 125.61 | 114.00 |
| 1 | M | 150 | ASP | CB-CG-OD2 | 6.39 | 124.05 | 118.30 |
| 1 | O | 183 | ASP | CB-CG-OD2 | 6.37 | 124.03 | 118.30 |
| 2 | H | 204 | ALA | N-CA-C | -6.34 | 93.88 | 111.00 |
| 3 | Z | 123 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 1 | L | 154 | ARG | NE-CZ-NH2 | -6.22 | 117.19 | 120.30 |
| 1 | M | 183 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 1 | O | 150 | ASP | CB-CG-OD2 | 6.19 | 123.87 | 118.30 |
| 2 | K | 31 | ASP | CB-CG-OD2 | 6.13 | 123.81 | 118.30 |
| 1 | O | 72 | LEU | CB-CG-CD1 | -6.10 | 100.62 | 111.00 |
| 2 | H | 203 | PRO | C-N-CA | 6.10 | 136.94 | 121.70 |
| 2 | H | 76 | ASP | CB-CG-OD2 | 6.06 | 123.75 | 118.30 |
| 2 | J | 139 | VAL | CB-CA-C | -6.04 | 99.92 | 111.40 |
| 3 | X | 123 | ASP | CB-CG-OD2 | 6.03 | 123.73 | 118.30 |
| 3 | Y | 75 | MET | CG-SD-CE | 5.98 | 109.76 | 100.20 |
| 3 | X | 48 | LEU | CA-CB-CG | 5.96 | 129.02 | 115.30 |
| 2 | J | 74 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 2 | J | 216 | ARG | N-CA-C | 5.91 | 126.95 | 111.00 |
| 2 | J | 143 | CYS | CA-CB-SG | -5.88 | 103.41 | 114.00 |
| 2 | H | 92 | ASP | CB-CG-OD1 | 5.86 | 123.57 | 118.30 |
| 2 | J | 69 | ARG | NE-CZ-NH1 | -5.81 | 117.40 | 120.30 |
| 1 | N | 119 | PRO | N-CD-CG | -5.80 | 94.50 | 103.20 |
| 3 | Z | 104 | LEU | CB-CG-CD1 | -5.80 | 101.14 | 111.00 |
| 3 | Y | 127 | ILE | CG1-CB-CG2 | -5.75 | 98.75 | 111.40 |
| 2 | K | 92 | ASP | CB-CG-OD2 | 5.72 | 123.45 | 118.30 |
| 3 | X | 135 | LEU | CA-CB-CG | -5.71 | 102.16 | 115.30 |
| 3 | X | 18 | ASP | CB-CG-OD2 | 5.69 | 123.42 | 118.30 |
| 2 | K | 52 | ARG | NE-CZ-NH2 | 5.66 | 123.13 | 120.30 |
| 3 | Z | 45 | ASP | CB-CG-OD2 | 5.65 | 123.38 | 118.30 |
| 2 | J | 166 | VAL | CB-CA-C | 5.64 | 122.12 | 111.40 |
| 3 | V | 134 | LEU | CB-CG-CD1 | -5.64 | 101.42 | 111.00 |
| 1 | L | 139 | TYR | CB-CG-CD2 | -5.62 | 117.63 | 121.00 |
| 1 | M | 191 | TYR | N-CA-C | -5.61 | 95.85 | 111.00 |
| 3 | X | 70 | LEU | CA-CB-CG | 5.60 | 128.18 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | J | 180 | LEU | CB-CG-CD1 | -5.60 | 101.48 | 111.00 |
| 2 | I | 151 | GLU | CA-CB-CG | -5.60 | 101.09 | 113.40 |
| 2 | J | 91 | GLU | N-CA-C | -5.58 | 95.94 | 111.00 |
| 2 | I | 44 | GLY | N-CA-C | -5.53 | 99.27 | 113.10 |
| 2 | J | 89 | ARG | NE-CZ-NH1 | 5.53 | 123.06 | 120.30 |
| 1 | M | 118 | PRO | N-CD-CG | -5.51 | 94.94 | 103.20 |
| 1 | N | 158 | VAL | CB-CA-C | -5.50 | 100.94 | 111.40 |
| 2 | J | 205 | SER | N-CA-C | 5.47 | 125.77 | 111.00 |
| 2 | J | 92 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 3 | X | 140 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 2 | H | 67 | LYS | CD-CE-NZ | 5.45 | 124.23 | 111.70 |
| 3 | X | 16 | LEU | CA-CB-CG | -5.44 | 102.79 | 115.30 |
| 1 | N | 169 | ASP | CB-CG-OD2 | 5.43 | 123.18 | 118.30 |
| 2 | K | 141 | LEU | CA-CB-CG | -5.42 | 102.84 | 115.30 |
| 2 | I | 54 | LYS | CD-CE-NZ | 5.41 | 124.15 | 111.70 |
| 3 | V | 144 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 3 | Z | 70 | LEU | CB-CG-CD2 | 5.40 | 120.17 | 111.00 |
| 1 | L | 144 | ASN | N-CA-C | 5.40 | 125.57 | 111.00 |
| 3 | Y | 81 | LEU | CB-CG-CD2 | -5.38 | 101.86 | 111.00 |
| 2 | K | 203 | PRO | N-CA-C | 5.32 | 125.93 | 112.10 |
| 2 | I | 89 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 3 | Y | 123 | ASP | CB-CG-OD2 | 5.32 | 123.08 | 118.30 |
| 1 | N | 45 | LEU | CB-CG-CD1 | -5.31 | 101.98 | 111.00 |
| 3 | V | 115 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 1 | L | 53 | LEU | CA-CB-CG | -5.30 | 103.11 | 115.30 |
| 2 | K | 143 | CYS | CA-CB-SG | -5.29 | 104.48 | 114.00 |
| 2 | J | 210 | ASP | CB-CG-OD2 | 5.27 | 123.05 | 118.30 |
| 1 | O | 8 | PRO | N-CD-CG | -5.27 | 95.30 | 103.20 |
| 2 | K | 168 | THR | CA-CB-CG2 | -5.26 | 105.03 | 112.40 |
| 2 | H | 114 | VAL | CB-CA-C | -5.26 | 101.40 | 111.40 |
| 1 | N | 144 | ASN | N-CA-C | 5.26 | 125.20 | 111.00 |
| 3 | Y | 99 | LEU | CA-CB-CG | 5.26 | 127.40 | 115.30 |
| 2 | J | 145 | VAL | CB-CA-C | 5.26 | 121.39 | 111.40 |
| 2 | J | 110 | THR | N-CA-CB | 5.25 | 120.28 | 110.30 |
| 3 | Y | 107 | LEU | CA-CB-CG | 5.25 | 127.37 | 115.30 |
| 3 | Z | 99 | LEU | CB-CG-CD2 | 5.25 | 119.92 | 111.00 |
| 2 | H | 89 | ARG | CG-CD-NE | 5.24 | 122.81 | 111.80 |
| 3 | Z | 135 | LEU | CA-CB-CG | -5.24 | 103.25 | 115.30 |
| 1 | O | 185 | TYR | N-CA-C | -5.20 | 96.97 | 111.00 |
| 1 | O | 53 | LEU | CB-CG-CD1 | 5.19 | 119.83 | 111.00 |
| 3 | Y | 25 | ARG | NE-CZ-NH2 | 5.18 | 122.89 | 120.30 |
| 1 | L | 3 | VAL | CB-CA-C | 5.18 | 121.24 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3 | X | 89 | LEU | CB-CG-CD2 | -5.17 | 102.21 | 111.00 |
| 1 | M | 53 | LEU | CA-CB-CG | -5.17 | 103.41 | 115.30 |
| 3 | Y | 54 | GLN | N-CA-C | -5.15 | 97.10 | 111.00 |
| 2 | H | 216 | ARG | NE-CZ-NH2 | -5.14 | 117.73 | 120.30 |
| 2 | I | 20 | LEU | CB-CG-CD1 | 5.11 | 119.69 | 111.00 |
| 2 | J | 18 | MET | CG-SD-CE | -5.10 | 92.03 | 100.20 |
| 2 | K | 11 | LEU | CA-CB-CG | 5.10 | 127.04 | 115.30 |
| 2 | H | 69 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 2 | K | 127 | LEU | CB-CG-CD2 | -5.08 | 102.37 | 111.00 |
| 2 | H | 100 | GLY | N-CA-C | 5.06 | 125.75 | 113.10 |
| 1 | M | 124 | LEU | CB-CG-CD2 | 5.06 | 119.60 | 111.00 |
| 2 | H | 217 | ASP | CB-CG-OD2 | 5.05 | 122.85 | 118.30 |
| 3 | Y | 136 | ARG | CB-CA-C | -5.04 | 100.33 | 110.40 |
| 1 | L | 181 | THR | OG1-CB-CG2 | -5.04 | 98.42 | 110.00 |
| 1 | M | 102 | LYS | N-CA-C | -5.02 | 97.45 | 111.00 |
| 1 | L | 164 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 1 | M | 204 | ILE | N-CA-C | -5.01 | 97.46 | 111.00 |
| 1 | O | 101 | THR | OG1-CB-CG2 | -5.01 | 98.47 | 110.00 |
| 1 | O | 133 | CYS | CA-CB-SG | -5.01 | 104.97 | 114.00 |

There are no chirality outliers.

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | H | 27 | PHE | Peptide |
| 2 | H | 99 | SER | Peptide |
| 2 | I | 138 | MET | Peptide |
| 2 | I | 175 | SER | Peptide |
| 2 | I | 203 | PRO | Peptide |
| 2 | I | 204 | ALA | Peptide |
| 2 | I | 7 | SER | Peptide |
| 2 | J | 115 | SER | Peptide |
| 2 | J | 133 | ALA | Peptide |
| 2 | J | 203 | PRO | Peptide |
| 2 | K | 109 | GLY | Peptide |
| 2 | K | 202 | HIS | Peptide |
| 1 | M | 61 | PHE | Peptide |
| 1 | M | 83 | ALA | Peptide |
| 1 | N | 168 | LYS | Peptide |
| 1 | N | 92 | GLY | Peptide |
| 3 | X | 49 | GLY | Peptide |
| 3 | Y | 53 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 3 | Z | 137 | GLY | Peptide |
| 3 | Z | 49 | GLY | Peptide |

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | L | 1638 | 0 | 1573 | 218 | 1 |
| 1 | M | 1632 | 0 | 1568 | 247 | 0 |
| 1 | N | 1632 | 0 | 1568 | 213 | 0 |
| 1 | O | 1638 | 0 | 1573 | 216 | 0 |
| 2 | H | 1630 | 0 | 1568 | 220 | 0 |
| 2 | I | 1630 | 0 | 1568 | 194 | 0 |
| 2 | J | 1630 | 0 | 1568 | 231 | 0 |
| 2 | K | 1630 | 0 | 1568 | 240 | 0 |
| 3 | V | 1090 | 0 | 1135 | 153 | 0 |
| 3 | X | 1049 | 0 | 1098 | 157 | 0 |
| 3 | Y | 1053 | 0 | 1101 | 160 | 0 |
| 3 | Z | 1045 | 0 | 1097 | 143 | 0 |
| 4 | H | 17 | 0 | 0 | 9 | 0 |
| 4 | I | 27 | 0 | 0 | 4 | 0 |
| 4 | J | 13 | 0 | 0 | 2 | 0 |
| 4 | K | 10 | 0 | 0 | 5 | 0 |
| 4 | L | 20 | 0 | 0 | 3 | 0 |
| 4 | M | 18 | 0 | 0 | 5 | 0 |
| 4 | N | 19 | 0 | 0 | 2 | 0 |
| 4 | O | 20 | 0 | 0 | 5 | 0 |
| 4 | V | 7 | 0 | 0 | 0 | 1 |
| 4 | X | 11 | 0 | 0 | 5 | 0 |
| 4 | Y | 3 | 0 | 0 | 0 | 0 |
| 4 | Z | 4 | 0 | 0 | 0 | 0 |
| All | All | 17466 | 0 | 16985 | 2256 | 1 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 66.

All (2256) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:N:11:MET:SD | 1:N:11:MET:CE | 2.03 | 1.46 |
| 1:L:11:MET:CE | 1:L:11:MET:SD | 2.04 | 1.45 |
| 2:J:85:MET:CE | 2:J:96:TYR:HE1 | 1.26 | 1.45 |
| 2:J:148:TYR:CE1 | 2:J:178:TYR:HB3 | 1.50 | 1.45 |
| 3:Z:55:MET:SD | 3:Z:55:MET:CE | 2.04 | 1.44 |
| 1:O:11:MET:SD | 1:O:11:MET:CE | 2.08 | 1.41 |
| 3:Y:75:MET:SD | 3:Y:75:MET:CE | 2.10 | 1.39 |
| 2:J:85:MET:CE | 2:J:96:TYR:CE1 | 2.09 | 1.36 |
| 1:O:150:ASP:OD2 | 1:O:188:HIS:HB3 | 1.33 | 1.28 |
| 2:J:85:MET:HE1 | 2:J:96:TYR:CE1 | 1.63 | 1.27 |
| 3:Z:14:LYS:O | 3:Z:18:ASP:HB2 | 1.26 | 1.27 |
| 3:Z:63:ILE:O | 3:Z:67:VAL:HG23 | 1.39 | 1.21 |
| 1:L:29:VAL:CG1 | 1:L:91:SER:HB2 | 1.71 | 1.20 |
| 1:O:90:ARG:NH2 | 2:K:102:SER:O | 1.74 | 1.19 |
| 1:N:167:SER:HB2 | 1:N:168:LYS:NZ | 1.56 | 1.18 |
| 2:J:122:PRO:HB3 | 2:J:148:TYR:HB3 | 1.22 | 1.17 |
| 2:J:148:TYR:CE1 | 2:J:178:TYR:CB | 2.27 | 1.16 |
| 1:L:185:TYR:CE1 | 1:L:191:TYR:HE1 | 1.63 | 1.16 |
| 1:L:197:HIS:ND1 | 1:L:199:THR:HB | 1.60 | 1.16 |
| 2:K:84:GLN:HA | 2:K:84:GLN:HE21 | 1.07 | 1.16 |
| 1:M:197:HIS:ND1 | 1:M:199:THR:HB | 1.61 | 1.15 |
| 2:J:85:MET:HE3 | 2:J:96:TYR:CE1 | 1.81 | 1.14 |
| 3:Z:56:GLU:OE2 | 3:Z:56:GLU:HA | 1.46 | 1.14 |
| 1:N:76:ARG:HG2 | 1:N:76:ARG:HH11 | 0.99 | 1.14 |
| 3:X:64:LEU:O | 3:X:68:THR:HG23 | 1.45 | 1.13 |
| 2:J:20:LEU:HD11 | 2:J:96:TYR:HD1 | 1.10 | 1.13 |
| 2:H:189:SER:CB | 4:H:224:HOH:O | 1.95 | 1.13 |
| 3:X:12:LEU:HB3 | 3:X:143:MET:HE1 | 1.20 | 1.12 |
| 2:K:89:ARG:HH11 | 2:K:89:ARG:HG3 | 1.06 | 1.12 |
| 1:M:150:ASP:OD2 | 1:M:188:HIS:HB3 | 1.50 | 1.11 |
| 2:K:38:ARG:HA | 2:K:95:ILE:O | 1.48 | 1.09 |
| 2:K:29:PHE:HB2 | 2:K:79:SER:HB3 | 1.33 | 1.09 |
| 1:L:110:ALA:O | 1:L:138:PHE:HA | 1.53 | 1.09 |
| 1:M:149:ILE:HD11 | 1:M:154:ARG:HD2 | 1.33 | 1.08 |
| 1:N:72:LEU:HD23 | 1:N:72:LEU:O | 1.53 | 1.08 |
| 3:X:51:TRP:CZ2 | 3:X:138:LYS:HE2 | 1.88 | 1.08 |
| 1:L:29:VAL:HG11 | 1:L:91:SER:HB2 | 1.32 | 1.07 |
| 3:X:41:LEU:CD1 | 3:X:127:ILE:HG22 | 1.84 | 1.07 |
| 2:J:95:ILE:HG23 | 2:J:111:LEU:HD23 | 1.35 | 1.07 |
| 1:O:32:MET:HB2 | 1:O:70:TYR:HD2 | 1.03 | 1.07 |
| 2:H:78:LYS:HB2 | 2:H:78:LYS:NZ | 1.65 | 1.07 |
| 3:X:17:ARG:HG3 | 3:X:17:ARG:HH11 | 1.18 | 1.07 |
| 2:H:189:SER:CA | 4:H:224:HOH:O | 2.00 | 1.06 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:29:PHE:HE1 | 2:J:34:MET:HE3 | 1.20 | 1.06 |
| 2:J:148:TYR:CE2 | 2:J:153:VAL:HB | 1.88 | 1.06 |
| 3:X:41:LEU:HD11 | 3:X:127:ILE:CG2 | 1.84 | 1.06 |
| 3:Y:10:ARG:HA | 3:Y:13:SER:OG | 1.56 | 1.06 |
| 1:N:119:PRO:HD3 | 1:N:131:VAL:HG23 | 1.37 | 1.05 |
| 2:J:130:GLY:O | 2:J:133:ALA:N | 1.89 | 1.05 |
| 1:M:6:GLN:HG2 | 1:M:23:CYS:HB2 | 1.30 | 1.05 |
| 2:K:70:PHE:CD1 | 2:K:85:MET:HB3 | 1.92 | 1.05 |
| 2:K:54:LYS:HE2 | 2:K:58:HIS:HE1 | 1.21 | 1.05 |
| 2:H:78:LYS:HB2 | 2:H:78:LYS:HZ2 | 1.12 | 1.05 |
| 1:L:7:SER:HB3 | 1:L:8:PRO:HD3 | 1.36 | 1.04 |
| 3:Y:8:ASP:OD1 | 3:Y:11:VAL:HG13 | 1.57 | 1.04 |
| 3:X:78:ARG:CG | 3:X:78:ARG:HH11 | 1.70 | 1.03 |
| 2:J:90:ALA:HA | 2:J:114:VAL:HG21 | 1.40 | 1.03 |
| 1:N:185:TYR:CE1 | 1:N:191:TYR:HE1 | 1.77 | 1.02 |
| 1:N:77:MET:HE3 | 1:N:81:ASP:HB2 | 1.40 | 1.02 |
| 2:I:153:VAL:HG23 | 2:I:201:ALA:O | 1.57 | 1.02 |
| 2:K:64:GLU:HA | 2:K:67:LYS:HG3 | 1.42 | 1.02 |
| 1:O:32:MET:HB2 | 1:O:70:TYR:CD2 | 1.95 | 1.01 |
| 3:X:78:ARG:HG2 | 3:X:78:ARG:NH1 | 1.54 | 1.01 |
| 3:X:112:LEU:HD12 | 3:X:113:PRO:HD2 | 1.39 | 1.01 |
| 2:J:51:ILE:HD13 | 2:J:74:ARG:HG2 | 1.41 | 1.00 |
| 2:J:153:VAL:HG23 | 2:J:202:HIS:HB2 | 1.38 | 1.00 |
| 2:J:89:ARG:HB3 | 2:J:91:GLU:OE1 | 1.60 | 1.00 |
| 2:H:12:VAL:O | 2:H:114:VAL:HA | 1.60 | 1.00 |
| 1:N:7:SER:CB | 1:N:22:THR:HB | 1.91 | 1.00 |
| 2:H:199:ASN:CB | 2:H:209:VAL:HG23 | 1.90 | 1.00 |
| 1:N:76:ARG:HG2 | 1:N:76:ARG:NH1 | 1.68 | 0.99 |
| 2:H:89:ARG:HD2 | 2:H:91:GLU:OE1 | 1.58 | 0.99 |
| 2:H:199:ASN:HB3 | 2:H:209:VAL:CG2 | 1.91 | 0.99 |
| 3:Y:136:ARG:HH22 | 3:Z:46:PHE:HD2 | 1.09 | 0.99 |
| 1:L:185:TYR:CE1 | 1:L:191:TYR:CE1 | 2.51 | 0.99 |
| 3:Y:130:SER:O | 3:Y:134:LEU:HD12 | 1.63 | 0.99 |
| 1:O:37:GLN:HE22 | 2:K:39:GLN:HE22 | 1.08 | 0.98 |
| 2:H:189:SER:HA | 4:H:224:HOH:O | 1.56 | 0.98 |
| 1:O:197:HIS:O | 1:O:199:THR:N | 1.96 | 0.98 |
| 3:X:12:LEU:HB3 | 3:X:143:MET:CE | 1.94 | 0.98 |
| 3:V:69:LEU:HD11 | 3:V:118:THR:HG21 | 1.42 | 0.98 |
| 2:J:124:VAL:HG11 | 2:J:200:VAL:HG21 | 1.46 | 0.97 |
| 1:N:7:SER:HB3 | 1:N:22:THR:HB | 1.01 | 0.97 |
| 2:J:20:LEU:HD11 | 2:J:96:TYR:CD1 | 2.00 | 0.96 |
| 1:L:185:TYR:CD1 | 1:L:191:TYR:HE1 | 1.83 | 0.96 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:131:VAL:N | 1:L:178:LEU:O | 1.98 | 0.96 |
| 1:M:48:TYR:CE1 | 3:X:113:PRO:HG2 | 1.99 | 0.96 |
| 2:J:70:PHE:HA | 2:J:84:GLN:O | 1.65 | 0.96 |
| 2:J:70:PHE:HD1 | 2:J:85:MET:HA | 1.29 | 0.96 |
| 2:K:84:GLN:CA | 2:K:84:GLN:HE21 | 1.78 | 0.96 |
| 1:N:7:SER:HB3 | 1:N:22:THR:CB | 1.95 | 0.96 |
| 2:H:203:PRO:HA | 4:H:228:HOH:O | 1.65 | 0.95 |
| 1:M:36:GLN:HB2 | 1:M:85:TYR:CE2 | 2.02 | 0.95 |
| 1:O:19:VAL:HG11 | 1:O:74:ILE:HD12 | 1.49 | 0.95 |
| 3:Z:64:LEU:O | 3:Z:68:THR:HG22 | 1.65 | 0.94 |
| 1:N:149:ILE:O | 1:N:190:SER:O | 1.83 | 0.94 |
| 2:J:51:ILE:HD13 | 2:J:74:ARG:CG | 1.97 | 0.94 |
| 2:J:29:PHE:CE1 | 2:J:34:MET:CE | 2.49 | 0.94 |
| 1:N:77:MET:CE | 1:N:81:ASP:HB2 | 1.97 | 0.94 |
| 3:Y:68:THR:HG22 | 3:Y:101:LEU:CD1 | 1.96 | 0.94 |
| 2:J:38:ARG:HB2 | 2:J:96:TYR:CE2 | 2.02 | 0.94 |
| 1:N:167:SER:HB2 | 1:N:168:LYS:HZ2 | 1.19 | 0.94 |
| 1:L:135:LEU:HD23 | 1:L:143:ILE:CD1 | 1.97 | 0.94 |
| 1:N:119:PRO:HD3 | 1:N:131:VAL:CG2 | 1.97 | 0.94 |
| 3:V:68:THR:HG22 | 3:V:101:LEU:HD11 | 1.50 | 0.93 |
| 2:K:66:VAL:O | 2:K:66:VAL:HG12 | 1.66 | 0.93 |
| 1:O:116:ILE:HG13 | 1:O:133:CYS:SG | 2.08 | 0.93 |
| 1:M:20:THR:HB | 1:M:73:THR:OG1 | 1.69 | 0.93 |
| 3:Z:56:GLU:CA | 3:Z:56:GLU:OE2 | 2.17 | 0.93 |
| 2:J:85:MET:HE1 | 2:J:96:TYR:HE1 | 0.77 | 0.93 |
| 2:K:54:LYS:HE2 | 2:K:58:HIS:CE1 | 2.03 | 0.93 |
| 1:N:72:LEU:HD23 | 1:N:72:LEU:C | 1.89 | 0.93 |
| 1:N:149:ILE:HG23 | 1:N:191:TYR:CE2 | 2.04 | 0.92 |
| 2:J:135:THR:HG23 | 4:J:221:HOH:O | 1.67 | 0.92 |
| 2:J:70:PHE:CE1 | 2:J:85:MET:HB3 | 2.04 | 0.92 |
| 1:O:132:VAL:HG11 | 2:K:127:LEU:HD13 | 1.52 | 0.92 |
| 2:H:78:LYS:HG3 | 2:H:78:LYS:O | 1.67 | 0.92 |
| 2:H:145:VAL:CG1 | 2:H:180:LEU:HD22 | 1.99 | 0.92 |
| 3:X:17:ARG:NH1 | 3:X:17:ARG:HG3 | 1.76 | 0.92 |
| 1:M:32:MET:HB2 | 1:M:70:TYR:CD2 | 2.03 | 0.91 |
| 3:X:41:LEU:HD11 | 3:X:127:ILE:HG22 | 0.94 | 0.91 |
| 1:L:194:GLU:HB3 | 1:L:205:VAL:HG22 | 1.51 | 0.91 |
| 2:I:124:VAL:HG21 | 2:I:200:VAL:HG21 | 1.48 | 0.91 |
| 2:H:78:LYS:CB | 2:H:78:LYS:NZ | 2.32 | 0.91 |
| 3:Y:136:ARG:NH2 | 3:Z:46:PHE:CD2 | 2.37 | 0.91 |
| 1:O:149:ILE:HG12 | 1:O:191:TYR:HE2 | 1.34 | 0.90 |
| 1:L:211:ASN:ND2 | 1:L:213:CYS:SG | 2.44 | 0.90 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:N:19:VAL:HG11 | 1:N:103:LEU:HD22 | 1.52 | 0.90 |
| 1:M:123:GLN:NE2 | 1:M:130:SER:OG | 2.03 | 0.90 |
| 2:J:29:PHE:CE1 | 2:J:34:MET:HE3 | 2.05 | 0.90 |
| 1:O:44:LYS:NZ | 1:O:44:LYS:HB2 | 1.86 | 0.90 |
| 1:N:185:TYR:CE1 | 1:N:191:TYR:CE1 | 2.60 | 0.90 |
| 2:H:66:VAL:CG1 | 2:H:70:PHE:CD2 | 2.54 | 0.90 |
| 2:I:27:PHE:CE2 | 2:I:29:PHE:HA | 2.07 | 0.90 |
| 1:N:147:TRP:CD1 | 1:N:158:VAL:HG11 | 2.07 | 0.90 |
| 2:J:33:TRP:H | 3:Y:111:GLN:HE22 | 1.17 | 0.90 |
| 1:N:2:VAL:O | 1:N:96:THR:HG21 | 1.72 | 0.89 |
| 3:Z:64:LEU:O | 3:Z:68:THR:CG2 | 2.21 | 0.89 |
| 3:X:112:LEU:HD12 | 3:X:113:PRO:CD | 2.02 | 0.89 |
| 2:I:56:ASN:H | 2:I:56:ASN:HD22 | 1.15 | 0.89 |
| 1:N:76:ARG:CG | 1:N:76:ARG:HH11 | 1.83 | 0.89 |
| 1:L:88:GLN:NE2 | 1:L:90:ARG:HD2 | 1.86 | 0.89 |
| 1:L:111:ALA:CB | 1:L:199:THR:HG21 | 2.02 | 0.89 |
| 3:Y:11:VAL:O | 3:Y:15:LEU:HB2 | 1.73 | 0.89 |
| 1:L:29:VAL:HG13 | 1:L:91:SER:HB2 | 1.53 | 0.88 |
| 2:J:148:TYR:HE2 | 2:J:153:VAL:HB | 1.31 | 0.88 |
| 2:K:153:VAL:HG23 | 2:K:202:HIS:HD2 | 1.38 | 0.88 |
| 3:X:74:VAL:HG11 | 3:X:94:SER:HB3 | 1.55 | 0.88 |
| 3:Z:107:LEU:O | 3:Z:107:LEU:HD23 | 1.72 | 0.88 |
| 1:L:2:VAL:O | 1:L:96:THR:HG21 | 1.73 | 0.88 |
| 3:X:51:TRP:HZ2 | 3:X:138:LYS:HE2 | 1.32 | 0.88 |
| 3:Y:63:ILE:O | 3:Y:67:VAL:HG23 | 1.73 | 0.88 |
| 2:I:216:ARG:HE | 3:Y:122:LYS:H | 1.21 | 0.88 |
| 1:L:84:THR:HG23 | 1:L:101:THR:H | 1.37 | 0.88 |
| 1:L:88:GLN:NE2 | 1:L:90:ARG:HH11 | 1.72 | 0.88 |
| 2:K:29:PHE:CB | 2:K:79:SER:HB3 | 2.04 | 0.88 |
| 2:J:216:ARG:HH22 | 3:X:123:ASP:HB3 | 1.39 | 0.88 |
| 1:M:76:ARG:HH11 | 1:M:76:ARG:HG2 | 1.39 | 0.88 |
| 2:I:120:THR:HG21 | 2:I:177:LEU:CD1 | 2.03 | 0.88 |
| 1:O:136:ASN:OD1 | 1:O:173:SER:HB3 | 1.74 | 0.87 |
| 2:K:40:SER:O | 2:K:44:GLY:HA2 | 1.75 | 0.87 |
| 1:N:186:GLU:HA | 1:N:210:ARG:NH1 | 1.90 | 0.87 |
| 1:L:185:TYR:HE1 | 1:L:191:TYR:CE1 | 1.92 | 0.87 |
| 1:M:120:SER:O | 1:M:122:GLU:N | 2.08 | 0.87 |
| 3:Y:105:GLN:NE2 | 3:Y:111:GLN:HG3 | 1.90 | 0.87 |
| 2:H:70:PHE:CE1 | 2:H:85:MET:HB3 | 2.07 | 0.87 |
| 1:L:88:GLN:HE22 | 1:L:90:ARG:HH11 | 0.89 | 0.87 |
| 2:J:38:ARG:HB2 | 2:J:96:TYR:CD2 | 2.09 | 0.86 |
| 3:Y:68:THR:HG22 | 3:Y:101:LEU:HD11 | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:J:6:GLU:OE2 | 2:J:97:TYR:HA | 1.74 | 0.86 |
| 1:N:36:GLN:HE21 | 1:N:85:TYR:HE2 | 1.24 | 0.86 |
| 3:V:69:LEU:HD11 | 3:V:118:THR:CG2 | 2.05 | 0.86 |
| 1:N:6:GLN:HE22 | 1:N:86:TYR:HA | 1.36 | 0.86 |
| 2:K:216:ARG:NH2 | 3:V:123:ASP:H | 1.74 | 0.85 |
| 2:J:90:ALA:HA | 2:J:114:VAL:CG2 | 2.07 | 0.85 |
| 2:I:149:PHE:HB2 | 2:I:177:LEU:CD2 | 2.07 | 0.85 |
| 1:N:19:VAL:HG11 | 1:N:103:LEU:CD2 | 2.07 | 0.85 |
| 1:N:189:ASN:ND2 | 1:N:210:ARG:H | 1.75 | 0.85 |
| 1:O:61:PHE:CE1 | 1:O:74:ILE:HG12 | 2.11 | 0.85 |
| 1:N:2:VAL:HG21 | 1:N:89:GLN:OE1 | 1.77 | 0.85 |
| 2:J:29:PHE:HE1 | 2:J:34:MET:CE | 1.86 | 0.85 |
| 3:Z:97:VAL:O | 3:Z:100:LEU:HB2 | 1.77 | 0.85 |
| 2:I:56:ASN:N | 2:I:56:ASN:HD22 | 1.74 | 0.84 |
| 2:J:146:LYS:HA | 2:J:179:THR:OG1 | 1.77 | 0.84 |
| 3:Y:116:GLY:O | 3:Y:118:THR:HG22 | 1.77 | 0.84 |
| 2:J:148:TYR:CD1 | 2:J:178:TYR:CB | 2.60 | 0.84 |
| 2:K:84:GLN:HA | 2:K:84:GLN:NE2 | 1.91 | 0.84 |
| 2:J:148:TYR:CD1 | 2:J:178:TYR:HB2 | 2.12 | 0.84 |
| 3:X:51:TRP:CZ2 | 3:X:138:LYS:CE | 2.60 | 0.84 |
| 1:N:79:ALA:HA | 1:N:105:ILE:HD13 | 1.59 | 0.84 |
| 2:H:66:VAL:HG11 | 2:H:70:PHE:CD2 | 2.13 | 0.84 |
| 1:L:88:GLN:HE22 | 1:L:90:ARG:NH1 | 1.74 | 0.84 |
| 3:Y:13:SER:O | 3:Y:14:LYS:C | 2.16 | 0.84 |
| 2:J:130:GLY:O | 2:J:133:ALA:CA | 2.25 | 0.84 |
| 2:J:122:PRO:CB | 2:J:148:TYR:HB3 | 2.07 | 0.83 |
| 3:Z:14:LYS:O | 3:Z:18:ASP:CB | 2.21 | 0.83 |
| 2:J:216:ARG:HG3 | 3:X:122:LYS:HG3 | 1.61 | 0.83 |
| 3:Z:41:LEU:HD11 | 3:Z:127:ILE:HG22 | 1.59 | 0.83 |
| 2:H:174:GLN:O | 2:H:176:ASP:N | 2.11 | 0.83 |
| 1:M:33:TYR:CD2 | 1:M:33:TYR:N | 2.40 | 0.83 |
| 2:K:39:GLN:HA | 2:K:44:GLY:O | 1.79 | 0.83 |
| 2:I:158:ASN:O | 2:I:160:GLY:N | 2.12 | 0.83 |
| 2:K:33:TRP:CE2 | 2:K:52:ARG:HG2 | 2.14 | 0.83 |
| 3:Y:130:SER:O | 3:Y:134:LEU:CD1 | 2.27 | 0.83 |
| 1:M:188:HIS:O | 1:M:210:ARG:CD | 2.27 | 0.83 |
| 1:L:154:ARG:O | 1:L:154:ARG:HG3 | 1.77 | 0.82 |
| 1:N:61:PHE:CE1 | 1:N:74:ILE:HG12 | 2.14 | 0.82 |
| 1:O:32:MET:SD | 1:O:88:GLN:O | 2.37 | 0.82 |
| 3:X:68:THR:HB | 4:X:170:HOH:O | 1.79 | 0.82 |
| 1:N:70:TYR:O | 1:N:71:SER:HB3 | 1.78 | 0.82 |
| 3:X:43:ALA:CB | 3:X:119:THR:HG23 | 2.09 | 0.82 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:I:22:CYS:O | 2:I:80:SER:HB3 | 1.80 | 0.82 |
| 3:Y:93:LEU:O | 3:Y:97:VAL:HG23 | 1.79 | 0.82 |
| 1:L:111:ALA:HB1 | 1:L:199:THR:HG21 | 1.61 | 0.82 |
