



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2017 – 07:24 AM EDT

PDB ID : 5D2L
Title : Crystal structure of TCR C7 in complex with HCMV NLV epitope presented by HLA-A2
Authors : Gao, M.; Mariuzza, R.A.
Deposited on : unknown
Resolution : 3.51 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20029824 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20029824 |

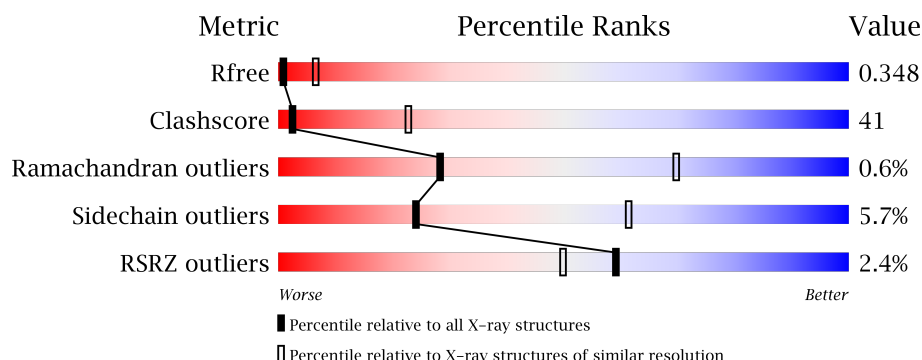
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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.




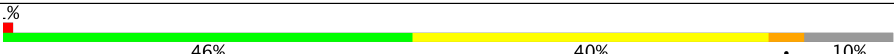
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1239 (3.64-3.40) |
| Clashscore | 112137 | 1007 (3.62-3.42) |
| Ramachandran outliers | 110173 | 1328 (3.64-3.40) |
| Sidechain outliers | 110143 | 1329 (3.64-3.40) |
| RSRZ outliers | 101464 | 1270 (3.64-3.40) |

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 276 | <div> <div>58%</div> <div>40%</div> <div>..</div> </div> |
| 1 | C | 276 | <div> <div>61%</div> <div>35%</div> <div>..</div> </div> |
| 1 | G | 276 | <div> <div>2%</div> <div>46%</div> <div>47%</div> <div>..</div> </div> |
| 1 | M | 276 | <div> <div>0%</div> <div>48%</div> <div>48%</div> <div>..</div> </div> |
| 2 | B | 100 | <div> <div>3%</div> <div>48%</div> <div>50%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | D | 100 |  |
| 2 | H | 100 |  |
| 2 | N | 100 |  |
| 3 | E | 205 |  |
| 3 | I | 205 |  |
| 3 | K | 205 |  |
| 3 | O | 205 |  |
| 4 | F | 245 |  |
| 4 | J | 245 |  |
| 4 | L | 245 |  |
| 4 | P | 245 |  |
| 5 | Q | 9 |  |
| 5 | R | 9 |  |
| 5 | T | 9 |  |
| 5 | U | 9 |  |

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HLA class I histocompatibility antigen, A-2 alpha chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2242 | 1401 | 408 | 424 | 9 | | | |
| 1 | G | 270 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2199 | 1379 | 395 | 416 | 9 | | | |
| 1 | M | 273 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2210 | 1379 | 401 | 421 | 9 | | | |
| 1 | C | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2242 | 1401 | 408 | 424 | 9 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| A | 0 | MET | - | initiating methionine | UNP P01892 |
| G | 0 | MET | - | initiating methionine | UNP P01892 |
| M | 0 | MET | - | initiating methionine | UNP P01892 |
| C | 0 | MET | - | initiating methionine | UNP P01892 |

- Molecule 2 is a protein called Beta-2-microglobulin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 522 | 140 | 158 | 3 | | | |
| 2 | H | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 777 | 494 | 128 | 152 | 3 | | | |
| 2 | N | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 825 | 524 | 138 | 159 | 4 | | | |
| 2 | D | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 827 | 527 | 137 | 159 | 4 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| B | 0 | MET | - | initiating methionine | UNP P61769 |
| H | 0 | MET | - | initiating methionine | UNP P61769 |
| N | 0 | MET | - | initiating methionine | UNP P61769 |
| D | 0 | MET | - | initiating methionine | UNP P61769 |

- Molecule 3 is a protein called C7 TCR alpha chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | I | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1404 | 878 | 227 | 293 | 6 | | | |
| 3 | K | 192 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1452 | 912 | 237 | 296 | 7 | | | |
| 3 | O | 187 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1435 | 900 | 234 | 294 | 7 | | | |
| 3 | E | 187 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1432 | 897 | 234 | 294 | 7 | | | |

- Molecule 4 is a protein called C7 TCR beta chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | J | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1759 | 1108 | 303 | 343 | 5 | | | |
| 4 | L | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1699 | 1064 | 299 | 331 | 5 | | | |
| 4 | P | 235 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1784 | 1122 | 306 | 351 | 5 | | | |
| 4 | F | 238 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1852 | 1163 | 323 | 361 | 5 | | | |

- Molecule 5 is a protein called ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 5 | Q | 9 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 64 | 42 | 10 | 11 | 1 | | | |
| 5 | U | 9 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 64 | 42 | 10 | 11 | 1 | | | |
| 5 | T | 9 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 64 | 42 | 10 | 11 | 1 | | | |
| 5 | R | 9 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 64 | 42 | 10 | 11 | 1 | | | |

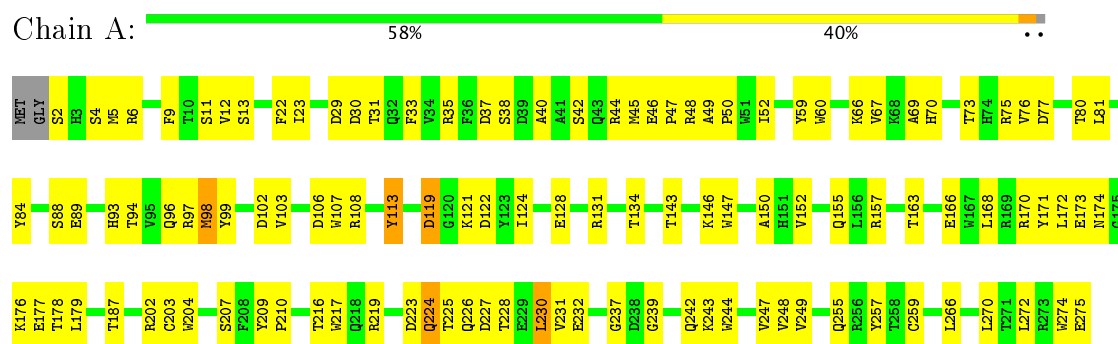
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 6 | A | 9 | Total O 9 9 | 0 | 0 |
| 6 | B | 1 | Total O 1 1 | 0 | 0 |
| 6 | I | 3 | Total O 3 3 | 0 | 0 |
| 6 | J | 2 | Total O 2 2 | 0 | 0 |
| 6 | G | 7 | Total O 7 7 | 0 | 0 |
| 6 | K | 2 | Total O 2 2 | 0 | 0 |
| 6 | M | 3 | Total O 3 3 | 0 | 0 |
| 6 | N | 5 | Total O 5 5 | 0 | 0 |
| 6 | O | 5 | Total O 5 5 | 0 | 0 |
| 6 | P | 5 | Total O 5 5 | 0 | 0 |
| 6 | C | 8 | Total O 8 8 | 0 | 0 |
| 6 | D | 2 | Total O 2 2 | 0 | 0 |
| 6 | E | 2 | Total O 2 2 | 0 | 0 |

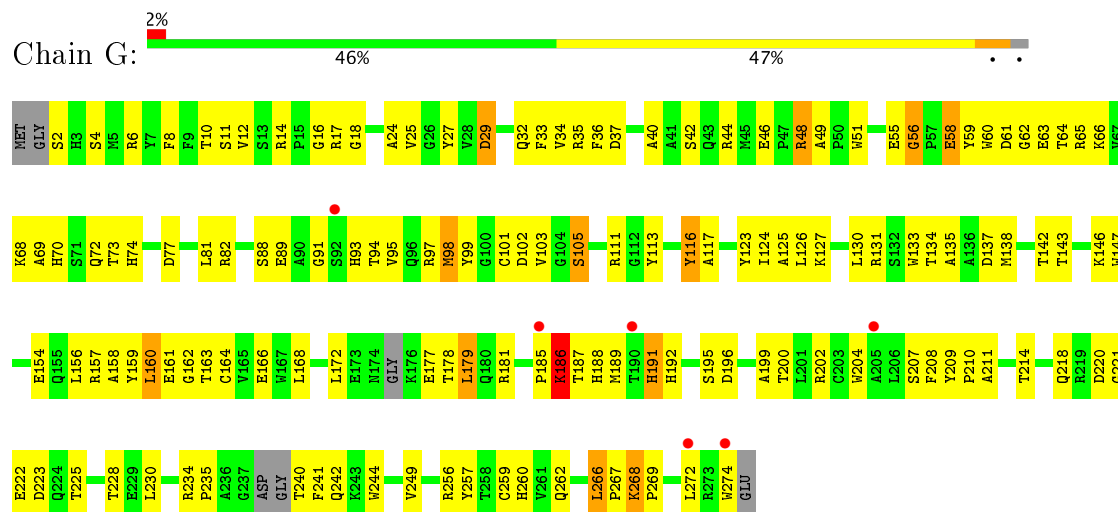
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

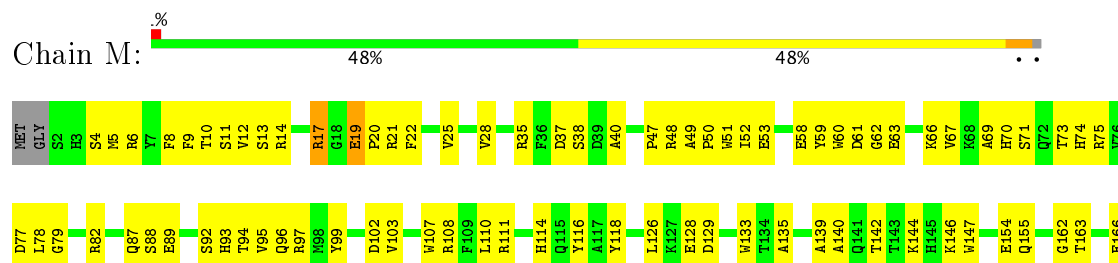
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



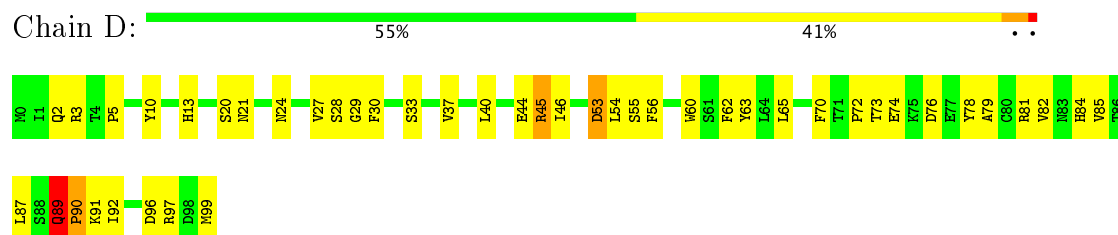
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



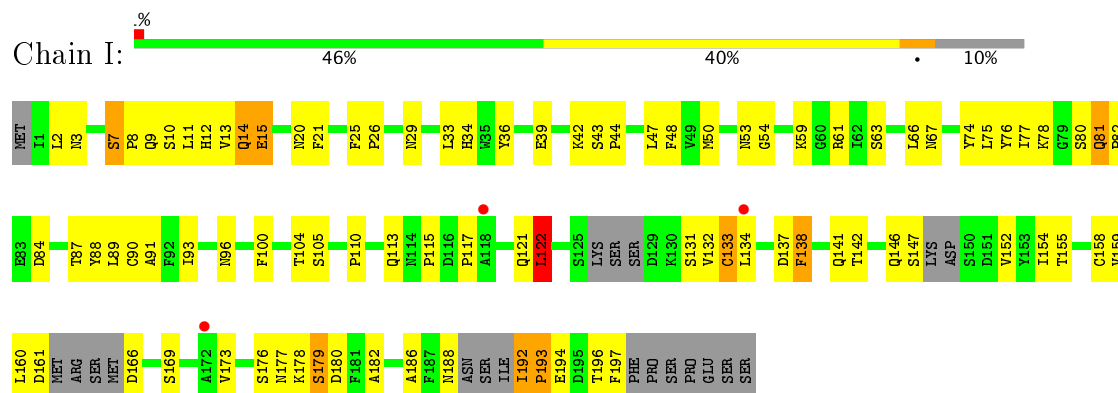
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