| 1:L:185:TYR:CD1 | 1:L:191:TYR:CE1 | 2.66 | 0.82 |
| 2:H:85:MET:HB2 | 2:H:88:LEU:HD11 | 1.61 | 0.82 |
| 3:Z:41:LEU:CD1 | 3:Z:127:ILE:HG22 | 2.10 | 0.82 |
| 2:H:166:VAL:HB | 2:H:184:VAL:HG23 | 1.61 | 0.82 |
| 1:N:3:VAL:H | 1:N:26:SER:HB3 | 1.42 | 0.82 |
| 1:N:119:PRO:CD | 1:N:131:VAL:CG2 | 2.57 | 0.81 |
| 1:M:107:ARG:NH2 | 1:N:78:GLU:OE2 | 2.13 | 0.81 |
| 3:Y:124:PRO:O | 3:Y:126:ALA:N | 2.13 | 0.81 |
| 2:K:33:TRP:H | 3:Z:111:GLN:HE22 | 1.24 | 0.81 |
| 1:M:22:THR:HG22 | 1:M:23:CYS:N | 1.95 | 0.81 |
| 3:X:132:GLN:HA | 3:X:135:LEU:HD12 | 1.62 | 0.81 |
| 1:O:117:PHE:N | 1:O:117:PHE:HD1 | 1.76 | 0.81 |
| 1:N:162:TRP:CE2 | 1:N:174:MET:HG3 | 2.15 | 0.81 |
| 3:Z:45:ASP:H | 3:Z:133:HIS:HE1 | 1.26 | 0.81 |
| 3:Z:71:LEU:HD12 | 3:Z:101:LEU:HD22 | 1.62 | 0.81 |
| 3:X:61:GLN:O | 3:X:64:LEU:N | 2.12 | 0.81 |
| 2:I:120:THR:HG21 | 2:I:177:LEU:HD11 | 1.60 | 0.81 |
| 1:O:44:LYS:HZ3 | 1:O:44:LYS:HB2 | 1.43 | 0.81 |
| 1:M:138:PHE:HE2 | 1:M:173:SER:HA | 1.46 | 0.81 |
| 2:H:66:VAL:HG13 | 2:H:70:PHE:CD2 | 2.14 | 0.81 |
| 3:V:81:LEU:HD12 | 3:V:87:SER:HB2 | 1.61 | 0.81 |
| 1:N:45:LEU:HD12 | 2:J:104:LEU:HD12 | 1.63 | 0.81 |
| 2:H:100:GLY:HA3 | 2:H:105:TYR:H | 1.45 | 0.81 |
| 3:Z:107:LEU:CD2 | 3:Z:107:LEU:O | 2.27 | 0.81 |
| 1:N:197:HIS:ND1 | 1:N:199:THR:HB | 1.95 | 0.81 |
| 3:Z:64:LEU:HD23 | 3:Z:112:LEU:HB2 | 1.60 | 0.81 |
| 1:M:188:HIS:O | 1:M:210:ARG:HD3 | 1.80 | 0.81 |
| 3:X:43:ALA:HB2 | 3:X:119:THR:HG23 | 1.62 | 0.81 |
| 2:K:70:PHE:CD1 | 2:K:85:MET:CB | 2.64 | 0.81 |
| 1:N:89:GLN:HE21 | 1:N:96:THR:HB | 1.46 | 0.81 |
| 3:X:63:ILE:O | 3:X:67:VAL:HG23 | 1.79 | 0.81 |
| 1:O:6:GLN:HE22 | 1:O:86:TYR:HA | 1.46 | 0.80 |
| 1:L:131:VAL:O | 1:L:147:TRP:CH2 | 2.34 | 0.80 |
| 1:N:167:SER:HB2 | 1:N:168:LYS:HZ1 | 1.43 | 0.80 |
| 1:M:138:PHE:CE2 | 1:M:173:SER:HA | 2.16 | 0.80 |
| 1:M:131:VAL:HG12 | 1:M:147:TRP:CH2 | 2.15 | 0.80 |
| 1:M:185:TYR:HD1 | 1:M:191:TYR:CZ | 2.00 | 0.80 |
| 3:V:125:ASN:N | 3:V:125:ASN:HD22 | 1.78 | 0.80 |
| 3:V:73:GLY:O | 3:V:76:ALA:HB3 | 1.82 | 0.80 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:216:ARG:NH2 | 3:X:123:ASP:HB3 | 1.96 | 0.80 |
| 2:I:134:GLN:HE22 | 3:Y:117:ARG:HB3 | 1.47 | 0.80 |
| 3:Y:131:PHE:CZ | 3:Y:135:LEU:HD11 | 2.16 | 0.80 |
| 2:K:146:LYS:HA | 2:K:179:THR:OG1 | 1.80 | 0.80 |
| 3:Z:141:PHE:O | 3:Z:145:VAL:HG23 | 1.82 | 0.80 |
| 2:K:100:GLY:O | 2:K:104:LEU:N | 2.15 | 0.80 |
| 1:M:37:GLN:HE22 | 2:I:39:GLN:HE22 | 1.29 | 0.80 |
| 1:N:185:TYR:HE1 | 1:N:191:TYR:CE1 | 1.99 | 0.80 |
| 3:V:42:PRO:HD3 | 3:V:70:LEU:HD23 | 1.61 | 0.80 |
| 1:O:107:ARG:HD2 | 1:O:170:SER:OG | 1.80 | 0.80 |
| 3:X:81:LEU:HD12 | 3:X:87:SER:HB2 | 1.64 | 0.80 |
| 2:J:70:PHE:HE1 | 2:J:85:MET:HB3 | 1.42 | 0.79 |
| 1:M:149:ILE:HD11 | 1:M:154:ARG:CD | 2.10 | 0.79 |
| 3:V:59:LYS:O | 3:V:63:ILE:HG13 | 1.83 | 0.79 |
| 2:J:37:VAL:HG22 | 2:J:47:TRP:HA | 1.65 | 0.79 |
| 1:L:72:LEU:HD23 | 1:L:72:LEU:O | 1.83 | 0.79 |
| 2:I:119:THR:HA | 2:I:149:PHE:O | 1.83 | 0.79 |
| 1:O:67:GLY:N | 1:O:70:TYR:HE1 | 1.81 | 0.79 |
| 2:K:51:ILE:HD11 | 2:K:74:ARG:HG2 | 1.64 | 0.79 |
| 2:K:213:ILE:HG23 | 2:K:214:VAL:N | 1.96 | 0.78 |
| 1:L:93:TYR:CE1 | 1:L:95:ARG:NH1 | 2.51 | 0.78 |
| 2:K:54:LYS:CE | 2:K:58:HIS:HE1 | 1.96 | 0.78 |
| 1:M:6:GLN:HE21 | 1:M:98:GLY:HA3 | 1.47 | 0.78 |
| 3:V:64:LEU:HD11 | 3:V:105:GLN:HG3 | 1.63 | 0.78 |
| 1:O:33:TYR:HB2 | 1:O:88:GLN:HB3 | 1.65 | 0.78 |
| 2:H:173:LEU:HD23 | 2:H:177:LEU:O | 1.84 | 0.78 |
| 2:H:56:ASN:HB3 | 4:H:218:HOH:O | 1.84 | 0.78 |
| 2:H:56:ASN:H | 2:H:56:ASN:HD22 | 1.32 | 0.78 |
| 2:H:64:GLU:HG2 | 2:H:67:LYS:HZ2 | 1.49 | 0.78 |
| 2:J:148:TYR:HE1 | 2:J:178:TYR:HB3 | 0.97 | 0.78 |
| 1:L:89:GLN:OE1 | 1:L:91:SER:HB3 | 1.84 | 0.78 |
| 1:M:45:LEU:HD22 | 1:M:46:TRP:N | 1.98 | 0.78 |
| 2:I:58:HIS:CD2 | 2:I:74:ARG:HD2 | 2.18 | 0.78 |
| 1:O:118:PRO:HB3 | 1:O:208:PHE:CE2 | 2.19 | 0.77 |
| 2:H:176:ASP:O | 2:H:177:LEU:HD23 | 1.84 | 0.77 |
| 1:N:35:PHE:N | 1:N:35:PHE:CD1 | 2.50 | 0.77 |
| 1:M:149:ILE:CD1 | 1:M:154:ARG:HD2 | 2.13 | 0.77 |
| 3:X:78:ARG:HG2 | 3:X:78:ARG:HH11 | 0.75 | 0.77 |
| 1:N:48:TYR:O | 1:N:52:ASN:HB2 | 1.84 | 0.77 |
| 2:H:84:GLN:HE21 | 2:H:84:GLN:CA | 1.98 | 0.77 |
| 2:J:156:THR:O | 2:J:199:ASN:N | 2.14 | 0.77 |
| 3:Z:35:LEU:N | 3:Z:122:LYS:O | 2.17 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:I:139:VAL:O | 2:I:185:THR:HG23 | 1.85 | 0.77 |
| 2:I:76:ASP:O | 2:I:79:SER:N | 2.15 | 0.77 |
| 2:H:157:TRP:CZ3 | 2:H:198:CYS:HB3 | 2.19 | 0.77 |
| 1:O:119:PRO:HG2 | 1:O:129:ALA:HB1 | 1.66 | 0.77 |
| 2:J:29:PHE:CD2 | 2:J:79:SER:HA | 2.20 | 0.77 |
| 1:L:36:GLN:HG3 | 1:L:85:TYR:CE2 | 2.19 | 0.77 |
| 1:L:7:SER:HB3 | 1:L:8:PRO:CD | 2.15 | 0.77 |
| 2:H:91:GLU:C | 2:H:93:THR:H | 1.88 | 0.77 |
| 1:O:77:MET:HE3 | 1:O:78:GLU:O | 1.84 | 0.77 |
| 1:O:33:TYR:N | 1:O:33:TYR:CD1 | 2.52 | 0.77 |
| 3:Z:12:LEU:HB2 | 3:Z:143:MET:SD | 2.24 | 0.77 |
| 1:N:189:ASN:ND2 | 1:N:210:ARG:N | 2.32 | 0.76 |
| 1:M:189:ASN:HA | 1:M:210:ARG:HG3 | 1.67 | 0.76 |
| 1:M:129:ALA:O | 1:M:179:THR:HG23 | 1.84 | 0.76 |
| 1:N:117:PHE:N | 1:N:117:PHE:CD1 | 2.47 | 0.76 |
| 2:I:75:ASP:OD1 | 2:I:75:ASP:C | 2.23 | 0.76 |
| 2:J:70:PHE:CD1 | 2:J:85:MET:HA | 2.17 | 0.76 |
| 3:Y:10:ARG:HA | 3:Y:13:SER:HG | 1.48 | 0.76 |
| 1:L:76:ARG:HH11 | 1:L:76:ARG:HB3 | 1.50 | 0.76 |
| 1:M:189:ASN:HA | 1:M:210:ARG:CG | 2.16 | 0.76 |
| 1:M:4:LEU:HD21 | 1:M:89:GLN:HG2 | 1.67 | 0.76 |
| 2:J:35:ASP:HB3 | 2:J:49:ALA:O | 1.84 | 0.76 |
| 2:H:33:TRP:H | 3:V:111:GLN:NE2 | 1.84 | 0.76 |
| 1:N:189:ASN:HD21 | 1:N:209:ASN:HB3 | 1.50 | 0.76 |
| 2:K:153:VAL:HG23 | 2:K:202:HIS:CD2 | 2.21 | 0.75 |
| 2:K:66:VAL:CG1 | 2:K:66:VAL:O | 2.35 | 0.75 |
| 2:K:66:VAL:HG11 | 2:K:70:PHE:CD2 | 2.21 | 0.75 |
| 1:M:45:LEU:HD22 | 1:M:45:LEU:C | 2.07 | 0.75 |
| 2:I:196:VAL:O | 2:I:196:VAL:CG2 | 2.34 | 0.75 |
| 3:V:69:LEU:CD1 | 3:V:118:THR:HG21 | 2.15 | 0.75 |
| 2:H:202:HIS:ND1 | 2:H:204:ALA:HB2 | 2.01 | 0.75 |
| 1:N:13:ALA:HB1 | 1:N:17:GLU:CD | 2.07 | 0.75 |
| 1:M:150:ASP:OD2 | 1:M:188:HIS:CB | 2.33 | 0.75 |
| 3:Y:64:LEU:O | 3:Y:68:THR:HG23 | 1.86 | 0.75 |
| 1:N:86:TYR:CD2 | 2:J:45:LEU:HD12 | 2.22 | 0.75 |
| 1:M:119:PRO:HA | 4:M:227:HOH:O | 1.87 | 0.75 |
| 2:H:85:MET:HE3 | 2:H:96:TYR:CZ | 2.22 | 0.75 |
| 1:N:33:TYR:CE1 | 1:N:90:ARG:HD3 | 2.22 | 0.75 |
| 2:J:139:VAL:HG12 | 2:J:139:VAL:O | 1.87 | 0.75 |
| 3:Z:101:LEU:O | 3:Z:105:GLN:HB2 | 1.87 | 0.74 |
| 1:L:111:ALA:HB2 | 1:L:199:THR:CG2 | 2.17 | 0.74 |
| 1:M:117:PHE:N | 1:M:117:PHE:CD1 | 2.55 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:119:PRO:HD3 | 1:M:131:VAL:HG22 | 1.69 | 0.74 |
| 2:H:56:ASN:HD22 | 2:H:56:ASN:N | 1.84 | 0.74 |
| 1:N:148:LYS:HE2 | 1:N:194:GLU:OE2 | 1.86 | 0.74 |
| 2:J:93:THR:HG23 | 2:J:113:THR:HA | 1.68 | 0.74 |
| 1:L:120:SER:O | 1:L:124:LEU:CD2 | 2.36 | 0.74 |
| 2:K:156:THR:O | 2:K:199:ASN:ND2 | 2.20 | 0.74 |
| 3:Y:84:THR:O | 3:Y:87:SER:N | 2.20 | 0.74 |
| 2:I:70:PHE:CD1 | 2:I:85:MET:HG2 | 2.21 | 0.74 |
| 2:I:58:HIS:HD2 | 2:I:74:ARG:HD2 | 1.49 | 0.74 |
| 1:N:88:GLN:NE2 | 1:N:90:ARG:HD2 | 2.02 | 0.74 |
| 2:K:140:THR:O | 2:K:141:LEU:HD23 | 1.86 | 0.74 |
| 2:K:148:TYR:O | 2:K:177:LEU:HD22 | 1.87 | 0.74 |
| 2:K:64:GLU:O | 2:K:66:VAL:N | 2.20 | 0.74 |
| 1:M:162:TRP:HE3 | 1:M:162:TRP:N | 1.84 | 0.74 |
| 2:J:120:THR:O | 2:J:148:TYR:HA | 1.87 | 0.74 |
| 3:Z:110:THR:O | 3:Z:110:THR:HG23 | 1.87 | 0.74 |
| 1:M:181:THR:HA | 4:M:215:HOH:O | 1.87 | 0.74 |
| 2:I:216:ARG:CD | 3:Y:122:LYS:HG3 | 2.16 | 0.74 |
| 1:O:77:MET:HE3 | 1:O:81:ASP:HB2 | 1.68 | 0.74 |
| 1:O:69:SER:C | 1:O:70:TYR:HD1 | 1.91 | 0.73 |
| 3:X:17:ARG:CG | 3:X:17:ARG:HH11 | 2.00 | 0.73 |
| 1:L:107:ARG:NH2 | 1:O:78:GLU:OE2 | 2.21 | 0.73 |
| 2:J:29:PHE:CE1 | 2:J:34:MET:HE2 | 2.24 | 0.73 |
| 2:H:75:ASP:OD1 | 2:H:77:SER:HB3 | 1.88 | 0.73 |
| 2:H:102:SER:HB2 | 3:V:111:GLN:HB2 | 1.71 | 0.73 |
| 1:M:7:SER:CB | 1:M:8:PRO:HD3 | 2.19 | 0.73 |
| 2:I:56:ASN:N | 2:I:56:ASN:ND2 | 2.37 | 0.73 |
| 1:O:147:TRP:CE3 | 1:O:192:THR:O | 2.42 | 0.73 |
| 1:L:135:LEU:HD23 | 1:L:143:ILE:HD13 | 1.71 | 0.73 |
| 1:M:162:TRP:CE3 | 1:M:162:TRP:N | 2.57 | 0.73 |
| 3:X:12:LEU:CB | 3:X:143:MET:CE | 2.67 | 0.73 |
| 2:K:89:ARG:NH1 | 2:K:89:ARG:HG3 | 1.86 | 0.73 |
| 2:I:145:VAL:HG13 | 2:I:180:LEU:O | 1.89 | 0.73 |
| 2:J:51:ILE:CD1 | 2:J:74:ARG:CG | 2.67 | 0.73 |
| 3:V:69:LEU:CD1 | 3:V:118:THR:CG2 | 2.66 | 0.73 |
| 2:I:66:VAL:HG22 | 2:I:70:PHE:CE2 | 2.24 | 0.72 |
| 3:Z:61:GLN:HG2 | 3:Z:112:LEU:CD2 | 2.19 | 0.72 |
| 3:X:134:LEU:O | 3:X:139:VAL:HG23 | 1.88 | 0.72 |
| 2:K:29:PHE:CE1 | 2:K:34:MET:HE2 | 2.23 | 0.72 |
| 1:O:117:PHE:N | 1:O:117:PHE:CD1 | 2.49 | 0.72 |
| 2:I:6:GLU:OE2 | 2:I:109:GLY:N | 2.21 | 0.72 |
| 1:L:4:LEU:HB2 | 1:L:97:PHE:O | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:166:ASP:HB3 | 1:L:169:ASP:O | 1.90 | 0.72 |
| 3:Z:71:LEU:HD12 | 3:Z:101:LEU:CD2 | 2.20 | 0.72 |
| 3:V:55:MET:H | 3:V:55:MET:HE2 | 1.55 | 0.72 |
| 2:J:88:LEU:HD23 | 2:J:92:ASP:OD2 | 1.89 | 0.72 |
| 2:H:66:VAL:HG11 | 2:H:70:PHE:HD2 | 1.55 | 0.72 |
| 2:H:69:ARG:NH2 | 2:H:92:ASP:OD2 | 2.21 | 0.72 |
| 1:M:132:VAL:HB | 1:M:177:THR:HG23 | 1.70 | 0.72 |
| 1:N:185:TYR:CD1 | 1:N:191:TYR:CE1 | 2.78 | 0.72 |
| 1:N:185:TYR:CD1 | 1:N:191:TYR:HE1 | 2.07 | 0.72 |
| 2:I:89:ARG:O | 2:I:92:ASP:HB2 | 1.90 | 0.71 |
| 1:L:111:ALA:HB1 | 1:L:112:PRO:HD2 | 1.72 | 0.71 |
| 2:I:145:VAL:HG22 | 2:I:145:VAL:O | 1.90 | 0.71 |
| 3:Y:115:ARG:HD2 | 3:Y:116:GLY:N | 2.06 | 0.71 |
| 2:H:47:TRP:HZ2 | 2:H:50:GLU:HB3 | 1.54 | 0.71 |
| 2:H:2:VAL:HA | 2:H:26:GLY:HA3 | 1.72 | 0.71 |
| 3:V:37:THR:O | 3:V:80:GLN:NE2 | 2.23 | 0.71 |
| 3:V:12:LEU:HD12 | 3:V:139:VAL:HG12 | 1.71 | 0.71 |
| 2:K:162:LEU:HD13 | 2:K:184:VAL:HG21 | 1.73 | 0.71 |
| 2:I:104:LEU:HG | 2:I:105:TYR:CE1 | 2.24 | 0.71 |
| 1:L:19:VAL:HB | 1:L:74:ILE:HB | 1.71 | 0.71 |
| 2:K:13:GLN:O | 2:K:14:PRO:O | 2.08 | 0.71 |
| 3:V:71:LEU:O | 3:V:75:MET:HG2 | 1.91 | 0.71 |
| 2:H:85:MET:HE3 | 2:H:96:TYR:CE1 | 2.25 | 0.71 |
| 2:J:86:ASN:O | 2:J:87:SER:C | 2.27 | 0.71 |
| 2:J:140:THR:HG23 | 2:J:185:THR:OG1 | 1.91 | 0.71 |
| 3:Y:10:ARG:O | 3:Y:13:SER:N | 2.24 | 0.71 |
| 3:Y:14:LYS:O | 3:Y:18:ASP:HB2 | 1.90 | 0.71 |
| 1:M:109:ASP:OD1 | 1:M:140:PRO:HD3 | 1.90 | 0.71 |
| 1:M:77:MET:SD | 1:M:105:ILE:HD12 | 2.31 | 0.71 |
| 3:Z:61:GLN:HG2 | 3:Z:112:LEU:HD23 | 1.73 | 0.71 |
| 1:M:192:THR:OG1 | 1:M:207:SER:OG | 2.08 | 0.71 |
| 1:N:167:SER:CB | 1:N:168:LYS:NZ | 2.47 | 0.71 |
| 1:M:169:ASP:OD2 | 1:M:171:THR:OG1 | 2.08 | 0.71 |
| 2:H:91:GLU:O | 2:H:93:THR:N | 2.24 | 0.71 |
| 2:H:95:ILE:HD13 | 2:H:111:LEU:HD23 | 1.73 | 0.71 |
| 2:H:166:VAL:HG22 | 2:H:166:VAL:O | 1.89 | 0.70 |
| 1:N:148:LYS:HA | 1:N:153:GLU:HA | 1.72 | 0.70 |
| 1:M:148:LYS:HA | 1:M:152:SER:O | 1.90 | 0.70 |
| 1:O:19:VAL:HG12 | 1:O:74:ILE:HB | 1.73 | 0.70 |
| 3:X:51:TRP:O | 3:X:54:GLN:HB2 | 1.92 | 0.70 |
| 3:Y:22:LEU:HD21 | 3:Y:92:GLN:HB3 | 1.73 | 0.70 |
| 1:O:19:VAL:CG1 | 1:O:74:ILE:HD12 | 2.19 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:13:ALA:HB2 | 1:M:19:VAL:HG21 | 1.71 | 0.70 |
| 1:L:6:GLN:NE2 | 1:L:87:CYS:H | 1.90 | 0.70 |
| 2:H:64:GLU:HG2 | 2:H:67:LYS:NZ | 2.06 | 0.70 |
| 1:O:147:TRP:CH2 | 1:O:193:CYS:HB2 | 2.26 | 0.70 |
| 2:K:120:THR:HG21 | 2:K:177:LEU:HD11 | 1.74 | 0.70 |
| 2:H:145:VAL:HG13 | 2:H:180:LEU:HD22 | 1.71 | 0.70 |
| 2:I:191:TRP:CD1 | 2:I:196:VAL:HG13 | 2.26 | 0.70 |
| 1:N:89:GLN:NE2 | 1:N:96:THR:HB | 2.07 | 0.70 |
| 1:M:1:GLN:O | 1:M:1:GLN:HG2 | 1.92 | 0.70 |
| 1:O:185:TYR:CD1 | 1:O:191:TYR:HE1 | 2.10 | 0.70 |
| 1:M:192:THR:HA | 1:M:207:SER:OG | 1.92 | 0.69 |
| 3:V:86:LEU:HD22 | 3:V:90:LEU:HG | 1.74 | 0.69 |
| 1:O:116:ILE:C | 1:O:117:PHE:HD1 | 1.95 | 0.69 |
| 2:J:187:PRO:O | 2:J:190:THR:OG1 | 2.09 | 0.69 |
| 2:K:33:TRP:H | 3:Z:111:GLN:NE2 | 1.90 | 0.69 |
| 1:O:149:ILE:HG12 | 1:O:191:TYR:CE2 | 2.24 | 0.69 |
| 1:M:76:ARG:NH1 | 1:M:76:ARG:HG2 | 2.07 | 0.69 |
| 2:K:29:PHE:CE1 | 2:K:34:MET:CE | 2.74 | 0.69 |
| 2:K:29:PHE:HB2 | 2:K:79:SER:CB | 2.17 | 0.69 |
| 1:N:106:LYS:HG3 | 1:N:106:LYS:O | 1.91 | 0.69 |
| 3:Z:131:PHE:O | 3:Z:134:LEU:HB2 | 1.91 | 0.69 |
| 2:H:138:MET:HE2 | 2:H:185:THR:HG22 | 1.72 | 0.69 |
| 2:J:212:LYS:O | 2:J:213:ILE:HG13 | 1.92 | 0.69 |
| 3:V:100:LEU:O | 3:V:103:ALA:HB3 | 1.92 | 0.69 |
| 1:M:60:ARG:NH1 | 1:M:81:ASP:OD2 | 2.26 | 0.69 |
| 3:Z:59:LYS:O | 3:Z:63:ILE:HG13 | 1.92 | 0.69 |
| 1:L:89:GLN:HE21 | 1:L:96:THR:CB | 2.06 | 0.69 |
| 2:K:66:VAL:HG21 | 2:K:70:PHE:CE2 | 2.28 | 0.69 |
| 2:I:191:TRP:HD1 | 2:I:196:VAL:HG13 | 1.58 | 0.69 |
| 1:L:119:PRO:HA | 4:L:223:HOH:O | 1.93 | 0.69 |
| 3:Z:46:PHE:CE1 | 3:Z:133:HIS:NE2 | 2.60 | 0.69 |
| 2:I:216:ARG:NE | 3:Y:122:LYS:H | 1.91 | 0.69 |
| 1:N:162:TRP:CH2 | 1:N:174:MET:HE2 | 2.28 | 0.69 |
| 1:L:37:GLN:HG2 | 1:L:38:LYS:N | 2.07 | 0.69 |
| 2:K:203:PRO:HB2 | 4:K:227:HOH:O | 1.93 | 0.69 |
| 2:H:51:ILE:HD12 | 2:H:74:ARG:CG | 2.22 | 0.69 |
| 3:Y:110:THR:OG1 | 3:Y:111:GLN:N | 2.26 | 0.69 |
| 2:K:202:HIS:ND1 | 2:K:204:ALA:HB2 | 2.08 | 0.68 |
| 1:N:110:ALA:HB3 | 1:N:139:TYR:N | 2.07 | 0.68 |
| 3:Z:73:GLY:O | 3:Z:76:ALA:HB3 | 1.93 | 0.68 |
| 1:L:154:ARG:HD2 | 1:L:156:ASN:O | 1.92 | 0.68 |
| 2:J:69:ARG:NH1 | 2:J:89:ARG:NH2 | 2.40 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:143:ILE:HG12 | 1:L:197:HIS:HB2 | 1.74 | 0.68 |
| 3:V:86:LEU:CD2 | 3:V:90:LEU:HG | 2.23 | 0.68 |
| 1:O:132:VAL:HB | 1:O:177:THR:HG23 | 1.74 | 0.68 |
| 2:H:123:SER:OG | 2:H:146:LYS:HB3 | 1.93 | 0.68 |
| 2:K:69:ARG:NH1 | 2:K:89:ARG:NH2 | 2.40 | 0.68 |
| 3:V:81:LEU:CD1 | 3:V:87:SER:HB2 | 2.23 | 0.68 |
| 3:X:12:LEU:CB | 3:X:143:MET:HE1 | 2.12 | 0.68 |
| 2:K:22:CYS:O | 2:K:80:SER:HA | 1.93 | 0.68 |
| 1:L:48:TYR:CE1 | 1:L:52:ASN:HB2 | 2.28 | 0.68 |
| 3:X:112:LEU:CD1 | 3:X:113:PRO:HD2 | 2.22 | 0.68 |
| 1:M:95:ARG:HG3 | 2:I:47:TRP:CD2 | 2.28 | 0.68 |
| 2:J:20:LEU:HD21 | 2:J:85:MET:SD | 2.34 | 0.68 |
| 1:O:67:GLY:N | 1:O:70:TYR:CE1 | 2.61 | 0.68 |
| 2:H:78:LYS:CB | 2:H:78:LYS:HZ3 | 2.06 | 0.68 |
| 3:V:100:LEU:HD22 | 3:V:104:LEU:HD11 | 1.75 | 0.68 |
| 2:I:188:SER:OG | 2:I:189:SER:N | 2.25 | 0.68 |
| 1:O:69:SER:O | 1:O:70:TYR:HD1 | 1.75 | 0.68 |
| 1:N:72:LEU:CD2 | 1:N:72:LEU:O | 2.39 | 0.68 |
| 3:V:125:ASN:H | 3:V:125:ASN:HD22 | 1.41 | 0.68 |
| 1:L:35:PHE:N | 1:L:35:PHE:CD1 | 2.59 | 0.68 |
| 2:K:119:THR:HG23 | 2:K:150:PRO:HD3 | 1.75 | 0.68 |
| 3:Z:64:LEU:CD2 | 3:Z:112:LEU:HB2 | 2.23 | 0.67 |
| 3:Y:13:SER:O | 3:Y:15:LEU:N | 2.26 | 0.67 |
| 1:L:75:SER:OG | 1:L:76:ARG:HG3 | 1.93 | 0.67 |
| 3:X:33:HIS:HB3 | 3:X:34:PRO:HD2 | 1.76 | 0.67 |
| 1:O:186:GLU:HB2 | 4:O:224:HOH:O | 1.94 | 0.67 |
| 1:L:149:ILE:O | 1:L:190:SER:O | 2.12 | 0.67 |
| 1:O:94:PRO:HB3 | 2:K:47:TRP:HZ3 | 1.59 | 0.67 |
| 3:X:85:CYS:O | 3:X:86:LEU:C | 2.32 | 0.67 |
| 2:H:199:ASN:HB3 | 2:H:209:VAL:HG23 | 0.94 | 0.67 |
| 3:X:64:LEU:O | 3:X:68:THR:CG2 | 2.34 | 0.67 |
| 2:K:100:GLY:HA3 | 2:K:105:TYR:HB2 | 1.75 | 0.67 |
| 1:M:22:THR:HG22 | 1:M:23:CYS:H | 1.59 | 0.67 |
| 1:M:109:ASP:HA | 1:M:139:TYR:O | 1.93 | 0.67 |
| 1:N:185:TYR:HE1 | 1:N:191:TYR:HE1 | 1.32 | 0.67 |
| 2:J:70:PHE:CE1 | 2:J:85:MET:CB | 2.77 | 0.67 |
| 3:Z:101:LEU:HD11 | 3:Z:105:GLN:HE22 | 1.60 | 0.67 |
| 1:N:119:PRO:CD | 1:N:131:VAL:HG22 | 2.25 | 0.67 |
| 1:N:3:VAL:N | 1:N:26:SER:HB3 | 2.10 | 0.67 |
| 1:L:6:GLN:HE22 | 1:L:87:CYS:H | 1.40 | 0.67 |
| 2:J:122:PRO:HB3 | 2:J:148:TYR:CB | 2.14 | 0.67 |
| 1:L:120:SER:O | 1:L:124:LEU:HD23 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:K:84:GLN:CA | 2:K:84:GLN:NE2 | 2.54 | 0.67 |
| 1:O:116:ILE:C | 1:O:117:PHE:CD1 | 2.68 | 0.67 |
| 1:L:84:THR:HG22 | 1:L:85:TYR:N | 2.07 | 0.67 |
| 1:L:84:THR:CG2 | 1:L:101:THR:H | 2.07 | 0.67 |
| 2:H:111:LEU:HD13 | 2:H:112:VAL:N | 2.10 | 0.67 |
| 1:N:184:GLU:O | 1:N:184:GLU:HG2 | 1.96 | 0.67 |
| 2:K:38:ARG:CA | 2:K:95:ILE:O | 2.35 | 0.66 |
| 1:N:118:PRO:HB3 | 1:N:208:PHE:CE2 | 2.30 | 0.66 |
| 2:H:93:THR:OG1 | 2:H:114:VAL:HG22 | 1.95 | 0.66 |
| 2:I:69:ARG:NH2 | 2:I:92:ASP:OD2 | 2.29 | 0.66 |
| 2:K:200:VAL:O | 2:K:208:LYS:N | 2.23 | 0.66 |
| 2:I:93:THR:OG1 | 2:I:114:VAL:N | 2.22 | 0.66 |
| 1:O:41:THR:HG23 | 1:O:42:SER:O | 1.95 | 0.66 |
| 1:N:2:VAL:HG21 | 1:N:89:GLN:CD | 2.16 | 0.66 |
| 3:Y:81:LEU:HD11 | 3:Y:86:LEU:HB3 | 1.76 | 0.66 |
| 2:J:157:TRP:CZ3 | 2:J:198:CYS:HB3 | 2.31 | 0.66 |
| 1:N:169:ASP:CG | 1:N:169:ASP:O | 2.34 | 0.66 |
| 2:H:216:ARG:NH2 | 3:Z:123:ASP:HB2 | 2.10 | 0.66 |
| 3:V:61:GLN:O | 3:V:65:GLY:N | 2.19 | 0.66 |
| 2:H:12:VAL:O | 2:H:114:VAL:CA | 2.41 | 0.66 |
| 1:N:33:TYR:O | 1:N:87:CYS:HA | 1.95 | 0.66 |
| 2:K:202:HIS:ND1 | 2:K:204:ALA:CB | 2.58 | 0.66 |
| 1:M:120:SER:O | 1:M:123:GLN:N | 2.27 | 0.66 |
| 3:Y:8:ASP:OD2 | 3:Y:10:ARG:CB | 2.43 | 0.66 |
| 2:H:207:THR:OG1 | 2:H:207:THR:O | 2.06 | 0.66 |
| 3:Z:97:VAL:O | 3:Z:100:LEU:CB | 2.43 | 0.66 |
| 3:Z:98:ARG:HA | 3:Z:101:LEU:HB2 | 1.77 | 0.66 |
| 2:I:174:GLN:O | 2:I:176:ASP:N | 2.28 | 0.66 |
| 1:L:105:ILE:HG13 | 1:L:106:LYS:N | 2.10 | 0.66 |
| 2:I:214:VAL:HG11 | 3:Y:40:LEU:CD2 | 2.26 | 0.66 |
| 1:O:185:TYR:CD1 | 1:O:191:TYR:CE1 | 2.84 | 0.66 |
| 2:I:196:VAL:O | 2:I:196:VAL:HG22 | 1.94 | 0.66 |
| 2:K:26:GLY:O | 2:K:27:PHE:HB3 | 1.95 | 0.66 |
| 1:L:149:ILE:HG13 | 1:L:154:ARG:HB3 | 1.77 | 0.66 |
| 1:L:107:ARG:HD3 | 1:L:139:TYR:CG | 2.31 | 0.66 |
| 3:Y:75:MET:HE3 | 3:Y:75:MET:HA | 1.79 | 0.65 |
| 1:M:185:TYR:CD1 | 1:M:191:TYR:CZ | 2.84 | 0.65 |
| 2:J:133:ALA:O | 2:J:134:GLN:HG2 | 1.96 | 0.65 |
| 1:N:194:GLU:HG2 | 1:N:205:VAL:HG23 | 1.77 | 0.65 |
| 2:I:64:GLU:HA | 2:I:67:LYS:HD3 | 1.77 | 0.65 |
| 3:V:140:ARG:O | 3:V:143:MET:HE2 | 1.94 | 0.65 |
| 2:H:191:TRP:CH2 | 2:H:214:VAL:HG13 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:31:TYR:HA | 1:M:50:THR:OG1 | 1.96 | 0.65 |
| 2:K:51:ILE:CD1 | 2:K:74:ARG:HD2 | 2.26 | 0.65 |
| 2:H:93:THR:OG1 | 2:H:114:VAL:CG2 | 2.44 | 0.65 |
| 3:V:12:LEU:HD12 | 3:V:139:VAL:CG1 | 2.26 | 0.65 |
| 1:M:32:MET:HB2 | 1:M:70:TYR:HD2 | 1.56 | 0.65 |
| 2:K:66:VAL:CG2 | 2:K:70:PHE:CE2 | 2.79 | 0.65 |
| 3:V:127:ILE:HG12 | 3:V:128:PHE:N | 2.10 | 0.65 |
| 1:N:45:LEU:HD12 | 2:J:104:LEU:CD1 | 2.27 | 0.65 |
| 1:O:90:ARG:HH21 | 2:K:102:SER:CB | 2.09 | 0.65 |
| 1:L:197:HIS:CE1 | 1:L:199:THR:HB | 2.30 | 0.65 |
| 1:L:157:GLY:O | 1:L:179:THR:HG22 | 1.96 | 0.65 |
| 2:I:33:TRP:CD1 | 2:I:53:SER:HB2 | 2.30 | 0.65 |
| 1:O:11:MET:HG3 | 1:O:103:LEU:CD1 | 2.27 | 0.65 |
| 1:L:194:GLU:CB | 1:L:205:VAL:HG22 | 2.24 | 0.65 |
| 1:N:117:PHE:N | 1:N:117:PHE:HD1 | 1.93 | 0.65 |
| 1:O:118:PRO:HB3 | 1:O:208:PHE:CZ | 2.31 | 0.65 |
| 1:N:169:ASP:OD2 | 1:N:169:ASP:O | 2.15 | 0.65 |
| 3:Z:43:ALA:HB2 | 3:Z:119:THR:HG23 | 1.78 | 0.65 |
| 1:N:167:SER:CB | 1:N:168:LYS:HZ2 | 2.01 | 0.65 |
| 1:N:192:THR:HG23 | 1:N:207:SER:HB2 | 1.77 | 0.65 |
| 1:O:192:THR:CG2 | 1:O:194:GLU:HG2 | 2.27 | 0.65 |
| 1:M:180:LEU:HD13 | 1:M:185:TYR:HB2 | 1.77 | 0.65 |
| 3:V:43:ALA:H | 3:V:118:THR:HA | 1.62 | 0.65 |
| 1:M:138:PHE:CD2 | 1:M:138:PHE:N | 2.63 | 0.65 |
| 1:L:209:ASN:HB3 | 1:L:213:CYS:SG | 2.37 | 0.65 |
| 1:L:111:ALA:CB | 1:L:199:THR:CG2 | 2.73 | 0.65 |
| 3:Y:15:LEU:O | 3:Y:19:SER:HB3 | 1.97 | 0.65 |