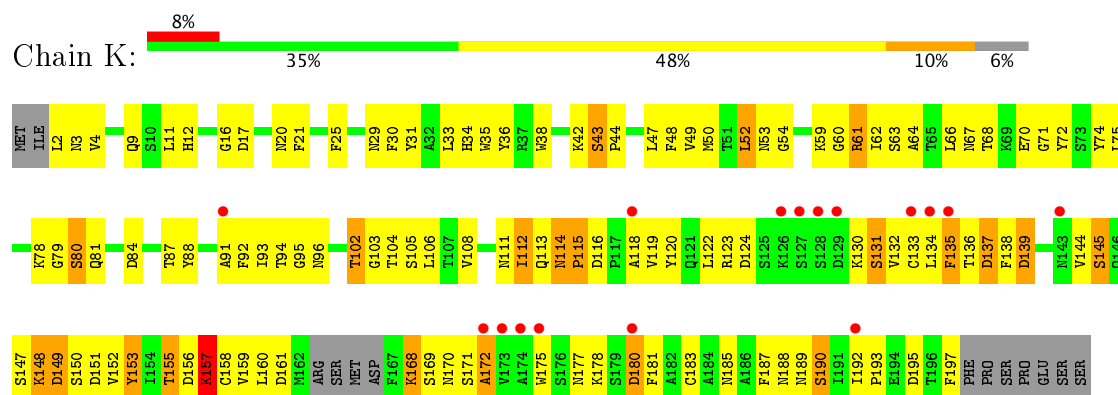
- Molecule 2: Beta-2-microglobulin



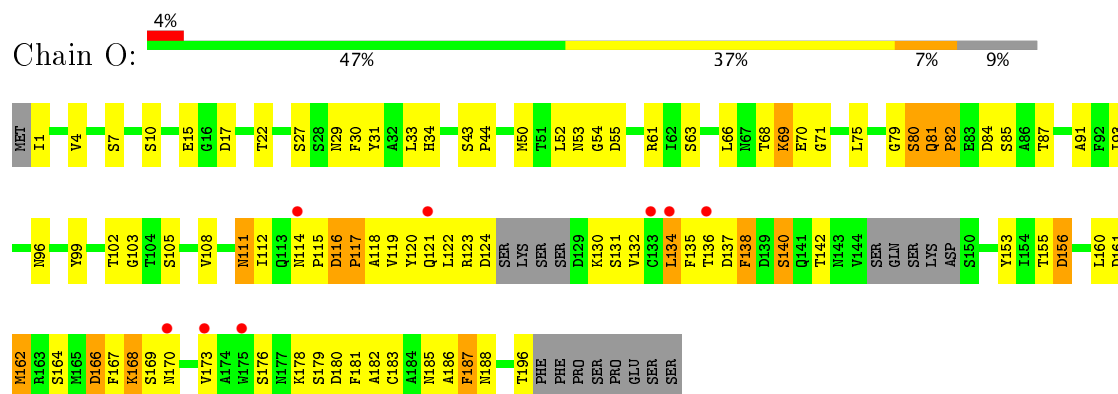
- Molecule 3: C7 TCR alpha chain



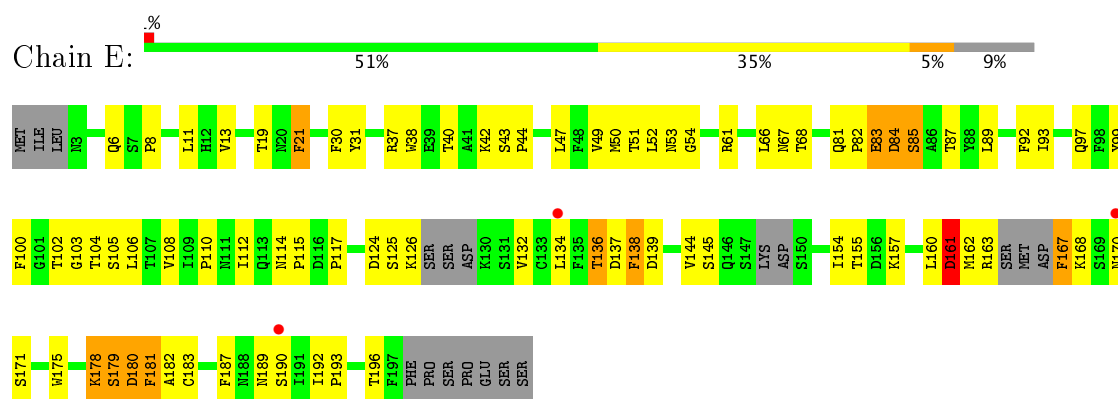
- Molecule 3: C7 TCR alpha chain



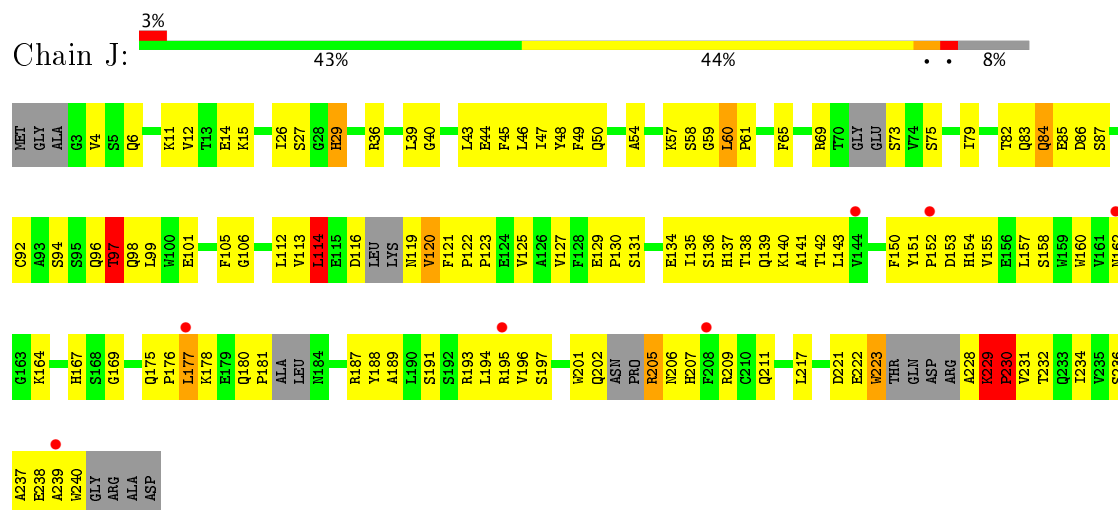
- Molecule 3: C7 TCR alpha chain



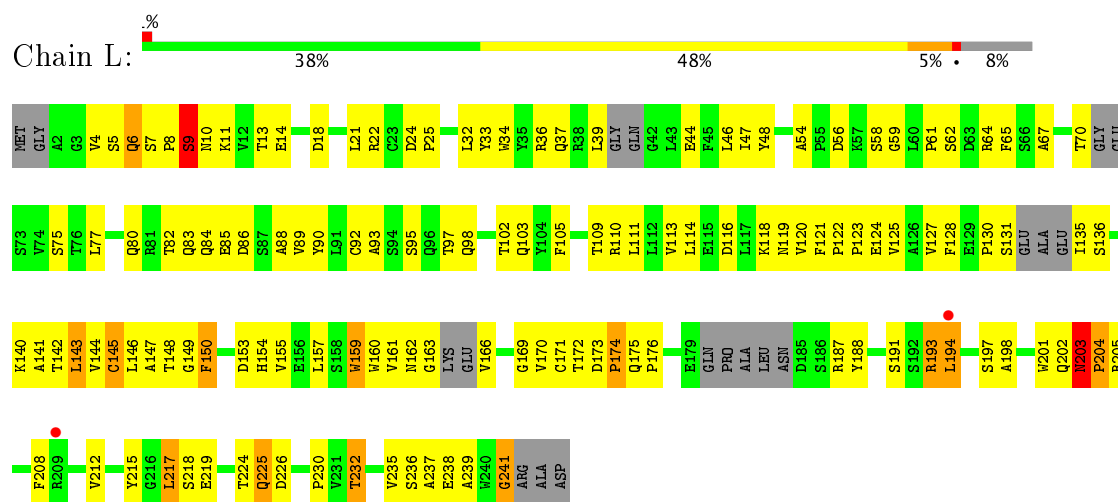
- Molecule 3: C7 TCR alpha chain



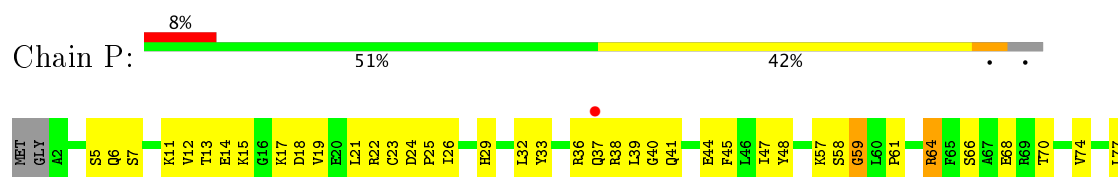
• Molecule 4: C7 TCR beta chain

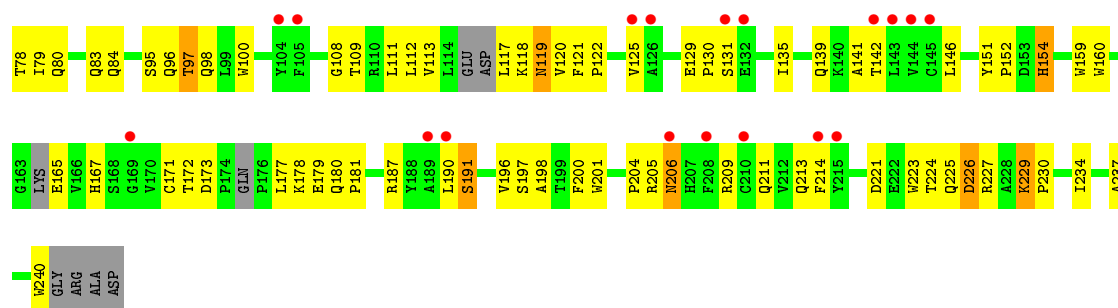


• Molecule 4: C7 TCR beta chain

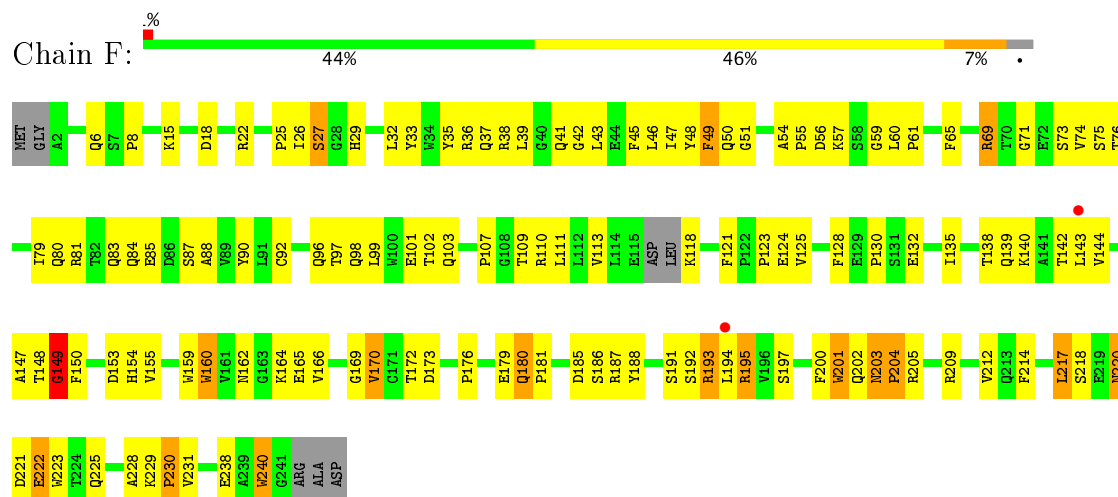


• Molecule 4: C7 TCR beta chain

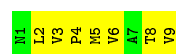




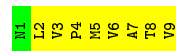
• Molecule 4: C7 TCR beta chain



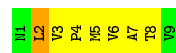
• Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL



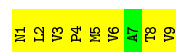
• Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL



• Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL



• Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 151.76Å 366.64Å 151.95Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.51 – 3.51 49.84 – 3.51 | Depositor EDS |
| % Data completeness (in resolution range) | 99.3 (49.51-3.51) 91.4 (49.84-3.51) | Depositor EDS |
| R_{merge} | 0.20 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.08 (at 3.48Å) | Xtriage |
| Refinement program | PHENIX 1.9_1692 | Depositor |
| R, R_{free} | 0.270 , 0.355 0.266 , 0.348 | Depositor DCC |
| R_{free} test set | 2469 reflections (5.08%) | DCC |
| Wilson B-factor (Å ²) | 81.7 | Xtriage |
| Anisotropy | 0.596 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 60.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 25272 | wwPDB-VP |
| Average B, all atoms (Å ²) | 80.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.13 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7879e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.47 | 0/2307 | 0.61 | 1/3132 (0.0%) |
| 1 | C | 0.46 | 0/2307 | 0.59 | 1/3132 (0.0%) |
| 1 | G | 0.53 | 1/2262 (0.0%) | 0.72 | 2/3072 (0.1%) |
| 1 | M | 0.42 | 0/2272 | 0.69 | 2/3085 (0.1%) |
| 2 | B | 0.43 | 0/845 | 0.66 | 0/1143 |
| 2 | D | 0.53 | 0/850 | 0.68 | 2/1151 (0.2%) |
| 2 | H | 0.44 | 0/798 | 0.64 | 0/1083 |
| 2 | N | 0.52 | 0/848 | 0.80 | 0/1150 |
| 3 | E | 0.46 | 0/1463 | 0.70 | 0/1987 |
| 3 | I | 0.54 | 0/1433 | 0.80 | 4/1946 (0.2%) |
| 3 | K | 0.56 | 1/1486 (0.1%) | 0.85 | 4/2018 (0.2%) |
| 3 | O | 0.54 | 2/1466 (0.1%) | 0.82 | 4/1992 (0.2%) |
| 4 | F | 0.54 | 1/1900 (0.1%) | 0.77 | 3/2586 (0.1%) |
| 4 | J | 0.50 | 2/1801 (0.1%) | 0.76 | 2/2448 (0.1%) |
| 4 | L | 0.52 | 0/1737 | 0.95 | 11/2362 (0.5%) |
| 4 | P | 0.43 | 0/1829 | 0.73 | 2/2494 (0.1%) |
| 5 | Q | 0.45 | 0/64 | 0.72 | 0/88 |
| 5 | R | 0.42 | 0/64 | 0.67 | 0/88 |
| 5 | T | 0.55 | 0/64 | 0.78 | 0/88 |
| 5 | U | 0.30 | 0/64 | 0.50 | 0/88 |
| All | All | 0.49 | 7/25860 (0.0%) | 0.74 | 38/35133 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | C | 0 | 1 |
| 1 | G | 0 | 4 |
| 2 | H | 0 | 1 |
| 2 | N | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | E | 0 | 3 |
| 3 | K | 0 | 5 |
| 3 | O | 0 | 3 |
| 4 | F | 0 | 3 |
| 4 | J | 0 | 2 |
| 4 | L | 0 | 5 |
| 4 | P | 0 | 3 |
| All | All | 0 | 32 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | J | 230 | PRO | N-CD | 5.28 | 1.55 | 1.47 |
| 1 | G | 267 | PRO | N-CD | 5.25 | 1.55 | 1.47 |
| 3 | K | 172 | ALA | CA-CB | -5.25 | 1.41 | 1.52 |
| 3 | O | 82 | PRO | N-CD | 5.13 | 1.55 | 1.47 |
| 3 | O | 117 | PRO | N-CD | 5.13 | 1.55 | 1.47 |
| 4 | F | 230 | PRO | N-CD | 5.08 | 1.54 | 1.47 |
| 4 | J | 61 | PRO | N-CD | 5.00 | 1.54 | 1.47 |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4 | L | 241 | GLY | N-CA-C | 12.45 | 144.23 | 113.10 |
| 3 | I | 7 | SER | C-N-CD | -11.91 | 94.40 | 120.60 |
| 4 | L | 149 | GLY | N-CA-C | 10.65 | 139.73 | 113.10 |
| 1 | G | 179 | LEU | N-CA-C | 8.08 | 132.81 | 111.00 |
| 3 | I | 192 | ILE | C-N-CD | 6.94 | 142.98 | 128.40 |
| 3 | K | 114 | ASN | C-N-CD | -6.57 | 106.14 | 120.60 |
| 4 | P | 146 | LEU | CA-CB-CG | 6.29 | 129.77 | 115.30 |
| 3 | K | 190 | SER | N-CA-C | -6.21 | 94.22 | 111.00 |
| 4 | L | 203 | ASN | C-N-CD | 6.09 | 141.20 | 128.40 |
| 2 | D | 2 | GLN | CA-CB-CG | 6.07 | 126.74 | 113.40 |
| 4 | L | 54 | ALA | C-N-CD | 6.06 | 141.13 | 128.40 |
| 4 | L | 174 | PRO | N-CA-CB | 6.04 | 110.55 | 103.30 |
| 3 | O | 162 | MET | CA-CB-CG | 6.02 | 123.54 | 113.30 |
| 3 | O | 43 | SER | C-N-CD | 6.00 | 141.01 | 128.40 |
| 2 | D | 89 | GLN | C-N-CD | 6.00 | 141.00 | 128.40 |
| 3 | I | 122 | LEU | N-CA-C | -5.97 | 94.88 | 111.00 |
| 4 | L | 194 | LEU | CA-CB-CG | 5.97 | 129.03 | 115.30 |
| 4 | J | 138 | THR | N-CA-C | 5.95 | 127.05 | 111.00 |
| 4 | L | 56 | ASP | N-CA-C | -5.94 | 94.97 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4 | P | 180 | GLN | C-N-CD | 5.93 | 140.85 | 128.40 |
| 4 | L | 157 | LEU | CA-CB-CG | 5.90 | 128.87 | 115.30 |
| 3 | I | 193 | PRO | CA-N-CD | -5.88 | 103.27 | 111.50 |
| 1 | M | 19 | GLU | C-N-CD | 5.81 | 140.61 | 128.40 |
| 4 | F | 229 | LYS | C-N-CD | 5.80 | 140.57 | 128.40 |
| 1 | M | 50 | PRO | N-CA-CB | 5.71 | 110.15 | 103.30 |
| 3 | O | 81 | GLN | C-N-CD | 5.69 | 140.35 | 128.40 |
| 3 | O | 116 | ASP | C-N-CD | 5.69 | 140.34 | 128.40 |
| 1 | G | 266 | LEU | C-N-CD | 5.65 | 140.27 | 128.40 |
| 4 | F | 149 | GLY | N-CA-C | -5.58 | 99.14 | 113.10 |
| 4 | L | 4 | VAL | N-CA-C | 5.55 | 125.99 | 111.00 |
| 3 | K | 43 | SER | C-N-CD | 5.47 | 139.89 | 128.40 |
| 4 | F | 204 | PRO | N-CA-C | 5.38 | 126.08 | 112.10 |
| 1 | A | 224 | GLN | CA-C-N | -5.38 | 105.37 | 117.20 |
| 4 | L | 225 | GLN | CA-CB-CG | 5.35 | 125.17 | 113.40 |
| 1 | C | 215 | LEU | CA-CB-CG | 5.07 | 126.95 | 115.30 |
| 3 | K | 157 | LYS | N-CA-C | 5.06 | 124.66 | 111.00 |
| 4 | J | 230 | PRO | CA-N-CD | -5.01 | 104.48 | 111.50 |
| 4 | L | 86 | ASP | N-CA-C | -5.00 | 97.50 | 111.00 |

There are no chirality outliers.

All (32) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 224 | GLN | Mainchain |
| 1 | C | 225 | THR | Peptide |
| 3 | E | 161 | ASP | Peptide |
| 3 | E | 181 | PHE | Peptide |
| 3 | E | 84 | ASP | Peptide |
| 4 | F | 149 | GLY | Peptide |
| 4 | F | 27 | SER | Peptide |
| 4 | F | 69 | ARG | Peptide |
| 1 | G | 105 | SER | Peptide |
| 1 | G | 160 | LEU | Mainchain |
| 1 | G | 186 | LYS | Peptide |
| 1 | G | 56 | GLY | Peptide |
| 2 | H | 17 | ASN | Peptide |
| 4 | J | 229 | LYS | Peptide |
| 4 | J | 97 | THR | Peptide |
| 3 | K | 130 | LYS | Peptide |
| 3 | K | 131 | SER | Peptide |
| 3 | K | 139 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 3 | K | 145 | SER | Peptide |
| 3 | K | 54 | GLY | Peptide |
| 4 | L | 136 | SER | Peptide |
| 4 | L | 204 | PRO | Peptide |
| 4 | L | 232 | THR | Peptide |
| 4 | L | 58 | SER | Peptide |
| 4 | L | 9 | SER | Peptide |
| 2 | N | 19 | LYS | Peptide |
| 3 | O | 111 | ASN | Peptide |
| 3 | O | 136 | THR | Peptide |
| 3 | O | 156 | ASP | Peptide |
| 4 | P | 206 | ASN | Peptide |
| 4 | P | 224 | THR | Peptide |
| 4 | P | 59 | GLY | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2242 | 0 | 2090 | 131 | 0 |
| 1 | C | 2242 | 0 | 2090 | 122 | 0 |
| 1 | G | 2199 | 0 | 2039 | 220 | 0 |
| 1 | M | 2210 | 0 | 2042 | 163 | 0 |
| 2 | B | 823 | 0 | 787 | 47 | 0 |
| 2 | D | 827 | 0 | 781 | 51 | 0 |
| 2 | H | 777 | 0 | 715 | 63 | 0 |
| 2 | N | 825 | 0 | 770 | 78 | 0 |
| 3 | E | 1432 | 0 | 1307 | 102 | 0 |
| 3 | I | 1404 | 0 | 1269 | 125 | 1 |
| 3 | K | 1452 | 0 | 1320 | 213 | 4 |
| 3 | O | 1435 | 0 | 1323 | 107 | 2 |
| 4 | F | 1852 | 0 | 1726 | 181 | 0 |
| 4 | J | 1759 | 0 | 1634 | 156 | 0 |
| 4 | L | 1699 | 0 | 1542 | 201 | 0 |
| 4 | P | 1784 | 0 | 1638 | 134 | 2 |
| 5 | Q | 64 | 0 | 74 | 12 | 0 |
| 5 | R | 64 | 0 | 74 | 12 | 0 |
| 5 | T | 64 | 0 | 74 | 13 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | U | 64 | 0 | 74 | 27 | 0 |
| 6 | A | 9 | 0 | 0 | 4 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 6 | C | 8 | 0 | 0 | 1 | 0 |
| 6 | D | 2 | 0 | 0 | 0 | 0 |
| 6 | E | 2 | 0 | 0 | 0 | 0 |
| 6 | G | 7 | 0 | 0 | 3 | 0 |
| 6 | I | 3 | 0 | 0 | 1 | 0 |
| 6 | J | 2 | 0 | 0 | 1 | 0 |
| 6 | K | 2 | 0 | 0 | 0 | 0 |
| 6 | M | 3 | 0 | 0 | 3 | 0 |
| 6 | N | 5 | 0 | 0 | 2 | 0 |
| 6 | O | 5 | 0 | 0 | 0 | 0 |
| 6 | P | 5 | 0 | 0 | 1 | 0 |
| All | All | 25272 | 0 | 23369 | 1971 | 5 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (1971) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:192:ILE:HG23 | 3:I:193:PRO:CD | 1.42 | 1.46 |
| 1:A:230:LEU:HD21 | 1:A:243:LYS:NZ | 1.27 | 1.43 |
| 3:K:175:TRP:CZ2 | 4:L:146:LEU:HD22 | 1.53 | 1.42 |
| 4:L:88:ALA:CB | 4:L:110:ARG:HG3 | 1.46 | 1.41 |
| 3:K:112:ILE:CG2 | 3:K:139:ASP:HB3 | 1.48 | 1.41 |
| 4:L:170:VAL:HA | 4:L:194:LEU:CD2 | 1.51 | 1.38 |
| 3:K:175:TRP:CZ2 | 4:L:146:LEU:HD13 | 1.57 | 1.38 |
| 3:K:38:TRP:CE3 | 3:K:44:PRO:HG3 | 1.59 | 1.38 |
| 4:P:112:LEU:CD1 | 4:P:154:HIS:CE1 | 2.05 | 1.38 |
| 1:C:202:ARG:CD | 1:C:244:TRP:HE1 | 1.37 | 1.35 |
| 3:I:192:ILE:CG2 | 3:I:193:PRO:HD3 | 1.57 | 1.35 |
| 1:G:98:MET:HE2 | 1:G:113:TYR:CD1 | 1.59 | 1.34 |
| 4:J:29:HIS:HD2 | 4:J:94:SER:CB | 1.40 | 1.34 |
| 3:K:61:ARG:HD2 | 3:K:78:LYS:O | 1.25 | 1.32 |
| 4:P:14:GLU:OE2 | 4:P:117:LEU:CD2 | 1.76 | 1.31 |
| 1:G:98:MET:CE | 1:G:113:TYR:CE1 | 2.15 | 1.30 |
| 2:N:13:HIS:CE1 | 4:F:81:ARG:NH2 | 1.99 | 1.29 |
| 2:D:44:GLU:OE2 | 2:D:46:ILE:HD11 | 1.28 | 1.28 |
| 3:K:138:PHE:HE1 | 3:K:157:LYS:CE | 1.45 | 1.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:8:PRO:O | 3:I:104:THR:HG23 | 1.23 | 1.27 |
| 1:A:102:ASP:CG | 1:A:113:TYR:OH | 1.73 | 1.26 |
| 1:G:192:HIS:CD2 | 1:G:202:ARG:HH21 | 1.51 | 1.26 |
| 4:F:170:VAL:CG1 | 4:F:194:LEU:HD13 | 1.64 | 1.26 |
| 1:G:98:MET:CE | 1:G:113:TYR:CD1 | 2.19 | 1.26 |
| 3:K:175:TRP:CZ2 | 4:L:146:LEU:CD2 | 2.19 | 1.25 |
| 1:A:4:SER:HB2 | 1:A:102:ASP:OD1 | 1.36 | 1.25 |
| 4:P:7:SER:OG | 4:P:22:ARG:HB3 | 1.35 | 1.25 |
| 1:A:230:LEU:CD2 | 1:A:243:LYS:NZ | 1.98 | 1.24 |
| 4:J:47:ILE:HD11 | 4:J:60:LEU:CD2 | 1.66 | 1.24 |
| 3:K:175:TRP:HZ2 | 4:L:146:LEU:CG | 1.52 | 1.21 |
| 1:G:97:ARG:NH1 | 5:U:6:VAL:CG1 | 2.01 | 1.21 |
| 4:L:88:ALA:HB3 | 4:L:110:ARG:CG | 1.70 | 1.20 |
| 3:K:175:TRP:CZ2 | 4:L:146:LEU:CD1 | 2.23 | 1.20 |
| 3:E:167:PHE:HD2 | 3:E:168:LYS:N | 1.39 | 1.20 |
| 1:G:97:ARG:HH11 | 5:U:6:VAL:CG1 | 1.52 | 1.19 |
| 3:O:138:PHE:CE1 | 3:O:142:THR:HG21 | 1.75 | 1.19 |
| 1:G:98:MET:HE1 | 1:G:113:TYR:CE1 | 1.76 | 1.19 |
| 3:K:136:THR:HG22 | 3:K:171:SER:HA | 1.23 | 1.19 |
| 1:G:97:ARG:HH11 | 5:U:6:VAL:HG11 | 1.08 | 1.19 |
| 3:K:112:ILE:CG2 | 3:K:139:ASP:CB | 2.21 | 1.17 |
| 3:K:138:PHE:CE1 | 3:K:157:LYS:CE | 2.27 | 1.17 |
| 4:J:29:HIS:CD2 | 4:J:94:SER:CB | 2.27 | 1.17 |
| 4:P:112:LEU:HD11 | 4:P:154:HIS:CE1 | 1.74 | 1.16 |
| 1:G:98:MET:HE2 | 1:G:113:TYR:CE1 | 1.80 | 1.16 |
| 1:G:97:ARG:NE | 1:G:116:TYR:HE1 | 1.41 | 1.16 |
| 3:I:122:LEU:CA | 3:I:132:VAL:O | 1.93 | 1.15 |
| 3:K:161:ASP:CG | 3:K:168:LYS:HD3 | 1.65 | 1.15 |
| 1:A:230:LEU:HD21 | 1:A:243:LYS:CE | 1.77 | 1.14 |
| 3:O:182:ALA:HB1 | 3:O:185:ASN:HB3 | 1.24 | 1.14 |
| 4:L:89:VAL:HG12 | 4:L:110:ARG:CB | 1.75 | 1.14 |
| 3:K:148:LYS:HB3 | 3:K:149:ASP:O | 1.46 | 1.14 |
| 4:L:89:VAL:HG12 | 4:L:110:ARG:HB2 | 1.27 | 1.14 |
| 3:K:138:PHE:CE1 | 3:K:157:LYS:HE2 | 1.84 | 1.13 |
| 1:G:16:GLY:HA3 | 1:G:17:ARG:HB2 | 1.29 | 1.12 |
| 1:C:202:ARG:HD3 | 1:C:244:TRP:HE1 | 1.01 | 1.12 |
| 2:N:40:LEU:HD23 | 2:N:43:GLY:HA3 | 1.13 | 1.12 |
| 4:L:83:GLN:HG3 | 4:L:84:GLN:H | 0.98 | 1.12 |
| 3:K:175:TRP:CE2 | 4:L:146:LEU:HD22 | 1.82 | 1.12 |
| 1:A:230:LEU:CD2 | 1:A:243:LYS:CE | 2.28 | 1.12 |
| 4:F:170:VAL:HG13 | 4:F:194:LEU:CD1 | 1.78 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:175:TRP:HZ2 | 4:L:146:LEU:CD2 | 1.58 | 1.11 |
| 4:J:29:HIS:HD2 | 4:J:94:SER:HB2 | 1.07 | 1.10 |
| 4:L:88:ALA:HB1 | 4:L:89:VAL:HA | 1.31 | 1.09 |
| 4:P:112:LEU:HD12 | 4:P:154:HIS:CE1 | 1.83 | 1.09 |
| 4:F:54:ALA:HB1 | 4:F:57:LYS:HE3 | 1.27 | 1.09 |
| 3:O:53:ASN:HB2 | 3:O:68:THR:HG23 | 1.33 | 1.09 |
| 3:K:175:TRP:HZ2 | 4:L:146:LEU:CD1 | 1.64 | 1.09 |
| 3:K:138:PHE:HE1 | 3:K:157:LYS:HE2 | 0.97 | 1.08 |
| 1:G:192:HIS:CD2 | 1:G:202:ARG:NH2 | 2.22 | 1.08 |
| 3:K:138:PHE:CE1 | 3:K:157:LYS:HE3 | 1.89 | 1.08 |
| 3:O:138:PHE:CE1 | 3:O:142:THR:CG2 | 2.35 | 1.07 |
| 4:F:218:SER:OG | 4:F:221:ASP:HB2 | 1.55 | 1.07 |
| 4:J:47:ILE:HD11 | 4:J:60:LEU:HD21 | 1.12 | 1.07 |
| 2:N:73:THR:CG2 | 2:N:76:ASP:OD1 | 2.01 | 1.07 |
| 3:E:136:THR:HG23 | 3:E:171:SER:HB2 | 1.14 | 1.07 |
| 1:G:2:SER:N | 1:G:105:SER:HG | 1.52 | 1.07 |
| 3:O:138:PHE:HE1 | 3:O:142:THR:CG2 | 1.68 | 1.07 |
| 1:A:4:SER:HB3 | 1:A:102:ASP:CG | 1.75 | 1.07 |
| 4:P:97:THR:HG22 | 4:P:98:GLN:HG2 | 1.37 | 1.07 |
| 4:J:141:ALA:HB3 | 4:J:196:VAL:O | 1.55 | 1.06 |
| 1:M:78:LEU:HD23 | 1:M:95:VAL:CG2 | 1.86 | 1.06 |
| 3:I:146:GLN:CD | 3:I:154:ILE:HG12 | 1.75 | 1.06 |
| 4:P:223:TRP:CH2 | 4:P:229:LYS:O | 2.09 | 1.06 |
| 1:G:97:ARG:NE | 1:G:116:TYR:CE1 | 2.15 | 1.06 |
| 1:C:202:ARG:CG | 1:C:244:TRP:HE1 | 1.68 | 1.05 |
| 1:C:202:ARG:HD3 | 1:C:244:TRP:NE1 | 1.69 | 1.05 |
| 3:K:112:ILE:HG23 | 3:K:139:ASP:HB3 | 1.10 | 1.05 |
| 4:L:88:ALA:CB | 4:L:110:ARG:CG | 2.27 | 1.05 |
| 4:J:29:HIS:CD2 | 4:J:94:SER:HB2 | 1.87 | 1.05 |
| 4:P:14:GLU:HG2 | 4:P:117:LEU:HG | 1.06 | 1.05 |
| 3:K:61:ARG:CD | 3:K:78:LYS:O | 2.04 | 1.05 |