| 2:K:13:GLN:O | 2:K:14:PRO:C | 2.35 | 0.65 |
| 2:J:54:LYS:O | 2:J:57:ASN:N | 2.29 | 0.64 |
| 2:I:29:PHE:HB3 | 2:I:79:SER:HB3 | 1.79 | 0.64 |
| 1:N:197:HIS:CE1 | 1:N:199:THR:HB | 2.32 | 0.64 |
| 1:L:47:ILE:HG22 | 1:L:48:TYR:N | 2.11 | 0.64 |
| 3:X:140:ARG:O | 3:X:144:LEU:HB2 | 1.97 | 0.64 |
| 2:K:152:PRO:HD2 | 4:K:227:HOH:O | 1.98 | 0.64 |
| 2:K:57:ASN:O | 2:K:59:ALA:N | 2.30 | 0.64 |
| 3:Z:45:ASP:H | 3:Z:133:HIS:CE1 | 2.14 | 0.64 |
| 2:K:122:PRO:HB3 | 2:K:148:TYR:HB3 | 1.78 | 0.64 |
| 1:O:15:PRO:HG3 | 1:O:105:ILE:HD11 | 1.79 | 0.64 |
| 2:K:102:SER:OG | 3:Z:111:GLN:HB2 | 1.98 | 0.64 |
| 1:M:88:GLN:HE22 | 1:M:90:ARG:HH11 | 1.45 | 0.64 |
| 2:H:198:CYS:SG | 2:H:198:CYS:O | 2.55 | 0.64 |
| 1:O:192:THR:HG23 | 1:O:194:GLU:HG2 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:N:64:SER:OG | 1:N:65:GLY:N | 2.28 | 0.64 |
| 1:O:131:VAL:N | 1:O:178:LEU:O | 2.26 | 0.64 |
| 1:N:31:TYR:HA | 1:N:50:THR:OG1 | 1.98 | 0.64 |
| 2:I:204:ALA:O | 2:I:206:SER:N | 2.29 | 0.64 |
| 2:K:69:ARG:HH11 | 2:K:89:ARG:NH2 | 1.93 | 0.64 |
| 2:J:191:TRP:CD1 | 2:J:192:PRO:HA | 2.33 | 0.64 |
| 2:J:38:ARG:HB2 | 2:J:96:TYR:HE2 | 1.60 | 0.64 |
| 2:K:51:ILE:HD13 | 2:K:74:ARG:HD2 | 1.79 | 0.64 |
| 2:J:60:ILE:C | 2:J:61:HIS:CD2 | 2.71 | 0.64 |
| 1:N:149:ILE:HG23 | 1:N:191:TYR:HE2 | 1.55 | 0.64 |
| 2:J:191:TRP:HA | 2:J:193:SER:N | 2.13 | 0.64 |
| 2:J:26:GLY:O | 2:J:27:PHE:HB3 | 1.97 | 0.64 |
| 2:H:138:MET:HE3 | 2:H:187:PRO:HA | 1.80 | 0.64 |
| 2:I:43:LYS:HB3 | 4:I:237:HOH:O | 1.97 | 0.64 |
| 1:M:147:TRP:O | 1:M:154:ARG:N | 2.31 | 0.64 |
| 2:J:51:ILE:CD1 | 2:J:74:ARG:HG3 | 2.26 | 0.64 |
| 2:H:69:ARG:O | 2:H:86:ASN:HB2 | 1.98 | 0.64 |
| 3:Y:124:PRO:O | 3:Y:125:ASN:C | 2.35 | 0.64 |
| 2:I:93:THR:HG1 | 2:I:114:VAL:H | 1.46 | 0.64 |
| 1:N:160:ASN:OD1 | 1:N:176:SER:OG | 2.10 | 0.64 |
| 3:Z:25:ARG:HG2 | 3:Z:28:GLN:OE1 | 1.98 | 0.64 |
| 3:Z:31:GLU:HB3 | 3:Z:33:HIS:CE1 | 2.33 | 0.64 |
| 1:L:14:SER:HB2 | 1:L:17:GLU:OE1 | 1.98 | 0.64 |
| 1:N:19:VAL:HG21 | 1:N:103:LEU:HD21 | 1.79 | 0.64 |
| 2:J:51:ILE:O | 2:J:52:ARG:O | 2.16 | 0.64 |
| 2:J:144:LEU:HD12 | 2:J:145:VAL:H | 1.62 | 0.64 |
| 1:M:60:ARG:HH12 | 1:M:81:ASP:CG | 2.00 | 0.64 |
| 2:J:191:TRP:CG | 2:J:192:PRO:HA | 2.32 | 0.64 |
| 1:M:22:THR:CG2 | 1:M:23:CYS:N | 2.62 | 0.63 |
| 3:V:41:LEU:O | 3:V:118:THR:HB | 1.98 | 0.63 |
| 1:O:189:ASN:HA | 1:O:210:ARG:HB2 | 1.80 | 0.63 |
| 1:M:61:PHE:CE1 | 1:M:74:ILE:CG1 | 2.81 | 0.63 |
| 2:J:20:LEU:CD1 | 2:J:96:TYR:HD1 | 2.00 | 0.63 |
| 2:J:51:ILE:CD1 | 2:J:74:ARG:HG2 | 2.23 | 0.63 |
| 2:H:70:PHE:CZ | 2:H:85:MET:HE1 | 2.33 | 0.63 |
| 2:I:57:ASN:O | 2:I:59:ALA:N | 2.31 | 0.63 |
| 3:Z:132:GLN:HA | 3:Z:135:LEU:HD12 | 1.80 | 0.63 |
| 1:L:89:GLN:HE21 | 1:L:96:THR:HB | 1.62 | 0.63 |
| 3:V:39:VAL:HG21 | 3:V:77:ALA:HB2 | 1.80 | 0.63 |
| 3:Y:134:LEU:O | 3:Y:139:VAL:N | 2.29 | 0.63 |
| 1:N:14:SER:N | 1:N:17:GLU:OE1 | 2.23 | 0.63 |
| 2:I:151:GLU:CB | 2:I:152:PRO:HA | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:K:69:ARG:NH2 | 2:K:92:ASP:OD2 | 2.31 | 0.63 |
| 1:L:7:SER:HB2 | 1:L:22:THR:CG2 | 2.28 | 0.63 |
| 2:H:38:ARG:NH2 | 2:H:70:PHE:HE2 | 1.95 | 0.63 |
| 2:H:46:GLU:HG3 | 2:H:46:GLU:O | 1.97 | 0.63 |
| 3:Y:116:GLY:O | 3:Y:118:THR:CG2 | 2.44 | 0.63 |
| 1:L:30:SER:HB3 | 1:L:31:TYR:CD2 | 2.33 | 0.63 |
| 3:Z:101:LEU:CD1 | 3:Z:105:GLN:NE2 | 2.62 | 0.63 |
| 2:K:88:LEU:HB3 | 2:K:114:VAL:HG11 | 1.81 | 0.63 |
| 3:Y:100:LEU:HD22 | 3:Y:100:LEU:O | 1.99 | 0.63 |
| 1:M:117:PHE:N | 1:M:117:PHE:HD1 | 1.96 | 0.63 |
| 1:M:11:MET:CE | 1:M:19:VAL:HG22 | 2.29 | 0.63 |
| 1:O:41:THR:HA | 4:O:226:HOH:O | 1.98 | 0.63 |
| 1:O:6:GLN:NE2 | 1:O:87:CYS:H | 1.95 | 0.63 |
| 2:K:51:ILE:CD1 | 2:K:74:ARG:HG2 | 2.29 | 0.63 |
| 2:I:173:LEU:HD22 | 2:I:176:ASP:HA | 1.79 | 0.63 |
| 3:V:42:PRO:CD | 3:V:70:LEU:HD23 | 2.29 | 0.63 |
| 1:N:35:PHE:N | 1:N:35:PHE:HD1 | 1.93 | 0.63 |
| 1:M:14:SER:O | 1:M:17:GLU:HB3 | 1.99 | 0.63 |
| 3:Z:110:THR:O | 3:Z:110:THR:CG2 | 2.47 | 0.63 |
| 3:Z:64:LEU:HD11 | 3:Z:105:GLN:HE21 | 1.63 | 0.63 |
| 3:Z:71:LEU:HD11 | 3:Z:98:ARG:HG2 | 1.81 | 0.63 |
| 1:L:135:LEU:HD23 | 1:L:143:ILE:HD12 | 1.80 | 0.63 |
| 2:J:124:VAL:HG11 | 2:J:200:VAL:CG2 | 2.27 | 0.63 |
| 2:H:145:VAL:HG11 | 2:H:180:LEU:HD22 | 1.79 | 0.63 |
| 1:N:188:HIS:O | 1:N:210:ARG:NH1 | 2.31 | 0.63 |
| 1:M:188:HIS:O | 1:M:210:ARG:HD2 | 1.98 | 0.62 |
| 1:M:33:TYR:HD2 | 1:M:33:TYR:N | 1.93 | 0.62 |
| 3:X:69:LEU:HD22 | 4:X:167:HOH:O | 1.98 | 0.62 |
| 1:O:150:ASP:OD2 | 1:O:188:HIS:CB | 2.28 | 0.62 |
| 1:L:88:GLN:HG2 | 1:L:89:GLN:N | 2.13 | 0.62 |
| 1:M:190:SER:O | 1:M:191:TYR:CG | 2.53 | 0.62 |
| 2:H:153:VAL:HG23 | 2:H:202:HIS:HB2 | 1.80 | 0.62 |
| 3:Z:71:LEU:CD1 | 3:Z:101:LEU:CD2 | 2.77 | 0.62 |
| 1:L:107:ARG:HD3 | 1:L:139:TYR:CB | 2.29 | 0.62 |
| 1:L:144:ASN:HB2 | 1:L:196:THR:O | 1.98 | 0.62 |
| 1:L:120:SER:O | 1:L:124:LEU:HD22 | 1.99 | 0.62 |
| 1:O:44:LYS:CB | 1:O:44:LYS:NZ | 2.61 | 0.62 |
| 1:M:37:GLN:HB2 | 1:M:43:PRO:HA | 1.81 | 0.62 |
| 1:O:203:PRO:O | 1:O:205:VAL:HG23 | 1.99 | 0.62 |
| 1:N:132:VAL:HG11 | 2:J:127:LEU:HD13 | 1.81 | 0.62 |
| 1:O:119:PRO:HG3 | 1:O:130:SER:N | 2.14 | 0.62 |
| 2:I:215:PRO:O | 3:Y:120:ALA:HB3 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:124:LEU:O | 1:O:125:THR:C | 2.36 | 0.62 |
| 1:O:49:SER:O | 1:O:51:SER:N | 2.32 | 0.62 |
| 1:L:7:SER:HB2 | 1:L:22:THR:HB | 1.82 | 0.62 |
| 2:H:176:ASP:HB3 | 4:H:226:HOH:O | 1.97 | 0.62 |
| 2:J:64:GLU:HG2 | 2:J:67:LYS:NZ | 2.15 | 0.62 |
| 3:V:93:LEU:O | 3:V:96:GLN:HB2 | 2.00 | 0.62 |
| 1:O:8:PRO:O | 1:O:101:THR:HG23 | 2.00 | 0.62 |
| 1:M:6:GLN:CG | 1:M:23:CYS:HB2 | 2.17 | 0.62 |
| 1:O:6:GLN:NE2 | 1:O:86:TYR:HA | 2.13 | 0.62 |
| 2:I:120:THR:HG21 | 2:I:177:LEU:HD13 | 1.80 | 0.62 |
| 1:M:78:GLU:O | 1:M:79:ALA:C | 2.38 | 0.62 |
| 3:V:40:LEU:N | 3:V:40:LEU:HD23 | 2.15 | 0.62 |
| 1:M:132:VAL:HG23 | 1:M:133:CYS:N | 2.14 | 0.62 |
| 1:O:120:SER:O | 1:O:123:GLN:N | 2.33 | 0.62 |
| 2:K:147:GLY:C | 2:K:177:LEU:HD13 | 2.20 | 0.62 |
| 1:M:162:TRP:HE3 | 1:M:162:TRP:H | 1.47 | 0.62 |
| 2:I:202:HIS:CE1 | 2:I:204:ALA:HB3 | 2.35 | 0.62 |
| 3:Z:111:GLN:O | 3:Z:112:LEU:HD13 | 2.00 | 0.61 |
| 1:N:72:LEU:CD2 | 1:N:72:LEU:C | 2.64 | 0.61 |
| 2:I:216:ARG:NH2 | 3:Y:121:HIS:HA | 2.15 | 0.61 |
| 2:K:172:VAL:O | 2:K:178:TYR:HA | 1.99 | 0.61 |
| 2:H:95:ILE:HD13 | 2:H:111:LEU:CD2 | 2.30 | 0.61 |
| 2:H:38:ARG:HH21 | 2:H:70:PHE:HE2 | 1.48 | 0.61 |
| 1:O:149:ILE:HG23 | 1:O:191:TYR:CE2 | 2.34 | 0.61 |
| 2:J:51:ILE:HD13 | 2:J:74:ARG:HG3 | 1.79 | 0.61 |
| 3:Y:22:LEU:HD12 | 3:Y:96:GLN:OE1 | 1.98 | 0.61 |
| 1:M:111:ALA:CB | 1:M:199:THR:HG21 | 2.30 | 0.61 |
| 1:M:185:TYR:HA | 1:M:191:TYR:OH | 2.01 | 0.61 |
| 3:Y:134:LEU:O | 3:Y:139:VAL:HB | 2.01 | 0.61 |
| 2:J:74:ARG:NE | 2:J:76:ASP:OD1 | 2.29 | 0.61 |
| 2:K:9:GLY:HA2 | 2:K:112:VAL:HG22 | 1.83 | 0.61 |
| 2:K:166:VAL:HG12 | 2:K:184:VAL:HG23 | 1.82 | 0.61 |
| 2:H:51:ILE:HD12 | 2:H:74:ARG:HG2 | 1.82 | 0.61 |
| 3:V:51:TRP:CZ2 | 3:V:138:LYS:HG2 | 2.36 | 0.61 |
| 1:M:119:PRO:HD3 | 1:M:131:VAL:CG2 | 2.30 | 0.61 |
| 1:L:169:ASP:OD2 | 1:L:171:THR:HG23 | 2.00 | 0.61 |
| 1:O:95:ARG:HG3 | 2:K:47:TRP:CG | 2.35 | 0.61 |
| 2:J:62:TYR:OH | 2:J:71:THR:HA | 2.00 | 0.61 |
| 1:L:116:ILE:HD12 | 1:L:193:CYS:HB3 | 1.83 | 0.61 |
| 1:O:19:VAL:HG12 | 1:O:74:ILE:CB | 2.31 | 0.61 |
| 2:K:101:TRP:CD1 | 3:Z:111:GLN:HB3 | 2.35 | 0.61 |
| 2:I:149:PHE:HB2 | 2:I:177:LEU:HD21 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:O:185:TYR:CE1 | 1:O:191:TYR:HE1 | 2.17 | 0.61 |
| 1:N:36:GLN:NE2 | 1:N:85:TYR:OH | 2.34 | 0.61 |
| 1:O:202:SER:O | 1:O:203:PRO:C | 2.39 | 0.61 |
| 3:Z:43:ALA:CB | 3:Z:119:THR:HG23 | 2.30 | 0.61 |
| 1:L:60:ARG:NH1 | 1:L:81:ASP:OD1 | 2.33 | 0.61 |
| 1:O:33:TYR:N | 1:O:33:TYR:HD1 | 1.97 | 0.61 |
| 3:Z:94:SER:OG | 3:Z:95:GLY:N | 2.32 | 0.61 |
| 1:M:123:GLN:NE2 | 1:M:130:SER:HG | 1.98 | 0.61 |
| 2:K:29:PHE:CD2 | 2:K:79:SER:HA | 2.36 | 0.61 |
| 2:I:29:PHE:HE2 | 2:I:76:ASP:HA | 1.66 | 0.61 |
| 3:Y:10:ARG:HA | 3:Y:13:SER:CB | 2.31 | 0.61 |
| 1:L:35:PHE:N | 1:L:35:PHE:HD1 | 1.98 | 0.61 |
| 2:H:151:GLU:HG2 | 2:H:152:PRO:HA | 1.82 | 0.61 |
| 3:V:33:HIS:HB3 | 3:V:34:PRO:HD2 | 1.82 | 0.61 |
| 2:J:129:PRO:HD2 | 2:J:191:TRP:HH2 | 1.64 | 0.60 |
| 1:M:136:ASN:HA | 1:M:173:SER:HB3 | 1.82 | 0.60 |
| 1:N:211:ASN:ND2 | 1:N:212:GLU:H | 1.98 | 0.60 |
| 1:L:189:ASN:ND2 | 1:L:211:ASN:OD1 | 2.34 | 0.60 |
| 1:L:84:THR:CG2 | 1:L:85:TYR:N | 2.64 | 0.60 |
| 3:V:102:GLY:O | 3:V:104:LEU:N | 2.35 | 0.60 |
| 1:M:70:TYR:O | 1:M:71:SER:HB3 | 2.02 | 0.60 |
| 1:M:6:GLN:NE2 | 1:M:87:CYS:H | 1.98 | 0.60 |
| 2:H:101:TRP:HB2 | 2:H:104:LEU:HB3 | 1.83 | 0.60 |
| 3:V:64:LEU:CD1 | 3:V:105:GLN:HG3 | 2.32 | 0.60 |
| 1:M:147:TRP:CG | 1:M:178:LEU:HD12 | 2.35 | 0.60 |
| 2:I:33:TRP:CE2 | 2:I:52:ARG:HG3 | 2.37 | 0.60 |
| 1:M:6:GLN:OE1 | 1:M:100:GLY:HA2 | 2.01 | 0.60 |
| 1:M:185:TYR:CE1 | 1:M:191:TYR:CE1 | 2.89 | 0.60 |
| 1:N:149:ILE:CG2 | 1:N:191:TYR:HE2 | 2.14 | 0.60 |
| 1:O:182:LYS:HD3 | 1:O:186:GLU:CD | 2.22 | 0.60 |
| 1:N:54:ALA:O | 1:N:57:VAL:HG23 | 2.01 | 0.60 |
| 2:I:61:HIS:CD2 | 2:I:61:HIS:N | 2.68 | 0.60 |
| 3:Z:61:GLN:HG3 | 3:Z:108:LEU:HD13 | 1.83 | 0.60 |
| 1:N:130:SER:HB3 | 1:N:179:THR:OG1 | 2.02 | 0.60 |
| 2:K:62:TYR:CE1 | 2:K:72:VAL:HG12 | 2.37 | 0.60 |
| 2:H:52:ARG:O | 2:H:58:HIS:HA | 2.00 | 0.60 |
| 3:Z:94:SER:O | 3:Z:98:ARG:HG3 | 2.02 | 0.60 |
| 1:M:70:TYR:N | 1:M:70:TYR:HD1 | 1.99 | 0.60 |
| 2:I:125:TYR:N | 2:I:144:LEU:O | 2.30 | 0.60 |
| 3:Z:31:GLU:OE1 | 3:Z:33:HIS:HE1 | 1.85 | 0.60 |
| 2:K:49:ALA:HA | 2:K:61:HIS:O | 2.02 | 0.60 |
| 1:L:29:VAL:HG11 | 1:L:91:SER:CB | 2.20 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:189:SER:HB3 | 4:H:224:HOH:O | 1.78 | 0.60 |
| 2:H:153:VAL:CG1 | 2:H:180:LEU:HD13 | 2.32 | 0.60 |
| 2:I:57:ASN:O | 2:I:58:HIS:C | 2.38 | 0.60 |
| 1:M:189:ASN:O | 1:M:209:ASN:HA | 2.02 | 0.60 |
| 3:Y:91:GLY:O | 3:Y:92:GLN:C | 2.38 | 0.60 |
| 1:O:53:LEU:HD22 | 1:O:57:VAL:HG11 | 1.83 | 0.60 |
| 3:X:23:HIS:CD2 | 3:X:23:HIS:O | 2.55 | 0.60 |
| 3:X:22:LEU:HD21 | 3:X:92:GLN:HE21 | 1.66 | 0.60 |
| 1:N:38:LYS:HD3 | 1:N:83:ALA:HB2 | 1.84 | 0.59 |
| 2:K:70:PHE:CD1 | 2:K:85:MET:HA | 2.37 | 0.59 |
| 1:M:118:PRO:HB3 | 1:M:208:PHE:CZ | 2.36 | 0.59 |
| 2:J:124:VAL:HA | 2:J:144:LEU:O | 2.03 | 0.59 |
| 1:O:185:TYR:CE1 | 1:O:191:TYR:CE1 | 2.90 | 0.59 |
| 2:H:84:GLN:HE21 | 2:H:84:GLN:HA | 1.66 | 0.59 |
| 2:K:199:ASN:HA | 2:K:208:LYS:O | 2.02 | 0.59 |
| 2:I:202:HIS:ND1 | 2:I:204:ALA:HB3 | 2.16 | 0.59 |
| 2:H:158:ASN:ND2 | 2:H:197:THR:H | 2.00 | 0.59 |
| 2:I:106:TRP:HA | 4:I:235:HOH:O | 2.01 | 0.59 |
| 3:V:100:LEU:HD22 | 3:V:104:LEU:CD1 | 2.33 | 0.59 |
| 3:X:12:LEU:HG | 3:X:12:LEU:O | 1.92 | 0.59 |
| 2:K:66:VAL:CG1 | 2:K:70:PHE:H | 2.16 | 0.59 |
| 3:Y:124:PRO:C | 3:Y:126:ALA:N | 2.52 | 0.59 |
| 1:L:106:LYS:O | 1:L:106:LYS:HG3 | 2.02 | 0.59 |
| 2:H:169:PHE:O | 4:H:233:HOH:O | 2.17 | 0.59 |
| 3:V:61:GLN:CD | 3:V:112:LEU:HD21 | 2.22 | 0.59 |
| 2:H:66:VAL:CG1 | 2:H:70:PHE:HB2 | 2.33 | 0.59 |
| 3:Y:136:ARG:NH1 | 3:Y:136:ARG:HB2 | 2.16 | 0.59 |
| 2:I:216:ARG:HE | 3:Y:122:LYS:N | 1.96 | 0.59 |
| 1:L:175:SER:N | 2:H:169:PHE:CE1 | 2.70 | 0.59 |
| 1:O:169:ASP:O | 1:O:169:ASP:OD2 | 2.19 | 0.59 |
| 2:J:57:ASN:O | 2:J:59:ALA:N | 2.36 | 0.59 |
| 3:Y:41:LEU:HD12 | 3:Y:121:HIS:CD2 | 2.38 | 0.59 |
| 1:N:33:TYR:HD2 | 1:N:48:TYR:HA | 1.67 | 0.59 |
| 2:I:33:TRP:HD1 | 2:I:53:SER:HB2 | 1.66 | 0.59 |
| 3:X:95:GLY:O | 3:X:98:ARG:HB2 | 2.02 | 0.59 |
| 3:Z:51:TRP:CH2 | 3:Z:138:LYS:HD3 | 2.37 | 0.59 |
| 2:K:66:VAL:CG1 | 2:K:70:PHE:CD2 | 2.86 | 0.59 |
| 2:K:37:VAL:HG13 | 2:K:46:GLU:O | 2.02 | 0.59 |
| 2:K:216:ARG:HH21 | 3:V:123:ASP:H | 1.49 | 0.59 |
| 1:N:147:TRP:CD1 | 1:N:158:VAL:CG1 | 2.85 | 0.59 |
| 2:K:202:HIS:HB3 | 2:K:206:SER:OG | 2.03 | 0.59 |
| 2:K:148:TYR:CE1 | 2:K:178:TYR:HB3 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:29:PHE:C | 2:H:29:PHE:CD2 | 2.75 | 0.59 |
| 3:Z:118:THR:O | 3:Z:119:THR:CG2 | 2.50 | 0.59 |
| 2:J:84:GLN:HE21 | 2:J:85:MET:N | 2.00 | 0.59 |
| 3:Y:136:ARG:HH11 | 3:Y:136:ARG:CB | 2.14 | 0.59 |
| 1:M:20:THR:HB | 1:M:73:THR:HG1 | 1.66 | 0.59 |
| 1:M:180:LEU:N | 1:M:180:LEU:HD12 | 2.17 | 0.59 |
| 3:Y:100:LEU:HD22 | 3:Y:104:LEU:HD11 | 1.85 | 0.59 |
| 1:N:123:GLN:HG3 | 2:J:125:TYR:CE2 | 2.38 | 0.59 |
| 2:I:158:ASN:O | 2:I:159:SER:C | 2.40 | 0.59 |
| 2:H:37:VAL:HG22 | 2:H:47:TRP:HA | 1.83 | 0.59 |
| 3:V:143:MET:HB2 | 3:V:149:THR:HG21 | 1.84 | 0.59 |
| 2:J:217:ASP:OD1 | 3:X:121:HIS:CE1 | 2.55 | 0.59 |
| 1:O:148:LYS:HA | 1:O:153:GLU:HA | 1.83 | 0.59 |
| 3:V:125:ASN:ND2 | 3:V:125:ASN:N | 2.51 | 0.59 |
| 1:M:88:GLN:HB2 | 1:M:97:PHE:CD1 | 2.38 | 0.59 |
| 2:H:138:MET:HE2 | 2:H:185:THR:CG2 | 2.33 | 0.59 |
| 3:Y:48:LEU:HB2 | 3:Y:51:TRP:HB3 | 1.85 | 0.59 |
| 1:M:192:THR:CA | 1:M:207:SER:OG | 2.51 | 0.58 |
| 2:I:148:TYR:O | 2:I:177:LEU:HD22 | 2.04 | 0.58 |
| 1:L:89:GLN:CG | 1:L:96:THR:HB | 2.33 | 0.58 |
| 2:J:56:ASN:N | 2:J:56:ASN:HD22 | 2.01 | 0.58 |
| 2:H:56:ASN:N | 2:H:56:ASN:ND2 | 2.50 | 0.58 |
| 1:O:48:TYR:CE2 | 3:Z:113:PRO:HG2 | 2.38 | 0.58 |
| 3:Y:70:LEU:HD22 | 3:Y:74:VAL:HG23 | 1.84 | 0.58 |
| 3:X:61:GLN:O | 3:X:62:ASP:C | 2.42 | 0.58 |
| 3:X:64:LEU:HD22 | 3:X:108:LEU:HD12 | 1.85 | 0.58 |
| 1:N:78:GLU:O | 1:N:81:ASP:HB2 | 2.03 | 0.58 |
| 2:I:148:TYR:CZ | 2:I:178:TYR:HB3 | 2.39 | 0.58 |
| 3:Z:118:THR:O | 3:Z:119:THR:HG22 | 2.03 | 0.58 |
| 1:L:14:SER:O | 1:L:17:GLU:HB3 | 2.03 | 0.58 |
| 1:O:154:ARG:NH2 | 1:O:184:GLU:OE1 | 2.35 | 0.58 |
| 2:J:70:PHE:CD1 | 2:J:85:MET:CB | 2.86 | 0.58 |
| 2:H:102:SER:O | 2:H:103:PHE:HB2 | 2.02 | 0.58 |
| 3:V:71:LEU:HD11 | 3:V:98:ARG:HG3 | 1.84 | 0.58 |
| 1:O:19:VAL:HG11 | 1:O:74:ILE:CD1 | 2.29 | 0.58 |
| 3:Y:100:LEU:HD12 | 3:Y:131:PHE:HE1 | 1.67 | 0.58 |
| 1:L:93:TYR:HE1 | 1:L:95:ARG:NH1 | 2.00 | 0.58 |
| 1:M:11:MET:HE2 | 1:M:19:VAL:HG22 | 1.84 | 0.58 |
| 2:H:216:ARG:HH22 | 3:Z:123:ASP:HB2 | 1.68 | 0.58 |
| 2:I:37:VAL:HG21 | 2:I:106:TRP:HH2 | 1.68 | 0.58 |
| 1:L:65:GLY:HA3 | 1:L:70:TYR:HA | 1.86 | 0.58 |
| 1:O:189:ASN:O | 1:O:210:ARG:N | 2.32 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:61:HIS:N | 2:J:61:HIS:CD2 | 2.70 | 0.58 |
| 1:L:153:GLU:HG2 | 1:L:155:GLN:HG2 | 1.86 | 0.58 |
| 2:H:191:TRP:CG | 2:H:192:PRO:HA | 2.39 | 0.58 |
| 1:M:70:TYR:N | 1:M:70:TYR:CD1 | 2.70 | 0.58 |
| 3:X:135:LEU:HA | 3:X:139:VAL:HB | 1.85 | 0.58 |
| 2:I:139:VAL:CG1 | 2:I:141:LEU:HD21 | 2.34 | 0.58 |
| 2:J:216:ARG:HG3 | 3:X:122:LYS:CG | 2.33 | 0.58 |
| 3:Y:12:LEU:HB3 | 3:Y:143:MET:SD | 2.44 | 0.58 |
| 3:V:67:VAL:O | 3:V:70:LEU:N | 2.36 | 0.58 |
| 1:M:88:GLN:HG2 | 1:M:89:GLN:N | 2.18 | 0.58 |
| 2:K:64:GLU:HG2 | 2:K:67:LYS:HD2 | 1.86 | 0.58 |
| 1:N:77:MET:CE | 1:N:81:ASP:CB | 2.77 | 0.58 |
| 2:I:29:PHE:CD2 | 2:I:79:SER:HA | 2.39 | 0.58 |
| 1:N:147:TRP:O | 1:N:154:ARG:N | 2.34 | 0.58 |
| 1:M:78:GLU:OE2 | 1:N:107:ARG:NH2 | 2.37 | 0.58 |
| 3:Z:119:THR:HG1 | 3:Z:121:HIS:HE2 | 1.47 | 0.58 |
| 1:O:61:PHE:HZ | 1:O:85:TYR:OH | 1.87 | 0.58 |
| 1:M:22:THR:CG2 | 1:M:23:CYS:H | 2.17 | 0.58 |
| 1:O:185:TYR:HD1 | 1:O:191:TYR:CE1 | 2.22 | 0.58 |
| 1:N:154:ARG:NH2 | 1:N:184:GLU:OE1 | 2.37 | 0.58 |
| 3:Y:41:LEU:HD12 | 3:Y:121:HIS:HD2 | 1.69 | 0.58 |
| 2:I:214:VAL:HG11 | 3:Y:40:LEU:HD21 | 1.86 | 0.58 |
| 2:H:20:LEU:HD23 | 2:H:20:LEU:N | 2.19 | 0.58 |
| 2:H:88:LEU:HB3 | 2:H:114:VAL:HG11 | 1.86 | 0.58 |
| 1:L:147:TRP:CD2 | 1:L:178:LEU:HD12 | 2.39 | 0.58 |
| 1:L:205:VAL:HG12 | 1:L:206:LYS:N | 2.19 | 0.58 |
| 1:O:44:LYS:HZ2 | 1:O:44:LYS:HB2 | 1.68 | 0.58 |
| 2:J:123:SER:N | 2:J:146:LYS:O | 2.37 | 0.58 |
| 2:H:120:THR:O | 2:H:148:TYR:HA | 2.03 | 0.58 |
| 1:N:139:TYR:CD2 | 1:N:140:PRO:HA | 2.37 | 0.58 |
| 1:L:65:GLY:CA | 1:L:70:TYR:HA | 2.34 | 0.57 |
| 3:X:70:LEU:O | 3:X:74:VAL:HG23 | 2.04 | 0.57 |
| 2:H:166:VAL:CG2 | 2:H:166:VAL:O | 2.51 | 0.57 |
| 1:O:77:MET:CE | 1:O:78:GLU:O | 2.51 | 0.57 |
| 2:K:56:ASN:O | 2:K:57:ASN:HB2 | 2.03 | 0.57 |
| 2:K:89:ARG:O | 2:K:114:VAL:HG21 | 2.03 | 0.57 |
| 2:H:114:VAL:O | 2:H:114:VAL:HG23 | 2.03 | 0.57 |
| 3:V:13:SER:O | 3:V:17:ARG:HD3 | 2.05 | 0.57 |
| 1:O:66:SER:C | 1:O:70:TYR:HE1 | 2.07 | 0.57 |
| 1:L:131:VAL:O | 1:L:147:TRP:CZ2 | 2.58 | 0.57 |
| 1:M:72:LEU:HD23 | 1:M:72:LEU:C | 2.25 | 0.57 |
| 3:V:145:VAL:HG13 | 3:V:145:VAL:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:120:SER:C | 1:M:122:GLU:H | 2.07 | 0.57 |
| 1:N:6:GLN:NE2 | 1:N:86:TYR:HA | 2.14 | 0.57 |
| 2:K:166:VAL:HG12 | 2:K:184:VAL:CG2 | 2.35 | 0.57 |
| 3:Z:22:LEU:HD11 | 3:Z:92:GLN:HB3 | 1.87 | 0.57 |
| 2:J:189:SER:O | 2:J:193:SER:HB2 | 2.04 | 0.57 |
| 1:M:84:THR:HA | 1:M:101:THR:O | 2.04 | 0.57 |
| 1:M:211:ASN:C | 1:M:212:GLU:HG3 | 2.25 | 0.57 |
| 1:N:149:ILE:CG2 | 1:N:191:TYR:CE2 | 2.81 | 0.57 |
| 3:V:87:SER:O | 3:V:89:LEU:N | 2.37 | 0.57 |
| 1:N:88:GLN:NE2 | 1:N:90:ARG:HH11 | 2.03 | 0.57 |
| 2:I:157:TRP:O | 2:I:158:ASN:HB2 | 2.04 | 0.57 |
| 3:V:143:MET:HB3 | 3:V:149:THR:HB | 1.87 | 0.57 |
| 1:O:116:ILE:CG1 | 1:O:133:CYS:SG | 2.89 | 0.57 |
| 1:O:132:VAL:HB | 1:O:177:THR:CG2 | 2.34 | 0.57 |
| 2:I:92:ASP:O | 2:I:96:TYR:OH | 2.17 | 0.57 |
| 1:L:10:ILE:HG12 | 1:L:102:LYS:HB3 | 1.85 | 0.57 |
| 1:M:91:SER:HB2 | 4:M:228:HOH:O | 2.04 | 0.57 |
| 3:Y:75:MET:SD | 3:Y:98:ARG:NH2 | 2.77 | 0.57 |
| 3:Y:12:LEU:O | 3:Y:16:LEU:HB2 | 2.05 | 0.57 |
| 1:N:207:SER:OG | 1:N:208:PHE:N | 2.35 | 0.57 |
| 3:V:41:LEU:HD22 | 3:V:127:ILE:HB | 1.86 | 0.57 |
| 3:V:41:LEU:HD11 | 3:V:127:ILE:HG22 | 1.86 | 0.57 |
| 1:M:35:PHE:N | 1:M:35:PHE:CD1 | 2.72 | 0.57 |
| 2:I:51:ILE:CD1 | 2:I:74:ARG:HG3 | 2.35 | 0.57 |
| 2:I:22:CYS:O | 2:I:80:SER:CB | 2.51 | 0.57 |
| 1:O:77:MET:CE | 1:O:81:ASP:HB2 | 2.33 | 0.57 |
| 2:H:9:GLY:HA2 | 2:H:112:VAL:HG22 | 1.86 | 0.57 |
| 2:H:36:TRP:CH2 | 2:H:98:CYS:HB2 | 2.40 | 0.57 |
| 2:J:172:VAL:O | 2:J:178:TYR:HA | 2.04 | 0.57 |
| 1:M:115:SER:O | 1:M:133:CYS:HA | 2.04 | 0.57 |
| 2:K:29:PHE:HZ | 2:K:81:VAL:HB | 1.69 | 0.57 |
| 2:J:124:VAL:CG1 | 2:J:200:VAL:HG21 | 2.28 | 0.57 |
| 1:L:117:PHE:CD1 | 1:L:117:PHE:N | 2.70 | 0.57 |
| 1:O:135:LEU:HD21 | 1:O:195:ALA:HB2 | 1.87 | 0.57 |
| 1:O:2:VAL:O | 1:O:96:THR:HG21 | 2.04 | 0.57 |
| 2:K:22:CYS:HB3 | 2:K:81:VAL:HG12 | 1.87 | 0.57 |
| 1:M:45:LEU:CD2 | 1:M:45:LEU:C | 2.73 | 0.57 |
| 3:V:12:LEU:HD21 | 3:V:140:ARG:HH21 | 1.70 | 0.57 |
| 1:L:105:ILE:HG13 | 1:L:106:LYS:H | 1.68 | 0.57 |
| 2:J:64:GLU:HG2 | 2:J:67:LYS:HZ2 | 1.70 | 0.57 |
| 1:L:173:SER:HB2 | 4:L:221:HOH:O | 2.03 | 0.57 |
| 3:Z:86:LEU:HD22 | 3:Z:90:LEU:HG | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:Z:64:LEU:CD1 | 3:Z:105:GLN:HE21 | 2.18 | 0.57 |
| 3:Y:124:PRO:C | 3:Y:126:ALA:H | 2.08 | 0.57 |
| 2:J:129:PRO:HD2 | 2:J:191:TRP:CH2 | 2.40 | 0.57 |
| 1:L:77:MET:HG3 | 1:L:78:GLU:N | 2.20 | 0.57 |
| 1:M:106:LYS:HG3 | 1:M:106:LYS:O | 2.03 | 0.57 |
| 2:I:139:VAL:HG11 | 2:I:141:LEU:HD21 | 1.87 | 0.56 |
| 2:J:130:GLY:O | 2:J:133:ALA:HA | 2.04 | 0.56 |
| 1:O:51:SER:HB3 | 1:O:63:GLY:O | 2.05 | 0.56 |
| 1:O:145:VAL:HG21 | 1:O:174:MET:HE2 | 1.87 | 0.56 |
| 1:M:185:TYR:CD1 | 1:M:191:TYR:CE1 | 2.93 | 0.56 |
| 3:X:78:ARG:HG3 | 3:X:90:LEU:HB3 | 1.86 | 0.56 |