| 2:B:37:VAL:HG12 | 2:B:82:VAL:HG22 | 1.10 | 1.05 |
| 1:M:19:GLU:OE1 | 1:M:19:GLU:N | 1.88 | 1.04 |
| 4:J:29:HIS:CD2 | 4:J:94:SER:OG | 2.09 | 1.04 |
| 2:N:73:THR:HG22 | 2:N:76:ASP:OD1 | 1.56 | 1.04 |
| 4:P:14:GLU:HG2 | 4:P:117:LEU:CG | 1.87 | 1.04 |
| 1:A:102:ASP:CG | 1:A:113:TYR:HH | 1.53 | 1.04 |
| 3:I:33:LEU:HD12 | 3:I:91:ALA:O | 1.58 | 1.04 |
| 4:P:112:LEU:HD11 | 4:P:154:HIS:HE1 | 1.10 | 1.04 |
| 4:J:113:VAL:O | 4:J:114:LEU:HG | 1.57 | 1.03 |
| 4:L:170:VAL:CA | 4:L:194:LEU:CD2 | 2.35 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:14:GLU:CG | 4:P:117:LEU:HG | 1.89 | 1.03 |
| 4:P:14:GLU:OE2 | 4:P:117:LEU:HD21 | 0.87 | 1.03 |
| 3:K:185:ASN:O | 3:K:188:ASN:ND2 | 1.91 | 1.03 |
| 1:M:20:PRO:HD2 | 1:M:75:ARG:CD | 1.89 | 1.03 |
| 4:P:14:GLU:CD | 4:P:117:LEU:HD21 | 1.77 | 1.03 |
| 4:J:136:SER:HA | 4:J:139:GLN:OE1 | 1.58 | 1.03 |
| 1:C:226:GLN:NE2 | 1:C:227:ASP:OD1 | 1.92 | 1.02 |
| 4:L:170:VAL:CA | 4:L:194:LEU:HD23 | 1.89 | 1.02 |
| 4:J:47:ILE:CD1 | 4:J:60:LEU:CD2 | 2.37 | 1.02 |
| 1:C:202:ARG:CD | 1:C:244:TRP:NE1 | 2.21 | 1.01 |
| 3:K:148:LYS:HB3 | 3:K:149:ASP:C | 1.79 | 1.01 |
| 4:L:204:PRO:HG3 | 4:L:241:GLY:HA3 | 1.42 | 1.01 |
| 4:J:194:LEU:HD23 | 4:J:195:ARG:N | 1.75 | 1.01 |
| 4:F:218:SER:OG | 4:F:221:ASP:CB | 2.07 | 1.01 |
| 4:P:223:TRP:CZ2 | 4:P:229:LYS:O | 2.13 | 1.01 |
| 1:M:82:ARG:NH1 | 1:M:93:HIS:HD2 | 1.56 | 1.01 |
| 3:E:136:THR:HG23 | 3:E:171:SER:CB | 1.89 | 1.01 |
| 3:E:136:THR:CG2 | 3:E:171:SER:CB | 2.40 | 1.00 |
| 1:M:78:LEU:HD23 | 1:M:95:VAL:HG23 | 1.41 | 1.00 |
| 1:A:4:SER:CB | 1:A:102:ASP:OD1 | 2.08 | 1.00 |
| 4:P:196:VAL:HG22 | 4:P:197:SER:H | 1.23 | 1.00 |
| 3:O:53:ASN:HB2 | 3:O:68:THR:CG2 | 1.89 | 1.00 |
| 4:J:47:ILE:CD1 | 4:J:60:LEU:HD23 | 1.91 | 0.99 |
| 3:E:181:PHE:HB2 | 3:E:182:ALA:HA | 1.44 | 0.99 |
| 1:M:66:LYS:HZ1 | 3:O:29:ASN:CG | 1.66 | 0.99 |
| 1:G:35:ARG:HH21 | 1:G:48:ARG:CG | 1.76 | 0.99 |
| 1:G:116:TYR:HD2 | 1:G:117:ALA:N | 1.61 | 0.98 |
| 3:K:175:TRP:HE1 | 4:L:146:LEU:HD21 | 1.25 | 0.98 |
| 4:P:112:LEU:HD12 | 4:P:154:HIS:NE2 | 1.78 | 0.97 |
| 1:A:4:SER:CB | 1:A:102:ASP:CG | 2.32 | 0.97 |
| 2:D:44:GLU:OE2 | 2:D:46:ILE:CD1 | 2.10 | 0.97 |
| 3:E:167:PHE:CD2 | 3:E:168:LYS:N | 2.18 | 0.97 |
| 3:E:192:ILE:HG22 | 3:E:193:PRO:CD | 1.94 | 0.97 |
| 1:G:82:ARG:HH21 | 1:G:89:GLU:N | 1.61 | 0.97 |
| 4:L:170:VAL:HG22 | 4:L:194:LEU:HD21 | 1.44 | 0.97 |
| 4:L:89:VAL:CG1 | 4:L:110:ARG:HB2 | 1.93 | 0.97 |
| 1:M:82:ARG:HH11 | 1:M:93:HIS:HD2 | 1.03 | 0.97 |
| 3:E:83:GLU:HA | 3:E:84:ASP:OD1 | 1.64 | 0.96 |
| 4:F:149:GLY:H | 4:F:150:PHE:HD2 | 1.14 | 0.96 |
| 1:G:98:MET:CE | 1:G:113:TYR:HE1 | 1.67 | 0.96 |
| 3:K:175:TRP:CH2 | 4:L:146:LEU:HD13 | 2.00 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:125:ALA:O | 1:G:134:THR:HG22 | 1.64 | 0.95 |
| 1:A:227:ASP:OD2 | 1:A:248:VAL:HG22 | 1.65 | 0.95 |
| 3:E:136:THR:CG2 | 3:E:171:SER:HB2 | 1.93 | 0.95 |
| 1:M:73:THR:HG21 | 5:T:6:VAL:HG23 | 1.44 | 0.95 |
| 4:F:54:ALA:HB1 | 4:F:57:LYS:CE | 1.96 | 0.95 |
| 1:A:230:LEU:CD2 | 1:A:243:LYS:HZ3 | 1.72 | 0.95 |
| 3:K:49:VAL:HG21 | 4:L:102:THR:HG22 | 1.47 | 0.95 |
| 4:F:159:TRP:HE1 | 4:F:192:SER:HG | 1.15 | 0.95 |
| 1:G:97:ARG:HG2 | 1:G:116:TYR:CD1 | 2.02 | 0.95 |
| 3:K:185:ASN:CG | 3:K:188:ASN:ND2 | 2.20 | 0.95 |
| 4:L:83:GLN:HG3 | 4:L:84:GLN:N | 1.82 | 0.95 |
| 2:H:22:PHE:CD2 | 2:H:68:THR:O | 2.20 | 0.95 |
| 4:L:97:THR:CB | 4:L:98:GLN:OE1 | 2.15 | 0.95 |
| 4:P:97:THR:CG2 | 4:P:98:GLN:HG2 | 1.96 | 0.94 |
| 1:G:2:SER:N | 1:G:105:SER:OG | 1.98 | 0.94 |
| 1:G:97:ARG:NH1 | 5:U:6:VAL:HG13 | 1.81 | 0.94 |
| 2:N:42:ASN:H | 2:N:43:GLY:HA2 | 1.32 | 0.94 |
| 1:G:187:THR:HB | 1:G:272:LEU:HD21 | 1.49 | 0.94 |
| 4:P:223:TRP:CZ2 | 4:P:225:GLN:NE2 | 2.34 | 0.94 |
| 3:I:14:GLN:OE1 | 3:I:14:GLN:N | 2.00 | 0.94 |
| 3:K:112:ILE:HG21 | 3:K:139:ASP:HB3 | 1.47 | 0.94 |
| 3:K:148:LYS:HB2 | 3:K:149:ASP:HA | 1.48 | 0.93 |
| 2:N:13:HIS:HE1 | 4:F:81:ARG:NH2 | 1.60 | 0.93 |
| 3:O:81:GLN:HB3 | 3:O:82:PRO:HD2 | 1.48 | 0.93 |
| 1:A:35:ARG:HD3 | 1:A:48:ARG:HE | 1.32 | 0.93 |
| 4:F:160:TRP:NE1 | 4:F:165:GLU:HA | 1.81 | 0.93 |
| 2:N:13:HIS:CE1 | 4:F:81:ARG:HH22 | 1.75 | 0.93 |
| 4:P:223:TRP:CH2 | 4:P:225:GLN:NE2 | 2.35 | 0.93 |
| 4:L:83:GLN:CG | 4:L:84:GLN:H | 1.80 | 0.93 |
| 3:K:192:ILE:HG13 | 3:K:193:PRO:HD2 | 1.50 | 0.93 |
| 2:N:13:HIS:CE1 | 4:F:81:ARG:HH21 | 1.74 | 0.93 |
| 4:L:191:SER:OG | 4:L:193:ARG:NH2 | 2.02 | 0.93 |
| 1:C:231:VAL:HG11 | 1:C:244:TRP:HE3 | 1.33 | 0.92 |
| 1:G:16:GLY:CA | 1:G:17:ARG:HB2 | 1.99 | 0.92 |
| 1:M:20:PRO:HD2 | 1:M:75:ARG:HD3 | 1.47 | 0.92 |
| 3:I:8:PRO:O | 3:I:104:THR:CG2 | 2.15 | 0.92 |
| 3:K:136:THR:HB | 3:K:170:ASN:O | 1.69 | 0.92 |
| 1:G:98:MET:HE2 | 1:G:113:TYR:HD1 | 1.29 | 0.91 |
| 1:M:219:ARG:HD3 | 1:M:224:GLN:NE2 | 1.86 | 0.91 |
| 4:P:160:TRP:HE3 | 4:P:209:ARG:HD2 | 1.34 | 0.91 |
| 1:C:4:SER:HB3 | 1:C:102:ASP:OD1 | 1.71 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:170:VAL:HA | 4:L:194:LEU:HD23 | 0.93 | 0.91 |
| 4:F:223:TRP:HH2 | 4:F:228:ALA:O | 1.54 | 0.91 |
| 3:K:112:ILE:HG23 | 3:K:139:ASP:CB | 1.95 | 0.91 |
| 4:F:170:VAL:HG13 | 4:F:194:LEU:HD13 | 0.94 | 0.91 |
| 4:J:135:ILE:HA | 4:J:140:LYS:O | 1.71 | 0.91 |
| 3:K:53:ASN:HA | 3:K:66:LEU:HD22 | 1.53 | 0.91 |
| 1:G:98:MET:HE1 | 1:G:113:TYR:HE1 | 1.11 | 0.91 |
| 3:K:136:THR:HG22 | 3:K:171:SER:CA | 2.00 | 0.91 |
| 1:C:131:ARG:HH11 | 1:C:131:ARG:HG3 | 1.35 | 0.90 |
| 1:G:35:ARG:HH21 | 1:G:48:ARG:HG2 | 1.36 | 0.90 |
| 2:N:4:THR:HG23 | 2:N:86:THR:HG21 | 1.51 | 0.90 |
| 4:F:149:GLY:HA3 | 4:F:150:PHE:HB3 | 1.53 | 0.90 |
| 3:K:175:TRP:CE2 | 4:L:146:LEU:CD2 | 2.49 | 0.90 |
| 4:L:202:GLN:CA | 4:L:204:PRO:HD2 | 2.01 | 0.90 |
| 3:O:138:PHE:CD1 | 3:O:142:THR:HG21 | 2.06 | 0.90 |
| 1:C:102:ASP:CG | 1:C:113:TYR:OH | 2.10 | 0.90 |
| 3:I:178:LYS:CG | 3:I:179:SER:OG | 2.19 | 0.90 |
| 3:K:161:ASP:CG | 3:K:168:LYS:CD | 2.39 | 0.90 |
| 1:G:162:GLY:O | 1:G:166:GLU:HG2 | 1.72 | 0.90 |
| 4:L:89:VAL:HG12 | 4:L:110:ARG:CG | 1.99 | 0.89 |
| 4:P:112:LEU:CD1 | 4:P:154:HIS:NE2 | 2.33 | 0.89 |
| 1:G:17:ARG:HH11 | 1:G:17:ARG:HG3 | 1.37 | 0.89 |
| 3:K:38:TRP:HE3 | 3:K:44:PRO:HG3 | 1.35 | 0.89 |
| 1:M:10:THR:HG21 | 2:N:54:LEU:HD22 | 1.53 | 0.89 |
| 1:C:100:GLY:O | 1:C:113:TYR:HD2 | 1.56 | 0.89 |
| 4:F:160:TRP:O | 4:F:209:ARG:HG2 | 1.73 | 0.89 |
| 2:H:24:ASN:HD21 | 2:H:65:LEU:HG | 1.38 | 0.89 |
| 4:F:193:ARG:HH11 | 4:F:193:ARG:HG3 | 1.38 | 0.89 |
| 1:M:188:HIS:HB2 | 1:M:204:TRP:HB2 | 1.55 | 0.89 |
| 3:I:138:PHE:HE1 | 3:I:142:THR:HG1 | 1.18 | 0.89 |
| 3:K:156:ASP:OD1 | 3:K:157:LYS:N | 2.06 | 0.88 |
| 1:A:230:LEU:HD21 | 1:A:243:LYS:HZ3 | 0.84 | 0.88 |
| 3:K:175:TRP:CZ2 | 4:L:146:LEU:CG | 2.45 | 0.88 |
| 1:M:82:ARG:NH1 | 1:M:93:HIS:CD2 | 2.41 | 0.88 |
| 2:N:40:LEU:CD2 | 2:N:43:GLY:HA3 | 2.02 | 0.88 |
| 3:K:161:ASP:OD1 | 3:K:168:LYS:CD | 2.20 | 0.88 |
| 3:K:144:VAL:HG23 | 3:K:157:LYS:NZ | 1.89 | 0.88 |
| 4:L:88:ALA:HB3 | 4:L:110:ARG:HG3 | 0.88 | 0.87 |
| 2:N:54:LEU:HD21 | 2:N:62:PHE:CD1 | 2.09 | 0.87 |
| 1:G:98:MET:CE | 1:G:113:TYR:HD1 | 1.75 | 0.87 |
| 1:C:202:ARG:CG | 1:C:244:TRP:NE1 | 2.37 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:88:ALA:HB1 | 4:L:110:ARG:HG3 | 1.57 | 0.87 |
| 3:O:138:PHE:CE1 | 3:O:142:THR:CB | 2.56 | 0.87 |
| 1:A:102:ASP:OD2 | 1:A:113:TYR:OH | 1.93 | 0.86 |
| 3:K:112:ILE:HG22 | 3:K:139:ASP:OD2 | 1.75 | 0.86 |
| 4:P:151:TYR:O | 4:P:214:PHE:CE1 | 2.27 | 0.86 |
| 2:N:13:HIS:HE1 | 4:F:81:ARG:HH22 | 1.12 | 0.86 |