| 1:N:189:ASN:HD22 | 1:N:210:ARG:N | 2.01 | 0.56 |
| 2:H:191:TRP:CD1 | 2:H:196:VAL:CG1 | 2.88 | 0.56 |
| 2:I:37:VAL:HG21 | 2:I:106:TRP:CH2 | 2.40 | 0.56 |
| 2:I:99:SER:HA | 4:I:235:HOH:O | 2.05 | 0.56 |
| 3:Y:85:CYS:O | 3:Y:88:SER:HB3 | 2.05 | 0.56 |
| 2:J:70:PHE:HD1 | 2:J:85:MET:CA | 2.11 | 0.56 |
| 1:O:19:VAL:HG12 | 1:O:74:ILE:CG1 | 2.36 | 0.56 |
| 1:L:185:TYR:O | 1:L:191:TYR:OH | 2.18 | 0.56 |
| 2:H:66:VAL:HG13 | 2:H:70:PHE:CG | 2.39 | 0.56 |
| 3:V:90:LEU:HD23 | 3:V:90:LEU:N | 2.15 | 0.56 |
| 1:N:89:GLN:HE21 | 1:N:96:THR:H | 1.52 | 0.56 |
| 2:H:51:ILE:CD1 | 2:H:74:ARG:CG | 2.83 | 0.56 |
| 1:O:7:SER:HB2 | 1:O:22:THR:HB | 1.87 | 0.56 |
| 1:O:145:VAL:HG11 | 1:O:176:SER:OG | 2.04 | 0.56 |
| 3:Y:144:LEU:O | 3:Y:146:GLY:N | 2.38 | 0.56 |
| 3:V:29:CYS:O | 3:V:30:PRO:O | 2.23 | 0.56 |
| 1:M:116:ILE:HD13 | 1:M:208:PHE:CD1 | 2.40 | 0.56 |
| 3:X:77:ALA:O | 3:X:78:ARG:C | 2.38 | 0.56 |
| 2:H:66:VAL:CG1 | 2:H:70:PHE:CG | 2.89 | 0.56 |
| 2:J:125:TYR:HB2 | 2:J:144:LEU:HB3 | 1.87 | 0.56 |
| 3:Z:107:LEU:CD2 | 3:Z:107:LEU:C | 2.73 | 0.56 |
| 2:K:213:ILE:HG12 | 2:K:214:VAL:H | 1.70 | 0.56 |
| 2:I:123:SER:O | 2:I:145:VAL:HA | 2.06 | 0.56 |
| 1:N:149:ILE:HG23 | 1:N:191:TYR:CD2 | 2.40 | 0.56 |
| 2:H:84:GLN:HE21 | 2:H:84:GLN:C | 2.08 | 0.56 |
| 1:M:181:THR:O | 1:M:182:LYS:C | 2.42 | 0.56 |
| 2:H:191:TRP:CD1 | 2:H:192:PRO:HA | 2.40 | 0.56 |
| 2:J:191:TRP:HA | 2:J:192:PRO:C | 2.25 | 0.56 |
| 3:Z:23:HIS:O | 3:Z:26:LEU:HB3 | 2.04 | 0.56 |
| 1:M:61:PHE:CE1 | 1:M:74:ILE:HG12 | 2.40 | 0.56 |
| 3:Y:73:GLY:HA2 | 3:Y:76:ALA:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:I:213:ILE:HG22 | 2:I:213:ILE:O | 2.05 | 0.56 |
| 1:L:147:TRP:HB3 | 1:L:178:LEU:HD12 | 1.88 | 0.56 |
| 1:L:213:CYS:HA | 3:Y:140:ARG:NH2 | 2.20 | 0.56 |
| 1:N:189:ASN:HD22 | 1:N:210:ARG:H | 1.49 | 0.56 |
| 2:H:33:TRP:N | 3:V:111:GLN:HE22 | 2.04 | 0.56 |
| 2:H:33:TRP:HD1 | 2:H:53:SER:HG | 1.53 | 0.56 |
| 1:L:2:VAL:HG23 | 4:L:232:HOH:O | 2.05 | 0.56 |
| 3:X:78:ARG:NH1 | 3:X:87:SER:OG | 2.34 | 0.56 |
| 1:N:77:MET:HE3 | 1:N:78:GLU:O | 2.06 | 0.56 |
| 2:H:90:ALA:HA | 2:H:114:VAL:CG2 | 2.36 | 0.56 |
| 1:L:164:ASP:O | 1:L:165:GLN:C | 2.40 | 0.56 |
| 1:M:124:LEU:O | 1:M:126:SER:N | 2.39 | 0.56 |
| 2:J:70:PHE:CD1 | 2:J:85:MET:CA | 2.88 | 0.56 |
| 1:N:119:PRO:HD2 | 1:N:131:VAL:CG2 | 2.36 | 0.56 |
| 1:M:48:TYR:CE1 | 3:X:113:PRO:CG | 2.82 | 0.56 |
| 2:I:74:ARG:HG2 | 2:I:74:ARG:HH11 | 1.71 | 0.56 |
| 2:I:22:CYS:HB3 | 2:I:81:VAL:O | 2.06 | 0.56 |
| 3:Z:101:LEU:CD1 | 3:Z:105:GLN:HE22 | 2.17 | 0.56 |
| 2:I:207:THR:O | 2:I:207:THR:OG1 | 2.24 | 0.56 |
| 1:O:132:VAL:HA | 1:O:177:THR:HA | 1.88 | 0.55 |
| 2:H:173:LEU:HD22 | 2:H:176:ASP:HA | 1.87 | 0.55 |
| 2:K:70:PHE:HD1 | 2:K:85:MET:HA | 1.71 | 0.55 |
| 1:N:90:ARG:O | 1:N:95:ARG:NH2 | 2.40 | 0.55 |
| 1:N:162:TRP:CD2 | 1:N:174:MET:HG3 | 2.41 | 0.55 |
| 2:H:138:MET:HA | 2:H:138:MET:HE3 | 1.86 | 0.55 |
| 1:M:174:MET:HG2 | 1:M:175:SER:N | 2.21 | 0.55 |
| 2:K:142:GLY:HA2 | 2:K:182:SER:O | 2.06 | 0.55 |
| 2:J:15:GLY:N | 2:J:88:LEU:O | 2.34 | 0.55 |
| 2:K:66:VAL:HG13 | 2:K:70:PHE:H | 1.72 | 0.55 |
| 2:K:70:PHE:CE1 | 2:K:85:MET:HB3 | 2.41 | 0.55 |
| 3:V:70:LEU:O | 3:V:74:VAL:HG23 | 2.06 | 0.55 |
| 3:Y:30:PRO:O | 3:Y:32:VAL:N | 2.39 | 0.55 |
| 1:O:76:ARG:HG2 | 1:O:76:ARG:NH1 | 2.20 | 0.55 |
| 2:J:20:LEU:N | 2:J:20:LEU:HD23 | 2.22 | 0.55 |
| 1:L:185:TYR:HD1 | 1:L:191:TYR:CE1 | 2.21 | 0.55 |
| 2:K:50:GLU:HG2 | 2:K:51:ILE:N | 2.21 | 0.55 |
| 2:H:153:VAL:HG12 | 2:H:180:LEU:HD13 | 1.89 | 0.55 |
| 1:M:53:LEU:HD11 | 1:M:61:PHE:O | 2.05 | 0.55 |
| 2:I:151:GLU:CG | 2:I:152:PRO:HA | 2.36 | 0.55 |
| 1:O:7:SER:OG | 1:O:8:PRO:HD3 | 2.06 | 0.55 |
| 3:Z:34:PRO:HA | 3:Z:124:PRO:HD2 | 1.89 | 0.55 |
| 1:L:154:ARG:CD | 1:L:156:ASN:O | 2.54 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:X:81:LEU:HD12 | 3:X:87:SER:CB | 2.34 | 0.55 |
| 2:J:90:ALA:N | 2:J:91:GLU:OE1 | 2.39 | 0.55 |
| 2:K:120:THR:O | 2:K:149:PHE:N | 2.35 | 0.55 |
| 3:V:147:GLY:O | 3:V:149:THR:N | 2.40 | 0.55 |
| 1:L:132:VAL:HB | 1:L:177:THR:HG23 | 1.89 | 0.55 |
| 1:O:90:ARG:HH21 | 2:K:102:SER:HB3 | 1.71 | 0.55 |
| 1:N:36:GLN:NE2 | 1:N:85:TYR:HE2 | 1.98 | 0.55 |
| 2:H:148:TYR:O | 2:H:178:TYR:HB2 | 2.06 | 0.55 |
| 1:O:108:ALA:O | 1:O:109:ASP:C | 2.43 | 0.55 |
| 1:L:3:VAL:H | 1:L:26:SER:CB | 2.20 | 0.55 |
| 1:L:114:VAL:HG12 | 1:L:115:SER:N | 2.20 | 0.55 |
| 1:M:114:VAL:HA | 1:M:134:PHE:O | 2.07 | 0.55 |
| 2:H:189:SER:O | 2:H:193:SER:OG | 2.19 | 0.55 |
| 1:M:116:ILE:CD1 | 1:M:208:PHE:HD1 | 2.20 | 0.55 |
| 2:K:51:ILE:HD11 | 2:K:74:ARG:CG | 2.36 | 0.55 |
| 3:Y:42:PRO:HD2 | 3:Y:130:SER:OG | 2.07 | 0.55 |
| 2:H:145:VAL:CG1 | 2:H:180:LEU:CD2 | 2.80 | 0.55 |
| 1:L:90:ARG:NH2 | 2:H:102:SER:O | 2.40 | 0.55 |
| 2:K:70:PHE:CZ | 2:K:85:MET:HE2 | 2.42 | 0.55 |
| 1:M:116:ILE:HD13 | 1:M:208:PHE:HD1 | 1.70 | 0.55 |
| 1:O:191:TYR:HB2 | 1:O:208:PHE:CE1 | 2.42 | 0.55 |
| 2:K:125:TYR:N | 2:K:144:LEU:O | 2.34 | 0.55 |
| 2:I:12:VAL:O | 2:I:114:VAL:HA | 2.07 | 0.55 |
| 1:O:147:TRP:HA | 1:O:192:THR:O | 2.06 | 0.55 |
| 3:Y:51:TRP:O | 3:Y:59:LYS:HD3 | 2.06 | 0.55 |
| 1:O:135:LEU:CD2 | 1:O:195:ALA:HB2 | 2.37 | 0.55 |
| 1:L:143:ILE:HG13 | 1:L:197:HIS:HD2 | 1.72 | 0.55 |
| 3:X:17:ARG:O | 3:X:21:VAL:HG23 | 2.05 | 0.55 |
| 3:Y:64:LEU:O | 3:Y:64:LEU:HD12 | 2.07 | 0.55 |
| 2:J:91:GLU:OE1 | 2:J:91:GLU:N | 2.40 | 0.55 |
| 2:J:85:MET:CE | 2:J:96:TYR:CZ | 2.86 | 0.55 |
| 3:Y:136:ARG:HH11 | 3:Y:136:ARG:HB2 | 1.70 | 0.55 |
| 2:K:175:SER:OG | 2:K:177:LEU:HB2 | 2.07 | 0.55 |
| 2:J:162:LEU:HD13 | 2:J:184:VAL:HG21 | 1.88 | 0.55 |
| 1:M:160:ASN:HB3 | 1:M:174:MET:CE | 2.37 | 0.55 |
| 1:M:7:SER:HB3 | 1:M:8:PRO:HD3 | 1.87 | 0.54 |
| 3:V:125:ASN:ND2 | 3:V:125:ASN:H | 2.06 | 0.54 |
| 2:H:4:LEU:HD12 | 2:H:107:GLY:H | 1.72 | 0.54 |
| 2:H:33:TRP:N | 3:V:111:GLN:NE2 | 2.53 | 0.54 |
| 1:O:69:SER:C | 1:O:70:TYR:CD1 | 2.77 | 0.54 |
| 1:M:111:ALA:HB2 | 1:M:199:THR:HG21 | 1.89 | 0.54 |
| 1:M:72:LEU:HD23 | 1:M:73:THR:N | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:N:189:ASN:ND2 | 1:N:209:ASN:HB3 | 2.22 | 0.54 |
| 1:N:197:HIS:ND1 | 1:N:199:THR:CB | 2.67 | 0.54 |
| 2:J:99:SER:OG | 2:J:103:PHE:HA | 2.06 | 0.54 |
| 2:J:36:TRP:HE1 | 2:J:81:VAL:HG22 | 1.73 | 0.54 |
| 1:N:137:ASN:N | 1:N:137:ASN:OD1 | 2.40 | 0.54 |
| 2:K:70:PHE:CD1 | 2:K:85:MET:CA | 2.90 | 0.54 |
| 3:X:125:ASN:O | 3:X:127:ILE:N | 2.41 | 0.54 |
| 3:Y:131:PHE:CE2 | 3:Y:135:LEU:HD11 | 2.42 | 0.54 |
| 2:I:148:TYR:O | 2:I:178:TYR:HB2 | 2.05 | 0.54 |
| 1:L:109:ASP:HA | 1:L:139:TYR:O | 2.08 | 0.54 |
| 2:H:138:MET:HE3 | 2:H:186:VAL:O | 2.07 | 0.54 |
| 1:M:124:LEU:C | 1:M:126:SER:H | 2.09 | 0.54 |
| 2:K:6:GLU:HA | 2:K:21:SER:O | 2.06 | 0.54 |
| 1:M:167:SER:C | 1:M:168:LYS:HE3 | 2.27 | 0.54 |
| 2:J:141:LEU:HD23 | 2:J:141:LEU:N | 2.22 | 0.54 |
| 1:N:119:PRO:HG3 | 1:N:185:TYR:CZ | 2.42 | 0.54 |
| 1:N:154:ARG:HD3 | 1:N:156:ASN:O | 2.08 | 0.54 |
| 2:J:197:THR:HG23 | 2:J:211:LYS:HB2 | 1.89 | 0.54 |
| 2:J:145:VAL:CG1 | 2:J:180:LEU:O | 2.56 | 0.54 |
| 1:O:94:PRO:HB3 | 2:K:47:TRP:CZ3 | 2.41 | 0.54 |
| 3:Y:51:TRP:O | 3:Y:59:LYS:HE2 | 2.08 | 0.54 |
| 2:H:6:GLU:OE2 | 2:H:108:GLN:OE1 | 2.25 | 0.54 |
| 3:Z:116:GLY:O | 3:Z:117:ARG:C | 2.44 | 0.54 |
| 1:M:180:LEU:HB3 | 1:M:184:GLU:OE2 | 2.07 | 0.54 |
| 2:H:38:ARG:NH2 | 2:H:70:PHE:CE2 | 2.76 | 0.54 |
| 2:K:191:TRP:CD1 | 2:K:196:VAL:CG1 | 2.90 | 0.54 |
| 2:J:143:CYS:O | 2:J:181:SER:HA | 2.08 | 0.54 |
| 3:X:16:LEU:HD11 | 3:X:136:ARG:HG2 | 1.90 | 0.54 |
| 2:H:88:LEU:HD23 | 2:H:92:ASP:CB | 2.37 | 0.54 |
| 2:H:89:ARG:HD2 | 2:H:91:GLU:CD | 2.25 | 0.54 |
| 3:V:35:LEU:HD22 | 3:V:122:LYS:O | 2.08 | 0.54 |
| 1:M:86:TYR:CD1 | 2:I:45:LEU:HD12 | 2.42 | 0.54 |
| 1:L:188:HIS:O | 1:L:210:ARG:HD3 | 2.08 | 0.54 |
| 3:Y:90:LEU:HD23 | 3:Y:93:LEU:HD12 | 1.90 | 0.54 |
| 1:O:119:PRO:HG3 | 1:O:130:SER:H | 1.73 | 0.54 |
| 1:L:165:GLN:HA | 1:L:171:THR:O | 2.08 | 0.54 |
| 2:J:129:PRO:CD | 2:J:191:TRP:CH2 | 2.91 | 0.54 |
| 1:N:211:ASN:ND2 | 1:N:212:GLU:N | 2.56 | 0.54 |
| 2:K:108:GLN:N | 2:K:108:GLN:OE1 | 2.39 | 0.54 |
| 3:X:14:LYS:O | 3:X:18:ASP:HB2 | 2.07 | 0.54 |
| 2:K:38:ARG:HB3 | 2:K:96:TYR:CE1 | 2.43 | 0.54 |
| 3:X:24:SER:O | 3:X:26:LEU:N | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:33:TRP:CG | 3:Y:111:GLN:NE2 | 2.76 | 0.54 |
| 2:I:215:PRO:O | 3:Y:120:ALA:CB | 2.56 | 0.54 |
| 2:J:64:GLU:OE2 | 2:J:67:LYS:HD2 | 2.08 | 0.54 |
| 2:H:125:TYR:HB2 | 2:H:144:LEU:HB3 | 1.90 | 0.54 |
| 1:N:79:ALA:CA | 1:N:105:ILE:HD13 | 2.36 | 0.54 |
| 2:H:51:ILE:HD12 | 2:H:74:ARG:HG3 | 1.88 | 0.54 |
| 1:M:174:MET:HE2 | 1:M:175:SER:O | 2.07 | 0.54 |
| 1:O:11:MET:CE | 1:O:11:MET:HB2 | 2.38 | 0.53 |
| 1:M:123:GLN:HG3 | 2:I:125:TYR:CE2 | 2.43 | 0.53 |
| 1:M:132:VAL:HG11 | 2:I:144:LEU:HD22 | 1.88 | 0.53 |
| 1:M:118:PRO:HG3 | 1:M:208:PHE:CE1 | 2.43 | 0.53 |
| 2:J:89:ARG:O | 2:J:114:VAL:HG21 | 2.08 | 0.53 |
| 2:H:149:PHE:HB2 | 2:H:177:LEU:CD2 | 2.38 | 0.53 |
| 2:H:100:GLY:HA3 | 2:H:105:TYR:N | 2.20 | 0.53 |
| 3:X:67:VAL:HG21 | 3:X:100:LEU:HD13 | 1.89 | 0.53 |
| 1:L:37:GLN:HG2 | 1:L:38:LYS:H | 1.73 | 0.53 |
| 1:L:77:MET:HE3 | 1:L:78:GLU:O | 2.07 | 0.53 |
| 1:N:41:THR:HG22 | 4:N:227:HOH:O | 2.07 | 0.53 |
| 1:L:184:GLU:HG3 | 1:L:187:ARG:NH1 | 2.23 | 0.53 |
| 1:M:185:TYR:O | 1:M:191:TYR:OH | 2.22 | 0.53 |
| 1:M:185:TYR:HD1 | 1:M:191:TYR:OH | 1.90 | 0.53 |
| 1:N:205:VAL:CG1 | 1:N:205:VAL:O | 2.56 | 0.53 |
| 2:I:33:TRP:H | 3:X:111:GLN:NE2 | 2.05 | 0.53 |
| 1:M:104:GLU:OE1 | 4:M:229:HOH:O | 2.19 | 0.53 |
| 1:L:49:SER:O | 1:L:51:SER:N | 2.41 | 0.53 |
| 1:L:20:THR:HB | 1:L:73:THR:HG23 | 1.90 | 0.53 |
| 1:N:135:LEU:HD21 | 1:N:195:ALA:HB2 | 1.90 | 0.53 |
| 3:Z:13:SER:O | 3:Z:14:LYS:C | 2.47 | 0.53 |
| 2:K:54:LYS:O | 2:K:57:ASN:N | 2.41 | 0.53 |
| 3:Y:14:LYS:O | 3:Y:18:ASP:N | 2.33 | 0.53 |
| 2:H:90:ALA:HA | 2:H:114:VAL:HG23 | 1.90 | 0.53 |
| 2:I:216:ARG:HD2 | 3:Y:122:LYS:HG3 | 1.90 | 0.53 |
| 1:N:111:ALA:HA | 1:N:199:THR:HG21 | 1.89 | 0.53 |
| 2:H:84:GLN:NE2 | 2:H:84:GLN:CA | 2.71 | 0.53 |
| 2:H:39:GLN:O | 2:H:95:ILE:HG12 | 2.08 | 0.53 |
| 2:J:127:LEU:HB2 | 2:J:142:GLY:HA3 | 1.90 | 0.53 |
| 2:J:3:LYS:O | 2:J:24:ALA:HA | 2.08 | 0.53 |
| 2:H:89:ARG:O | 2:H:92:ASP:N | 2.42 | 0.53 |
| 1:L:147:TRP:CE3 | 1:L:178:LEU:HD12 | 2.43 | 0.53 |
| 2:I:54:LYS:NZ | 2:I:58:HIS:HE1 | 2.06 | 0.53 |
| 1:L:75:SER:OG | 1:L:76:ARG:N | 2.38 | 0.53 |
| 2:J:189:SER:O | 2:J:193:SER:CB | 2.57 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:V:43:ALA:N | 3:V:118:THR:HA | 2.23 | 0.53 |
| 2:K:123:SER:O | 2:K:146:LYS:N | 2.36 | 0.53 |
| 3:Z:31:GLU:OE1 | 3:Z:33:HIS:CE1 | 2.62 | 0.53 |
| 1:N:120:SER:O | 1:N:121:SER:C | 2.46 | 0.53 |
| 2:J:56:ASN:N | 2:J:56:ASN:ND2 | 2.56 | 0.53 |
| 2:J:145:VAL:HG13 | 2:J:180:LEU:O | 2.08 | 0.53 |
| 1:L:21:ILE:HD12 | 1:L:72:LEU:HD22 | 1.91 | 0.53 |
| 2:H:196:VAL:O | 2:H:196:VAL:HG22 | 2.08 | 0.53 |
| 2:K:70:PHE:CG | 2:K:85:MET:HB3 | 2.42 | 0.53 |
| 3:Y:15:LEU:HD23 | 3:Y:135:LEU:HD21 | 1.89 | 0.53 |
| 1:N:178:LEU:HD22 | 1:N:180:LEU:CD2 | 2.39 | 0.53 |
| 2:I:216:ARG:HH21 | 3:Y:122:LYS:N | 2.05 | 0.53 |
| 2:H:40:SER:OG | 2:H:43:LYS:HB3 | 2.08 | 0.53 |
| 3:Z:15:LEU:O | 3:Z:19:SER:HB3 | 2.08 | 0.53 |
| 3:X:56:GLU:HB3 | 4:X:174:HOH:O | 2.09 | 0.53 |
| 3:X:9:LEU:O | 3:X:11:VAL:N | 2.42 | 0.53 |
| 1:M:111:ALA:HB2 | 1:M:199:THR:CG2 | 2.39 | 0.53 |
| 1:M:132:VAL:HG23 | 1:M:133:CYS:H | 1.71 | 0.53 |
| 2:J:197:THR:HA | 2:J:211:LYS:HA | 1.90 | 0.53 |
| 3:Z:101:LEU:HD11 | 3:Z:105:GLN:NE2 | 2.22 | 0.53 |
| 2:J:69:ARG:HH11 | 2:J:89:ARG:NH2 | 2.05 | 0.53 |
| 3:Y:133:HIS:CD2 | 3:Z:46:PHE:CD2 | 2.97 | 0.53 |
| 3:Y:35:LEU:N | 3:Y:122:LYS:O | 2.31 | 0.53 |
| 2:H:138:MET:CE | 2:H:185:THR:HG22 | 2.38 | 0.53 |
| 3:Z:87:SER:O | 3:Z:88:SER:C | 2.47 | 0.53 |
| 2:K:66:VAL:HG21 | 2:K:70:PHE:CD2 | 2.44 | 0.53 |
| 1:M:192:THR:OG1 | 1:M:207:SER:CB | 2.56 | 0.53 |
| 3:X:123:ASP:O | 3:X:125:ASN:N | 2.42 | 0.53 |
| 2:I:158:ASN:C | 2:I:160:GLY:N | 2.62 | 0.53 |
| 3:Z:93:LEU:HG | 3:Z:128:PHE:CD1 | 2.44 | 0.53 |
| 1:O:84:THR:HA | 1:O:101:THR:O | 2.08 | 0.53 |
| 1:O:36:GLN:HG2 | 1:O:37:GLN:N | 2.24 | 0.52 |
| 3:X:90:LEU:HD11 | 3:X:127:ILE:HD11 | 1.91 | 0.52 |
| 1:L:7:SER:CB | 1:L:22:THR:HB | 2.39 | 0.52 |
| 1:N:130:SER:HA | 1:N:179:THR:HA | 1.91 | 0.52 |
| 3:V:55:MET:O | 3:V:59:LYS:HG3 | 2.10 | 0.52 |
| 2:I:206:SER:C | 2:I:207:THR:HG22 | 2.29 | 0.52 |
| 1:M:61:PHE:CE1 | 1:M:74:ILE:HG13 | 2.43 | 0.52 |
| 2:H:72:VAL:HG22 | 2:H:73:SER:N | 2.24 | 0.52 |
| 2:K:39:GLN:OE1 | 2:K:97:TYR:OH | 2.24 | 0.52 |
| 1:N:121:SER:O | 1:N:124:LEU:N | 2.35 | 0.52 |
| 1:M:123:GLN:CD | 1:M:130:SER:HG | 2.13 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:K:38:ARG:NH1 | 2:K:46:GLU:OE1 | 2.30 | 0.52 |
| 1:L:7:SER:HB2 | 1:L:22:THR:CB | 2.39 | 0.52 |
| 1:M:86:TYR:CE1 | 2:I:45:LEU:HD12 | 2.44 | 0.52 |
| 2:H:202:HIS:CE1 | 2:H:204:ALA:HB2 | 2.44 | 0.52 |
| 1:N:70:TYR:N | 1:N:70:TYR:CD1 | 2.75 | 0.52 |
| 2:K:87:SER:O | 2:K:87:SER:OG | 2.24 | 0.52 |
| 1:L:111:ALA:HB2 | 1:L:199:THR:OG1 | 2.10 | 0.52 |
| 1:M:35:PHE:O | 1:M:85:TYR:HA | 2.10 | 0.52 |
| 2:I:27:PHE:HE2 | 2:I:29:PHE:HA | 1.66 | 0.52 |
| 1:O:107:ARG:HG3 | 1:O:108:ALA:N | 2.24 | 0.52 |
| 1:O:147:TRP:CD1 | 1:O:158:VAL:HG12 | 2.45 | 0.52 |
| 3:Z:29:CYS:SG | 3:Z:89:LEU:HD12 | 2.49 | 0.52 |
| 2:J:70:PHE:CE1 | 2:J:85:MET:HG2 | 2.44 | 0.52 |
| 1:M:7:SER:OG | 1:M:8:PRO:CD | 2.58 | 0.52 |
| 1:M:132:VAL:CG2 | 1:M:133:CYS:N | 2.72 | 0.52 |
| 3:Y:100:LEU:O | 3:Y:100:LEU:CD2 | 2.57 | 0.52 |
| 2:K:191:TRP:CD1 | 2:K:192:PRO:HA | 2.44 | 0.52 |
| 3:Y:81:LEU:CD1 | 3:Y:86:LEU:HB3 | 2.40 | 0.52 |
| 2:J:158:ASN:HB2 | 2:J:162:LEU:HB2 | 1.91 | 0.52 |
| 1:O:76:ARG:HH11 | 1:O:76:ARG:CG | 2.23 | 0.52 |
| 2:K:52:ARG:HD2 | 2:K:59:ALA:HB3 | 1.90 | 0.52 |
| 1:L:149:ILE:HG22 | 1:L:150:ASP:N | 2.25 | 0.52 |
| 2:K:70:PHE:HZ | 2:K:92:ASP:OD2 | 1.92 | 0.52 |
| 2:I:149:PHE:HB2 | 2:I:177:LEU:HD23 | 1.87 | 0.52 |
| 2:H:91:GLU:C | 2:H:93:THR:N | 2.51 | 0.52 |
| 2:H:89:ARG:CD | 2:H:91:GLU:OE1 | 2.46 | 0.52 |
| 1:O:166:ASP:OD2 | 1:O:169:ASP:HB3 | 2.09 | 0.52 |
| 3:Y:72:GLU:O | 3:Y:76:ALA:N | 2.38 | 0.52 |
| 1:O:88:GLN:NE2 | 1:O:90:ARG:HH11 | 2.08 | 0.52 |
| 3:X:68:THR:HG22 | 3:X:101:LEU:CD1 | 2.39 | 0.52 |
| 1:M:190:SER:O | 1:M:191:TYR:CD1 | 2.62 | 0.52 |
| 3:X:124:PRO:O | 3:X:127:ILE:HG12 | 2.10 | 0.52 |
| 2:K:216:ARG:NE | 3:V:122:LYS:H | 2.07 | 0.52 |
| 2:H:175:SER:O | 2:H:175:SER:OG | 2.26 | 0.52 |
| 3:Y:91:GLY:O | 3:Y:94:SER:N | 2.38 | 0.52 |
| 3:X:86:LEU:C | 3:X:86:LEU:HD22 | 2.30 | 0.52 |
| 1:M:160:ASN:HB3 | 1:M:174:MET:HE2 | 1.91 | 0.52 |
| 1:O:28:SER:O | 1:O:29:VAL:CG1 | 2.58 | 0.52 |
| 3:Z:93:LEU:HG | 3:Z:128:PHE:CE1 | 2.44 | 0.52 |
| 1:N:49:SER:O | 1:N:50:THR:HB | 2.09 | 0.52 |
| 3:X:17:ARG:CG | 3:X:17:ARG:NH1 | 2.59 | 0.52 |
| 1:M:138:PHE:HD2 | 1:M:138:PHE:N | 2.07 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:213:ILE:HD13 | 3:X:37:THR:HG23 | 1.92 | 0.52 |
| 3:Z:26:LEU:CD1 | 3:Z:32:VAL:HG11 | 2.40 | 0.52 |
| 1:O:114:VAL:HG13 | 1:O:135:LEU:HG | 1.92 | 0.52 |
| 3:X:68:THR:HG22 | 3:X:101:LEU:HD13 | 1.92 | 0.52 |
| 1:N:6:GLN:HE22 | 1:N:86:TYR:CA | 2.17 | 0.52 |
| 1:N:6:GLN:NE2 | 1:N:87:CYS:H | 2.08 | 0.52 |
| 2:H:122:PRO:HB3 | 2:H:148:TYR:HB3 | 1.91 | 0.52 |
| 2:I:22:CYS:O | 2:I:80:SER:HA | 2.10 | 0.52 |
| 3:V:16:LEU:O | 3:V:19:SER:HB3 | 2.09 | 0.52 |
| 2:K:4:LEU:HD11 | 2:K:105:TYR:HB3 | 1.92 | 0.51 |
| 2:H:70:PHE:CD1 | 2:H:85:MET:HA | 2.44 | 0.51 |
| 2:I:39:GLN:HB3 | 2:I:95:ILE:HG13 | 1.93 | 0.51 |
| 2:H:127:LEU:HD21 | 2:H:144:LEU:HB2 | 1.91 | 0.51 |
| 1:M:179:THR:CG2 | 1:M:180:LEU:N | 2.73 | 0.51 |
| 3:X:20:HIS:O | 3:X:24:SER:N | 2.38 | 0.51 |
| 1:L:84:THR:HG23 | 1:L:101:THR:N | 2.16 | 0.51 |
| 1:O:201:THR:O | 1:O:203:PRO:HD3 | 2.09 | 0.51 |
| 2:H:158:ASN:HD21 | 2:H:197:THR:H | 1.58 | 0.51 |
| 1:N:163:THR:HG23 | 1:N:164:ASP:O | 2.10 | 0.51 |
| 3:X:115:ARG:HG3 | 3:X:116:GLY:N | 2.26 | 0.51 |
| 1:O:161:SER:C | 1:O:162:TRP:CE3 | 2.84 | 0.51 |
| 1:O:19:VAL:CG1 | 1:O:74:ILE:CD1 | 2.88 | 0.51 |
| 2:H:150:PRO:O | 2:H:202:HIS:NE2 | 2.40 | 0.51 |
| 1:L:212:GLU:CG | 2:H:131:SER:HB2 | 2.40 | 0.51 |
| 1:M:37:GLN:CG | 1:M:38:LYS:N | 2.73 | 0.51 |
| 1:O:109:ASP:OD1 | 1:O:140:PRO:HD3 | 2.11 | 0.51 |
| 1:N:35:PHE:HD1 | 1:N:35:PHE:H | 1.57 | 0.51 |
| 2:K:93:THR:HA | 2:K:112:VAL:O | 2.10 | 0.51 |
| 1:L:114:VAL:HG21 | 1:L:204:ILE:HG22 | 1.92 | 0.51 |
| 3:Y:57:GLU:O | 3:Y:60:ALA:HB3 | 2.11 | 0.51 |
| 3:V:44:VAL:O | 3:V:44:VAL:HG12 | 2.10 | 0.51 |
| 1:O:88:GLN:NE2 | 1:O:90:ARG:NH1 | 2.59 | 0.51 |
| 2:K:51:ILE:CD1 | 2:K:74:ARG:CD | 2.89 | 0.51 |
| 2:J:54:LYS:NZ | 2:J:58:HIS:HE1 | 2.08 | 0.51 |
| 2:H:38:ARG:HB3 | 2:H:48:VAL:HG21 | 1.93 | 0.51 |
| 3:V:123:ASP:OD1 | 3:V:125:ASN:ND2 | 2.42 | 0.51 |
| 2:J:2:VAL:HG23 | 2:J:27:PHE:CD1 | 2.45 | 0.51 |
| 2:J:35:ASP:OD1 | 2:J:50:GLU:HB2 | 2.11 | 0.51 |
| 2:I:8:GLY:C | 2:I:9:GLY:O | 2.49 | 0.51 |
| 2:J:29:PHE:CD2 | 2:J:79:SER:CA | 2.92 | 0.51 |
| 2:J:56:ASN:H | 2:J:56:ASN:HD22 | 1.56 | 0.51 |
| 3:V:66:ALA:O | 3:V:67:VAL:C | 2.49 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:214:VAL:HG12 | 2:H:215:PRO:HD3 | 1.92 | 0.51 |
| 1:M:163:THR:HG23 | 1:M:164:ASP:O | 2.11 | 0.51 |
| 2:I:91:GLU:CD | 2:I:91:GLU:H | 2.13 | 0.51 |
| 2:K:187:PRO:O | 2:K:189:SER:N | 2.44 | 0.51 |
| 1:N:118:PRO:HA | 1:N:131:VAL:HG22 | 1.93 | 0.51 |
| 2:I:29:PHE:CE2 | 2:I:76:ASP:HA | 2.45 | 0.51 |
| 3:Z:107:LEU:O | 3:Z:107:LEU:HD22 | 2.09 | 0.51 |
| 2:I:157:TRP:CZ3 | 2:I:184:VAL:HG11 | 2.46 | 0.51 |
| 1:L:52:ASN:ND2 | 3:V:115:ARG:HD3 | 2.26 | 0.51 |
| 3:X:116:GLY:O | 3:X:118:THR:HG22 | 2.10 | 0.51 |
| 2:K:66:VAL:HG22 | 2:K:70:PHE:CE2 | 2.46 | 0.51 |
| 2:H:64:GLU:OE2 | 2:H:67:LYS:HD2 | 2.10 | 0.51 |
| 3:V:140:ARG:HA | 3:V:143:MET:HE1 | 1.92 | 0.51 |
| 1:O:182:LYS:HD3 | 1:O:186:GLU:OE1 | 2.11 | 0.51 |
| 1:O:62:ARG:HG3 | 1:O:62:ARG:HH11 | 1.76 | 0.51 |
| 3:X:131:PHE:CE1 | 3:X:135:LEU:HD11 | 2.45 | 0.51 |
| 1:M:116:ILE:CD1 | 1:M:208:PHE:CD1 | 2.93 | 0.51 |
| 1:M:107:ARG:HH12 | 1:M:169:ASP:HB2 | 1.74 | 0.51 |
| 2:H:70:PHE:CD1 | 2:H:85:MET:HB3 | 2.44 | 0.51 |
| 1:O:118:PRO:HG3 | 1:O:208:PHE:CD2 | 2.46 | 0.51 |
| 2:I:57:ASN:C | 2:I:59:ALA:N | 2.63 | 0.51 |
| 1:N:33:TYR:CD2 | 1:N:48:TYR:HA | 2.45 | 0.51 |
| 2:J:157:TRP:O | 2:J:158:ASN:C | 2.46 | 0.51 |
| 1:L:77:MET:HE3 | 1:L:81:ASP:HB2 | 1.93 | 0.51 |
| 1:N:211:ASN:HD22 | 1:N:212:GLU:N | 2.09 | 0.51 |
| 2:K:38:ARG:HB3 | 2:K:96:TYR:CD1 | 2.46 | 0.51 |
| 2:K:74:ARG:HB3 | 2:K:81:VAL:HG23 | 1.91 | 0.51 |
| 2:I:51:ILE:HD11 | 2:I:74:ARG:HG3 | 1.92 | 0.51 |
| 3:Z:41:LEU:HD13 | 3:Z:127:ILE:HG22 | 1.89 | 0.51 |
| 3:X:43:ALA:HB1 | 3:X:119:THR:HG23 | 1.89 | 0.51 |
| 1:M:38:LYS:NZ | 1:M:80:GLU:O | 2.44 | 0.51 |
| 2:K:12:VAL:O | 2:K:114:VAL:HA | 2.11 | 0.51 |
| 2:H:89:ARG:O | 2:H:90:ALA:C | 2.48 | 0.51 |
| 2:I:51:ILE:HD13 | 2:I:74:ARG:CG | 2.41 | 0.51 |
| 1:O:47:ILE:HG12 | 1:O:53:LEU:HD23 | 1.93 | 0.51 |
| 2:K:187:PRO:HD2 | 2:K:190:THR:OG1 | 2.10 | 0.51 |
| 1:L:29:VAL:O | 1:L:70:TYR:OH | 2.28 | 0.50 |
| 2:J:2:VAL:HG11 | 2:J:105:TYR:CE1 | 2.46 | 0.50 |
| 3:Z:135:LEU:HA | 3:Z:139:VAL:HB | 1.92 | 0.50 |
| 1:O:48:TYR:O | 1:O:52:ASN:HB2 | 2.11 | 0.50 |
| 1:M:165:GLN:HG2 | 1:M:172:TYR:CE1 | 2.46 | 0.50 |
| 2:I:84:GLN:C | 2:I:84:GLN:HE21 | 2.15 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:147:TRP:CZ3 | 1:M:193:CYS:HB3 | 2.46 | 0.50 |
| 2:J:28:THR:HG22 | 2:J:30:SER:OG | 2.11 | 0.50 |
| 1:O:149:ILE:CG1 | 1:O:191:TYR:HE2 | 2.17 | 0.50 |
| 2:H:64:GLU:CG | 2:H:67:LYS:NZ | 2.72 | 0.50 |
| 1:N:14:SER:O | 1:N:17:GLU:HB3 | 2.12 | 0.50 |
| 2:I:151:GLU:CB | 2:I:152:PRO:CA | 2.89 | 0.50 |
| 3:Z:57:GLU:HG3 | 3:Z:108:LEU:HD21 | 1.93 | 0.50 |
| 1:L:149:ILE:O | 1:L:190:SER:OG | 2.25 | 0.50 |
| 1:N:105:ILE:N | 1:N:165:GLN:OE1 | 2.42 | 0.50 |
| 3:V:81:LEU:HD12 | 3:V:87:SER:CB | 2.38 | 0.50 |
| 3:V:87:SER:C | 3:V:89:LEU:H | 2.13 | 0.50 |
| 3:X:67:VAL:CG2 | 3:X:100:LEU:HD13 | 2.41 | 0.50 |
| 1:L:47:ILE:CG2 | 1:L:48:TYR:N | 2.73 | 0.50 |
| 1:L:106:LYS:O | 1:L:106:LYS:CG | 2.59 | 0.50 |
| 2:H:52:ARG:HD2 | 2:H:59:ALA:HB3 | 1.93 | 0.50 |
| 1:L:149:ILE:HD13 | 1:L:191:TYR:CE2 | 2.47 | 0.50 |
| 1:L:143:ILE:HG13 | 1:L:197:HIS:CD2 | 2.46 | 0.50 |
| 2:J:54:LYS:HZ2 | 2:J:58:HIS:HE1 | 1.59 | 0.50 |
| 2:H:88:LEU:HD23 | 2:H:92:ASP:HB2 | 1.93 | 0.50 |
| 3:Y:36:PRO:HD2 | 3:Y:80:GLN:OE1 | 2.12 | 0.50 |
| 1:M:189:ASN:HD21 | 1:M:209:ASN:HB3 | 1.77 | 0.50 |
| 2:J:29:PHE:O | 2:J:31:ASP:N | 2.44 | 0.50 |
| 2:J:54:LYS:O | 2:J:56:ASN:N | 2.44 | 0.50 |
| 1:N:35:PHE:HE2 | 2:J:103:PHE:HB3 | 1.77 | 0.50 |
| 2:H:29:PHE:HE2 | 2:H:74:ARG:HE | 1.59 | 0.50 |
| 2:H:216:ARG:HD2 | 2:H:217:ASP:N | 2.26 | 0.50 |
| 3:V:93:LEU:HD23 | 3:V:93:LEU:C | 2.32 | 0.50 |
| 1:O:134:PHE:CE1 | 2:K:183:SER:HB3 | 2.46 | 0.50 |
| 2:J:4:LEU:HD12 | 2:J:107:GLY:N | 2.26 | 0.50 |
| 1:L:123:GLN:OE1 | 1:L:130:SER:N | 2.44 | 0.50 |
| 3:Z:51:TRP:CZ3 | 3:Z:138:LYS:HE2 | 2.46 | 0.50 |
| 1:M:22:THR:HG23 | 1:M:70:TYR:O | 2.11 | 0.50 |
| 2:I:145:VAL:CG2 | 2:I:145:VAL:O | 2.59 | 0.50 |
| 3:Y:68:THR:CG2 | 3:Y:101:LEU:HD11 | 2.37 | 0.50 |
| 3:Y:44:VAL:HG11 | 3:Z:46:PHE:CE2 | 2.47 | 0.50 |
| 2:J:99:SER:HB2 | 2:J:105:TYR:O | 2.12 | 0.50 |
| 2:H:191:TRP:CD1 | 2:H:196:VAL:HG13 | 2.47 | 0.50 |
| 1:O:169:ASP:O | 1:O:171:THR:N | 2.45 | 0.50 |
| 3:X:116:GLY:O | 3:X:118:THR:CG2 | 2.60 | 0.50 |
| 2:K:186:VAL:HB | 2:K:187:PRO:CD | 2.42 | 0.50 |
| 2:K:75:ASP:OD1 | 2:K:75:ASP:C | 2.50 | 0.50 |
| 3:Z:64:LEU:HD11 | 3:Z:105:GLN:NE2 | 2.25 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:K:29:PHE:CD1 | 2:K:79:SER:O | 2.64 | 0.50 |
| 2:K:29:PHE:CG | 2:K:79:SER:HA | 2.47 | 0.50 |
| 2:K:29:PHE:HE1 | 2:K:34:MET:HE3 | 1.77 | 0.50 |
| 1:N:2:VAL:CG2 | 1:N:89:GLN:CD | 2.80 | 0.50 |
| 3:X:42:PRO:HG2 | 3:X:70:LEU:HB2 | 1.92 | 0.50 |
| 1:M:115:SER:CB | 1:M:117:PHE:HE1 | 2.24 | 0.50 |
| 2:K:38:ARG:CB | 2:K:96:TYR:CE1 | 2.95 | 0.50 |
| 2:K:29:PHE:O | 2:K:31:ASP:N | 2.45 | 0.50 |
| 2:J:157:TRP:C | 2:J:159:SER:N | 2.63 | 0.50 |
| 3:Z:91:GLY:O | 3:Z:93:LEU:N | 2.44 | 0.50 |
| 2:I:206:SER:O | 2:I:207:THR:HG22 | 2.11 | 0.50 |
| 3:V:22:LEU:CD1 | 3:V:96:GLN:NE2 | 2.75 | 0.50 |
| 1:N:82:ALA:O | 1:N:83:ALA:HB2 | 2.11 | 0.50 |
| 1:O:154:ARG:HD3 | 1:O:156:ASN:O | 2.11 | 0.50 |
| 1:M:21:ILE:O | 1:M:71:SER:HB2 | 2.12 | 0.50 |
| 1:M:169:ASP:O | 1:M:169:ASP:OD2 | 2.29 | 0.50 |
| 1:N:61:PHE:HE1 | 1:N:74:ILE:HG12 | 1.72 | 0.50 |
| 2:K:202:HIS:ND1 | 2:K:204:ALA:HB3 | 2.27 | 0.50 |
| 1:N:194:GLU:HG2 | 1:N:205:VAL:CG2 | 2.40 | 0.50 |
| 3:V:139:VAL:O | 3:V:140:ARG:C | 2.50 | 0.50 |
| 2:H:138:MET:HA | 2:H:138:MET:CE | 2.41 | 0.50 |
| 3:V:49:GLY:O | 3:V:51:TRP:N | 2.45 | 0.50 |
| 3:X:91:GLY:O | 3:X:92:GLN:C | 2.49 | 0.50 |
| 1:N:19:VAL:HB | 1:N:74:ILE:HD12 | 1.94 | 0.49 |
| 1:N:42:SER:HB3 | 2:J:97:TYR:CE2 | 2.47 | 0.49 |
| 2:H:205:SER:O | 2:H:207:THR:HG22 | 2.12 | 0.49 |
| 3:Z:24:SER:O | 3:Z:26:LEU:N | 2.45 | 0.49 |
| 2:J:64:GLU:O | 2:J:67:LYS:HB2 | 2.12 | 0.49 |
| 3:Y:52:LYS:HZ1 | 3:Y:145:VAL:HG23 | 1.76 | 0.49 |
| 2:J:81:VAL:CG2 | 2:J:82:TYR:N | 2.75 | 0.49 |
| 3:Z:56:GLU:N | 3:Z:56:GLU:OE2 | 2.45 | 0.49 |
| 1:L:149:ILE:HG22 | 1:L:150:ASP:H | 1.76 | 0.49 |
| 1:M:149:ILE:HG23 | 1:M:191:TYR:CE2 | 2.46 | 0.49 |
| 1:M:89:GLN:HA | 4:M:222:HOH:O | 2.11 | 0.49 |
| 1:O:28:SER:O | 1:O:29:VAL:HG13 | 2.12 | 0.49 |
| 3:X:134:LEU:C | 3:X:139:VAL:HG23 | 2.32 | 0.49 |
| 3:Y:100:LEU:HD22 | 3:Y:104:LEU:CD1 | 2.41 | 0.49 |
| 3:V:127:ILE:O | 3:V:128:PHE:C | 2.51 | 0.49 |
| 2:I:69:ARG:HH22 | 2:I:92:ASP:CG | 2.15 | 0.49 |
| 1:L:37:GLN:O | 1:L:83:ALA:HB1 | 2.12 | 0.49 |
| 3:X:9:LEU:C | 3:X:11:VAL:N | 2.66 | 0.49 |
| 1:M:117:PHE:HE2 | 2:I:141:LEU:HA | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:N:36:GLN:HB2 | 1:N:85:TYR:CE2 | 2.48 | 0.49 |
| 2:K:155:VAL:CG1 | 2:K:168:THR:HG21 | 2.43 | 0.49 |
| 2:H:137:SER:O | 2:H:188:SER:HB3 | 2.12 | 0.49 |
| 2:I:117:ALA:O | 2:I:118:LYS:HD3 | 2.11 | 0.49 |
| 2:H:101:TRP:CB | 2:H:104:LEU:HB3 | 2.43 | 0.49 |
| 1:M:7:SER:CB | 1:M:8:PRO:CD | 2.87 | 0.49 |
| 3:X:132:GLN:OE1 | 3:X:136:ARG:NH2 | 2.45 | 0.49 |
| 2:J:28:THR:HB | 2:J:31:ASP:HB2 | 1.94 | 0.49 |
| 1:M:107:ARG:HH11 | 1:M:170:SER:N | 2.10 | 0.49 |
| 1:N:36:GLN:NE2 | 1:N:85:TYR:CE2 | 2.60 | 0.49 |
| 1:L:77:MET:HG3 | 1:L:78:GLU:O | 2.12 | 0.49 |
| 1:O:161:SER:OG | 2:K:170:PRO:HD2 | 2.12 | 0.49 |
| 1:M:21:ILE:HG22 | 1:M:22:THR:O | 2.12 | 0.49 |
| 2:K:66:VAL:HG11 | 2:K:70:PHE:CG | 2.48 | 0.49 |
| 2:J:29:PHE:C | 2:J:31:ASP:H | 2.15 | 0.49 |
| 1:N:116:ILE:C | 1:N:117:PHE:CD1 | 2.86 | 0.49 |
| 2:J:90:ALA:H | 2:J:91:GLU:CD | 2.16 | 0.49 |
| 1:N:205:VAL:HG12 | 1:N:205:VAL:O | 2.12 | 0.49 |
| 1:L:116:ILE:C | 1:L:117:PHE:CD1 | 2.86 | 0.49 |
| 2:K:60:ILE:CG2 | 2:K:72:VAL:HG13 | 2.42 | 0.49 |
| 1:L:3:VAL:H | 1:L:26:SER:HB3 | 1.77 | 0.49 |
| 3:Y:45:ASP:OD1 | 3:Y:45:ASP:N | 2.45 | 0.49 |
| 3:Z:52:LYS:HG2 | 3:Z:141:PHE:HE1 | 1.78 | 0.49 |
| 1:N:183:ASP:O | 1:N:187:ARG:HG3 | 2.12 | 0.49 |
| 2:I:216:ARG:NE | 3:Y:122:LYS:HG3 | 2.27 | 0.49 |
| 2:I:64:GLU:O | 2:I:66:VAL:N | 2.38 | 0.49 |
| 2:J:214:VAL:HG11 | 3:X:40:LEU:HD21 | 1.94 | 0.49 |
| 3:X:95:GLY:HA2 | 3:X:98:ARG:HD2 | 1.95 | 0.49 |
| 1:O:5:THR:O | 1:O:5:THR:HG22 | 2.12 | 0.49 |
| 2:J:66:VAL:HG13 | 2:J:70:PHE:CD2 | 2.48 | 0.49 |
| 3:X:73:GLY:O | 3:X:74:VAL:C | 2.49 | 0.49 |
| 3:Y:77:ALA:O | 3:Y:78:ARG:C | 2.50 | 0.49 |
| 2:K:169:PHE:HD2 | 2:K:181:SER:O | 1.96 | 0.49 |
| 2:J:70:PHE:CD1 | 2:J:85:MET:HG2 | 2.48 | 0.49 |
| 3:V:64:LEU:HD13 | 3:V:105:GLN:N | 2.28 | 0.49 |
| 3:X:137:GLY:O | 3:X:140:ARG:N | 2.46 | 0.49 |
| 3:Y:133:HIS:O | 3:Y:137:GLY:N | 2.44 | 0.49 |
| 2:H:146:LYS:HG2 | 2:H:179:THR:OG1 | 2.13 | 0.49 |
| 1:N:110:ALA:HB3 | 1:N:138:PHE:C | 2.33 | 0.49 |
| 2:H:33:TRP:H | 3:V:111:GLN:HE22 | 1.53 | 0.49 |
| 2:H:151:GLU:OE2 | 2:H:171:ALA:CB | 2.61 | 0.49 |
| 2:H:52:ARG:O | 2:H:58:HIS:HD2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:47:ILE:HG12 | 1:O:53:LEU:CD2 | 2.43 | 0.49 |
| 2:J:38:ARG:HA | 2:J:95:ILE:O | 2.13 | 0.48 |
| 2:H:101:TRP:O | 2:H:103:PHE:N | 2.46 | 0.48 |
| 1:O:83:ALA:HB3 | 1:O:85:TYR:CE1 | 2.48 | 0.48 |
| 1:O:33:TYR:CZ | 1:O:90:ARG:HD3 | 2.48 | 0.48 |
| 2:K:89:ARG:O | 2:K:114:VAL:CG2 | 2.61 | 0.48 |
| 1:O:4:LEU:HD12 | 1:O:87:CYS:O | 2.13 | 0.48 |
| 2:K:29:PHE:CE1 | 2:K:34:MET:HE3 | 2.48 | 0.48 |
| 3:V:42:PRO:HD2 | 3:V:130:SER:OG | 2.13 | 0.48 |
| 2:H:149:PHE:HB2 | 2:H:177:LEU:HD22 | 1.95 | 0.48 |
| 1:L:174:MET:HG3 | 1:L:174:MET:O | 2.13 | 0.48 |
| 1:M:34:TRP:HB2 | 1:M:47:ILE:HB | 1.94 | 0.48 |
| 2:H:70:PHE:CZ | 2:H:85:MET:CE | 2.96 | 0.48 |
| 3:Y:133:HIS:CD2 | 3:Z:46:PHE:HD2 | 2.31 | 0.48 |
| 1:N:123:GLN:NE2 | 1:N:130:SER:OG | 2.38 | 0.48 |
| 1:M:48:TYR:CZ | 3:X:113:PRO:HG2 | 2.46 | 0.48 |
| 2:I:20:LEU:HD13 | 2:I:96:TYR:HB2 | 1.95 | 0.48 |
| 2:H:216:ARG:CD | 2:H:217:ASP:N | 2.76 | 0.48 |
| 2:I:35:ASP:OD1 | 2:I:50:GLU:HB2 | 2.12 | 0.48 |
| 3:Y:26:LEU:O | 3:Y:28:GLN:N | 2.46 | 0.48 |
| 3:V:95:GLY:O | 3:V:98:ARG:HB2 | 2.13 | 0.48 |
| 1:N:167:SER:CB | 1:N:168:LYS:HZ1 | 2.20 | 0.48 |
| 1:L:160:ASN:HB3 | 1:L:174:MET:HE3 | 1.94 | 0.48 |
| 2:K:89:ARG:HB2 | 2:K:92:ASP:OD1 | 2.13 | 0.48 |
| 2:K:89:ARG:O | 2:K:114:VAL:HB | 2.13 | 0.48 |
| 2:I:158:ASN:ND2 | 2:I:197:THR:H | 2.11 | 0.48 |
| 3:V:11:VAL:HG23 | 3:V:12:LEU:H | 1.78 | 0.48 |
| 1:L:61:PHE:CE1 | 1:L:74:ILE:HG12 | 2.49 | 0.48 |
| 3:Y:52:LYS:NZ | 3:Y:145:VAL:HG23 | 2.28 | 0.48 |
| 3:V:8:ASP:OD1 | 3:V:8:ASP:N | 2.46 | 0.48 |
| 1:N:37:GLN:N | 1:N:84:THR:O | 2.41 | 0.48 |
| 2:J:51:ILE:C | 2:J:52:ARG:O | 2.50 | 0.48 |
| 1:O:197:HIS:O | 1:O:199:THR:HB | 2.14 | 0.48 |
| 1:M:33:TYR:H | 1:M:33:TYR:HD2 | 1.60 | 0.48 |
| 2:I:22:CYS:O | 2:I:80:SER:CA | 2.62 | 0.48 |
| 1:O:147:TRP:HD1 | 1:O:158:VAL:HG12 | 1.77 | 0.48 |
| 3:V:22:LEU:HG | 3:V:96:GLN:HE22 | 1.77 | 0.48 |
| 2:J:81:VAL:HG22 | 2:J:82:TYR:N | 2.28 | 0.48 |
| 1:M:103:LEU:HD12 | 1:M:104:GLU:N | 2.28 | 0.48 |
| 1:M:113:THR:H | 1:M:136:ASN:H | 1.61 | 0.48 |
| 2:K:191:TRP:CZ2 | 2:K:214:VAL:HG13 | 2.49 | 0.48 |
| 3:Z:91:GLY:O | 3:Z:92:GLN:C | 2.52 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:214:VAL:HA | 2:J:215:PRO:HD3 | 1.72 | 0.48 |
| 3:Z:82:GLY:HA3 | 3:Z:83:PRO:HD3 | 1.68 | 0.48 |
| 1:M:179:THR:HG22 | 1:M:180:LEU:N | 2.27 | 0.48 |
| 3:Y:104:LEU:O | 3:Y:105:GLN:C | 2.49 | 0.48 |
| 2:H:89:ARG:O | 2:H:114:VAL:HG21 | 2.14 | 0.48 |
| 2:H:202:HIS:ND1 | 2:H:204:ALA:CB | 2.75 | 0.48 |
| 1:O:62:ARG:HG3 | 1:O:62:ARG:NH1 | 2.28 | 0.48 |
| 3:Z:56:GLU:OE1 | 3:Z:145:VAL:HB | 2.13 | 0.48 |
| 1:O:19:VAL:CG1 | 1:O:74:ILE:CG1 | 2.92 | 0.48 |
| 1:O:29:VAL:O | 1:O:67:GLY:HA2 | 2.14 | 0.48 |
| 2:K:29:PHE:C | 2:K:31:ASP:H | 2.17 | 0.48 |
| 1:L:147:TRP:CD1 | 1:L:158:VAL:HG11 | 2.49 | 0.48 |
| 2:H:180:LEU:HD23 | 2:H:180:LEU:C | 2.34 | 0.48 |
| 1:M:18:LYS:HG3 | 1:M:19:VAL:N | 2.28 | 0.48 |
| 1:N:139:TYR:CG | 1:N:140:PRO:HA | 2.49 | 0.48 |
| 2:I:206:SER:C | 2:I:207:THR:CG2 | 2.82 | 0.48 |
| 3:X:126:ALA:O | 3:X:130:SER:HB2 | 2.14 | 0.48 |
| 2:K:90:ALA:HA | 2:K:114:VAL:HG23 | 1.96 | 0.48 |
| 1:L:147:TRP:CG | 1:L:178:LEU:HD12 | 2.49 | 0.48 |
| 1:L:212:GLU:HG2 | 2:H:131:SER:HB2 | 1.94 | 0.48 |
| 1:N:86:TYR:CD2 | 2:J:45:LEU:CD1 | 2.94 | 0.48 |
| 1:N:33:TYR:CD1 | 1:N:90:ARG:HD3 | 2.49 | 0.48 |
| 2:H:173:LEU:HA | 2:H:177:LEU:O | 2.14 | 0.48 |
| 2:H:138:MET:CE | 2:H:186:VAL:O | 2.62 | 0.48 |
| 1:L:122:GLU:CD | 1:L:122:GLU:H | 2.16 | 0.48 |
| 3:Z:54:GLN:HB2 | 3:Z:59:LYS:HG3 | 1.96 | 0.48 |
| 1:O:35:PHE:O | 1:O:85:TYR:HA | 2.13 | 0.48 |
| 1:M:7:SER:OG | 1:M:8:PRO:N | 2.42 | 0.48 |
| 1:M:180:LEU:H | 1:M:180:LEU:HD12 | 1.78 | 0.48 |
| 1:M:37:GLN:OE1 | 1:M:43:PRO:HD3 | 2.13 | 0.48 |
| 3:X:120:ALA:O | 3:X:121:HIS:CD2 | 2.67 | 0.48 |
| 2:J:81:VAL:CG2 | 2:J:82:TYR:H | 2.27 | 0.48 |
| 2:K:17:SER:HA | 2:K:88:LEU:HD12 | 1.95 | 0.47 |
| 3:X:35:LEU:HD21 | 3:X:77:ALA:CB | 2.43 | 0.47 |
| 1:N:119:PRO:HG3 | 1:N:185:TYR:CE2 | 2.48 | 0.47 |
| 2:I:120:THR:O | 2:I:149:PHE:N | 2.39 | 0.47 |
| 1:L:147:TRP:CE2 | 1:L:178:LEU:HB2 | 2.49 | 0.47 |
| 2:I:216:ARG:HH21 | 3:Y:121:HIS:CA | 2.27 | 0.47 |
| 1:M:95:ARG:HG3 | 2:I:47:TRP:CG | 2.48 | 0.47 |
| 1:M:137:ASN:H | 1:M:173:SER:CB | 2.26 | 0.47 |
| 2:J:157:TRP:CH2 | 2:J:198:CYS:HB3 | 2.49 | 0.47 |
| 3:Z:128:PHE:O | 3:Z:131:PHE:HB3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:H:51:ILE:CD1 | 2:H:74:ARG:HG3 | 2.44 | 0.47 |
| 3:V:112:LEU:N | 3:V:112:LEU:CD1 | 2.77 | 0.47 |
| 1:O:90:ARG:CZ | 2:K:103:PHE:HD2 | 2.26 | 0.47 |
| 1:M:34:TRP:CZ3 | 1:M:87:CYS:HB3 | 2.49 | 0.47 |
| 1:M:6:GLN:HE22 | 1:M:87:CYS:H | 1.61 | 0.47 |
| 1:M:147:TRP:CD2 | 1:M:178:LEU:HD12 | 2.48 | 0.47 |
| 1:M:154:ARG:HG3 | 1:M:155:GLN:N | 2.28 | 0.47 |
| 2:H:17:SER:HB3 | 2:H:86:ASN:OD1 | 2.14 | 0.47 |
| 3:V:41:LEU:CD2 | 3:V:127:ILE:HB | 2.44 | 0.47 |
| 3:Y:90:LEU:HA | 3:Y:90:LEU:HD23 | 1.65 | 0.47 |
| 3:Y:123:ASP:HA | 3:Y:124:PRO:HD2 | 1.64 | 0.47 |
| 3:Y:123:ASP:O | 3:Y:126:ALA:CB | 2.61 | 0.47 |
| 1:O:107:ARG:NE | 1:O:108:ALA:O | 2.42 | 0.47 |
| 1:O:7:SER:CB | 1:O:22:THR:HB | 2.45 | 0.47 |
| 2:J:75:ASP:C | 2:J:75:ASP:OD1 | 2.52 | 0.47 |
| 2:H:102:SER:HB2 | 3:V:111:GLN:H | 1.79 | 0.47 |
| 1:M:111:ALA:HB1 | 1:M:112:PRO:HD2 | 1.95 | 0.47 |
| 1:L:84:THR:HG23 | 1:L:101:THR:O | 2.14 | 0.47 |
| 2:J:47:TRP:O | 2:J:63:ALA:HB2 | 2.14 | 0.47 |
| 2:J:102:SER:O | 2:J:103:PHE:HB2 | 2.14 | 0.47 |
| 3:Y:78:ARG:NH1 | 3:Y:87:SER:O | 2.46 | 0.47 |
| 1:N:109:ASP:OD1 | 1:N:140:PRO:HD3 | 2.15 | 0.47 |
| 1:L:48:TYR:CE1 | 1:L:52:ASN:CB | 2.97 | 0.47 |
| 2:I:102:SER:HB2 | 3:X:111:GLN:HB2 | 1.97 | 0.47 |
| 3:Y:70:LEU:HD22 | 3:Y:74:VAL:CG2 | 2.43 | 0.47 |
| 1:O:174:MET:HG2 | 1:O:174:MET:O | 2.11 | 0.47 |
| 1:O:58:PRO:O | 1:O:61:PHE:HB2 | 2.13 | 0.47 |
| 1:L:111:ALA:HB1 | 1:L:112:PRO:CD | 2.44 | 0.47 |
| 3:X:90:LEU:HD23 | 3:X:90:LEU:N | 2.29 | 0.47 |
| 2:H:159:SER:HA | 2:H:199:ASN:HD21 | 1.79 | 0.47 |
| 3:X:23:HIS:HD2 | 3:X:23:HIS:O | 1.96 | 0.47 |
| 1:O:174:MET:HA | 2:K:169:PHE:HE1 | 1.79 | 0.47 |
| 3:Y:30:PRO:O | 3:Y:31:GLU:C | 2.53 | 0.47 |
| 3:V:24:SER:O | 3:V:26:LEU:N | 2.47 | 0.47 |
| 1:O:37:GLN:HE21 | 1:O:86:TYR:HE2 | 1.63 | 0.47 |
| 2:I:148:TYR:CE1 | 2:I:178:TYR:O | 2.67 | 0.47 |
| 2:I:56:ASN:C | 2:I:57:ASN:ND2 | 2.68 | 0.47 |
| 2:H:64:GLU:CG | 2:H:67:LYS:HZ2 | 2.24 | 0.47 |
| 2:K:13:GLN:C | 2:K:14:PRO:O | 2.52 | 0.47 |
| 2:K:17:SER:OG | 2:K:86:ASN:HA | 2.14 | 0.47 |
| 1:M:115:SER:HB2 | 1:M:117:PHE:HE1 | 1.78 | 0.47 |
| 1:M:185:TYR:HE1 | 1:M:191:TYR:CE1 | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:X:39:VAL:HG11 | 3:X:77:ALA:N | 2.30 | 0.47 |
| 3:Y:43:ALA:HB2 | 3:Y:119:THR:OG1 | 2.13 | 0.47 |
| 3:Y:124:PRO:HA | 3:Y:127:ILE:HD13 | 1.96 | 0.47 |
| 2:I:8:GLY:O | 2:I:9:GLY:O | 2.32 | 0.47 |
| 2:K:33:TRP:CZ2 | 2:K:52:ARG:HG2 | 2.48 | 0.47 |
| 2:K:64:GLU:C | 2:K:66:VAL:H | 2.18 | 0.47 |
| 2:K:38:ARG:HH11 | 2:K:46:GLU:CD | 2.18 | 0.47 |
| 2:J:124:VAL:HG21 | 2:J:208:LYS:CB | 2.44 | 0.47 |
| 1:M:36:GLN:HB2 | 1:M:85:TYR:HE2 | 1.69 | 0.47 |
| 1:N:89:GLN:NE2 | 1:N:96:THR:H | 2.13 | 0.47 |
| 2:I:216:ARG:CG | 3:Y:122:LYS:HG3 | 2.44 | 0.47 |
| 1:N:34:TRP:HA | 1:N:86:TYR:O | 2.14 | 0.47 |
| 1:M:88:GLN:NE2 | 1:M:90:ARG:HH11 | 2.10 | 0.47 |
| 3:V:52:LYS:O | 3:V:52:LYS:HG3 | 2.14 | 0.47 |
| 2:K:214:VAL:O | 3:V:38:PRO:HG2 | 2.15 | 0.47 |
| 1:O:119:PRO:HA | 4:O:214:HOH:O | 2.14 | 0.47 |
| 1:N:106:LYS:HA | 1:N:139:TYR:OH | 2.15 | 0.47 |
| 2:H:186:VAL:HB | 2:H:190:THR:OG1 | 2.15 | 0.47 |
| 2:K:203:PRO:CB | 4:K:227:HOH:O | 2.58 | 0.47 |
| 1:L:53:LEU:H | 1:L:53:LEU:HG | 1.60 | 0.47 |
| 1:O:121:SER:HA | 1:O:124:LEU:HB2 | 1.96 | 0.47 |
| 1:O:89:GLN:OE1 | 1:O:91:SER:HB3 | 2.14 | 0.47 |
| 1:L:136:ASN:ND2 | 2:H:167:HIS:HD2 | 2.12 | 0.47 |
| 3:Y:71:LEU:HD23 | 3:Y:71:LEU:O | 2.15 | 0.47 |
| 2:K:57:ASN:C | 2:K:59:ALA:H | 2.18 | 0.47 |
| 2:H:66:VAL:O | 2:H:66:VAL:HG12 | 2.14 | 0.47 |
| 2:I:216:ARG:HH21 | 3:Y:122:LYS:H | 1.61 | 0.47 |
| 1:M:84:THR:HA | 1:M:102:LYS:HA | 1.97 | 0.47 |
| 2:I:111:LEU:HD13 | 2:I:113:THR:OG1 | 2.14 | 0.47 |
| 1:L:4:LEU:HD21 | 1:L:89:GLN:HB3 | 1.97 | 0.47 |
| 3:Z:64:LEU:O | 3:Z:68:THR:HG23 | 2.12 | 0.47 |
| 1:M:6:GLN:NE2 | 1:M:98:GLY:HA3 | 2.22 | 0.47 |
| 2:K:89:ARG:O | 2:K:114:VAL:CB | 2.63 | 0.47 |
| 2:K:141:LEU:HD11 | 2:K:191:TRP:CD2 | 2.49 | 0.47 |
| 2:K:156:THR:OG1 | 2:K:199:ASN:ND2 | 2.47 | 0.47 |
| 2:I:85:MET:HE2 | 2:I:88:LEU:HD21 | 1.96 | 0.47 |
| 2:K:8:GLY:O | 2:K:9:GLY:O | 2.33 | 0.47 |
| 1:L:117:PHE:HD1 | 1:L:117:PHE:N | 2.13 | 0.47 |
| 2:I:211:LYS:O | 2:I:212:LYS:C | 2.52 | 0.47 |
| 2:J:148:TYR:O | 2:J:178:TYR:HB2 | 2.15 | 0.47 |
| 3:X:87:SER:O | 3:X:90:LEU:HB2 | 2.14 | 0.47 |
| 2:I:51:ILE:CD1 | 2:I:74:ARG:CG | 2.92 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:39:GLN:HA | 2:H:44:GLY:O | 2.15 | 0.47 |
| 2:I:214:VAL:HG11 | 3:Y:40:LEU:HD23 | 1.96 | 0.47 |
| 1:N:132:VAL:HG11 | 2:J:127:LEU:CD1 | 2.45 | 0.47 |
| 2:K:93:THR:OG1 | 2:K:113:THR:HA | 2.15 | 0.47 |
| 2:K:60:ILE:HG23 | 2:K:72:VAL:HG13 | 1.96 | 0.47 |
| 2:K:155:VAL:O | 2:K:155:VAL:HG22 | 2.14 | 0.47 |
| 1:L:88:GLN:OE1 | 2:H:103:PHE:CD2 | 2.68 | 0.46 |
| 1:M:7:SER:HB2 | 1:M:22:THR:HB | 1.98 | 0.46 |
| 2:K:90:ALA:O | 2:K:92:ASP:N | 2.48 | 0.46 |
| 1:M:192:THR:HG1 | 1:M:207:SER:CB | 2.27 | 0.46 |
| 3:X:51:TRP:O | 3:X:54:GLN:CB | 2.63 | 0.46 |
| 1:L:107:ARG:HB2 | 1:L:108:ALA:H | 1.43 | 0.46 |
| 3:X:33:HIS:HB3 | 3:X:34:PRO:CD | 2.42 | 0.46 |
| 1:O:131:VAL:HB | 1:O:178:LEU:HB3 | 1.96 | 0.46 |
| 3:Z:25:ARG:NH2 | 3:Z:89:LEU:HD21 | 2.30 | 0.46 |
| 2:K:49:ALA:HB1 | 2:K:72:VAL:HG11 | 1.97 | 0.46 |
| 1:O:76:ARG:CG | 1:O:76:ARG:NH1 | 2.79 | 0.46 |
| 2:J:83:LEU:HD22 | 2:J:84:GLN:N | 2.30 | 0.46 |
| 3:V:69:LEU:HD13 | 3:V:118:THR:HG22 | 1.97 | 0.46 |
| 2:H:123:SER:O | 2:H:145:VAL:HA | 2.15 | 0.46 |
| 2:H:36:TRP:CZ3 | 2:H:98:CYS:HB2 | 2.50 | 0.46 |
| 1:N:120:SER:HB3 | 2:J:126:PRO:HD2 | 1.96 | 0.46 |
| 3:Z:9:LEU:C | 3:Z:11:VAL:H | 2.17 | 0.46 |
| 1:O:35:PHE:CD1 | 1:O:35:PHE:N | 2.83 | 0.46 |
| 3:X:90:LEU:CD2 | 3:X:90:LEU:N | 2.76 | 0.46 |
| 2:J:33:TRP:CD1 | 3:Y:111:GLN:NE2 | 2.83 | 0.46 |
| 1:L:209:ASN:HD22 | 1:L:213:CYS:HB2 | 1.80 | 0.46 |
| 1:M:76:ARG:NH1 | 1:M:76:ARG:CG | 2.78 | 0.46 |
| 3:Y:52:LYS:HE2 | 3:Y:141:PHE:HB3 | 1.98 | 0.46 |
| 2:K:197:THR:HG23 | 2:K:211:LYS:HA | 1.98 | 0.46 |
| 3:X:93:LEU:O | 3:X:96:GLN:HB2 | 2.15 | 0.46 |
| 3:Z:71:LEU:CD1 | 3:Z:101:LEU:HD23 | 2.44 | 0.46 |
| 3:X:129:LEU:O | 3:X:131:PHE:N | 2.48 | 0.46 |
| 2:K:66:VAL:CG1 | 2:K:70:PHE:CG | 2.99 | 0.46 |
| 2:K:4:LEU:HB3 | 2:K:22:CYS:SG | 2.55 | 0.46 |
| 1:N:21:ILE:HB | 1:N:72:LEU:HD22 | 1.97 | 0.46 |
| 1:M:33:TYR:CD1 | 1:M:90:ARG:NH1 | 2.84 | 0.46 |
| 3:Y:52:LYS:HZ3 | 3:Y:59:LYS:NZ | 2.14 | 0.46 |
| 1:O:160:ASN:N | 1:O:160:ASN:OD1 | 2.48 | 0.46 |
| 1:O:43:PRO:HG2 | 2:K:106:TRP:CZ3 | 2.51 | 0.46 |
| 2:J:70:PHE:CA | 2:J:84:GLN:O | 2.49 | 0.46 |
| 1:N:89:GLN:HG3 | 1:N:89:GLN:H | 1.64 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:N:32:MET:HG3 | 1:N:33:TYR:O | 2.15 | 0.46 |
| 3:Z:12:LEU:CB | 3:Z:143:MET:SD | 3.01 | 0.46 |
| 2:J:140:THR:OG1 | 2:J:185:THR:HG23 | 2.15 | 0.46 |
| 3:V:9:LEU:O | 3:V:9:LEU:HD23 | 2.15 | 0.46 |
| 2:J:38:ARG:HD3 | 2:J:43:LYS:NZ | 2.30 | 0.46 |
| 1:L:124:LEU:HD11 | 1:L:185:TYR:CD2 | 2.50 | 0.46 |
| 1:M:8:PRO:O | 1:M:8:PRO:CD | 2.63 | 0.46 |
| 3:X:39:VAL:HG21 | 3:X:77:ALA:HB2 | 1.98 | 0.46 |
| 2:H:89:ARG:O | 2:H:91:GLU:N | 2.48 | 0.46 |
| 2:K:177:LEU:HD23 | 2:K:177:LEU:HA | 1.66 | 0.46 |
| 3:X:86:LEU:O | 3:X:86:LEU:HD22 | 2.15 | 0.46 |
| 2:I:151:GLU:HB3 | 2:I:152:PRO:CA | 2.45 | 0.46 |
| 1:O:7:SER:OG | 1:O:8:PRO:CD | 2.64 | 0.46 |
| 3:Y:25:ARG:O | 3:Y:26:LEU:C | 2.54 | 0.46 |
| 1:M:143:ILE:O | 1:M:143:ILE:CG2 | 2.63 | 0.46 |
| 3:V:42:PRO:O | 3:V:43:ALA:O | 2.34 | 0.46 |
| 1:M:37:GLN:NE2 | 2:I:39:GLN:HE22 | 2.04 | 0.46 |
| 1:M:45:LEU:CD2 | 1:M:46:TRP:N | 2.74 | 0.46 |
| 1:L:163:THR:HG23 | 1:L:164:ASP:O | 2.16 | 0.46 |
| 1:L:48:TYR:CE2 | 3:V:113:PRO:HG3 | 2.51 | 0.46 |
| 3:Y:31:GLU:HB3 | 3:Y:33:HIS:HE1 | 1.80 | 0.46 |
| 1:N:136:ASN:O | 1:N:137:ASN:C | 2.53 | 0.46 |
| 1:L:184:GLU:O | 1:L:185:TYR:C | 2.53 | 0.46 |
| 3:X:90:LEU:HD11 | 3:X:127:ILE:CD1 | 2.46 | 0.46 |