| 3:K:135:PHE:HZ | 3:K:192:ILE:CD1 | 1.88 | 0.86 |
| 1:G:116:TYR:CD2 | 1:G:117:ALA:N | 2.43 | 0.86 |
| 3:I:146:GLN:OE1 | 3:I:154:ILE:CD1 | 2.24 | 0.86 |
| 1:G:16:GLY:HA3 | 1:G:17:ARG:CB | 2.05 | 0.86 |
| 3:K:175:TRP:NE1 | 4:L:146:LEU:HD21 | 1.90 | 0.86 |
| 1:M:215:LEU:HD21 | 1:M:261:VAL:HG22 | 1.55 | 0.86 |
| 1:M:82:ARG:HH11 | 1:M:93:HIS:CD2 | 1.93 | 0.85 |
| 1:A:230:LEU:HD23 | 1:A:243:LYS:CE | 2.03 | 0.85 |
| 4:P:7:SER:OG | 4:P:22:ARG:CB | 2.22 | 0.85 |
| 3:O:80:SER:O | 3:O:81:GLN:NE2 | 2.09 | 0.85 |
| 3:O:61:ARG:NH1 | 3:O:84:ASP:OD2 | 2.09 | 0.85 |
| 4:F:121:PHE:CE2 | 4:F:187:ARG:NH2 | 2.44 | 0.85 |
| 3:E:178:LYS:O | 3:E:179:SER:OG | 1.95 | 0.85 |
| 3:I:146:GLN:OE1 | 3:I:154:ILE:HD11 | 1.75 | 0.85 |
| 3:E:38:TRP:HD1 | 3:E:44:PRO:HG3 | 1.41 | 0.85 |
| 4:F:110:ARG:NH2 | 4:F:154:HIS:CD2 | 2.45 | 0.85 |
| 2:N:2:GLN:NE2 | 2:N:85:VAL:HB | 1.91 | 0.85 |
| 1:C:226:GLN:OE1 | 1:C:227:ASP:N | 2.09 | 0.84 |
| 3:E:136:THR:CG2 | 3:E:171:SER:HB3 | 2.06 | 0.84 |
| 4:L:127:VAL:HG11 | 4:L:239:ALA:HB2 | 1.57 | 0.84 |
| 1:G:225:THR:O | 6:G:301:HOH:O | 1.95 | 0.84 |
| 1:A:42:SER:OG | 1:A:44:ARG:HG2 | 1.77 | 0.84 |
| 4:F:201:TRP:C | 4:F:204:PRO:HD3 | 1.97 | 0.84 |
| 4:F:96:GLN:O | 4:F:97:THR:OG1 | 1.94 | 0.84 |
| 3:I:15:GLU:OE2 | 6:I:301:HOH:O | 1.94 | 0.84 |
| 3:O:119:VAL:HA | 3:O:134:LEU:O | 1.77 | 0.84 |
| 1:M:9:PHE:HB2 | 1:M:97:ARG:HB3 | 1.60 | 0.84 |
| 3:K:175:TRP:NE1 | 4:L:146:LEU:CD2 | 2.40 | 0.84 |
| 4:J:223:TRP:CE3 | 4:J:223:TRP:HA | 2.13 | 0.83 |
| 3:K:120:TYR:HH | 4:L:135:ILE:N | 1.76 | 0.83 |
| 4:F:54:ALA:CB | 4:F:57:LYS:HE3 | 2.07 | 0.83 |
| 4:L:161:VAL:HG23 | 4:L:166:VAL:HG11 | 1.59 | 0.83 |
| 4:F:160:TRP:HE1 | 4:F:165:GLU:HA | 1.37 | 0.83 |
| 3:O:53:ASN:CB | 3:O:68:THR:HG23 | 2.06 | 0.83 |
| 1:C:45:MET:H | 1:C:64:THR:HG22 | 1.41 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:39:LEU:HD12 | 4:P:39:LEU:O | 1.77 | 0.83 |
| 2:D:79:ALA:HB1 | 2:D:92:ILE:HD11 | 1.59 | 0.83 |
| 4:F:26:ILE:O | 4:F:27:SER:OG | 1.96 | 0.83 |
| 1:G:125:ALA:HB3 | 1:G:134:THR:CG2 | 2.08 | 0.83 |
| 4:F:197:SER:HB3 | 4:F:200:PHE:HB2 | 1.60 | 0.83 |
| 1:G:218:GLN:HB3 | 1:G:223:ASP:HA | 1.59 | 0.83 |
| 4:J:84:GLN:NE2 | 1:G:177:GLU:OE1 | 2.11 | 0.83 |
| 4:J:129:GLU:HG3 | 4:J:130:PRO:HD2 | 1.59 | 0.83 |
| 3:E:192:ILE:HG22 | 3:E:193:PRO:HD2 | 1.60 | 0.83 |
| 4:J:194:LEU:CD2 | 4:J:196:VAL:HG23 | 2.08 | 0.82 |
| 1:G:58:GLU:O | 1:G:62:GLY:N | 2.13 | 0.82 |
| 4:L:150:PHE:CE1 | 4:L:188:TYR:O | 2.33 | 0.82 |
| 3:I:178:LYS:HG2 | 3:I:179:SER:HG | 1.44 | 0.82 |
| 2:N:12:ARG:O | 2:N:13:HIS:CG | 2.32 | 0.82 |
| 3:O:138:PHE:CE1 | 3:O:142:THR:HB | 2.14 | 0.82 |
| 1:M:66:LYS:NZ | 3:O:29:ASN:CG | 2.32 | 0.82 |
| 3:E:30:PHE:HD2 | 3:E:92:PHE:CE2 | 1.98 | 0.82 |
| 4:F:46:LEU:O | 4:F:59:GLY:HA3 | 1.80 | 0.82 |
| 1:C:100:GLY:O | 1:C:113:TYR:CD2 | 2.32 | 0.82 |
| 2:D:54:LEU:HD21 | 2:D:62:PHE:CD1 | 2.13 | 0.82 |
| 3:E:136:THR:HA | 3:E:138:PHE:HE1 | 1.45 | 0.82 |
| 3:K:38:TRP:CE3 | 3:K:44:PRO:CG | 2.55 | 0.82 |
| 4:P:160:TRP:HD1 | 4:P:165:GLU:HG3 | 1.44 | 0.82 |
| 1:A:230:LEU:CD2 | 1:A:243:LYS:HZ1 | 1.90 | 0.81 |
| 4:L:123:PRO:HG3 | 4:L:150:PHE:HD2 | 1.43 | 0.81 |
| 3:K:148:LYS:CB | 3:K:149:ASP:C | 2.49 | 0.81 |
| 3:E:178:LYS:C | 3:E:179:SER:OG | 2.11 | 0.81 |
| 3:I:194:GLU:O | 3:I:196:THR:CG2 | 2.28 | 0.81 |
| 1:C:192:HIS:CE1 | 1:C:202:ARG:HH12 | 1.98 | 0.81 |
| 3:K:161:ASP:OD1 | 3:K:168:LYS:HD2 | 1.81 | 0.81 |
| 1:C:225:THR:O | 1:C:228:THR:HG22 | 1.79 | 0.81 |
| 3:I:178:LYS:C | 3:I:179:SER:OG | 2.16 | 0.81 |
| 2:B:17:ASN:ND2 | 2:B:74:GLU:OE1 | 2.14 | 0.81 |
| 2:B:37:VAL:CG1 | 2:B:82:VAL:HG22 | 2.04 | 0.81 |
| 3:I:178:LYS:HG2 | 3:I:179:SER:OG | 1.79 | 0.80 |
| 4:J:160:TRP:CZ3 | 4:J:211:GLN:CB | 2.64 | 0.80 |
| 4:P:112:LEU:CG | 4:P:154:HIS:CE1 | 2.63 | 0.80 |
| 4:P:19:VAL:HG22 | 4:P:79:ILE:HG12 | 1.63 | 0.80 |
| 3:E:136:THR:HG22 | 3:E:171:SER:HB3 | 1.63 | 0.80 |
| 1:G:14:ARG:O | 1:G:18:GLY:HA3 | 1.80 | 0.80 |
| 3:O:122:LEU:HD22 | 4:P:130:PRO:HA | 1.64 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:4:SER:CB | 1:C:102:ASP:OD1 | 2.29 | 0.80 |
| 3:E:138:PHE:O | 3:E:139:ASP:C | 2.16 | 0.79 |
| 1:G:192:HIS:HD2 | 1:G:202:ARG:NH2 | 1.69 | 0.79 |
| 1:A:223:ASP:O | 1:A:225:THR:HG23 | 1.82 | 0.79 |
| 3:I:138:PHE:CD1 | 3:I:142:THR:OG1 | 2.35 | 0.79 |
| 1:C:234:ARG:NH2 | 1:C:242:GLN:OE1 | 2.12 | 0.79 |
| 4:F:223:TRP:CZ3 | 4:F:230:PRO:HD2 | 2.18 | 0.79 |
| 2:H:70:PHE:HE1 | 2:H:78:TYR:CD1 | 2.00 | 0.79 |
| 1:M:220:ASP:OD1 | 6:M:301:HOH:O | 2.01 | 0.79 |
| 3:K:49:VAL:HG21 | 4:L:102:THR:CG2 | 2.13 | 0.79 |
| 4:F:110:ARG:NH2 | 4:F:154:HIS:HD2 | 1.80 | 0.78 |
| 3:O:81:GLN:HB3 | 3:O:82:PRO:CD | 2.12 | 0.78 |
| 1:G:125:ALA:HB3 | 1:G:134:THR:HG21 | 1.64 | 0.78 |
| 3:I:146:GLN:CD | 3:I:154:ILE:CG1 | 2.52 | 0.78 |
| 4:J:27:SER:OG | 6:J:301:HOH:O | 2.00 | 0.78 |
| 4:P:178:LYS:HA | 4:P:187:ARG:O | 1.81 | 0.78 |
| 3:I:192:ILE:HG23 | 3:I:193:PRO:HD3 | 0.78 | 0.78 |
| 3:K:38:TRP:CZ3 | 3:K:42:LYS:O | 2.35 | 0.78 |
| 4:F:149:GLY:N | 4:F:150:PHE:HD2 | 1.81 | 0.78 |
| 3:K:112:ILE:HG22 | 3:K:139:ASP:CG | 2.05 | 0.78 |
| 4:L:25:PRO:HG3 | 4:L:32:LEU:HD13 | 1.65 | 0.78 |
| 4:L:64:ARG:O | 4:L:80:GLN:NE2 | 2.17 | 0.78 |
| 3:K:175:TRP:HE1 | 4:L:146:LEU:CD2 | 1.96 | 0.78 |
| 3:E:49:VAL:CG2 | 4:F:102:THR:HG22 | 2.13 | 0.78 |
| 1:G:133:TRP:CZ3 | 1:G:147:TRP:CZ3 | 2.72 | 0.78 |
| 3:K:144:VAL:HG23 | 3:K:157:LYS:HZ1 | 1.46 | 0.78 |
| 2:N:73:THR:HG21 | 2:N:76:ASP:OD1 | 1.81 | 0.78 |
| 3:I:115:PRO:CB | 3:I:137:ASP:OD2 | 2.32 | 0.77 |
| 3:K:148:LYS:CB | 3:K:149:ASP:CA | 2.61 | 0.77 |
| 1:C:93:HIS:ND1 | 1:C:118:TYR:OH | 2.14 | 0.77 |
| 3:K:49:VAL:CG2 | 4:L:102:THR:HG22 | 2.15 | 0.77 |
| 2:B:37:VAL:HG21 | 2:B:66:TYR:CE1 | 2.19 | 0.77 |
| 1:C:72:GLN:HG3 | 4:F:55:PRO:HB2 | 1.66 | 0.77 |
| 3:I:178:LYS:HG3 | 3:I:179:SER:OG | 1.83 | 0.77 |
| 4:J:60:LEU:O | 4:J:60:LEU:HD12 | 1.83 | 0.77 |
| 1:M:192:HIS:O | 1:M:200:THR:OG1 | 2.02 | 0.77 |
| 1:C:66:LYS:NZ | 5:R:1:ASN:OD1 | 2.18 | 0.77 |
| 1:M:87:GLN:OE1 | 1:M:93:HIS:NE2 | 2.17 | 0.77 |
| 2:N:42:ASN:O | 6:N:101:HOH:O | 2.01 | 0.77 |
| 3:O:138:PHE:HD1 | 3:O:142:THR:OG1 | 1.67 | 0.77 |
| 4:F:97:THR:OG1 | 4:F:98:GLN:HG2 | 1.85 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:42:ASN:N | 2:N:43:GLY:HA2 | 1.96 | 0.77 |
| 4:J:217:LEU:HD13 | 4:J:221:ASP:HB3 | 1.67 | 0.77 |
| 4:L:170:VAL:CG2 | 4:L:194:LEU:HD21 | 2.15 | 0.77 |
| 1:A:187:THR:HB | 1:A:272:LEU:HD11 | 1.67 | 0.77 |
| 2:D:87:LEU:HD13 | 2:D:90:PRO:HA | 1.66 | 0.77 |
| 4:F:217:LEU:CD1 | 4:F:218:SER:H | 1.97 | 0.77 |
| 1:G:188:HIS:HB3 | 1:G:204:TRP:HB2 | 1.66 | 0.77 |
| 1:G:220:ASP:OD2 | 1:G:256:ARG:CZ | 2.32 | 0.77 |
| 3:K:138:PHE:CZ | 3:K:157:LYS:HE3 | 2.19 | 0.77 |
| 1:M:78:LEU:CD2 | 1:M:95:VAL:HG23 | 2.13 | 0.77 |
| 4:J:84:GLN:HA | 4:J:113:VAL:HG21 | 1.67 | 0.77 |
| 3:I:138:PHE:CE1 | 3:I:142:THR:OG1 | 2.38 | 0.76 |
| 4:P:14:GLU:H | 4:P:17:LYS:HZ1 | 1.33 | 0.76 |
| 1:G:218:GLN:HB2 | 1:G:222:GLU:O | 1.86 | 0.76 |
| 1:A:4:SER:HB3 | 1:A:102:ASP:OD2 | 1.84 | 0.76 |
| 4:F:132:GLU:HG3 | 4:F:135:ILE:HG21 | 1.68 | 0.76 |
| 4:P:7:SER:HG | 4:P:22:ARG:HB3 | 1.51 | 0.76 |
| 4:F:159:TRP:O | 4:F:166:VAL:HB | 1.84 | 0.76 |
| 2:N:30:PHE:CE1 | 2:N:62:PHE:HB2 | 2.20 | 0.76 |
| 1:C:235:PRO:O | 2:D:10:TYR:OH | 2.01 | 0.76 |
| 1:G:133:TRP:CZ3 | 1:G:147:TRP:CE3 | 2.72 | 0.76 |
| 4:L:143:LEU:HD12 | 4:L:144:VAL:N | 2.00 | 0.76 |
| 3:K:161:ASP:OD1 | 3:K:168:LYS:HD3 | 1.83 | 0.76 |