| 2:J:135:THR:CG2 | 4:J:221:HOH:O | 2.39 | 0.46 |
| 1:N:88:GLN:HE22 | 1:N:90:ARG:HH11 | 1.64 | 0.46 |
| 2:I:43:LYS:HG3 | 4:I:241:HOH:O | 2.15 | 0.46 |
| 2:H:72:VAL:CG2 | 2:H:73:SER:N | 2.79 | 0.46 |
| 3:V:75:MET:O | 3:V:76:ALA:C | 2.52 | 0.46 |
| 1:M:8:PRO:O | 1:M:8:PRO:HD2 | 2.16 | 0.46 |
| 2:I:149:PHE:CB | 2:I:177:LEU:HD21 | 2.44 | 0.46 |
| 3:V:86:LEU:O | 3:V:89:LEU:HB2 | 2.16 | 0.46 |
| 3:X:63:ILE:O | 3:X:63:ILE:HG22 | 2.15 | 0.46 |
| 1:M:57:VAL:O | 2:J:137:SER:OG | 2.25 | 0.46 |
| 2:H:216:ARG:HD3 | 2:H:217:ASP:H | 1.80 | 0.46 |
| 2:K:187:PRO:O | 2:K:188:SER:C | 2.52 | 0.46 |
| 1:O:33:TYR:CE2 | 1:O:90:ARG:HD3 | 2.51 | 0.46 |
| 1:N:131:VAL:N | 1:N:178:LEU:O | 2.36 | 0.46 |
| 1:N:79:ALA:C | 1:N:81:ASP:H | 2.20 | 0.46 |
| 1:O:111:ALA:HA | 1:O:112:PRO:HD2 | 1.58 | 0.46 |
| 2:H:174:GLN:HB3 | 2:H:175:SER:H | 1.66 | 0.46 |
| 1:L:47:ILE:HG12 | 1:L:53:LEU:HD23 | 1.99 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:V:16:LEU:HA | 3:V:16:LEU:HD23 | 1.64 | 0.46 |
| 2:K:62:TYR:OH | 2:K:71:THR:HA | 2.15 | 0.46 |
| 1:L:175:SER:HB3 | 2:H:169:PHE:CD1 | 2.50 | 0.46 |
| 1:O:62:ARG:HB3 | 4:O:230:HOH:O | 2.16 | 0.46 |
| 3:V:97:VAL:O | 3:V:97:VAL:HG12 | 2.16 | 0.46 |
| 2:I:13:GLN:O | 2:I:14:PRO:C | 2.53 | 0.46 |
| 3:Z:111:GLN:O | 3:Z:112:LEU:CD1 | 2.64 | 0.45 |
| 3:Y:14:LYS:O | 3:Y:18:ASP:CB | 2.60 | 0.45 |
| 2:I:78:LYS:HB2 | 2:I:78:LYS:HE3 | 1.59 | 0.45 |
| 2:I:18:MET:SD | 2:I:112:VAL:HG22 | 2.56 | 0.45 |
| 3:V:144:LEU:HB3 | 3:V:145:VAL:H | 1.47 | 0.45 |
| 2:J:160:GLY:O | 2:J:163:SER:HB3 | 2.15 | 0.45 |
| 3:X:15:LEU:HD23 | 3:X:135:LEU:CD2 | 2.47 | 0.45 |
| 1:M:118:PRO:HG3 | 1:M:208:PHE:CD1 | 2.50 | 0.45 |
| 3:V:38:PRO:HB3 | 3:V:120:ALA:HB1 | 1.98 | 0.45 |
| 1:L:107:ARG:NE | 1:L:108:ALA:O | 2.36 | 0.45 |
| 2:I:196:VAL:O | 2:I:196:VAL:HG23 | 2.16 | 0.45 |
| 1:L:37:GLN:NE2 | 1:L:86:TYR:HE2 | 2.14 | 0.45 |
| 2:J:22:CYS:C | 2:J:80:SER:HB3 | 2.37 | 0.45 |
| 2:K:83:LEU:HD23 | 2:K:83:LEU:HA | 1.45 | 0.45 |
| 1:O:103:LEU:HA | 1:O:103:LEU:HD12 | 1.32 | 0.45 |
| 1:L:191:TYR:HD1 | 1:L:208:PHE:CZ | 2.34 | 0.45 |
| 3:Z:100:LEU:O | 3:Z:104:LEU:HD12 | 2.16 | 0.45 |
| 3:X:99:LEU:O | 3:X:103:ALA:N | 2.49 | 0.45 |
| 2:J:95:ILE:CG2 | 2:J:111:LEU:HD23 | 2.25 | 0.45 |
| 2:K:69:ARG:HH11 | 2:K:89:ARG:HH22 | 1.61 | 0.45 |
| 1:N:21:ILE:HG12 | 1:N:101:THR:HG21 | 1.98 | 0.45 |
| 2:H:78:LYS:O | 2:H:78:LYS:CG | 2.51 | 0.45 |
| 3:V:87:SER:C | 3:V:89:LEU:N | 2.70 | 0.45 |
| 1:M:36:GLN:HB2 | 1:M:85:TYR:CD2 | 2.50 | 0.45 |
| 1:N:184:GLU:O | 1:N:184:GLU:CG | 2.62 | 0.45 |
| 1:L:36:GLN:HG3 | 1:L:85:TYR:HE2 | 1.79 | 0.45 |
| 3:Y:90:LEU:CD2 | 3:Y:93:LEU:HD12 | 2.47 | 0.45 |
| 2:I:191:TRP:CD1 | 2:I:192:PRO:HA | 2.52 | 0.45 |
| 1:M:164:ASP:O | 1:M:165:GLN:C | 2.51 | 0.45 |
| 3:V:101:LEU:O | 3:V:102:GLY:O | 2.34 | 0.45 |
| 3:V:105:GLN:NE2 | 3:V:111:GLN:HG2 | 2.32 | 0.45 |
| 3:X:64:LEU:HA | 3:X:104:LEU:HD13 | 1.98 | 0.45 |
| 2:K:89:ARG:NH1 | 2:K:89:ARG:CG | 2.67 | 0.45 |
| 2:J:69:ARG:NH1 | 2:J:89:ARG:HH21 | 2.12 | 0.45 |
| 2:I:104:LEU:HD22 | 3:X:113:PRO:HB3 | 1.99 | 0.45 |
| 2:K:216:ARG:NH1 | 3:V:121:HIS:HD1 | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:V:86:LEU:HD11 | 3:V:124:PRO:HB3 | 1.97 | 0.45 |
| 2:H:111:LEU:HD22 | 2:H:111:LEU:HA | 1.45 | 0.45 |
| 3:V:14:LYS:HA | 3:V:17:ARG:HH11 | 1.82 | 0.45 |
| 3:X:29:CYS:HB2 | 3:X:32:VAL:HG13 | 1.98 | 0.45 |
| 3:X:17:ARG:H | 3:X:17:ARG:HG2 | 1.34 | 0.45 |
| 2:K:216:ARG:HD2 | 2:K:217:ASP:N | 2.32 | 0.45 |
| 1:M:77:MET:CE | 1:M:81:ASP:HB2 | 2.47 | 0.45 |
| 1:N:169:ASP:OD2 | 1:N:171:THR:HG23 | 2.17 | 0.45 |
| 2:I:99:SER:OG | 2:I:103:PHE:HA | 2.17 | 0.45 |
| 1:M:124:LEU:CD1 | 1:M:128:GLY:O | 2.65 | 0.45 |
| 3:Y:62:ASP:OD1 | 3:Y:62:ASP:N | 2.49 | 0.45 |
| 3:V:64:LEU:O | 3:V:68:THR:HG23 | 2.16 | 0.45 |
| 3:Z:62:ASP:O | 3:Z:66:ALA:N | 2.50 | 0.45 |
| 2:K:22:CYS:O | 2:K:80:SER:CA | 2.64 | 0.45 |
| 3:X:78:ARG:CG | 3:X:78:ARG:NH1 | 2.42 | 0.45 |
| 3:V:85:CYS:O | 3:V:89:LEU:HD13 | 2.17 | 0.45 |
| 2:K:145:VAL:HG21 | 2:K:153:VAL:HG11 | 1.98 | 0.45 |
| 2:K:199:ASN:HB3 | 2:K:209:VAL:HG23 | 1.98 | 0.45 |
| 2:K:62:TYR:CZ | 2:K:72:VAL:HG12 | 2.52 | 0.45 |
| 1:O:47:ILE:HD12 | 1:O:72:LEU:HD12 | 1.98 | 0.45 |
| 3:V:8:ASP:H | 3:V:151:CYS:CB | 2.29 | 0.45 |
| 3:V:8:ASP:H | 3:V:151:CYS:HB3 | 1.82 | 0.45 |
| 3:Z:52:LYS:HG2 | 3:Z:141:PHE:CE1 | 2.52 | 0.45 |
| 3:X:15:LEU:HD23 | 3:X:135:LEU:HD21 | 1.99 | 0.45 |
| 2:I:173:LEU:CD2 | 2:I:176:ASP:HA | 2.46 | 0.45 |
| 2:J:51:ILE:O | 2:J:52:ARG:C | 2.55 | 0.45 |
| 3:V:69:LEU:CD1 | 3:V:118:THR:HG22 | 2.47 | 0.45 |
| 1:N:147:TRP:NE1 | 1:N:158:VAL:CG1 | 2.79 | 0.45 |
| 1:O:112:PRO:HD3 | 1:O:138:PHE:HB3 | 1.98 | 0.45 |
| 1:O:53:LEU:HD23 | 1:O:53:LEU:HA | 1.78 | 0.45 |
| 3:V:78:ARG:O | 3:V:79:GLY:O | 2.35 | 0.45 |
| 1:O:35:PHE:HE1 | 1:O:88:GLN:HB2 | 1.82 | 0.45 |
| 3:X:70:LEU:HD22 | 3:X:74:VAL:HG23 | 1.99 | 0.45 |
| 2:K:120:THR:HA | 2:K:121:PRO:HD2 | 1.81 | 0.45 |
| 1:N:65:GLY:O | 1:N:66:SER:HB3 | 2.16 | 0.45 |
| 2:I:202:HIS:CE1 | 2:I:204:ALA:CB | 3.00 | 0.45 |
| 1:M:160:ASN:CG | 1:M:174:MET:CE | 2.86 | 0.45 |
| 1:O:137:ASN:HA | 1:O:172:TYR:O | 2.17 | 0.45 |
| 2:K:70:PHE:HD1 | 2:K:85:MET:CA | 2.29 | 0.45 |
| 3:V:89:LEU:O | 3:V:92:GLN:N | 2.50 | 0.45 |
| 2:H:120:THR:N | 2:H:149:PHE:O | 2.48 | 0.45 |
| 3:Z:143:MET:HG2 | 3:Z:143:MET:H | 1.59 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:29:PHE:CG | 2:H:79:SER:HA | 2.51 | 0.45 |
| 1:O:21:ILE:HG12 | 1:O:101:THR:HG21 | 1.98 | 0.45 |
| 1:N:38:LYS:HG3 | 1:N:39:PRO:HD2 | 1.99 | 0.45 |
| 1:L:103:LEU:HD12 | 1:L:103:LEU:HA | 1.80 | 0.45 |
| 3:X:131:PHE:O | 3:X:134:LEU:HB2 | 2.17 | 0.44 |
| 2:K:37:VAL:O | 2:K:97:TYR:N | 2.42 | 0.44 |
| 3:Y:16:LEU:HD23 | 3:Y:16:LEU:HA | 1.77 | 0.44 |
| 2:I:119:THR:HG22 | 2:I:149:PHE:O | 2.17 | 0.44 |
| 1:O:138:PHE:CE2 | 1:O:173:SER:HA | 2.52 | 0.44 |
| 1:M:7:SER:OG | 1:M:8:PRO:HD3 | 2.17 | 0.44 |
| 3:X:132:GLN:O | 3:X:134:LEU:N | 2.50 | 0.44 |
| 2:K:38:ARG:CB | 2:K:96:TYR:CD1 | 3.00 | 0.44 |
| 2:K:38:ARG:HD3 | 2:K:46:GLU:OE1 | 2.17 | 0.44 |
| 2:J:54:LYS:NZ | 2:J:58:HIS:CE1 | 2.86 | 0.44 |
| 1:N:110:ALA:HB3 | 1:N:138:PHE:HA | 1.98 | 0.44 |
| 2:I:151:GLU:HB3 | 2:I:152:PRO:HA | 1.98 | 0.44 |
| 2:K:48:VAL:O | 2:K:62:TYR:HA | 2.17 | 0.44 |
| 2:I:21:SER:HA | 2:I:82:TYR:CD2 | 2.52 | 0.44 |
| 1:L:154:ARG:HE | 1:L:154:ARG:HB2 | 1.45 | 0.44 |
| 3:Z:46:PHE:CE1 | 3:Z:133:HIS:CD2 | 3.05 | 0.44 |
| 2:J:200:VAL:HG22 | 2:J:208:LYS:O | 2.18 | 0.44 |
| 2:K:202:HIS:CE1 | 2:K:204:ALA:HB2 | 2.52 | 0.44 |
| 2:K:140:THR:C | 2:K:141:LEU:HD23 | 2.37 | 0.44 |
| 2:H:19:LYS:HD3 | 2:H:84:GLN:HG2 | 2.00 | 0.44 |
| 2:I:88:LEU:HB3 | 2:I:114:VAL:HG11 | 1.97 | 0.44 |
| 1:L:86:TYR:CG | 2:H:45:LEU:HD12 | 2.52 | 0.44 |
| 3:X:38:PRO:HB2 | 3:X:120:ALA:HB1 | 2.00 | 0.44 |
| 3:X:69:LEU:CD2 | 4:X:167:HOH:O | 2.62 | 0.44 |
| 1:M:12:SER:HB2 | 1:M:104:GLU:HB2 | 2.00 | 0.44 |
| 3:Z:63:ILE:HD12 | 3:Z:142:LEU:HD22 | 2.00 | 0.44 |
| 3:V:61:GLN:HG2 | 3:V:108:LEU:HD22 | 2.00 | 0.44 |
| 3:V:75:MET:O | 3:V:79:GLY:N | 2.34 | 0.44 |
| 2:K:57:ASN:C | 2:K:59:ALA:N | 2.70 | 0.44 |
| 2:J:155:VAL:HA | 2:J:199:ASN:O | 2.18 | 0.44 |
| 1:O:132:VAL:CG2 | 1:O:133:CYS:N | 2.79 | 0.44 |
| 1:L:189:ASN:O | 1:L:210:ARG:N | 2.46 | 0.44 |
| 2:I:24:ALA:HB1 | 2:I:27:PHE:CE1 | 2.52 | 0.44 |
| 3:Y:127:ILE:HD13 | 3:Y:127:ILE:HG23 | 1.50 | 0.44 |
| 1:O:120:SER:O | 1:O:122:GLU:N | 2.50 | 0.44 |
| 2:J:71:THR:HG22 | 2:J:71:THR:O | 2.18 | 0.44 |
| 3:V:33:HIS:CB | 3:V:34:PRO:HD2 | 2.47 | 0.44 |
| 3:Y:73:GLY:HA2 | 3:Y:76:ALA:CB | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:51:SER:HB3 | 1:L:63:GLY:O | 2.17 | 0.44 |
| 1:L:88:GLN:HE22 | 1:L:90:ARG:HD2 | 1.78 | 0.44 |
| 3:X:16:LEU:HA | 3:X:16:LEU:HD23 | 1.38 | 0.44 |
| 1:M:208:PHE:CD2 | 1:M:209:ASN:N | 2.86 | 0.44 |
| 1:O:4:LEU:HA | 1:O:24:SER:O | 2.18 | 0.44 |
| 3:X:123:ASP:C | 3:X:125:ASN:N | 2.70 | 0.44 |
| 3:Y:8:ASP:C | 3:Y:10:ARG:H | 2.20 | 0.44 |
| 1:N:77:MET:CE | 1:N:78:GLU:O | 2.65 | 0.44 |
| 3:Y:63:ILE:HG22 | 3:Y:67:VAL:CG2 | 2.47 | 0.44 |
| 3:Y:114:PRO:O | 3:Y:115:ARG:HB3 | 2.18 | 0.44 |
| 3:V:52:LYS:HD2 | 3:V:59:LYS:NZ | 2.32 | 0.44 |
| 1:O:203:PRO:O | 1:O:205:VAL:N | 2.51 | 0.44 |
| 1:L:165:GLN:HG2 | 1:L:165:GLN:H | 1.62 | 0.44 |
| 3:V:40:LEU:N | 3:V:40:LEU:CD2 | 2.81 | 0.44 |
| 1:O:76:ARG:HH11 | 1:O:76:ARG:HG2 | 1.81 | 0.44 |
| 2:J:203:PRO:HA | 2:J:205:SER:H | 1.83 | 0.44 |
| 2:I:62:TYR:OH | 2:I:71:THR:HA | 2.18 | 0.44 |
| 2:J:120:THR:HG21 | 2:J:177:LEU:HD21 | 1.99 | 0.44 |
| 3:Z:95:GLY:O | 3:Z:99:LEU:HD23 | 2.17 | 0.44 |
| 3:X:12:LEU:HD12 | 3:X:135:LEU:HB3 | 1.99 | 0.44 |
| 2:I:216:ARG:HH21 | 3:Y:121:HIS:HA | 1.82 | 0.44 |
| 1:N:162:TRP:CH2 | 1:N:174:MET:CE | 2.99 | 0.44 |
| 2:K:187:PRO:O | 2:K:190:THR:OG1 | 2.30 | 0.44 |
| 1:O:163:THR:HG23 | 1:O:164:ASP:O | 2.18 | 0.44 |
| 2:J:40:SER:HB3 | 2:J:43:LYS:HE3 | 2.00 | 0.44 |
| 3:V:100:LEU:O | 3:V:101:LEU:C | 2.55 | 0.44 |
| 1:O:4:LEU:CD1 | 1:O:87:CYS:O | 2.66 | 0.44 |
| 3:X:90:LEU:HA | 3:X:90:LEU:HD22 | 1.52 | 0.44 |
| 1:N:119:PRO:CD | 1:N:131:VAL:HG23 | 2.20 | 0.44 |
| 1:M:137:ASN:OD1 | 1:M:137:ASN:N | 2.50 | 0.44 |
| 2:I:38:ARG:NH1 | 2:I:46:GLU:OE1 | 2.49 | 0.44 |
| 1:N:1:GLN:OE1 | 1:N:1:GLN:O | 2.36 | 0.44 |
| 1:L:48:TYR:CD1 | 1:L:52:ASN:HB2 | 2.52 | 0.44 |
| 1:N:107:ARG:NH1 | 1:N:169:ASP:OD2 | 2.51 | 0.44 |
| 2:H:216:ARG:CD | 2:H:217:ASP:H | 2.29 | 0.44 |
| 1:O:52:ASN:CG | 3:Z:115:ARG:CZ | 2.86 | 0.44 |
| 2:I:21:SER:HG | 2:I:82:TYR:HE2 | 1.65 | 0.44 |
| 2:K:132:ALA:O | 2:K:133:ALA:C | 2.56 | 0.44 |
| 1:M:47:ILE:HD13 | 1:M:63:GLY:N | 2.32 | 0.44 |
| 2:J:130:GLY:C | 2:J:133:ALA:H | 2.18 | 0.44 |
| 2:K:216:ARG:NH2 | 3:V:123:ASP:N | 2.54 | 0.44 |
| 1:O:109:ASP:OD1 | 1:O:140:PRO:CD | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:V:149:THR:OG1 | 3:V:150:LEU:N | 2.50 | 0.44 |
| 3:V:96:GLN:HA | 3:V:99:LEU:HD12 | 1.99 | 0.44 |
| 1:L:32:MET:HB2 | 1:L:70:TYR:CD2 | 2.53 | 0.44 |
| 1:M:116:ILE:C | 1:M:117:PHE:CD1 | 2.91 | 0.44 |
| 1:M:189:ASN:CA | 1:M:210:ARG:HG3 | 2.42 | 0.44 |
| 2:K:51:ILE:HD13 | 2:K:51:ILE:HG21 | 1.69 | 0.44 |
| 1:N:89:GLN:HE21 | 1:N:96:THR:CB | 2.25 | 0.44 |
| 1:N:32:MET:HB2 | 1:N:70:TYR:CD2 | 2.53 | 0.44 |
| 2:I:39:GLN:OE1 | 2:I:97:TYR:OH | 2.23 | 0.44 |
| 2:I:38:ARG:HA | 2:I:95:ILE:O | 2.18 | 0.44 |
| 2:J:157:TRP:CD1 | 2:J:166:VAL:HG21 | 2.53 | 0.44 |
| 1:L:38:LYS:HA | 1:L:39:PRO:HD2 | 1.80 | 0.44 |
| 1:L:48:TYR:HE1 | 1:L:52:ASN:HD22 | 1.66 | 0.44 |
| 2:H:6:GLU:OE1 | 2:H:98:CYS:HB3 | 2.18 | 0.44 |
| 2:J:117:ALA:HB3 | 2:J:149:PHE:CE2 | 2.53 | 0.44 |
| 3:Z:98:ARG:HA | 3:Z:101:LEU:CB | 2.47 | 0.43 |
| 3:X:36:PRO:HG2 | 3:X:80:GLN:HB3 | 2.00 | 0.43 |
| 1:M:48:TYR:CD1 | 3:X:113:PRO:CG | 3.00 | 0.43 |
| 2:J:155:VAL:HB | 2:J:200:VAL:HG12 | 2.00 | 0.43 |
| 3:Y:63:ILE:HG22 | 3:Y:67:VAL:HG21 | 2.00 | 0.43 |
| 2:I:192:PRO:O | 2:I:193:SER:O | 2.35 | 0.43 |
| 3:V:19:SER:O | 3:V:22:LEU:N | 2.51 | 0.43 |
| 3:Z:51:TRP:CD1 | 3:Z:51:TRP:C | 2.91 | 0.43 |
| 1:L:64:SER:OG | 1:L:65:GLY:N | 2.50 | 0.43 |
| 1:O:90:ARG:HH21 | 2:K:102:SER:HB2 | 1.81 | 0.43 |
| 1:N:166:ASP:O | 1:N:167:SER:C | 2.56 | 0.43 |
| 1:L:119:PRO:HB2 | 1:L:124:LEU:CD2 | 2.48 | 0.43 |
| 3:Z:46:PHE:HD1 | 3:Z:46:PHE:HA | 1.71 | 0.43 |
| 1:O:191:TYR:CB | 1:O:208:PHE:CE1 | 3.00 | 0.43 |
| 1:O:118:PRO:CB | 1:O:208:PHE:CE2 | 2.96 | 0.43 |
| 1:L:211:ASN:O | 1:L:212:GLU:HB2 | 2.18 | 0.43 |
| 1:N:109:ASP:OD1 | 1:N:109:ASP:N | 2.49 | 0.43 |
| 1:O:95:ARG:HG2 | 1:O:95:ARG:H | 1.52 | 0.43 |
| 3:Z:119:THR:OG1 | 3:Z:121:HIS:NE2 | 2.42 | 0.43 |
| 3:Z:26:LEU:O | 3:Z:29:CYS:HB2 | 2.18 | 0.43 |
| 3:Z:26:LEU:HD11 | 3:Z:32:VAL:HG11 | 1.99 | 0.43 |
| 3:Z:30:PRO:O | 3:Z:31:GLU:C | 2.57 | 0.43 |
| 2:J:22:CYS:O | 2:J:80:SER:HA | 2.18 | 0.43 |
| 2:J:39:GLN:HB3 | 2:J:95:ILE:HG12 | 2.00 | 0.43 |
| 2:I:124:VAL:HA | 2:I:144:LEU:O | 2.18 | 0.43 |
| 3:Y:115:ARG:HD2 | 3:Y:116:GLY:CA | 2.48 | 0.43 |
| 3:Z:127:ILE:HD13 | 3:Z:127:ILE:HG21 | 1.68 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:94:PRO:HA | 2:H:47:TRP:CZ3 | 2.52 | 0.43 |
| 1:M:11:MET:HE2 | 1:M:19:VAL:CG2 | 2.48 | 0.43 |
| 2:I:152:PRO:O | 2:I:152:PRO:CD | 2.66 | 0.43 |
| 2:J:23:ALA:HA | 2:J:80:SER:HA | 1.99 | 0.43 |
| 2:J:148:TYR:HD1 | 2:J:148:TYR:H | 1.66 | 0.43 |
| 3:Y:75:MET:HA | 3:Y:75:MET:CE | 2.47 | 0.43 |
| 3:V:104:LEU:O | 3:V:108:LEU:HD12 | 2.18 | 0.43 |
| 1:M:187:ARG:O | 1:M:187:ARG:HG2 | 2.18 | 0.43 |
| 1:M:73:THR:HG22 | 1:M:73:THR:O | 2.17 | 0.43 |
| 3:Y:115:ARG:CD | 3:Y:116:GLY:N | 2.79 | 0.43 |
| 1:L:61:PHE:CD1 | 1:L:74:ILE:HG12 | 2.54 | 0.43 |
| 1:N:110:ALA:CB | 1:N:138:PHE:HA | 2.49 | 0.43 |
| 3:Z:119:THR:HG1 | 3:Z:121:HIS:CD2 | 2.35 | 0.43 |
| 3:X:108:LEU:HD23 | 3:X:108:LEU:HA | 1.43 | 0.43 |
| 1:M:123:GLN:HE22 | 1:M:130:SER:HG | 1.51 | 0.43 |
| 1:O:118:PRO:CG | 1:O:208:PHE:CD2 | 3.01 | 0.43 |
| 2:I:158:ASN:C | 2:I:160:GLY:H | 2.21 | 0.43 |
| 1:O:46:TRP:HA | 1:O:46:TRP:CE3 | 2.52 | 0.43 |
| 2:I:36:TRP:NE1 | 2:I:83:LEU:HG | 2.34 | 0.43 |
| 1:M:7:SER:HB3 | 1:M:22:THR:H | 1.82 | 0.43 |
| 3:X:129:LEU:O | 3:X:132:GLN:N | 2.51 | 0.43 |
| 1:M:185:TYR:CA | 1:M:191:TYR:OH | 2.67 | 0.43 |
| 2:H:93:THR:OG1 | 2:H:114:VAL:HG23 | 2.15 | 0.43 |
| 2:I:51:ILE:HD13 | 2:I:74:ARG:HG3 | 2.00 | 0.43 |
| 1:M:97:PHE:HE2 | 2:I:47:TRP:N | 2.15 | 0.43 |
| 3:X:100:LEU:HD22 | 3:X:100:LEU:O | 2.18 | 0.43 |
| 3:Y:51:TRP:C | 3:Y:53:THR:N | 2.72 | 0.43 |
| 3:X:134:LEU:HD23 | 3:X:134:LEU:HA | 1.84 | 0.43 |
| 1:M:147:TRP:CE3 | 1:M:192:THR:O | 2.72 | 0.43 |
| 3:X:51:TRP:CE2 | 3:X:138:LYS:HE3 | 2.53 | 0.43 |
| 3:X:51:TRP:CZ2 | 3:X:138:LYS:HE3 | 2.51 | 0.43 |
| 3:Y:11:VAL:O | 3:Y:15:LEU:HD22 | 2.18 | 0.43 |
| 3:Y:139:VAL:O | 3:Y:143:MET:HG3 | 2.19 | 0.43 |
| 2:J:89:ARG:O | 2:J:114:VAL:HG11 | 2.18 | 0.43 |
| 2:H:18:MET:O | 2:H:85:MET:N | 2.52 | 0.43 |
| 3:V:123:ASP:HA | 3:V:124:PRO:HD3 | 1.81 | 0.43 |
| 1:M:46:TRP:CE2 | 1:M:57:VAL:HG13 | 2.53 | 0.43 |
| 2:I:9:GLY:HA2 | 2:I:18:MET:SD | 2.58 | 0.43 |
| 2:H:37:VAL:HG12 | 2:H:37:VAL:O | 2.19 | 0.43 |
| 1:L:114:VAL:HG21 | 1:L:204:ILE:CG2 | 2.48 | 0.43 |
| 3:V:26:LEU:O | 3:V:27:SER:C | 2.57 | 0.43 |
| 2:J:174:GLN:HB3 | 2:J:175:SER:H | 1.46 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:33:TRP:CZ3 | 3:V:110:THR:HA | 2.53 | 0.43 |
| 3:X:132:GLN:C | 3:X:134:LEU:N | 2.72 | 0.43 |
| 2:I:4:LEU:HD23 | 2:I:24:ALA:HB2 | 2.01 | 0.43 |
| 3:Y:86:LEU:HD23 | 3:Y:86:LEU:HA | 1.72 | 0.43 |
| 1:L:79:ALA:HA | 1:L:105:ILE:HD13 | 2.01 | 0.43 |
| 3:Y:52:LYS:NZ | 3:Y:145:VAL:CG2 | 2.82 | 0.43 |
| 3:Z:75:MET:HA | 3:Z:75:MET:HE3 | 2.00 | 0.43 |
| 1:N:44:LYS:HE3 | 1:N:44:LYS:HB2 | 1.53 | 0.43 |
| 1:O:180:LEU:HD12 | 1:O:180:LEU:C | 2.39 | 0.43 |
| 2:H:104:LEU:HG | 2:H:104:LEU:O | 2.18 | 0.43 |
| 3:Z:61:GLN:O | 3:Z:65:GLY:N | 2.35 | 0.43 |
| 1:M:189:ASN:HD22 | 1:M:210:ARG:N | 2.16 | 0.43 |
| 3:X:137:GLY:O | 3:X:138:LYS:C | 2.57 | 0.43 |
| 3:X:41:LEU:HD13 | 3:X:127:ILE:HA | 2.01 | 0.43 |
| 2:I:177:LEU:HD23 | 2:I:177:LEU:HA | 1.41 | 0.43 |
| 2:I:54:LYS:O | 2:I:55:VAL:C | 2.57 | 0.43 |
| 1:O:123:GLN:HG3 | 2:K:125:TYR:CE2 | 2.54 | 0.43 |
| 1:N:94:PRO:HA | 2:J:47:TRP:CZ3 | 2.54 | 0.43 |
| 2:H:84:GLN:NE2 | 2:H:84:GLN:HA | 2.33 | 0.43 |
| 2:K:175:SER:O | 2:K:176:ASP:C | 2.57 | 0.43 |
| 2:K:149:PHE:HB2 | 2:K:177:LEU:CD2 | 2.49 | 0.43 |
| 1:O:194:GLU:HB3 | 1:O:205:VAL:HG13 | 2.00 | 0.43 |
| 3:V:140:ARG:HA | 3:V:143:MET:CE | 2.48 | 0.43 |
| 2:J:162:LEU:HA | 2:J:162:LEU:HD23 | 1.79 | 0.43 |
| 2:J:186:VAL:HG23 | 2:J:187:PRO:O | 2.18 | 0.43 |
| 1:N:169:ASP:OD2 | 1:N:169:ASP:C | 2.56 | 0.43 |
| 3:V:15:LEU:O | 3:V:16:LEU:C | 2.56 | 0.43 |
| 2:K:33:TRP:CZ3 | 3:Z:110:THR:HA | 2.53 | 0.43 |
| 3:Z:61:GLN:O | 3:Z:62:ASP:C | 2.58 | 0.43 |
| 2:K:51:ILE:HD11 | 2:K:74:ARG:CD | 2.49 | 0.43 |
| 3:V:74:VAL:HG22 | 3:V:127:ILE:HG13 | 2.01 | 0.43 |
| 3:Y:37:THR:HG22 | 3:Y:38:PRO:O | 2.18 | 0.43 |
| 3:Z:12:LEU:HD13 | 3:Z:143:MET:SD | 2.59 | 0.43 |
| 3:X:30:PRO:O | 3:X:31:GLU:C | 2.57 | 0.43 |
| 1:M:54:ALA:O | 1:M:56:GLY:N | 2.52 | 0.43 |
| 1:N:175:SER:HB3 | 2:J:169:PHE:CE1 | 2.54 | 0.43 |
| 3:V:75:MET:O | 3:V:77:ALA:N | 2.52 | 0.42 |
| 3:Z:101:LEU:HD12 | 3:Z:105:GLN:NE2 | 2.34 | 0.42 |
| 1:N:58:PRO:O | 1:N:61:PHE:HB2 | 2.20 | 0.42 |
| 3:V:70:LEU:HA | 3:V:70:LEU:HD23 | 1.82 | 0.42 |
| 2:K:124:VAL:HA | 2:K:144:LEU:O | 2.19 | 0.42 |
| 3:X:37:THR:HA | 3:X:38:PRO:HD3 | 1.71 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:I:36:TRP:CD1 | 2:I:83:LEU:HG | 2.54 | 0.42 |
| 1:N:125:THR:HG22 | 1:N:125:THR:O | 2.19 | 0.42 |
| 3:X:12:LEU:HD22 | 3:X:143:MET:SD | 2.60 | 0.42 |
| 1:O:117:PHE:HA | 1:O:118:PRO:HD3 | 1.66 | 0.42 |
| 3:Y:115:ARG:HD2 | 3:Y:115:ARG:C | 2.40 | 0.42 |
| 3:Y:123:ASP:O | 3:Y:124:PRO:C | 2.57 | 0.42 |
| 2:I:93:THR:HG23 | 2:I:112:VAL:O | 2.19 | 0.42 |
| 3:Z:119:THR:O | 3:Z:121:HIS:HD2 | 2.02 | 0.42 |
| 2:J:111:LEU:HD22 | 2:J:111:LEU:HA | 1.73 | 0.42 |
| 3:V:64:LEU:HB2 | 3:V:104:LEU:HB3 | 1.99 | 0.42 |
| 3:V:78:ARG:O | 3:V:79:GLY:C | 2.57 | 0.42 |
| 2:J:77:SER:C | 2:J:79:SER:H | 2.21 | 0.42 |
| 2:J:54:LYS:O | 2:J:55:VAL:C | 2.54 | 0.42 |
| 1:N:118:PRO:HB3 | 1:N:208:PHE:CZ | 2.54 | 0.42 |
| 3:V:90:LEU:HD21 | 3:V:128:PHE:CE2 | 2.54 | 0.42 |
| 3:V:90:LEU:O | 3:V:94:SER:HB3 | 2.19 | 0.42 |
| 1:O:185:TYR:CE1 | 1:O:210:ARG:HG3 | 2.54 | 0.42 |
| 1:O:185:TYR:HE1 | 1:O:191:TYR:CE1 | 2.37 | 0.42 |
| 2:K:122:PRO:CB | 2:K:148:TYR:HB3 | 2.47 | 0.42 |
| 2:J:184:VAL:HG22 | 2:J:185:THR:N | 2.33 | 0.42 |
| 2:K:25:SER:O | 2:K:27:PHE:HD1 | 2.03 | 0.42 |
| 2:H:214:VAL:HG12 | 2:H:215:PRO:CD | 2.49 | 0.42 |
| 2:K:9:GLY:HA2 | 2:K:112:VAL:CG2 | 2.48 | 0.42 |
| 3:V:97:VAL:HA | 3:V:131:PHE:CZ | 2.53 | 0.42 |
| 1:N:18:LYS:HA | 1:N:75:SER:O | 2.19 | 0.42 |
| 1:N:27:SER:O | 1:N:28:SER:C | 2.58 | 0.42 |
| 2:K:45:LEU:HD23 | 2:K:45:LEU:HA | 1.74 | 0.42 |
| 1:L:33:TYR:CE1 | 1:L:90:ARG:HD3 | 2.54 | 0.42 |
| 1:M:189:ASN:O | 1:M:210:ARG:N | 2.45 | 0.42 |
| 3:Y:13:SER:O | 3:Y:16:LEU:N | 2.52 | 0.42 |
| 1:N:162:TRP:CZ2 | 1:N:174:MET:CE | 3.02 | 0.42 |
| 1:N:1:GLN:N | 1:N:94:PRO:HD2 | 2.34 | 0.42 |
| 3:Y:26:LEU:C | 3:Y:28:GLN:N | 2.73 | 0.42 |
| 2:J:151:GLU:HA | 2:J:152:PRO:HA | 1.68 | 0.42 |
| 2:J:11:LEU:O | 2:J:12:VAL:HG13 | 2.19 | 0.42 |
| 1:O:104:GLU:HB3 | 4:O:217:HOH:O | 2.19 | 0.42 |
| 3:Z:51:TRP:HZ2 | 3:Z:63:ILE:HD11 | 1.85 | 0.42 |
| 1:M:50:THR:HG23 | 1:M:70:TYR:CD2 | 2.55 | 0.42 |
| 2:K:90:ALA:O | 2:K:114:VAL:HG23 | 2.20 | 0.42 |
| 3:X:87:SER:O | 3:X:89:LEU:N | 2.52 | 0.42 |
| 2:I:149:PHE:CG | 2:I:150:PRO:HA | 2.55 | 0.42 |
| 1:L:76:ARG:NH1 | 1:L:76:ARG:HB3 | 2.27 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:139:TYR:CG | 1:M:140:PRO:HA | 2.55 | 0.42 |
| 1:L:6:GLN:HE22 | 1:L:87:CYS:N | 2.13 | 0.42 |
| 1:O:20:THR:O | 1:O:20:THR:HG23 | 2.18 | 0.42 |
| 2:J:177:LEU:HA | 2:J:177:LEU:HD23 | 1.82 | 0.42 |
| 1:O:188:HIS:N | 1:O:188:HIS:CD2 | 2.88 | 0.42 |
| 1:O:70:TYR:N | 1:O:70:TYR:CD1 | 2.87 | 0.42 |
| 2:K:38:ARG:CD | 2:K:46:GLU:HG2 | 2.49 | 0.42 |
| 2:K:29:PHE:CB | 2:K:79:SER:CB | 2.87 | 0.42 |
| 2:K:216:ARG:HH21 | 3:V:123:ASP:N | 2.13 | 0.42 |
| 3:Y:86:LEU:O | 3:Y:89:LEU:N | 2.53 | 0.42 |
| 1:O:124:LEU:HA | 1:O:124:LEU:HD12 | 1.92 | 0.42 |
| 3:V:22:LEU:O | 3:V:23:HIS:C | 2.56 | 0.42 |
| 3:X:22:LEU:CD2 | 3:X:92:GLN:HE21 | 2.32 | 0.42 |
| 2:I:19:LYS:HG3 | 2:I:84:GLN:HB2 | 2.00 | 0.42 |
| 1:M:143:ILE:HG23 | 1:M:143:ILE:O | 2.18 | 0.42 |
| 2:I:60:ILE:HG21 | 2:I:62:TYR:CE2 | 2.54 | 0.42 |
| 2:K:3:LYS:HD2 | 4:K:224:HOH:O | 2.19 | 0.42 |
| 2:J:8:GLY:C | 2:J:9:GLY:O | 2.56 | 0.42 |
| 3:Z:101:LEU:O | 3:Z:102:GLY:C | 2.58 | 0.42 |
| 1:M:132:VAL:CG1 | 2:I:144:LEU:HD22 | 2.49 | 0.42 |
| 2:H:151:GLU:OE2 | 2:H:171:ALA:HB2 | 2.19 | 0.42 |
| 1:O:46:TRP:HB3 | 1:O:47:ILE:H | 1.62 | 0.42 |
| 1:L:114:VAL:CG1 | 1:L:115:SER:N | 2.82 | 0.42 |
| 3:Z:75:MET:HE3 | 3:Z:75:MET:CA | 2.49 | 0.42 |
| 2:I:98:CYS:O | 2:I:98:CYS:SG | 2.77 | 0.42 |
| 3:V:78:ARG:HD2 | 3:V:91:GLY:N | 2.34 | 0.42 |
| 1:O:88:GLN:HE22 | 1:O:90:ARG:NH1 | 2.17 | 0.42 |
| 3:Y:43:ALA:H | 3:Y:118:THR:HA | 1.85 | 0.42 |
| 2:K:141:LEU:HD23 | 2:K:141:LEU:HA | 1.55 | 0.42 |
| 1:L:48:TYR:CE2 | 3:V:113:PRO:CG | 3.03 | 0.42 |
| 1:L:14:SER:O | 1:L:15:PRO:C | 2.56 | 0.42 |
| 1:O:7:SER:CB | 1:O:8:PRO:HD3 | 2.49 | 0.42 |
| 2:I:19:LYS:HG3 | 2:I:84:GLN:HA | 2.01 | 0.42 |
| 3:Y:26:LEU:C | 3:Y:28:GLN:H | 2.21 | 0.42 |
| 2:I:62:TYR:CZ | 2:I:72:VAL:HG12 | 2.55 | 0.42 |
| 1:L:65:GLY:HA2 | 1:L:70:TYR:HA | 2.01 | 0.42 |
| 1:L:135:LEU:HB2 | 1:L:174:MET:HG2 | 2.00 | 0.42 |
| 3:X:123:ASP:OD2 | 3:X:125:ASN:HB2 | 2.20 | 0.42 |
| 3:X:17:ARG:O | 3:X:20:HIS:HB2 | 2.19 | 0.42 |
| 3:Y:101:LEU:O | 3:Y:104:LEU:N | 2.53 | 0.42 |
| 2:J:134:GLN:HB3 | 2:J:136:ASN:HD21 | 1.84 | 0.42 |
| 3:Z:100:LEU:HA | 3:Z:100:LEU:HD23 | 1.58 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:Z:96:GLN:O | 3:Z:97:VAL:C | 2.58 | 0.42 |
| 1:L:43:PRO:HD2 | 2:H:106:TRP:CE3 | 2.54 | 0.42 |
| 1:M:37:GLN:O | 1:M:83:ALA:HB1 | 2.20 | 0.42 |
| 1:O:202:SER:O | 1:O:204:ILE:N | 2.53 | 0.42 |
| 3:Z:121:HIS:ND1 | 3:Z:126:ALA:HB1 | 2.35 | 0.42 |
| 2:K:183:SER:OG | 2:K:183:SER:O | 2.37 | 0.42 |
| 2:K:157:TRP:CZ3 | 2:K:198:CYS:HB3 | 2.55 | 0.42 |
| 2:K:129:PRO:O | 2:K:215:PRO:HG3 | 2.19 | 0.42 |
| 2:H:211:LYS:O | 2:H:213:ILE:HG12 | 2.20 | 0.42 |
| 1:M:185:TYR:CD1 | 1:M:191:TYR:OH | 2.73 | 0.42 |
| 2:H:122:PRO:CB | 2:H:148:TYR:HB3 | 2.50 | 0.42 |
| 3:Y:125:ASN:O | 3:Y:129:LEU:HB2 | 2.19 | 0.42 |
| 2:J:86:ASN:O | 2:J:87:SER:O | 2.36 | 0.42 |
| 3:X:31:GLU:HB3 | 3:X:33:HIS:CE1 | 2.55 | 0.42 |
| 1:N:107:ARG:HG3 | 1:N:108:ALA:N | 2.34 | 0.42 |
| 1:O:169:ASP:O | 1:O:169:ASP:CG | 2.57 | 0.42 |
| 2:I:200:VAL:HG23 | 2:I:208:LYS:O | 2.19 | 0.41 |
| 1:M:211:ASN:O | 1:M:212:GLU:HB2 | 2.20 | 0.41 |
| 3:X:35:LEU:HA | 3:X:36:PRO:HD2 | 1.76 | 0.41 |
| 1:N:86:TYR:CG | 2:J:45:LEU:HD12 | 2.55 | 0.41 |
| 2:H:176:ASP:CB | 4:H:226:HOH:O | 2.62 | 0.41 |
| 2:K:123:SER:HB3 | 2:K:125:TYR:OH | 2.19 | 0.41 |
| 1:O:107:ARG:CG | 1:O:108:ALA:N | 2.77 | 0.41 |
| 2:K:192:PRO:O | 2:K:193:SER:C | 2.58 | 0.41 |
| 1:L:76:ARG:CB | 1:L:76:ARG:HH11 | 2.27 | 0.41 |
| 2:J:213:ILE:HG23 | 2:J:214:VAL:HG23 | 2.01 | 0.41 |
| 1:M:78:GLU:CD | 1:N:107:ARG:HH22 | 2.24 | 0.41 |
| 2:H:216:ARG:HH22 | 3:Z:123:ASP:CB | 2.31 | 0.41 |
| 3:V:93:LEU:O | 3:V:96:GLN:CB | 2.67 | 0.41 |
| 1:L:114:VAL:CG2 | 1:L:204:ILE:HG21 | 2.50 | 0.41 |
| 1:O:31:TYR:HA | 1:O:50:THR:OG1 | 2.19 | 0.41 |
| 2:J:13:GLN:O | 2:J:14:PRO:C | 2.56 | 0.41 |
| 2:J:38:ARG:NH2 | 2:J:92:ASP:HA | 2.34 | 0.41 |
| 2:H:33:TRP:HD1 | 2:H:53:SER:OG | 2.02 | 0.41 |
| 3:Z:108:LEU:HA | 3:Z:108:LEU:HD23 | 1.65 | 0.41 |
| 1:M:166:ASP:HB3 | 1:M:169:ASP:O | 2.19 | 0.41 |
| 3:V:66:ALA:O | 3:V:69:LEU:N | 2.52 | 0.41 |
| 2:I:76:ASP:O | 2:I:78:LYS:N | 2.53 | 0.41 |
| 2:H:40:SER:O | 2:H:44:GLY:HA2 | 2.20 | 0.41 |
| 1:L:37:GLN:HE21 | 1:L:86:TYR:HE2 | 1.67 | 0.41 |
| 3:Z:123:ASP:C | 3:Z:125:ASN:N | 2.71 | 0.41 |
| 3:V:26:LEU:O | 3:V:28:GLN:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:130:GLY:C | 2:H:132:ALA:H | 2.23 | 0.41 |
| 2:J:38:ARG:HB2 | 2:J:96:TYR:HD2 | 1.72 | 0.41 |
| 1:L:33:TYR:CD1 | 1:L:90:ARG:HD3 | 2.55 | 0.41 |
| 1:L:89:GLN:NE2 | 1:L:96:THR:HB | 2.32 | 0.41 |
| 3:Z:108:LEU:O | 3:Z:110:THR:HG22 | 2.20 | 0.41 |
| 1:M:184:GLU:HG3 | 1:M:187:ARG:HH12 | 1.85 | 0.41 |
| 2:J:56:ASN:OD1 | 3:Y:105:GLN:HB3 | 2.20 | 0.41 |
| 2:J:135:THR:C | 2:J:136:ASN:O | 2.57 | 0.41 |
| 3:V:128:PHE:O | 3:V:132:GLN:HG3 | 2.20 | 0.41 |
| 1:O:94:PRO:CB | 2:K:47:TRP:CZ3 | 3.03 | 0.41 |
| 2:K:27:PHE:CG | 2:K:27:PHE:O | 2.73 | 0.41 |
| 1:O:174:MET:HA | 2:K:169:PHE:CE1 | 2.56 | 0.41 |
| 2:K:7:SER:O | 2:K:21:SER:N | 2.47 | 0.41 |
| 2:K:157:TRP:O | 2:K:158:ASN:C | 2.57 | 0.41 |
| 3:Y:112:LEU:HA | 3:Y:113:PRO:HD3 | 1.79 | 0.41 |
| 1:M:211:ASN:O | 1:M:212:GLU:CB | 2.68 | 0.41 |
| 1:L:147:TRP:CB | 1:L:178:LEU:HD12 | 2.50 | 0.41 |
| 1:O:189:ASN:ND2 | 1:O:210:ARG:N | 2.67 | 0.41 |
| 1:M:57:VAL:HA | 1:M:58:PRO:HD3 | 1.83 | 0.41 |
| 2:I:214:VAL:HA | 2:I:215:PRO:HD3 | 1.84 | 0.41 |
| 2:I:35:ASP:O | 2:I:99:SER:N | 2.39 | 0.41 |
| 3:Y:70:LEU:O | 3:Y:74:VAL:HG23 | 2.20 | 0.41 |
| 1:O:18:LYS:HG3 | 1:O:75:SER:O | 2.20 | 0.41 |
| 2:K:52:ARG:HB3 | 2:K:56:ASN:HB2 | 2.02 | 0.41 |
| 1:L:110:ALA:O | 1:L:138:PHE:CA | 2.45 | 0.41 |
| 3:X:143:MET:HG3 | 3:X:143:MET:H | 1.60 | 0.41 |
| 2:K:40:SER:CB | 2:K:42:GLU:H | 2.34 | 0.41 |
| 2:J:29:PHE:C | 2:J:31:ASP:N | 2.73 | 0.41 |
| 1:L:178:LEU:HD23 | 1:L:179:THR:N | 2.36 | 0.41 |
| 1:M:90:ARG:CA | 1:M:95:ARG:HH21 | 2.33 | 0.41 |
| 1:L:169:ASP:C | 1:L:169:ASP:OD2 | 2.58 | 0.41 |
| 1:N:132:VAL:HB | 1:N:177:THR:HG23 | 2.01 | 0.41 |
| 3:V:22:LEU:HD12 | 3:V:96:GLN:NE2 | 2.36 | 0.41 |
| 1:N:135:LEU:CD2 | 1:N:195:ALA:HB2 | 2.50 | 0.41 |
| 2:K:158:ASN:HA | 2:K:158:ASN:HD22 | 1.50 | 0.41 |
| 1:L:159:LEU:HD23 | 1:L:159:LEU:HA | 1.84 | 0.41 |
| 3:Z:140:ARG:C | 3:Z:142:LEU:N | 2.73 | 0.41 |
| 1:L:185:TYR:HE1 | 1:L:191:TYR:CD1 | 2.33 | 0.41 |
| 1:L:135:LEU:O | 1:L:138:PHE:HE2 | 2.04 | 0.41 |
| 2:I:122:PRO:HA | 2:I:146:LYS:O | 2.20 | 0.41 |
| 2:J:216:ARG:NE | 3:X:122:LYS:H | 2.18 | 0.41 |
| 2:H:157:TRP:CE3 | 2:H:198:CYS:HB3 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:Y:86:LEU:O | 3:Y:87:SER:C | 2.59 | 0.41 |
| 1:L:35:PHE:HB3 | 1:L:44:LYS:O | 2.21 | 0.41 |
| 3:Z:141:PHE:O | 3:Z:142:LEU:C | 2.56 | 0.41 |
| 3:X:16:LEU:HD11 | 3:X:136:ARG:CG | 2.50 | 0.41 |
| 2:K:40:SER:HB2 | 2:K:42:GLU:H | 1.85 | 0.41 |
| 2:J:89:ARG:CB | 2:J:91:GLU:OE1 | 2.49 | 0.41 |
| 2:H:70:PHE:HD1 | 2:H:85:MET:HA | 1.85 | 0.41 |
| 1:N:184:GLU:HG3 | 1:N:187:ARG:NH2 | 2.36 | 0.41 |
| 1:L:52:ASN:ND2 | 3:V:115:ARG:HH11 | 2.19 | 0.41 |
| 1:O:134:PHE:CZ | 2:K:183:SER:HB3 | 2.56 | 0.41 |
| 1:L:114:VAL:HG23 | 1:L:204:ILE:HG21 | 2.02 | 0.41 |
| 1:N:125:THR:CG2 | 1:N:125:THR:O | 2.68 | 0.41 |
| 3:X:72:GLU:OE1 | 3:X:114:PRO:HG3 | 2.21 | 0.41 |
| 1:M:204:ILE:HD13 | 1:M:204:ILE:N | 2.36 | 0.41 |
| 3:Z:59:LYS:NZ | 3:Z:145:VAL:HG21 | 2.36 | 0.41 |
| 3:X:123:ASP:C | 3:X:125:ASN:H | 2.23 | 0.41 |
| 3:V:123:ASP:OD1 | 3:V:124:PRO:HD2 | 2.21 | 0.41 |
| 1:O:116:ILE:CA | 1:O:117:PHE:HD1 | 2.33 | 0.41 |
| 3:Y:63:ILE:O | 3:Y:67:VAL:CG2 | 2.59 | 0.41 |
| 1:M:4:LEU:N | 1:M:4:LEU:HD23 | 2.36 | 0.41 |
| 2:H:2:VAL:O | 2:H:2:VAL:HG22 | 2.20 | 0.41 |
| 2:I:38:ARG:HB2 | 2:I:96:TYR:CD1 | 2.56 | 0.41 |
| 2:K:174:GLN:HB3 | 2:K:175:SER:H | 1.27 | 0.41 |
| 1:M:1:GLN:O | 1:M:1:GLN:CG | 2.65 | 0.41 |
| 3:X:69:LEU:O | 3:X:69:LEU:HD22 | 2.21 | 0.41 |
| 1:L:141:LYS:HG3 | 1:L:172:TYR:CD1 | 2.56 | 0.41 |
| 1:N:104:GLU:HB3 | 4:N:216:HOH:O | 2.21 | 0.41 |
| 1:O:45:LEU:O | 1:O:54:ALA:HB3 | 2.21 | 0.41 |
| 2:J:70:PHE:CE1 | 2:J:85:MET:CG | 3.03 | 0.41 |
| 1:L:181:THR:OG1 | 1:L:184:GLU:HB2 | 2.21 | 0.41 |
| 1:M:49:SER:O | 1:M:51:SER:N | 2.54 | 0.41 |
| 2:I:122:PRO:HB2 | 2:I:145:VAL:HG23 | 2.03 | 0.41 |
| 2:I:123:SER:HB2 | 2:I:125:TYR:CE2 | 2.56 | 0.41 |
| 2:K:51:ILE:O | 2:K:51:ILE:HG23 | 2.20 | 0.41 |
| 3:X:35:LEU:HD21 | 3:X:77:ALA:HB1 | 2.01 | 0.41 |
| 3:Y:135:LEU:HA | 3:Y:139:VAL:HB | 2.02 | 0.41 |
| 3:Y:10:ARG:O | 3:Y:13:SER:CA | 2.69 | 0.41 |
| 3:Y:8:ASP:O | 3:Y:11:VAL:HG22 | 2.21 | 0.41 |
| 1:N:116:ILE:HD11 | 1:N:208:PHE:HD1 | 1.85 | 0.41 |
| 2:I:176:ASP:O | 2:I:177:LEU:HG | 2.21 | 0.41 |
| 2:I:148:TYR:CE2 | 2:I:153:VAL:HG12 | 2.56 | 0.41 |
| 2:J:51:ILE:HD11 | 2:J:74:ARG:HG3 | 1.99 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:V:41:LEU:HD13 | 3:V:127:ILE:HA | 2.03 | 0.41 |
| 2:J:171:ALA:HB2 | 2:J:180:LEU:HD12 | 2.01 | 0.41 |
| 3:Y:38:PRO:HG3 | 3:Y:122:LYS:HG2 | 2.01 | 0.41 |
| 1:M:137:ASN:H | 1:M:173:SER:HB3 | 1.86 | 0.41 |
| 2:H:2:VAL:HG21 | 2:H:105:TYR:CG | 2.56 | 0.41 |
| 1:M:38:LYS:HA | 1:M:39:PRO:HD2 | 1.68 | 0.41 |
| 1:L:139:TYR:CA | 1:L:140:PRO:O | 2.69 | 0.41 |
| 3:Y:22:LEU:HD21 | 3:Y:92:GLN:CB | 2.45 | 0.41 |
| 1:L:6:GLN:HE22 | 1:L:86:TYR:HA | 1.85 | 0.41 |
| 2:H:138:MET:CE | 2:H:187:PRO:HA | 2.49 | 0.41 |
| 1:L:34:TRP:C | 1:L:35:PHE:CD1 | 2.94 | 0.41 |
| 3:Y:51:TRP:O | 3:Y:52:LYS:C | 2.59 | 0.41 |
| 2:K:168:THR:HG22 | 2:K:169:PHE:N | 2.36 | 0.41 |
| 1:O:162:TRP:O | 2:K:170:PRO:HG2 | 2.20 | 0.41 |
| 2:H:83:LEU:HD23 | 2:H:83:LEU:HA | 1.48 | 0.41 |
| 2:H:54:LYS:HB2 | 2:H:54:LYS:HE2 | 1.90 | 0.41 |
| 2:J:196:VAL:O | 2:J:196:VAL:HG22 | 2.20 | 0.41 |
| 3:X:25:ARG:HH11 | 3:X:25:ARG:HG3 | 1.86 | 0.41 |
| 1:L:29:VAL:HG12 | 1:L:30:SER:H | 1.86 | 0.41 |
| 2:K:64:GLU:C | 2:K:66:VAL:N | 2.71 | 0.41 |
| 2:J:28:THR:O | 2:J:29:PHE:C | 2.58 | 0.41 |
| 1:L:147:TRP:CE3 | 1:L:178:LEU:CD1 | 3.04 | 0.41 |
| 3:Z:35:LEU:HA | 3:Z:36:PRO:HD2 | 1.99 | 0.41 |
| 1:O:147:TRP:HE3 | 1:O:192:THR:O | 2.01 | 0.41 |
| 1:L:144:ASN:O | 1:L:195:ALA:HA | 2.21 | 0.41 |
| 3:V:49:GLY:C | 3:V:51:TRP:H | 2.25 | 0.41 |
| 1:O:11:MET:CG | 1:O:103:LEU:CD1 | 2.97 | 0.40 |
| 3:V:75:MET:CE | 3:V:98:ARG:HH22 | 2.34 | 0.40 |
| 2:K:54:LYS:O | 2:K:57:ASN:HA | 2.21 | 0.40 |
| 1:M:31:TYR:HB3 | 1:M:49:SER:HA | 2.02 | 0.40 |
| 1:M:35:PHE:O | 1:M:86:TYR:N | 2.54 | 0.40 |
| 3:V:93:LEU:C | 3:V:93:LEU:CD2 | 2.90 | 0.40 |
| 3:Z:116:GLY:O | 3:Z:117:ARG:O | 2.39 | 0.40 |
| 2:K:66:VAL:CG2 | 2:K:70:PHE:CD2 | 3.03 | 0.40 |
| 2:J:6:GLU:H | 2:J:6:GLU:HG2 | 1.52 | 0.40 |
| 1:O:147:TRP:CZ3 | 1:O:193:CYS:HB2 | 2.56 | 0.40 |
| 2:H:24:ALA:HB3 | 2:H:29:PHE:HD1 | 1.87 | 0.40 |
| 2:H:141:LEU:CD1 | 2:H:196:VAL:HG11 | 2.51 | 0.40 |
| 1:O:145:VAL:HG11 | 1:O:176:SER:CB | 2.51 | 0.40 |
| 3:X:109:GLY:O | 4:X:166:HOH:O | 2.22 | 0.40 |
| 1:O:44:LYS:HZ3 | 1:O:44:LYS:CB | 2.23 | 0.40 |
| 2:I:216:ARG:HE | 3:Y:122:LYS:HG3 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:X:100:LEU:O | 3:X:103:ALA:HB3 | 2.22 | 0.40 |
| 2:H:157:TRP:CZ3 | 2:H:198:CYS:CB | 3.00 | 0.40 |
| 2:I:70:PHE:CE1 | 2:I:85:MET:HE2 | 2.56 | 0.40 |
| 3:X:69:LEU:HA | 3:X:69:LEU:HD23 | 1.87 | 0.40 |
| 3:Z:86:LEU:HD11 | 3:Z:124:PRO:HG3 | 2.03 | 0.40 |
| 2:J:33:TRP:N | 3:Y:111:GLN:HE22 | 2.00 | 0.40 |
| 1:N:116:ILE:HG21 | 1:N:206:LYS:O | 2.22 | 0.40 |
| 1:N:19:VAL:HG11 | 1:N:103:LEU:HD21 | 1.99 | 0.40 |
| 1:N:19:VAL:HG23 | 1:N:77:MET:HB2 | 2.03 | 0.40 |
| 2:K:216:ARG:HH22 | 3:V:123:ASP:CB | 2.34 | 0.40 |
| 2:I:216:ARG:NH2 | 3:Y:122:LYS:H | 2.18 | 0.40 |
| 1:N:124:LEU:C | 1:N:126:SER:H | 2.24 | 0.40 |
| 2:K:78:LYS:HA | 4:K:219:HOH:O | 2.21 | 0.40 |
| 3:X:71:LEU:HA | 3:X:71:LEU:HD23 | 1.68 | 0.40 |
| 3:Z:141:PHE:HA | 3:Z:144:LEU:HB2 | 2.02 | 0.40 |
| 3:V:98:ARG:O | 3:V:101:LEU:HB3 | 2.21 | 0.40 |
| 1:O:19:VAL:CG1 | 1:O:74:ILE:HG13 | 2.51 | 0.40 |
| 1:M:31:TYR:CE2 | 3:X:61:GLN:NE2 | 2.90 | 0.40 |
| 1:M:189:ASN:ND2 | 1:M:211:ASN:ND2 | 2.69 | 0.40 |
| 1:M:192:THR:OG1 | 1:M:207:SER:HB2 | 2.20 | 0.40 |
| 1:N:185:TYR:HD1 | 1:N:191:TYR:CE1 | 2.35 | 0.40 |
| 2:H:105:TYR:O | 2:H:106:TRP:CD1 | 2.75 | 0.40 |
| 1:M:46:TRP:O | 1:M:57:VAL:HG21 | 2.21 | 0.40 |
| 2:I:66:VAL:O | 2:I:68:GLY:N | 2.55 | 0.40 |
| 1:M:162:TRP:O | 2:I:170:PRO:HD2 | 2.20 | 0.40 |
| 2:I:6:GLU:OE2 | 2:I:109:GLY:CA | 2.69 | 0.40 |
| 3:X:120:ALA:O | 3:X:121:HIS:CG | 2.74 | 0.40 |
| 2:J:214:VAL:HG23 | 3:X:38:PRO:HD2 | 2.04 | 0.40 |
| 1:O:134:PHE:C | 1:O:135:LEU:HD12 | 2.42 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|----------------|----------------------|-------------|----------|
| 1:L:62:ARG:NH2 | 4:V:165:HOH:O[1_545] | 2.19 | 0.01 |

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

of similar resolution. 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 | L | 211/213 (99%) | 178 (84%) | 28 (13%) | 5 (2%) | 9 | 53 |
| 1 | M | 210/213 (99%) | 179 (85%) | 20 (10%) | 11 (5%) | 3 | 27 |
| 1 | N | 210/213 (99%) | 177 (84%) | 20 (10%) | 13 (6%) | 2 | 21 |
| 1 | O | 211/213 (99%) | 175 (83%) | 24 (11%) | 12 (6%) | 3 | 24 |
| 2 | H | 215/217 (99%) | 175 (81%) | 24 (11%) | 16 (7%) | 2 | 15 |
| 2 | I | 215/217 (99%) | 170 (79%) | 25 (12%) | 20 (9%) | 1 | 9 |
| 2 | J | 215/217 (99%) | 166 (77%) | 31 (14%) | 18 (8%) | 1 | 12 |
| 2 | K | 215/217 (99%) | 165 (77%) | 30 (14%) | 20 (9%) | 1 | 9 |
| 3 | V | 143/163 (88%) | 88 (62%) | 32 (22%) | 23 (16%) | 0 | 1 |
| 3 | X | 136/163 (83%) | 98 (72%) | 19 (14%) | 19 (14%) | 0 | 2 |
| 3 | Y | 137/163 (84%) | 92 (67%) | 33 (24%) | 12 (9%) | 1 | 11 |
| 3 | Z | 136/163 (83%) | 89 (65%) | 31 (23%) | 16 (12%) | 1 | 4 |
| All | All | 2254/2372 (95%) | 1752 (78%) | 317 (14%) | 185 (8%) | 1 | 13 |

All (185) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 7 | SER |
| 1 | L | 107 | ARG |
| 1 | L | 212 | GLU |
| 2 | H | 28 | THR |
| 2 | H | 133 | ALA |
| 2 | H | 175 | SER |
| 2 | H | 176 | ASP |
| 2 | H | 204 | ALA |
| 1 | M | 121 | SER |
| 2 | I | 65 | SER |
| 2 | I | 67 | LYS |
| 2 | I | 101 | TRP |
| 2 | I | 159 | SER |
| 2 | I | 175 | SER |
| 2 | I | 184 | VAL |
| 2 | I | 193 | SER |
| 2 | I | 204 | ALA |
| 2 | I | 205 | SER |
| 1 | N | 28 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 71 | SER |
| 1 | N | 167 | SER |
| 1 | N | 170 | SER |
| 2 | J | 30 | SER |
| 2 | J | 52 | ARG |
| 2 | J | 55 | VAL |
| 2 | J | 65 | SER |
| 2 | J | 116 | ALA |
| 2 | J | 131 | SER |
| 2 | J | 204 | ALA |
| 1 | O | 198 | LYS |
| 2 | K | 9 | GLY |
| 2 | K | 27 | PHE |
| 2 | K | 57 | ASN |
| 2 | K | 58 | HIS |
| 2 | K | 65 | SER |
| 2 | K | 203 | PRO |
| 3 | V | 11 | VAL |
| 3 | V | 30 | PRO |
| 3 | V | 43 | ALA |
| 3 | V | 50 | GLU |
| 3 | V | 54 | GLN |
| 3 | V | 80 | GLN |
| 3 | V | 103 | ALA |
| 3 | V | 145 | VAL |
| 3 | V | 148 | SER |
| 3 | X | 10 | ARG |
| 3 | X | 11 | VAL |
| 3 | X | 31 | GLU |
| 3 | X | 88 | SER |
| 3 | X | 130 | SER |
| 3 | Y | 13 | SER |
| 3 | Y | 31 | GLU |
| 3 | Y | 43 | ALA |
| 3 | Y | 85 | CYS |
| 3 | Z | 50 | GLU |
| 3 | Z | 138 | LYS |
| 2 | H | 92 | ASP |
| 2 | H | 107 | GLY |
| 2 | H | 132 | ALA |
| 1 | M | 125 | THR |
| 1 | M | 167 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 191 | TYR |
| 2 | I | 9 | GLY |
| 2 | I | 131 | SER |
| 1 | N | 109 | ASP |
| 1 | N | 125 | THR |
| 1 | N | 137 | ASN |
| 2 | J | 16 | GLY |
| 2 | J | 27 | PHE |
| 2 | J | 89 | ARG |
| 2 | J | 216 | ARG |
| 1 | O | 121 | SER |
| 1 | O | 170 | SER |
| 1 | O | 212 | GLU |
| 2 | K | 14 | PRO |
| 2 | K | 26 | GLY |
| 2 | K | 28 | THR |
| 2 | K | 55 | VAL |
| 2 | K | 87 | SER |
| 2 | K | 91 | GLU |
| 2 | K | 117 | ALA |
| 2 | K | 176 | ASP |
| 2 | K | 204 | ALA |
| 3 | V | 27 | SER |
| 3 | V | 31 | GLU |
| 3 | V | 79 | GLY |
| 3 | V | 87 | SER |
| 3 | V | 88 | SER |
| 3 | V | 91 | GLY |
| 3 | V | 102 | GLY |
| 3 | V | 138 | LYS |
| 3 | V | 144 | LEU |
| 3 | V | 146 | GLY |
| 3 | X | 25 | ARG |
| 3 | X | 27 | SER |
| 3 | X | 44 | VAL |
| 3 | X | 62 | ASP |
| 3 | X | 87 | SER |
| 3 | X | 103 | ALA |
| 3 | X | 133 | HIS |
| 3 | X | 138 | LYS |
| 3 | Y | 125 | ASN |
| 3 | Z | 10 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Z | 25 | ARG |
| 3 | Z | 92 | GLN |
| 2 | H | 14 | PRO |
| 2 | H | 90 | ALA |
| 2 | H | 203 | PRO |
| 1 | M | 39 | PRO |
| 1 | M | 67 | GLY |
| 2 | I | 14 | PRO |
| 2 | I | 77 | SER |
| 2 | I | 163 | SER |
| 2 | I | 176 | ASP |
| 1 | N | 122 | GLU |
| 2 | J | 136 | ASN |
| 2 | J | 176 | ASP |
| 1 | O | 7 | SER |
| 1 | O | 149 | ILE |
| 1 | O | 203 | PRO |
| 1 | O | 204 | ILE |
| 2 | K | 59 | ALA |
| 2 | K | 119 | THR |
| 3 | V | 34 | PRO |
| 3 | V | 49 | GLY |
| 3 | V | 76 | ALA |
| 3 | V | 141 | PHE |
| 3 | X | 34 | PRO |
| 3 | Y | 9 | LEU |
| 3 | Y | 14 | LYS |
| 3 | Y | 27 | SER |
| 3 | Y | 140 | ARG |
| 3 | Y | 145 | VAL |
| 3 | Z | 56 | GLU |
| 3 | Z | 82 | GLY |
| 3 | Z | 91 | GLY |
| 3 | Z | 94 | SER |
| 3 | Z | 129 | LEU |
| 1 | L | 15 | PRO |
| 1 | M | 8 | PRO |
| 1 | M | 59 | ALA |
| 1 | M | 149 | ILE |
| 2 | I | 66 | VAL |
| 2 | I | 150 | PRO |
| 1 | N | 45 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 49 | SER |
| 2 | J | 42 | GLU |
| 2 | J | 215 | PRO |
| 1 | O | 23 | CYS |
| 1 | O | 55 | SER |
| 2 | K | 30 | SER |
| 3 | X | 126 | ALA |
| 3 | X | 129 | LEU |
| 3 | X | 144 | LEU |
| 3 | Y | 82 | GLY |
| 3 | Z | 31 | GLU |
| 3 | Z | 110 | THR |
| 3 | Z | 117 | ARG |
| 1 | L | 149 | ILE |
| 2 | H | 131 | SER |
| 1 | M | 79 | ALA |
| 2 | I | 158 | ASN |
| 1 | N | 165 | GLN |
| 2 | J | 133 | ALA |
| 2 | J | 193 | SER |
| 2 | K | 159 | SER |
| 2 | H | 159 | SER |
| 2 | H | 207 | THR |
| 2 | I | 100 | GLY |
| 1 | N | 39 | PRO |
| 3 | X | 36 | PRO |
| 3 | X | 61 | GLN |
| 3 | Z | 65 | GLY |
| 2 | H | 41 | PRO |
| 1 | O | 202 | SER |
| 1 | M | 151 | GLY |
| 1 | N | 8 | PRO |
| 2 | K | 122 | PRO |
| 3 | Y | 102 | GLY |
| 3 | Z | 49 | GLY |
| 3 | Z | 102 | GLY |
| 2 | J | 152 | PRO |
| 1 | O | 40 | GLY |
| 2 | I | 130 | GLY |
| 2 | H | 152 | 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 X-ray entries followed by that with respect to entries of similar resolution. 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 | L | 186/186 (100%) | 121 (65%) | 65 (35%) | 0 | 1 |
| 1 | M | 185/186 (100%) | 118 (64%) | 67 (36%) | 0 | 1 |
| 1 | N | 185/186 (100%) | 121 (65%) | 64 (35%) | 0 | 1 |
| 1 | O | 186/186 (100%) | 117 (63%) | 69 (37%) | 0 | 0 |
| 2 | H | 182/185 (98%) | 115 (63%) | 67 (37%) | 0 | 1 |
| 2 | I | 182/185 (98%) | 108 (59%) | 74 (41%) | 0 | 0 |
| 2 | J | 182/185 (98%) | 109 (60%) | 73 (40%) | 0 | 0 |
| 2 | K | 182/185 (98%) | 115 (63%) | 67 (37%) | 0 | 1 |
| 3 | V | 122/138 (88%) | 73 (60%) | 49 (40%) | 0 | 0 |
| 3 | X | 117/138 (85%) | 74 (63%) | 43 (37%) | 0 | 1 |
| 3 | Y | 117/138 (85%) | 72 (62%) | 45 (38%) | 0 | 0 |
| 3 | Z | 116/138 (84%) | 74 (64%) | 42 (36%) | 0 | 1 |
| All | All | 1942/2036 (95%) | 1217 (63%) | 725 (37%) | 0 | 0 |

All (725) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 1 | GLN |
| 1 | L | 2 | VAL |
| 1 | L | 3 | VAL |
| 1 | L | 5 | THR |
| 1 | L | 11 | MET |
| 1 | L | 12 | SER |
| 1 | L | 18 | LYS |
| 1 | L | 20 | THR |
| 1 | L | 22 | THR |
| 1 | L | 27 | SER |
| 1 | L | 29 | VAL |
| 1 | L | 35 | PHE |
| 1 | L | 38 | LYS |
| 1 | L | 42 | SER |
| 1 | L | 44 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 45 | LEU |
| 1 | L | 55 | SER |
| 1 | L | 60 | ARG |
| 1 | L | 68 | THR |
| 1 | L | 72 | LEU |