| 1:A:230:LEU:HD21 | 1:A:243:LYS:HE2 | 1.68 | 0.76 |
| 2:D:76:ASP:HB3 | 2:D:78:TYR:HE1 | 1.50 | 0.76 |
| 3:K:185:ASN:CG | 3:K:188:ASN:HD22 | 1.89 | 0.76 |
| 4:L:143:LEU:HD12 | 4:L:144:VAL:H | 1.50 | 0.76 |
| 2:N:54:LEU:HD21 | 2:N:62:PHE:HD1 | 1.51 | 0.76 |
| 3:O:53:ASN:CB | 3:O:68:THR:CG2 | 2.62 | 0.75 |
| 2:B:89:GLN:HB2 | 2:B:90:PRO:HD2 | 1.68 | 0.75 |
| 2:H:24:ASN:OD1 | 2:H:65:LEU:HD23 | 1.86 | 0.75 |
| 3:K:17:ASP:O | 3:K:80:SER:OG | 2.04 | 0.75 |
| 4:P:223:TRP:HZ2 | 4:P:225:GLN:HE21 | 1.30 | 0.75 |
| 2:D:44:GLU:HG2 | 2:D:46:ILE:HG12 | 1.67 | 0.75 |
| 3:K:135:PHE:CZ | 3:K:192:ILE:CD1 | 2.70 | 0.75 |
| 1:G:97:ARG:NH1 | 5:U:6:VAL:HG11 | 1.84 | 0.75 |
| 1:A:122:ASP:OD1 | 2:B:60:TRP:NE1 | 2.20 | 0.75 |
| 4:J:223:TRP:HE3 | 4:J:223:TRP:HA | 1.47 | 0.75 |
| 3:K:59:LYS:HD2 | 3:K:60:GLY:H | 1.50 | 0.75 |
| 4:J:113:VAL:O | 4:J:114:LEU:CG | 2.35 | 0.75 |
| 1:G:17:ARG:NH1 | 1:G:17:ARG:HG3 | 1.99 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:151:TYR:O | 4:P:214:PHE:CZ | 2.40 | 0.75 |
| 4:J:57:LYS:O | 4:J:59:GLY:N | 2.17 | 0.75 |
| 1:M:20:PRO:HD2 | 1:M:75:ARG:HD2 | 1.67 | 0.75 |
| 4:P:122:PRO:HD3 | 4:P:230:PRO:HG3 | 1.69 | 0.75 |
| 3:E:84:ASP:HB3 | 3:E:85:SER:HB2 | 1.69 | 0.75 |
| 4:F:142:THR:HA | 4:F:195:ARG:HB2 | 1.66 | 0.75 |
| 1:G:97:ARG:HH12 | 5:U:6:VAL:CG1 | 1.99 | 0.75 |
| 3:K:31:TYR:HD1 | 5:U:4:PRO:HB2 | 1.52 | 0.75 |
| 4:P:14:GLU:HB2 | 4:P:17:LYS:HE3 | 1.69 | 0.75 |
| 1:A:96:GLN:OE1 | 2:B:60:TRP:CE3 | 2.39 | 0.75 |
| 3:E:49:VAL:HG21 | 4:F:102:THR:HG22 | 1.67 | 0.75 |
| 1:G:192:HIS:CD2 | 1:G:202:ARG:HD2 | 2.21 | 0.75 |
| 4:J:29:HIS:CD2 | 4:J:94:SER:C | 2.59 | 0.75 |
| 3:K:185:ASN:C | 3:K:188:ASN:HD22 | 1.90 | 0.75 |
| 1:A:230:LEU:CD2 | 1:A:243:LYS:HE2 | 2.13 | 0.74 |
| 4:P:112:LEU:CG | 4:P:154:HIS:NE2 | 2.50 | 0.74 |
| 1:A:102:ASP:OD1 | 1:A:113:TYR:OH | 1.93 | 0.74 |
| 4:L:153:ASP:HB2 | 4:L:188:TYR:CD2 | 2.22 | 0.74 |
| 1:C:192:HIS:ND1 | 1:C:202:ARG:NH1 | 2.30 | 0.74 |
| 3:K:148:LYS:HB2 | 3:K:149:ASP:CA | 2.17 | 0.74 |
| 1:C:131:ARG:HG3 | 1:C:131:ARG:NH1 | 1.98 | 0.74 |
| 3:E:136:THR:CA | 3:E:138:PHE:HE1 | 2.00 | 0.74 |
| 4:P:112:LEU:HG | 4:P:154:HIS:NE2 | 2.02 | 0.74 |
| 3:O:53:ASN:HB2 | 3:O:68:THR:CB | 2.17 | 0.74 |
| 3:E:97:GLN:NE2 | 3:E:99:TYR:OH | 2.20 | 0.74 |
| 4:F:218:SER:OG | 4:F:221:ASP:HB3 | 1.86 | 0.74 |
| 4:F:223:TRP:CH2 | 4:F:228:ALA:O | 2.39 | 0.74 |
| 3:K:135:PHE:CZ | 3:K:192:ILE:HG12 | 2.23 | 0.74 |
| 4:P:112:LEU:CD1 | 4:P:154:HIS:HE1 | 1.71 | 0.74 |
| 1:A:93:HIS:ND1 | 1:A:119:ASP:OD1 | 2.20 | 0.74 |
| 4:J:47:ILE:CG1 | 4:J:60:LEU:HD23 | 2.18 | 0.74 |
| 4:L:88:ALA:CB | 4:L:89:VAL:HA | 2.03 | 0.74 |
| 1:C:66:LYS:HD2 | 5:R:4:PRO:HA | 1.67 | 0.74 |
| 3:K:25:PHE:CZ | 3:K:71:GLY:HA2 | 2.22 | 0.74 |
| 3:K:192:ILE:HG13 | 3:K:193:PRO:CD | 2.17 | 0.74 |
| 3:K:93:ILE:HG22 | 5:U:5:MET:HE1 | 1.70 | 0.74 |
| 1:A:33:PHE:HD1 | 1:A:52:ILE:HD12 | 1.52 | 0.73 |
| 3:O:138:PHE:CD1 | 3:O:142:THR:CB | 2.71 | 0.73 |
| 4:F:205:ARG:HA | 4:F:240:TRP:CH2 | 2.23 | 0.73 |
| 3:I:48:PHE:HE1 | 3:I:59:LYS:HG3 | 1.52 | 0.73 |
| 1:C:35:ARG:HD2 | 2:D:53:ASP:CG | 2.08 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:192:ILE:CG2 | 3:E:193:PRO:HD3 | 2.17 | 0.73 |
| 4:J:178:LYS:HD2 | 4:J:188:TYR:CE1 | 2.23 | 0.73 |
| 3:O:138:PHE:HE1 | 3:O:142:THR:CB | 1.96 | 0.73 |
| 1:A:202:ARG:HG3 | 1:A:244:TRP:HE1 | 1.53 | 0.73 |
| 4:F:201:TRP:O | 4:F:204:PRO:CD | 2.36 | 0.73 |
| 1:G:186:LYS:O | 1:G:186:LYS:HG3 | 1.87 | 0.73 |
| 1:G:192:HIS:HD2 | 1:G:202:ARG:HH21 | 0.87 | 0.73 |
| 1:M:259:CYS:HB3 | 1:M:272:LEU:HB2 | 1.70 | 0.73 |
| 1:G:214:THR:O | 1:G:214:THR:HG23 | 1.89 | 0.73 |
| 2:H:21:ASN:OD1 | 2:H:22:PHE:N | 2.22 | 0.73 |
| 3:I:194:GLU:O | 3:I:196:THR:HG23 | 1.89 | 0.73 |
| 2:B:36:GLU:HB2 | 2:B:83:ASN:HB3 | 1.71 | 0.73 |
| 3:E:192:ILE:CG2 | 3:E:193:PRO:CD | 2.66 | 0.73 |
| 3:I:192:ILE:CG2 | 3:I:193:PRO:CD | 2.36 | 0.73 |
| 4:J:129:GLU:CG | 4:J:130:PRO:HD2 | 2.18 | 0.73 |
| 4:P:159:TRP:CD1 | 4:P:209:ARG:O | 2.41 | 0.73 |
| 1:C:202:ARG:HE | 1:C:244:TRP:HZ2 | 1.33 | 0.72 |
| 1:G:191:HIS:O | 1:G:191:HIS:ND1 | 2.20 | 0.72 |
| 4:L:10:ASN:HB2 | 4:L:154:HIS:NE2 | 2.04 | 0.72 |
| 1:C:225:THR:O | 1:C:228:THR:N | 2.16 | 0.72 |
| 2:H:37:VAL:HG23 | 2:H:81:ARG:O | 1.88 | 0.72 |
| 3:I:146:GLN:NE2 | 3:I:154:ILE:HG12 | 2.04 | 0.72 |
| 4:J:116:ASP:HB3 | 4:J:119:ASN:N | 2.05 | 0.72 |
| 3:K:138:PHE:O | 3:K:139:ASP:OD1 | 2.07 | 0.72 |
| 4:L:173:ASP:OD2 | 4:L:191:SER:OG | 2.07 | 0.72 |
| 1:A:99:TYR:OH | 5:Q:3:VAL:HG12 | 1.90 | 0.72 |
| 4:L:202:GLN:C | 4:L:204:PRO:HD2 | 2.09 | 0.72 |
| 4:P:18:ASP:OD2 | 2:D:20:SER:OG | 2.08 | 0.72 |
| 3:E:42:LYS:HD2 | 3:E:43:SER:H | 1.55 | 0.72 |
| 4:F:160:TRP:O | 4:F:209:ARG:CG | 2.37 | 0.72 |
| 4:J:194:LEU:HD22 | 4:J:196:VAL:HG23 | 1.70 | 0.72 |
| 3:K:34:HIS:HB2 | 3:K:91:ALA:HB3 | 1.71 | 0.72 |
| 1:A:5:MET:HB2 | 1:A:168:LEU:HD13 | 1.70 | 0.72 |
| 4:F:150:PHE:CE1 | 4:F:155:VAL:HG11 | 2.23 | 0.72 |
| 1:C:235:PRO:HD2 | 2:D:10:TYR:OH | 1.89 | 0.72 |
| 3:K:2:LEU:HB3 | 3:K:3:ASN:HA | 1.70 | 0.72 |
| 4:L:88:ALA:HB1 | 4:L:89:VAL:CA | 2.15 | 0.72 |
| 3:I:117:PRO:HB2 | 3:I:196:THR:HB | 1.71 | 0.72 |
| 3:K:9:GLN:HA | 3:K:104:THR:HA | 1.70 | 0.72 |
| 4:L:202:GLN:HA | 4:L:204:PRO:HD2 | 1.70 | 0.72 |
| 4:P:196:VAL:HG22 | 4:P:197:SER:N | 2.02 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:89:GLN:HG3 | 2:D:90:PRO:HD2 | 1.72 | 0.72 |
| 4:J:98:GLN:HB2 | 4:J:101:GLU:OE1 | 1.90 | 0.72 |
| 1:M:96:GLN:NE2 | 2:N:31:HIS:HE1 | 1.87 | 0.72 |
| 1:M:59:TYR:OH | 1:M:171:TYR:OH | 2.06 | 0.71 |
| 4:J:114:LEU:N | 4:J:114:LEU:HD12 | 2.03 | 0.71 |
| 1:M:197:HIS:O | 1:M:198:GLU:HG2 | 1.90 | 0.71 |
| 1:M:224:GLN:OE1 | 1:M:227:ASP:HB3 | 1.90 | 0.71 |
| 3:O:70:GLU:N | 3:O:71:GLY:HA2 | 2.05 | 0.71 |
| 4:P:160:TRP:CE3 | 4:P:209:ARG:HD2 | 2.22 | 0.71 |
| 4:J:29:HIS:NE2 | 4:J:94:SER:O | 2.22 | 0.71 |
| 3:E:30:PHE:HD2 | 3:E:92:PHE:HE2 | 1.39 | 0.71 |
| 4:J:178:LYS:HD2 | 4:J:188:TYR:HE1 | 1.55 | 0.71 |
| 1:M:89:GLU:HG2 | 1:M:89:GLU:O | 1.90 | 0.71 |
| 4:F:170:VAL:HA | 4:F:194:LEU:HD12 | 1.72 | 0.71 |
| 1:M:87:GLN:OE1 | 1:M:93:HIS:CE1 | 2.44 | 0.71 |
| 1:A:223:ASP:O | 1:A:225:THR:CG2 | 2.38 | 0.71 |
| 2:N:12:ARG:O | 2:N:13:HIS:ND1 | 2.23 | 0.71 |
| 2:H:24:ASN:HD21 | 2:H:65:LEU:CG | 2.03 | 0.70 |
| 2:H:24:ASN:OD1 | 2:H:65:LEU:CD2 | 2.39 | 0.70 |
| 3:E:112:ILE:HG22 | 3:E:115:PRO:HD3 | 1.73 | 0.70 |
| 4:F:84:GLN:CD | 4:F:85:GLU:H | 1.93 | 0.70 |
| 3:K:102:THR:OG1 | 3:K:103:GLY:N | 2.23 | 0.70 |
| 3:E:178:LYS:O | 3:E:180:ASP:N | 2.21 | 0.70 |
| 3:I:194:GLU:O | 3:I:196:THR:HG22 | 1.91 | 0.70 |
| 4:P:112:LEU:HG | 4:P:154:HIS:CE1 | 2.26 | 0.70 |
| 1:A:230:LEU:HD23 | 1:A:243:LYS:HE3 | 1.71 | 0.70 |
| 4:P:151:TYR:O | 4:P:214:PHE:HE1 | 1.75 | 0.70 |
| 2:D:33:SER:HB3 | 2:D:62:PHE:CD2 | 2.25 | 0.70 |
| 4:F:217:LEU:HD13 | 4:F:218:SER:H | 1.54 | 0.70 |
| 4:L:160:TRP:NE1 | 4:L:163:GLY:O | 2.23 | 0.70 |
| 4:F:121:PHE:HE2 | 4:F:187:ARG:HH21 | 1.37 | 0.70 |
| 1:G:192:HIS:CG | 1:G:202:ARG:NH2 | 2.60 | 0.70 |
| 3:K:112:ILE:CG2 | 3:K:139:ASP:CG | 2.59 | 0.70 |
| 1:M:95:VAL:CG1 | 1:M:116:TYR:CE1 | 2.74 | 0.70 |
| 1:M:66:LYS:CE | 3:O:29:ASN:ND2 | 2.54 | 0.70 |
| 1:A:59:TYR:HH | 1:A:171:TYR:HH | 1.40 | 0.70 |
| 1:C:218:GLN:HG2 | 1:C:260:HIS:CD2 | 2.27 | 0.70 |
| 4:L:89:VAL:HG12 | 4:L:110:ARG:HG3 | 1.73 | 0.70 |
| 3:O:155:THR:HG23 | 4:P:173:ASP:OD2 | 1.91 | 0.70 |
| 4:P:119:ASN:HB3 | 4:P:151:TYR:CD2 | 2.27 | 0.70 |
| 1:C:231:VAL:HG11 | 1:C:244:TRP:CE3 | 2.24 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:L:204:PRO:CG | 4:L:241:GLY:HA3 | 2.19 | 0.69 |
| 2:N:4:THR:CG2 | 2:N:86:THR:HG21 | 2.22 | 0.69 |
| 3:E:136:THR:HA | 3:E:138:PHE:CE1 | 2.27 | 0.69 |
| 3:K:50:MET:HB3 | 3:K:66:LEU:HD12 | 1.73 | 0.69 |
| 2:N:57:SER:O | 2:N:59:ASP:N | 2.24 | 0.69 |
| 4:P:25:PRO:HD3 | 4:P:32:LEU:HD21 | 1.74 | 0.69 |
| 4:J:160:TRP:HB2 | 4:J:209:ARG:CB | 2.23 | 0.69 |
| 3:K:35:TRP:HE1 | 3:K:75:LEU:HD22 | 1.56 | 0.69 |
| 3:K:59:LYS:HD2 | 3:K:60:GLY:N | 2.07 | 0.69 |
| 4:L:202:GLN:HA | 4:L:202:GLN:OE1 | 1.90 | 0.69 |
| 3:O:34:HIS:HB2 | 3:O:91:ALA:HB3 | 1.72 | 0.69 |
| 4:L:9:SER:O | 4:L:10:ASN:OD1 | 2.09 | 0.69 |
| 4:L:127:VAL:CG1 | 4:L:239:ALA:HB2 | 2.22 | 0.69 |
| 2:D:24:ASN:HB3 | 2:D:65:LEU:HD11 | 1.73 | 0.69 |
| 4:F:201:TRP:O | 4:F:204:PRO:HD3 | 1.93 | 0.69 |
| 1:G:24:ALA:HB3 | 1:G:36:PHE:HB3 | 1.74 | 0.69 |
| 3:I:122:LEU:CA | 3:I:132:VAL:H | 2.05 | 0.69 |
| 3:K:148:LYS:CB | 3:K:149:ASP:HA | 2.20 | 0.69 |
| 4:L:170:VAL:HA | 4:L:194:LEU:HD21 | 1.69 | 0.69 |
| 4:L:33:TYR:HB2 | 4:L:93:ALA:HB3 | 1.73 | 0.69 |
| 4:L:88:ALA:HB1 | 4:L:110:ARG:HA | 1.75 | 0.69 |
| 2:B:24:ASN:HB3 | 2:B:65:LEU:HD11 | 1.74 | 0.69 |
| 4:L:125:VAL:HB | 4:L:237:ALA:HB2 | 1.73 | 0.69 |
| 1:A:99:TYR:CZ | 5:Q:3:VAL:HG12 | 2.26 | 0.69 |
| 3:I:161:ASP:OD2 | 3:I:166:ASP:N | 2.25 | 0.69 |
| 3:O:138:PHE:HD1 | 3:O:142:THR:HG1 | 1.37 | 0.69 |
| 4:P:160:TRP:CD1 | 4:P:165:GLU:HG3 | 2.27 | 0.69 |
| 2:H:71:THR:OG1 | 2:H:72:PRO:HD3 | 1.92 | 0.68 |
| 4:J:47:ILE:HG13 | 4:J:60:LEU:HD23 | 1.74 | 0.68 |
| 1:M:219:ARG:NH2 | 1:M:222:GLU:OE1 | 2.26 | 0.68 |
| 4:F:98:GLN:NE2 | 4:F:98:GLN:HA | 2.08 | 0.68 |
| 1:G:159:TYR:CD1 | 1:G:163:THR:OG1 | 2.46 | 0.68 |
| 1:G:35:ARG:HE | 1:G:48:ARG:HG3 | 1.56 | 0.68 |
| 3:I:146:GLN:NE2 | 3:I:154:ILE:CG1 | 2.57 | 0.68 |
| 4:J:85:GLU:O | 4:J:87:SER:N | 2.27 | 0.68 |
| 1:G:192:HIS:HB2 | 1:G:202:ARG:HH22 | 1.57 | 0.68 |
| 1:M:22:PHE:H | 1:M:38:SER:HB2 | 1.56 | 0.68 |
| 2:H:22:PHE:HD2 | 2:H:68:THR:O | 1.75 | 0.68 |
| 3:I:117:PRO:O | 3:I:196:THR:O | 2.12 | 0.68 |
| 1:G:162:GLY:O | 1:G:166:GLU:CG | 2.41 | 0.68 |
| 3:I:34:HIS:HB2 | 3:I:91:ALA:HB3 | 1.73 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:5:MET:HB3 | 1:M:168:LEU:HD13 | 1.75 | 0.68 |
| 3:K:112:ILE:HG22 | 3:K:139:ASP:CB | 2.21 | 0.68 |
| 4:L:114:LEU:HD23 | 4:L:116:ASP:H | 1.59 | 0.68 |
| 4:L:10:ASN:HB2 | 4:L:154:HIS:CE1 | 2.28 | 0.68 |
| 4:L:36:ARG:HB3 | 4:L:89:VAL:O | 1.94 | 0.68 |
| 1:G:98:MET:HE3 | 1:G:99:TYR:HA | 1.76 | 0.68 |
| 4:L:90:TYR:N | 4:L:109:THR:O | 2.22 | 0.68 |
| 1:M:200:THR:HG22 | 1:M:248:VAL:HA | 1.75 | 0.68 |
| 1:C:27:TYR:CE2 | 1:C:32:GLN:HB2 | 2.28 | 0.68 |
| 3:K:131:SER:HG | 4:L:128:PHE:HD1 | 1.41 | 0.68 |
| 4:J:153:ASP:O | 4:J:155:VAL:N | 2.26 | 0.67 |
| 3:O:53:ASN:CB | 3:O:68:THR:OG1 | 2.43 | 0.67 |
| 3:I:146:GLN:HE22 | 3:I:154:ILE:HD13 | 1.57 | 0.67 |
| 4:L:123:PRO:HG3 | 4:L:150:PHE:CD2 | 2.27 | 0.67 |
| 1:M:21:ARG:HG3 | 1:M:38:SER:HB3 | 1.76 | 0.67 |
| 1:C:10:THR:HG21 | 2:D:54:LEU:HD22 | 1.75 | 0.67 |
| 3:E:50:MET:HB3 | 3:E:66:LEU:HD12 | 1.75 | 0.67 |
| 1:G:6:ARG:HB3 | 1:G:8:PHE:HE2 | 1.60 | 0.67 |
| 4:L:62:SER:CA | 4:L:65:PHE:CE2 | 2.78 | 0.67 |
| 3:K:148:LYS:CB | 3:K:149:ASP:O | 2.34 | 0.67 |
| 4:J:113:VAL:C | 4:J:114:LEU:HG | 2.14 | 0.67 |
| 4:L:47:ILE:HD11 | 4:L:67:ALA:HB3 | 1.77 | 0.67 |
| 3:O:117:PRO:HB2 | 3:O:196:THR:HA | 1.77 | 0.67 |
| 1:A:121:LYS:HE3 | 2:B:1:ILE:HD13 | 1.77 | 0.67 |
| 4:F:98:GLN:HB2 | 4:F:101:GLU:OE1 | 1.95 | 0.67 |
| 1:G:55:GLU:O | 1:G:59:TYR:HB3 | 1.95 | 0.67 |
| 3:K:123:ARG:HA | 3:K:131:SER:OG | 1.94 | 0.67 |
| 3:O:134:LEU:HD13 | 3:O:173:VAL:HG12 | 1.75 | 0.67 |
| 3:E:132:VAL:HG22 | 3:E:175:TRP:HB3 | 1.75 | 0.67 |
| 3:K:11:LEU:HB3 | 3:K:106:LEU:HD13 | 1.76 | 0.67 |
| 3:O:160:LEU:O | 3:O:168:LYS:HA | 1.95 | 0.67 |
| 1:A:42:SER:OG | 1:A:44:ARG:CG | 2.42 | 0.67 |
| 4:P:14:GLU:OE2 | 4:P:117:LEU:CG | 2.40 | 0.67 |
| 3:K:112:ILE:HG21 | 3:K:139:ASP:CB | 2.13 | 0.66 |
| 2:N:47:GLU:HG3 | 2:N:47:GLU:O | 1.94 | 0.66 |
| 1:G:143:THR:HB | 5:U:9:VAL:HG23 | 1.76 | 0.66 |
| 1:G:66:LYS:HD2 | 5:U:4:PRO:HA | 1.76 | 0.66 |
| 1:M:66:LYS:HZ2 | 3:O:29:ASN:HB2 | 1.60 | 0.66 |
| 4:P:204:PRO:HB2 | 4:P:205:ARG:HA | 1.78 | 0.66 |
| 4:F:170:VAL:CG1 | 4:F:194:LEU:CD1 | 2.53 | 0.66 |
| 1:M:78:LEU:HD23 | 1:M:95:VAL:HG21 | 1.74 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:135:PHE:HZ | 3:K:192:ILE:CG1 | 2.08 | 0.66 |
| 3:K:144:VAL:CG2 | 3:K:157:LYS:NZ | 2.57 | 0.66 |
| 1:M:133:TRP:HB2 | 1:M:144:LYS:HG3 | 1.77 | 0.66 |
| 3:O:138:PHE:CD1 | 3:O:142:THR:OG1 | 2.48 | 0.66 |
| 4:P:26:ILE:HB | 4:P:29:HIS:CD2 | 2.30 | 0.66 |
| 3:I:178:LYS:C | 3:I:179:SER:HG | 1.98 | 0.66 |
| 4:J:206:ASN:OD1 | 4:J:207:HIS:N | 2.28 | 0.66 |
| 3:E:181:PHE:CB | 3:E:182:ALA:HA | 2.20 | 0.66 |
| 3:E:84:ASP:HA | 3:E:85:SER:OG | 1.95 | 0.66 |
| 4:F:79:ILE:O | 4:F:79:ILE:HG13 | 1.96 | 0.66 |
| 3:O:53:ASN:HB2 | 3:O:68:THR:OG1 | 1.96 | 0.66 |
| 3:E:84:ASP:HB3 | 3:E:85:SER:O | 1.95 | 0.66 |
| 4:J:223:TRP:CZ2 | 4:J:228:ALA:O | 2.49 | 0.66 |
| 4:F:165:GLU:O | 4:F:166:VAL:HG23 | 1.95 | 0.65 |
| 1:G:35:ARG:CG | 1:G:46:GLU:HB3 | 2.26 | 0.65 |
| 3:I:13:VAL:C | 3:I:14:GLN:OE1 | 2.33 | 0.65 |
| 1:A:255:GLN:NE2 | 6:A:301:HOH:O | 2.11 | 0.65 |
| 3:E:124:ASP:HB3 | 4:F:128:PHE:HA | 1.75 | 0.65 |
| 4:F:98:GLN:HE21 | 4:F:98:GLN:HA | 1.61 | 0.65 |
| 3:K:135:PHE:HZ | 3:K:192:ILE:HD11 | 1.62 | 0.65 |
| 4:L:170:VAL:HG22 | 4:L:194:LEU:CD2 | 2.21 | 0.65 |
| 4:F:6:GLN:HB3 | 4:F:107:PRO:HD2 | 1.77 | 0.65 |
| 3:I:160:LEU:HD12 | 3:I:169:SER:HB2 | 1.77 | 0.65 |
| 4:J:65:PHE:HA | 4:J:79:ILE:HG22 | 1.78 | 0.65 |
| 3:K:151:ASP:CG | 3:K:177:ASN:H | 1.99 | 0.65 |
| 1:M:77:ASP:OD2 | 5:T:8:THR:HB | 1.97 | 0.65 |
| 3:O:15:GLU:OE1 | 3:O:168:LYS:NZ | 2.29 | 0.65 |
| 4:P:100:TRP:HH2 | 5:T:7:ALA:HB2 | 1.61 | 0.65 |
| 2:B:29:GLY:HA2 | 2:B:61:SER:HB2 | 1.79 | 0.65 |
| 3:E:82:PRO:O | 3:E:85:SER:OG | 2.08 | 0.65 |
| 3:K:185:ASN:O | 3:K:188:ASN:CB | 2.44 | 0.65 |
| 1:M:237:GLY:O | 1:M:238:ASP:HB2 | 1.94 | 0.65 |
| 3:O:17:ASP:O | 3:O:80:SER:OG | 2.15 | 0.65 |
| 1:G:97:ARG:CG | 1:G:116:TYR:CD1 | 2.80 | 0.65 |
| 1:M:87:GLN:OE1 | 1:M:93:HIS:CD2 | 2.50 | 0.65 |
| 2:N:81:ARG:HG3 | 2:N:92:ILE:HG13 | 1.76 | 0.65 |
| 3:O:138:PHE:CD1 | 3:O:142:THR:CG2 | 2.75 | 0.65 |
| 4:F:195:ARG:HH11 | 4:F:195:ARG:HG2 | 1.61 | 0.65 |
| 4:L:159:TRP:CZ2 | 4:L:194:LEU:HG | 2.32 | 0.65 |
| 4:F:160:TRP:CD1 | 4:F:165:GLU:HA | 2.31 | 0.65 |
| 1:C:202:ARG:NE | 1:C:244:TRP:HZ2 | 1.94 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:5:SER:HB2 | 4:L:24:ASP:HB3 | 1.79 | 0.65 |
| 2:N:2:GLN:NE2 | 2:N:85:VAL:CG2 | 2.60 | 0.65 |
| 1:G:137:ASP:OD1 | 1:G:138:MET:N | 2.25 | 0.64 |
| 1:G:98:MET:HE1 | 1:G:99:TYR:C | 2.18 | 0.64 |
| 2:H:17:ASN:OD1 | 2:H:97:ARG:NH1 | 2.30 | 0.64 |
| 3:I:192:ILE:HG23 | 3:I:193:PRO:N | 2.13 | 0.64 |
| 3:I:178:LYS:O | 3:I:180:ASP:N | 2.25 | 0.64 |
| 4:J:26:ILE:HG22 | 4:J:27:SER:H | 1.63 | 0.64 |
| 1:M:35:ARG:HD3 | 1:M:48:ARG:HH11 | 1.61 | 0.64 |
| 1:M:95:VAL:CG1 | 1:M:116:TYR:HE1 | 2.10 | 0.64 |
| 3:O:118:ALA:HB1 | 3:O:120:TYR:CE1 | 2.32 | 0.64 |
| 4:P:11:LYS:NZ | 4:P:19:VAL:HB | 2.12 | 0.64 |
| 1:C:187:THR:C | 1:C:188:HIS:ND1 | 2.50 | 0.64 |
| 1:M:37:ASP:HB3 | 1:M:40:ALA:HB2 | 1.80 | 0.64 |
| 2:B:37:VAL:HG21 | 2:B:66:TYR:CZ | 2.32 | 0.64 |
| 3:E:82:PRO:HA | 3:E:108:VAL:HG21 | 1.78 | 0.64 |
| 2:H:72:PRO:HB2 | 2:H:78:TYR:OH | 1.98 | 0.64 |