| 1 | L | 73 | THR |
| 1 | L | 76 | ARG |
| 1 | L | 77 | MET |
| 1 | L | 90 | ARG |
| 1 | L | 95 | ARG |
| 1 | L | 104 | GLU |
| 1 | L | 105 | ILE |
| 1 | L | 106 | LYS |
| 1 | L | 107 | ARG |
| 1 | L | 115 | SER |
| 1 | L | 116 | ILE |
| 1 | L | 117 | PHE |
| 1 | L | 118 | PRO |
| 1 | L | 120 | SER |
| 1 | L | 123 | GLN |
| 1 | L | 124 | LEU |
| 1 | L | 132 | VAL |
| 1 | L | 133 | CYS |
| 1 | L | 143 | ILE |
| 1 | L | 145 | VAL |
| 1 | L | 146 | LYS |
| 1 | L | 149 | ILE |
| 1 | L | 152 | SER |
| 1 | L | 154 | ARG |
| 1 | L | 162 | TRP |
| 1 | L | 163 | THR |
| 1 | L | 165 | GLN |
| 1 | L | 168 | LYS |
| 1 | L | 169 | ASP |
| 1 | L | 171 | THR |
| 1 | L | 173 | SER |
| 1 | L | 175 | SER |
| 1 | L | 180 | LEU |
| 1 | L | 181 | THR |
| 1 | L | 182 | LYS |
| 1 | L | 190 | SER |
| 1 | L | 192 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 193 | CYS |
| 1 | L | 194 | GLU |
| 1 | L | 199 | THR |
| 1 | L | 201 | THR |
| 1 | L | 202 | SER |
| 1 | L | 204 | ILE |
| 1 | L | 211 | ASN |
| 1 | L | 213 | CYS |
| 2 | H | 3 | LYS |
| 2 | H | 4 | LEU |
| 2 | H | 12 | VAL |
| 2 | H | 13 | GLN |
| 2 | H | 21 | SER |
| 2 | H | 28 | THR |
| 2 | H | 29 | PHE |
| 2 | H | 30 | SER |
| 2 | H | 35 | ASP |
| 2 | H | 38 | ARG |
| 2 | H | 42 | GLU |
| 2 | H | 50 | GLU |
| 2 | H | 51 | ILE |
| 2 | H | 54 | LYS |
| 2 | H | 56 | ASN |
| 2 | H | 57 | ASN |
| 2 | H | 64 | GLU |
| 2 | H | 67 | LYS |
| 2 | H | 69 | ARG |
| 2 | H | 71 | THR |
| 2 | H | 74 | ARG |
| 2 | H | 78 | LYS |
| 2 | H | 79 | SER |
| 2 | H | 80 | SER |
| 2 | H | 83 | LEU |
| 2 | H | 84 | GLN |
| 2 | H | 85 | MET |
| 2 | H | 87 | SER |
| 2 | H | 88 | LEU |
| 2 | H | 89 | ARG |
| 2 | H | 95 | ILE |
| 2 | H | 98 | CYS |
| 2 | H | 99 | SER |
| 2 | H | 101 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | H | 102 | SER |
| 2 | H | 108 | GLN |
| 2 | H | 110 | THR |
| 2 | H | 111 | LEU |
| 2 | H | 113 | THR |
| 2 | H | 114 | VAL |
| 2 | H | 121 | PRO |
| 2 | H | 124 | VAL |
| 2 | H | 136 | ASN |
| 2 | H | 139 | VAL |
| 2 | H | 141 | LEU |
| 2 | H | 146 | LYS |
| 2 | H | 155 | VAL |
| 2 | H | 156 | THR |
| 2 | H | 159 | SER |
| 2 | H | 161 | SER |
| 2 | H | 162 | LEU |
| 2 | H | 166 | VAL |
| 2 | H | 172 | VAL |
| 2 | H | 174 | GLN |
| 2 | H | 175 | SER |
| 2 | H | 180 | LEU |
| 2 | H | 188 | SER |
| 2 | H | 195 | THR |
| 2 | H | 196 | VAL |
| 2 | H | 198 | CYS |
| 2 | H | 199 | ASN |
| 2 | H | 206 | SER |
| 2 | H | 207 | THR |
| 2 | H | 213 | ILE |
| 2 | H | 214 | VAL |
| 2 | H | 216 | ARG |
| 2 | H | 217 | ASP |
| 1 | M | 1 | GLN |
| 1 | M | 3 | VAL |
| 1 | M | 7 | SER |
| 1 | M | 11 | MET |
| 1 | M | 12 | SER |
| 1 | M | 18 | LYS |
| 1 | M | 20 | THR |
| 1 | M | 23 | CYS |
| 1 | M | 24 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 30 | SER |
| 1 | M | 33 | TYR |
| 1 | M | 36 | GLN |
| 1 | M | 38 | LYS |
| 1 | M | 41 | THR |
| 1 | M | 45 | LEU |
| 1 | M | 62 | ARG |
| 1 | M | 68 | THR |
| 1 | M | 73 | THR |
| 1 | M | 76 | ARG |
| 1 | M | 77 | MET |
| 1 | M | 81 | ASP |
| 1 | M | 88 | GLN |
| 1 | M | 90 | ARG |
| 1 | M | 95 | ARG |
| 1 | M | 97 | PHE |
| 1 | M | 105 | ILE |
| 1 | M | 106 | LYS |
| 1 | M | 113 | THR |
| 1 | M | 115 | SER |
| 1 | M | 116 | ILE |
| 1 | M | 117 | PHE |
| 1 | M | 120 | SER |
| 1 | M | 124 | LEU |
| 1 | M | 126 | SER |
| 1 | M | 130 | SER |
| 1 | M | 132 | VAL |
| 1 | M | 137 | ASN |
| 1 | M | 138 | PHE |
| 1 | M | 142 | ASP |
| 1 | M | 143 | ILE |
| 1 | M | 146 | LYS |
| 1 | M | 150 | ASP |
| 1 | M | 153 | GLU |
| 1 | M | 154 | ARG |
| 1 | M | 155 | GLN |
| 1 | M | 156 | ASN |
| 1 | M | 162 | TRP |
| 1 | M | 163 | THR |
| 1 | M | 165 | GLN |
| 1 | M | 166 | ASP |
| 1 | M | 168 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 170 | SER |
| 1 | M | 174 | MET |
| 1 | M | 175 | SER |
| 1 | M | 177 | THR |
| 1 | M | 180 | LEU |
| 1 | M | 181 | THR |
| 1 | M | 182 | LYS |
| 1 | M | 189 | ASN |
| 1 | M | 192 | THR |
| 1 | M | 194 | GLU |
| 1 | M | 196 | THR |
| 1 | M | 198 | LYS |
| 1 | M | 199 | THR |
| 1 | M | 208 | PHE |
| 1 | M | 210 | ARG |
| 1 | M | 211 | ASN |
| 2 | I | 3 | LYS |
| 2 | I | 4 | LEU |
| 2 | I | 6 | GLU |
| 2 | I | 7 | SER |
| 2 | I | 12 | VAL |
| 2 | I | 13 | GLN |
| 2 | I | 19 | LYS |
| 2 | I | 22 | CYS |
| 2 | I | 28 | THR |
| 2 | I | 38 | ARG |
| 2 | I | 40 | SER |
| 2 | I | 52 | ARG |
| 2 | I | 53 | SER |
| 2 | I | 55 | VAL |
| 2 | I | 56 | ASN |
| 2 | I | 57 | ASN |
| 2 | I | 61 | HIS |
| 2 | I | 67 | LYS |
| 2 | I | 71 | THR |
| 2 | I | 74 | ARG |
| 2 | I | 75 | ASP |
| 2 | I | 77 | SER |
| 2 | I | 78 | LYS |
| 2 | I | 79 | SER |
| 2 | I | 80 | SER |
| 2 | I | 88 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I | 91 | GLU |
| 2 | I | 95 | ILE |
| 2 | I | 98 | CYS |
| 2 | I | 99 | SER |
| 2 | I | 102 | SER |
| 2 | I | 108 | GLN |
| 2 | I | 110 | THR |
| 2 | I | 111 | LEU |
| 2 | I | 112 | VAL |
| 2 | I | 113 | THR |
| 2 | I | 115 | SER |
| 2 | I | 118 | LYS |
| 2 | I | 119 | THR |
| 2 | I | 123 | SER |
| 2 | I | 134 | GLN |
| 2 | I | 136 | ASN |
| 2 | I | 138 | MET |
| 2 | I | 139 | VAL |
| 2 | I | 141 | LEU |
| 2 | I | 144 | LEU |
| 2 | I | 145 | VAL |
| 2 | I | 146 | LYS |
| 2 | I | 150 | PRO |
| 2 | I | 153 | VAL |
| 2 | I | 154 | THR |
| 2 | I | 155 | VAL |
| 2 | I | 159 | SER |
| 2 | I | 162 | LEU |
| 2 | I | 164 | SER |
| 2 | I | 172 | VAL |
| 2 | I | 173 | LEU |
| 2 | I | 174 | GLN |
| 2 | I | 178 | TYR |
| 2 | I | 179 | THR |
| 2 | I | 180 | LEU |
| 2 | I | 189 | SER |
| 2 | I | 193 | SER |
| 2 | I | 194 | GLU |
| 2 | I | 195 | THR |
| 2 | I | 198 | CYS |
| 2 | I | 199 | ASN |
| 2 | I | 200 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I | 206 | SER |
| 2 | I | 207 | THR |
| 2 | I | 209 | VAL |
| 2 | I | 211 | LYS |
| 2 | I | 213 | ILE |
| 2 | I | 216 | ARG |
| 1 | N | 1 | GLN |
| 1 | N | 2 | VAL |
| 1 | N | 7 | SER |
| 1 | N | 10 | ILE |
| 1 | N | 12 | SER |
| 1 | N | 14 | SER |
| 1 | N | 17 | GLU |
| 1 | N | 26 | SER |
| 1 | N | 30 | SER |
| 1 | N | 35 | PHE |
| 1 | N | 38 | LYS |
| 1 | N | 39 | PRO |
| 1 | N | 41 | THR |
| 1 | N | 42 | SER |
| 1 | N | 44 | LYS |
| 1 | N | 45 | LEU |
| 1 | N | 49 | SER |
| 1 | N | 62 | ARG |
| 1 | N | 64 | SER |
| 1 | N | 68 | THR |
| 1 | N | 72 | LEU |
| 1 | N | 76 | ARG |
| 1 | N | 77 | MET |
| 1 | N | 86 | TYR |
| 1 | N | 95 | ARG |
| 1 | N | 102 | LYS |
| 1 | N | 104 | GLU |
| 1 | N | 105 | ILE |
| 1 | N | 106 | LYS |
| 1 | N | 115 | SER |
| 1 | N | 116 | ILE |
| 1 | N | 117 | PHE |
| 1 | N | 120 | SER |
| 1 | N | 121 | SER |
| 1 | N | 124 | LEU |
| 1 | N | 130 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 132 | VAL |
| 1 | N | 137 | ASN |
| 1 | N | 144 | ASN |
| 1 | N | 146 | LYS |
| 1 | N | 153 | GLU |
| 1 | N | 155 | GLN |
| 1 | N | 158 | VAL |
| 1 | N | 162 | TRP |
| 1 | N | 163 | THR |
| 1 | N | 164 | ASP |
| 1 | N | 165 | GLN |
| 1 | N | 167 | SER |
| 1 | N | 168 | LYS |
| 1 | N | 169 | ASP |
| 1 | N | 171 | THR |
| 1 | N | 174 | MET |
| 1 | N | 176 | SER |
| 1 | N | 179 | THR |
| 1 | N | 180 | LEU |
| 1 | N | 181 | THR |
| 1 | N | 190 | SER |
| 1 | N | 194 | GLU |
| 1 | N | 201 | THR |
| 1 | N | 204 | ILE |
| 1 | N | 205 | VAL |
| 1 | N | 206 | LYS |
| 1 | N | 210 | ARG |
| 1 | N | 211 | ASN |
| 2 | J | 3 | LYS |
| 2 | J | 4 | LEU |
| 2 | J | 5 | GLU |
| 2 | J | 6 | GLU |
| 2 | J | 7 | SER |
| 2 | J | 11 | LEU |
| 2 | J | 12 | VAL |
| 2 | J | 13 | GLN |
| 2 | J | 18 | MET |
| 2 | J | 20 | LEU |
| 2 | J | 30 | SER |
| 2 | J | 31 | ASP |
| 2 | J | 35 | ASP |
| 2 | J | 38 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | J | 40 | SER |
| 2 | J | 54 | LYS |
| 2 | J | 55 | VAL |
| 2 | J | 56 | ASN |
| 2 | J | 57 | ASN |
| 2 | J | 61 | HIS |
| 2 | J | 65 | SER |
| 2 | J | 67 | LYS |
| 2 | J | 69 | ARG |
| 2 | J | 71 | THR |
| 2 | J | 74 | ARG |
| 2 | J | 75 | ASP |
| 2 | J | 77 | SER |
| 2 | J | 78 | LYS |
| 2 | J | 80 | SER |
| 2 | J | 81 | VAL |
| 2 | J | 83 | LEU |
| 2 | J | 85 | MET |
| 2 | J | 92 | ASP |
| 2 | J | 95 | ILE |
| 2 | J | 99 | SER |
| 2 | J | 102 | SER |
| 2 | J | 108 | GLN |
| 2 | J | 110 | THR |
| 2 | J | 111 | LEU |
| 2 | J | 113 | THR |
| 2 | J | 114 | VAL |
| 2 | J | 115 | SER |
| 2 | J | 123 | SER |
| 2 | J | 124 | VAL |
| 2 | J | 131 | SER |
| 2 | J | 136 | ASN |
| 2 | J | 137 | SER |
| 2 | J | 138 | MET |
| 2 | J | 139 | VAL |
| 2 | J | 144 | LEU |
| 2 | J | 148 | TYR |
| 2 | J | 151 | GLU |
| 2 | J | 153 | VAL |
| 2 | J | 156 | THR |
| 2 | J | 158 | ASN |
| 2 | J | 159 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | J | 162 | LEU |
| 2 | J | 166 | VAL |
| 2 | J | 172 | VAL |
| 2 | J | 173 | LEU |
| 2 | J | 174 | GLN |
| 2 | J | 175 | SER |
| 2 | J | 179 | THR |
| 2 | J | 183 | SER |
| 2 | J | 194 | GLU |
| 2 | J | 195 | THR |
| 2 | J | 196 | VAL |
| 2 | J | 199 | ASN |
| 2 | J | 200 | VAL |
| 2 | J | 206 | SER |
| 2 | J | 210 | ASP |
| 2 | J | 216 | ARG |
| 2 | J | 217 | ASP |
| 1 | O | 1 | GLN |
| 1 | O | 2 | VAL |
| 1 | O | 12 | SER |
| 1 | O | 14 | SER |
| 1 | O | 18 | LYS |
| 1 | O | 19 | VAL |
| 1 | O | 20 | THR |
| 1 | O | 24 | SER |
| 1 | O | 30 | SER |
| 1 | O | 33 | TYR |
| 1 | O | 38 | LYS |
| 1 | O | 41 | THR |
| 1 | O | 42 | SER |
| 1 | O | 44 | LYS |
| 1 | O | 45 | LEU |
| 1 | O | 46 | TRP |
| 1 | O | 51 | SER |
| 1 | O | 55 | SER |
| 1 | O | 60 | ARG |
| 1 | O | 61 | PHE |
| 1 | O | 62 | ARG |
| 1 | O | 64 | SER |
| 1 | O | 71 | SER |
| 1 | O | 73 | THR |
| 1 | O | 76 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 77 | MET |
| 1 | O | 80 | GLU |
| 1 | O | 90 | ARG |
| 1 | O | 91 | SER |
| 1 | O | 95 | ARG |
| 1 | O | 102 | LYS |
| 1 | O | 113 | THR |
| 1 | O | 114 | VAL |
| 1 | O | 115 | SER |
| 1 | O | 116 | ILE |
| 1 | O | 117 | PHE |
| 1 | O | 120 | SER |
| 1 | O | 122 | GLU |
| 1 | O | 124 | LEU |
| 1 | O | 133 | CYS |
| 1 | O | 143 | ILE |
| 1 | O | 145 | VAL |
| 1 | O | 146 | LYS |
| 1 | O | 155 | GLN |
| 1 | O | 163 | THR |
| 1 | O | 164 | ASP |
| 1 | O | 165 | GLN |
| 1 | O | 166 | ASP |
| 1 | O | 168 | LYS |
| 1 | O | 171 | THR |
| 1 | O | 174 | MET |
| 1 | O | 177 | THR |
| 1 | O | 178 | LEU |
| 1 | O | 180 | LEU |
| 1 | O | 181 | THR |
| 1 | O | 182 | LYS |
| 1 | O | 184 | GLU |
| 1 | O | 188 | HIS |
| 1 | O | 189 | ASN |
| 1 | O | 190 | SER |
| 1 | O | 192 | THR |
| 1 | O | 193 | CYS |
| 1 | O | 194 | GLU |
| 1 | O | 196 | THR |
| 1 | O | 204 | ILE |
| 1 | O | 206 | LYS |
| 1 | O | 210 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 211 | ASN |
| 1 | O | 212 | GLU |
| 2 | K | 2 | VAL |
| 2 | K | 4 | LEU |
| 2 | K | 5 | GLU |
| 2 | K | 7 | SER |
| 2 | K | 11 | LEU |
| 2 | K | 12 | VAL |
| 2 | K | 13 | GLN |
| 2 | K | 19 | LYS |
| 2 | K | 21 | SER |
| 2 | K | 28 | THR |
| 2 | K | 31 | ASP |
| 2 | K | 38 | ARG |
| 2 | K | 46 | GLU |
| 2 | K | 55 | VAL |
| 2 | K | 60 | ILE |
| 2 | K | 64 | GLU |
| 2 | K | 65 | SER |
| 2 | K | 69 | ARG |
| 2 | K | 73 | SER |
| 2 | K | 75 | ASP |
| 2 | K | 78 | LYS |
| 2 | K | 79 | SER |
| 2 | K | 80 | SER |
| 2 | K | 83 | LEU |
| 2 | K | 84 | GLN |
| 2 | K | 85 | MET |
| 2 | K | 87 | SER |
| 2 | K | 89 | ARG |
| 2 | K | 93 | THR |
| 2 | K | 95 | ILE |
| 2 | K | 108 | GLN |
| 2 | K | 110 | THR |
| 2 | K | 111 | LEU |
| 2 | K | 113 | THR |
| 2 | K | 115 | SER |
| 2 | K | 118 | LYS |
| 2 | K | 119 | THR |
| 2 | K | 123 | SER |
| 2 | K | 124 | VAL |
| 2 | K | 136 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | K | 144 | LEU |
| 2 | K | 151 | GLU |
| 2 | K | 153 | VAL |
| 2 | K | 155 | VAL |
| 2 | K | 156 | THR |
| 2 | K | 158 | ASN |
| 2 | K | 162 | LEU |
| 2 | K | 164 | SER |
| 2 | K | 167 | HIS |
| 2 | K | 172 | VAL |
| 2 | K | 173 | LEU |
| 2 | K | 177 | LEU |
| 2 | K | 179 | THR |
| 2 | K | 180 | LEU |
| 2 | K | 181 | SER |
| 2 | K | 185 | THR |
| 2 | K | 194 | GLU |
| 2 | K | 195 | THR |
| 2 | K | 196 | VAL |
| 2 | K | 198 | CYS |
| 2 | K | 199 | ASN |
| 2 | K | 205 | SER |
| 2 | K | 206 | SER |
| 2 | K | 209 | VAL |
| 2 | K | 210 | ASP |
| 2 | K | 214 | VAL |
| 2 | K | 216 | ARG |
| 3 | V | 8 | ASP |
| 3 | V | 12 | LEU |
| 3 | V | 13 | SER |
| 3 | V | 15 | LEU |
| 3 | V | 16 | LEU |
| 3 | V | 17 | ARG |
| 3 | V | 24 | SER |
| 3 | V | 28 | GLN |
| 3 | V | 31 | GLU |
| 3 | V | 32 | VAL |
| 3 | V | 35 | LEU |
| 3 | V | 37 | THR |
| 3 | V | 40 | LEU |
| 3 | V | 41 | LEU |
| 3 | V | 46 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | V | 48 | LEU |
| 3 | V | 50 | GLU |
| 3 | V | 55 | MET |
| 3 | V | 57 | GLU |
| 3 | V | 62 | ASP |
| 3 | V | 70 | LEU |
| 3 | V | 71 | LEU |
| 3 | V | 78 | ARG |
| 3 | V | 81 | LEU |
| 3 | V | 84 | THR |
| 3 | V | 86 | LEU |
| 3 | V | 87 | SER |
| 3 | V | 88 | SER |
| 3 | V | 94 | SER |
| 3 | V | 98 | ARG |
| 3 | V | 99 | LEU |
| 3 | V | 100 | LEU |
| 3 | V | 107 | LEU |
| 3 | V | 110 | THR |
| 3 | V | 115 | ARG |
| 3 | V | 117 | ARG |
| 3 | V | 122 | LYS |
| 3 | V | 125 | ASN |
| 3 | V | 127 | ILE |
| 3 | V | 129 | LEU |
| 3 | V | 130 | SER |
| 3 | V | 134 | LEU |
| 3 | V | 140 | ARG |
| 3 | V | 141 | PHE |
| 3 | V | 143 | MET |
| 3 | V | 144 | LEU |
| 3 | V | 148 | SER |
| 3 | V | 150 | LEU |
| 3 | V | 151 | CYS |
| 3 | X | 11 | VAL |
| 3 | X | 12 | LEU |
| 3 | X | 16 | LEU |
| 3 | X | 17 | ARG |
| 3 | X | 18 | ASP |
| 3 | X | 19 | SER |
| 3 | X | 24 | SER |
| 3 | X | 25 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | X | 28 | GLN |
| 3 | X | 31 | GLU |
| 3 | X | 32 | VAL |
| 3 | X | 40 | LEU |
| 3 | X | 48 | LEU |
| 3 | X | 50 | GLU |
| 3 | X | 51 | TRP |
| 3 | X | 53 | THR |
| 3 | X | 54 | GLN |
| 3 | X | 62 | ASP |
| 3 | X | 68 | THR |
| 3 | X | 69 | LEU |
| 3 | X | 70 | LEU |
| 3 | X | 71 | LEU |
| 3 | X | 72 | GLU |
| 3 | X | 75 | MET |
| 3 | X | 78 | ARG |
| 3 | X | 81 | LEU |
| 3 | X | 86 | LEU |
| 3 | X | 89 | LEU |
| 3 | X | 90 | LEU |
| 3 | X | 93 | LEU |
| 3 | X | 96 | GLN |
| 3 | X | 100 | LEU |
| 3 | X | 106 | SER |
| 3 | X | 107 | LEU |
| 3 | X | 110 | THR |
| 3 | X | 112 | LEU |
| 3 | X | 115 | ARG |
| 3 | X | 127 | ILE |
| 3 | X | 129 | LEU |
| 3 | X | 135 | LEU |
| 3 | X | 136 | ARG |
| 3 | X | 143 | MET |
| 3 | X | 144 | LEU |
| 3 | Y | 9 | LEU |
| 3 | Y | 12 | LEU |
| 3 | Y | 15 | LEU |
| 3 | Y | 17 | ARG |
| 3 | Y | 19 | SER |
| 3 | Y | 22 | LEU |
| 3 | Y | 26 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Y | 27 | SER |
| 3 | Y | 35 | LEU |
| 3 | Y | 44 | VAL |
| 3 | Y | 45 | ASP |
| 3 | Y | 48 | LEU |
| 3 | Y | 52 | LYS |
| 3 | Y | 53 | THR |
| 3 | Y | 54 | GLN |
| 3 | Y | 55 | MET |
| 3 | Y | 56 | GLU |
| 3 | Y | 68 | THR |
| 3 | Y | 69 | LEU |
| 3 | Y | 70 | LEU |
| 3 | Y | 71 | LEU |
| 3 | Y | 72 | GLU |
| 3 | Y | 75 | MET |
| 3 | Y | 81 | LEU |
| 3 | Y | 85 | CYS |
| 3 | Y | 87 | SER |
| 3 | Y | 89 | LEU |
| 3 | Y | 93 | LEU |
| 3 | Y | 96 | GLN |
| 3 | Y | 99 | LEU |
| 3 | Y | 100 | LEU |
| 3 | Y | 105 | GLN |
| 3 | Y | 106 | SER |
| 3 | Y | 107 | LEU |
| 3 | Y | 110 | THR |
| 3 | Y | 111 | GLN |
| 3 | Y | 112 | LEU |
| 3 | Y | 115 | ARG |
| 3 | Y | 117 | ARG |
| 3 | Y | 119 | THR |
| 3 | Y | 127 | ILE |
| 3 | Y | 129 | LEU |
| 3 | Y | 140 | ARG |
| 3 | Y | 143 | MET |
| 3 | Y | 144 | LEU |
| 3 | Z | 9 | LEU |
| 3 | Z | 11 | VAL |
| 3 | Z | 12 | LEU |
| 3 | Z | 15 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Z | 17 | ARG |
| 3 | Z | 19 | SER |
| 3 | Z | 22 | LEU |
| 3 | Z | 25 | ARG |
| 3 | Z | 26 | LEU |
| 3 | Z | 32 | VAL |
| 3 | Z | 35 | LEU |
| 3 | Z | 37 | THR |
| 3 | Z | 44 | VAL |
| 3 | Z | 46 | PHE |
| 3 | Z | 48 | LEU |
| 3 | Z | 50 | GLU |
| 3 | Z | 52 | LYS |
| 3 | Z | 55 | MET |
| 3 | Z | 56 | GLU |
| 3 | Z | 57 | GLU |
| 3 | Z | 62 | ASP |
| 3 | Z | 68 | THR |
| 3 | Z | 69 | LEU |
| 3 | Z | 70 | LEU |
| 3 | Z | 80 | GLN |
| 3 | Z | 81 | LEU |
| 3 | Z | 84 | THR |
| 3 | Z | 86 | LEU |
| 3 | Z | 87 | SER |
| 3 | Z | 93 | LEU |
| 3 | Z | 94 | SER |
| 3 | Z | 99 | LEU |
| 3 | Z | 100 | LEU |
| 3 | Z | 105 | GLN |
| 3 | Z | 107 | LEU |
| 3 | Z | 112 | LEU |
| 3 | Z | 115 | ARG |
| 3 | Z | 118 | THR |
| 3 | Z | 127 | ILE |
| 3 | Z | 129 | LEU |
| 3 | Z | 140 | ARG |
| 3 | Z | 143 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 1 | GLN |
| 1 | L | 6 | GLN |
| 1 | L | 37 | GLN |
| 1 | L | 88 | GLN |
| 1 | L | 189 | ASN |
| 1 | L | 211 | ASN |
| 2 | H | 13 | GLN |
| 2 | H | 56 | ASN |
| 2 | H | 57 | ASN |
| 2 | H | 84 | GLN |
| 2 | H | 158 | ASN |
| 2 | H | 174 | GLN |
| 2 | H | 199 | ASN |
| 1 | M | 1 | GLN |
| 1 | M | 6 | GLN |
| 1 | M | 37 | GLN |
| 1 | M | 88 | GLN |
| 1 | M | 155 | GLN |
| 1 | M | 165 | GLN |
| 1 | M | 188 | HIS |
| 1 | M | 189 | ASN |
| 1 | M | 211 | ASN |
| 2 | I | 13 | GLN |
| 2 | I | 56 | ASN |
| 2 | I | 57 | ASN |
| 2 | I | 58 | HIS |
| 2 | I | 61 | HIS |
| 2 | I | 84 | GLN |
| 2 | I | 134 | GLN |
| 2 | I | 158 | ASN |
| 2 | I | 199 | ASN |
| 1 | N | 6 | GLN |
| 1 | N | 36 | GLN |
| 1 | N | 37 | GLN |
| 1 | N | 88 | GLN |
| 1 | N | 89 | GLN |
| 1 | N | 155 | GLN |
| 1 | N | 189 | ASN |
| 1 | N | 211 | ASN |
| 2 | J | 58 | HIS |
| 2 | J | 61 | HIS |
| 2 | J | 84 | GLN |
| 2 | J | 134 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | J | 136 | ASN |
| 2 | J | 158 | ASN |
| 2 | J | 199 | ASN |
| 1 | O | 6 | GLN |
| 1 | O | 37 | GLN |
| 1 | O | 88 | GLN |
| 1 | O | 155 | GLN |
| 1 | O | 188 | HIS |
| 1 | O | 189 | ASN |
| 2 | K | 58 | HIS |
| 2 | K | 84 | GLN |
| 2 | K | 158 | ASN |
| 3 | V | 23 | HIS |
| 3 | V | 111 | GLN |
| 3 | V | 125 | ASN |
| 3 | X | 20 | HIS |
| 3 | X | 23 | HIS |
| 3 | X | 28 | GLN |
| 3 | X | 92 | GLN |
| 3 | Y | 111 | GLN |
| 3 | Y | 121 | HIS |
| 3 | Y | 133 | HIS |
| 3 | Z | 20 | HIS |
| 3 | Z | 33 | HIS |
| 3 | Z | 61 | GLN |
| 3 | Z | 105 | GLN |
| 3 | Z | 111 | GLN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | L | 213/213 (100%) | -0.53 | 0 100 100 | 5, 23, 37, 46 | 0 |
| 1 | M | 212/213 (99%) | -0.51 | 0 100 100 | 5, 25, 40, 46 | 0 |
| 1 | N | 212/213 (99%) | -0.51 | 0 100 100 | 8, 26, 41, 49 | 0 |
| 1 | O | 213/213 (100%) | -0.45 | 0 100 100 | 7, 29, 50, 73 | 0 |
| 2 | H | 217/217 (100%) | -0.53 | 0 100 100 | 5, 23, 38, 63 | 0 |
| 2 | I | 217/217 (100%) | -0.49 | 0 100 100 | 10, 27, 44, 52 | 0 |
| 2 | J | 217/217 (100%) | -0.49 | 0 100 100 | 8, 24, 46, 67 | 0 |
| 2 | K | 217/217 (100%) | -0.39 | 0 100 100 | 13, 34, 54, 63 | 0 |
| 3 | V | 145/163 (88%) | -0.32 | 1 (0%) 84 42 | 8, 38, 81, 88 | 0 |
| 3 | X | 138/163 (84%) | -0.40 | 0 100 100 | 9, 32, 74, 83 | 0 |
| 3 | Y | 139/163 (85%) | -0.44 | 0 100 100 | 8, 27, 63, 70 | 0 |
| 3 | Z | 138/163 (84%) | -0.34 | 0 100 100 | 8, 41, 65, 77 | 0 |
| All | All | 2278/2372 (96%) | -0.46 | 1 (0%) 100 100 | 5, 27, 56, 88 | 0 |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | V | 7 | CYS | 2.1 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.