| 3:I:132:VAL:CG1 | 3:I:173:VAL:HG13 | 2.28 | 0.64 |
| 3:I:160:LEU:CD2 | 4:J:169:GLY:O | 2.46 | 0.64 |
| 4:J:194:LEU:HD23 | 4:J:195:ARG:H | 1.61 | 0.64 |
| 4:L:90:TYR:HB2 | 4:L:109:THR:HG23 | 1.79 | 0.64 |
| 1:M:219:ARG:HG3 | 1:M:257:TYR:CE2 | 2.32 | 0.64 |
| 1:M:58:GLU:HA | 1:M:61:ASP:HB3 | 1.79 | 0.64 |
| 3:I:146:GLN:CD | 3:I:154:ILE:CD1 | 2.66 | 0.64 |
| 1:G:27:TYR:OH | 2:H:63:TYR:OH | 2.12 | 0.64 |
| 4:L:103:GLN:HG2 | 4:L:105:PHE:HE1 | 1.63 | 0.64 |
| 3:I:7:SER:CB | 3:I:8:PRO:HD3 | 2.28 | 0.64 |
| 4:L:97:THR:CB | 4:L:98:GLN:CD | 2.66 | 0.64 |
| 1:A:81:LEU:HG | 5:Q:9:VAL:HG21 | 1.80 | 0.64 |
| 4:F:170:VAL:HG12 | 4:F:194:LEU:HD13 | 1.76 | 0.64 |
| 4:J:127:VAL:HG11 | 4:J:239:ALA:HB2 | 1.79 | 0.64 |
| 4:L:161:VAL:HG23 | 4:L:166:VAL:CG1 | 2.27 | 0.64 |
| 3:E:53:ASN:HB2 | 3:E:68:THR:HB | 1.79 | 0.64 |
| 3:I:138:PHE:HE1 | 3:I:142:THR:O | 1.81 | 0.64 |
| 3:K:16:GLY:N | 3:K:80:SER:O | 2.31 | 0.64 |
| 4:L:161:VAL:CG2 | 4:L:166:VAL:HG11 | 2.27 | 0.64 |
| 1:A:35:ARG:HD2 | 2:B:53:ASP:OD1 | 1.98 | 0.63 |
| 4:F:121:PHE:CD2 | 4:F:187:ARG:NH2 | 2.66 | 0.63 |
| 3:K:135:PHE:CE1 | 3:K:138:PHE:HB3 | 2.33 | 0.63 |
| 1:C:120:GLY:O | 2:D:3:ARG:NH2 | 2.32 | 0.63 |
| 1:G:234:ARG:HG3 | 1:G:242:GLN:HB2 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:70:PHE:CE1 | 2:H:78:TYR:CE1 | 2.86 | 0.63 |
| 3:I:141:GLN:O | 3:I:141:GLN:HG3 | 1.98 | 0.63 |
| 1:C:202:ARG:NE | 1:C:244:TRP:CZ2 | 2.66 | 0.63 |
| 4:J:129:GLU:CD | 4:J:130:PRO:CD | 2.66 | 0.63 |
| 1:G:97:ARG:NH1 | 5:U:6:VAL:HG12 | 2.10 | 0.63 |
| 3:I:194:GLU:C | 3:I:196:THR:HG23 | 2.18 | 0.63 |
| 4:J:97:THR:HB | 4:J:98:GLN:HG2 | 1.80 | 0.63 |
| 4:L:150:PHE:CE1 | 4:L:188:TYR:C | 2.72 | 0.63 |
| 4:L:191:SER:CB | 4:L:193:ARG:HH21 | 2.12 | 0.63 |
| 3:O:140:SER:C | 3:O:142:THR:H | 2.02 | 0.63 |
| 3:O:138:PHE:HE1 | 3:O:142:THR:HB | 1.58 | 0.63 |
| 1:A:80:THR:HG23 | 5:Q:9:VAL:HG23 | 1.79 | 0.63 |
| 4:F:173:ASP:OD2 | 4:F:191:SER:OG | 2.17 | 0.63 |
| 4:F:159:TRP:NE1 | 4:F:192:SER:OG | 2.19 | 0.63 |
| 4:F:200:PHE:O | 4:F:204:PRO:HB3 | 1.99 | 0.63 |
| 2:H:5:PRO:HB3 | 2:H:30:PHE:HB3 | 1.78 | 0.63 |
| 4:J:83:GLN:HG2 | 4:J:84:GLN:H | 1.63 | 0.63 |
| 4:L:218:SER:OG | 4:L:218:SER:O | 2.12 | 0.63 |
| 2:N:2:GLN:NE2 | 2:N:85:VAL:CB | 2.60 | 0.63 |
| 1:M:146:LYS:HZ2 | 4:P:97:THR:HG1 | 1.47 | 0.63 |
| 1:G:77:ASP:OD1 | 1:G:97:ARG:NH2 | 2.32 | 0.63 |
| 3:I:196:THR:OG1 | 3:I:197:PHE:N | 2.32 | 0.63 |
| 4:J:238:GLU:HG3 | 4:J:239:ALA:N | 2.14 | 0.63 |
| 4:L:201:TRP:C | 4:L:204:PRO:CD | 2.67 | 0.63 |
| 4:F:230:PRO:O | 4:F:231:VAL:CG2 | 2.47 | 0.62 |
| 1:G:192:HIS:HB2 | 1:G:202:ARG:NH2 | 2.12 | 0.62 |
| 2:H:11:SER:HB2 | 2:H:95:TRP:HZ2 | 1.63 | 0.62 |
| 1:M:12:VAL:HG22 | 1:M:94:THR:HG23 | 1.81 | 0.62 |
| 3:O:123:ARG:HG2 | 3:O:124:ASP:H | 1.64 | 0.62 |
| 3:O:180:ASP:OD1 | 3:O:182:ALA:HB2 | 1.98 | 0.62 |
| 3:I:10:SER:O | 3:I:11:LEU:HD23 | 1.99 | 0.62 |
| 3:K:38:TRP:HZ3 | 3:K:42:LYS:O | 1.81 | 0.62 |
| 4:F:165:GLU:O | 4:F:166:VAL:CG2 | 2.46 | 0.62 |
| 4:F:193:ARG:CG | 4:F:193:ARG:HH11 | 2.09 | 0.62 |
| 2:H:70:PHE:CE1 | 2:H:78:TYR:CD1 | 2.87 | 0.62 |
| 3:I:33:LEU:CD1 | 3:I:91:ALA:O | 2.42 | 0.62 |
| 3:O:33:LEU:HB3 | 3:O:50:MET:HB2 | 1.81 | 0.62 |
| 4:F:195:ARG:CG | 4:F:195:ARG:HH11 | 2.13 | 0.62 |
| 1:G:126:LEU:HD11 | 1:G:130:LEU:HA | 1.82 | 0.62 |
| 3:K:161:ASP:CB | 3:K:168:LYS:HD3 | 2.29 | 0.62 |
| 4:P:21:LEU:HB2 | 4:P:77:LEU:HB3 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:F:47:ILE:HG22 | 4:F:48:TYR:N | 2.13 | 0.62 |
| 1:M:20:PRO:CD | 1:M:75:ARG:HD2 | 2.29 | 0.62 |
| 1:A:96:GLN:OE1 | 2:B:60:TRP:HE3 | 1.83 | 0.62 |
| 1:C:102:ASP:OD1 | 1:C:113:TYR:OH | 2.10 | 0.62 |
| 3:E:38:TRP:CD1 | 3:E:44:PRO:HG3 | 2.29 | 0.62 |
| 3:K:115:PRO:HB3 | 3:K:139:ASP:OD2 | 2.00 | 0.62 |
| 2:H:24:ASN:CG | 2:H:65:LEU:HD21 | 2.20 | 0.62 |
| 3:I:146:GLN:NE2 | 3:I:154:ILE:HD13 | 2.15 | 0.62 |
| 4:L:119:ASN:OD1 | 4:L:187:ARG:NH2 | 2.33 | 0.62 |
| 1:G:73:THR:HG21 | 5:U:6:VAL:HG12 | 1.82 | 0.62 |
| 3:I:15:GLU:O | 3:I:15:GLU:HG3 | 1.99 | 0.61 |
| 4:L:161:VAL:HG13 | 4:L:208:PHE:HA | 1.81 | 0.61 |
| 1:C:213:ILE:HG13 | 1:C:263:HIS:HB2 | 1.82 | 0.61 |
| 1:G:133:TRP:CE3 | 1:G:147:TRP:HE3 | 2.18 | 0.61 |
| 4:L:153:ASP:HB2 | 4:L:188:TYR:HD2 | 1.64 | 0.61 |
| 3:O:183:CYS:O | 3:O:186:ALA:HB2 | 2.00 | 0.61 |
| 4:P:64:ARG:HH11 | 4:P:64:ARG:CG | 2.13 | 0.61 |
| 1:A:22:PHE:H | 1:A:38:SER:HB3 | 1.65 | 0.61 |
| 4:F:132:GLU:CG | 4:F:135:ILE:HG21 | 2.31 | 0.61 |
| 4:J:234:ILE:HD12 | 4:J:234:ILE:O | 1.99 | 0.61 |
| 3:K:185:ASN:ND2 | 3:K:188:ASN:ND2 | 2.48 | 0.61 |
| 2:N:73:THR:HG23 | 2:N:75:LYS:H | 1.64 | 0.61 |
| 3:E:181:PHE:HB2 | 3:E:182:ALA:CA | 2.25 | 0.61 |
| 3:K:185:ASN:O | 3:K:188:ASN:N | 2.30 | 0.61 |
| 1:M:103:VAL:HA | 1:M:108:ARG:O | 2.01 | 0.61 |
| 1:C:197:HIS:ND1 | 1:C:198:GLU:HG3 | 2.16 | 0.61 |
| 3:K:185:ASN:O | 3:K:188:ASN:HB3 | 2.01 | 0.61 |
| 2:N:59:ASP:HB3 | 2:N:61:SER:OG | 2.01 | 0.61 |
| 2:B:36:GLU:CB | 2:B:83:ASN:HB3 | 2.29 | 0.61 |
| 2:N:81:ARG:HD3 | 2:N:92:ILE:HG12 | 1.83 | 0.61 |
| 4:P:14:GLU:CD | 4:P:117:LEU:CD2 | 2.53 | 0.61 |
| 2:D:89:GLN:HG3 | 2:D:90:PRO:CD | 2.31 | 0.61 |
| 3:E:126:LYS:HD2 | 3:E:126:LYS:N | 2.16 | 0.61 |
| 1:M:47:PRO:HB3 | 1:M:60:TRP:CH2 | 2.36 | 0.61 |
| 4:F:25:PRO:HG2 | 4:F:73:SER:HB2 | 1.81 | 0.60 |
| 4:L:161:VAL:HG12 | 4:L:162:ASN:N | 2.16 | 0.60 |
| 1:G:27:TYR:CD1 | 1:G:32:GLN:NE2 | 2.66 | 0.60 |
| 2:H:44:GLU:OE1 | 4:F:71:GLY:HA2 | 2.00 | 0.60 |
| 2:N:81:ARG:HD3 | 2:N:92:ILE:CG1 | 2.30 | 0.60 |
| 1:A:73:THR:HG23 | 3:I:96:ASN:HD21 | 1.67 | 0.60 |
| 2:D:87:LEU:HD13 | 2:D:89:GLN:O | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:218:GLN:OE1 | 1:G:221:GLY:HA2 | 2.01 | 0.60 |
| 3:I:13:VAL:HG23 | 3:I:15:GLU:H | 1.66 | 0.60 |
| 2:D:82:VAL:O | 2:D:90:PRO:HB2 | 2.02 | 0.60 |
| 1:G:207:SER:HA | 1:G:240:THR:HB | 1.83 | 0.60 |
| 1:G:99:TYR:CZ | 5:U:3:VAL:HG12 | 2.37 | 0.60 |
| 3:I:87:THR:HA | 3:I:105:SER:HA | 1.83 | 0.60 |
| 4:L:150:PHE:O | 4:L:150:PHE:HD1 | 1.84 | 0.60 |
| 1:A:231:VAL:O | 1:A:231:VAL:HG23 | 2.00 | 0.60 |
| 1:C:187:THR:HB | 1:C:272:LEU:HD11 | 1.81 | 0.60 |
| 1:M:195:SER:O | 1:M:197:HIS:ND1 | 2.34 | 0.60 |
| 2:D:30:PHE:HE1 | 2:D:62:PHE:HB2 | 1.66 | 0.60 |
| 1:G:56:GLY:HA2 | 1:G:60:TRP:CE2 | 2.36 | 0.60 |
| 1:G:6:ARG:HB2 | 1:G:27:TYR:HB2 | 1.83 | 0.60 |
| 1:M:95:VAL:HG13 | 1:M:116:TYR:CE1 | 2.37 | 0.60 |
| 1:A:93:HIS:HB3 | 1:A:119:ASP:OD1 | 2.02 | 0.60 |
| 1:G:159:TYR:HD1 | 1:G:163:THR:OG1 | 1.84 | 0.60 |
| 1:G:35:ARG:NH2 | 1:G:48:ARG:CG | 2.58 | 0.60 |
| 4:J:129:GLU:CG | 4:J:130:PRO:CD | 2.79 | 0.60 |
| 3:K:68:THR:HG22 | 3:K:68:THR:O | 2.02 | 0.60 |
| 4:F:222:GLU:HG2 | 4:F:223:TRP:N | 2.15 | 0.60 |
| 1:G:123:TYR:CE2 | 1:G:143:THR:HG21 | 2.37 | 0.60 |
| 4:F:125:VAL:HG22 | 4:F:147:ALA:HA | 1.84 | 0.59 |
| 4:F:170:VAL:CA | 4:F:194:LEU:HD12 | 2.32 | 0.59 |
| 4:F:197:SER:CB | 4:F:200:PHE:HB2 | 2.30 | 0.59 |
| 4:F:88:ALA:HB3 | 4:F:90:TYR:CE1 | 2.37 | 0.59 |
| 1:G:195:SER:CB | 1:G:196:ASP:HA | 2.32 | 0.59 |
| 2:H:70:PHE:CZ | 2:H:78:TYR:CE2 | 2.90 | 0.59 |
| 4:J:129:GLU:CD | 4:J:130:PRO:HD2 | 2.22 | 0.59 |
| 4:J:12:VAL:HG22 | 4:J:154:HIS:CE1 | 2.37 | 0.59 |
| 2:N:2:GLN:HE21 | 2:N:85:VAL:HB | 1.65 | 0.59 |
| 1:C:81:LEU:HG | 5:R:9:VAL:HG21 | 1.83 | 0.59 |
| 2:D:45:ARG:O | 2:D:45:ARG:HG2 | 2.00 | 0.59 |
| 1:G:97:ARG:CG | 1:G:116:TYR:CE1 | 2.85 | 0.59 |
| 3:I:74:TYR:HB3 | 3:I:76:TYR:HE1 | 1.66 | 0.59 |
| 4:J:223:TRP:HZ2 | 4:J:228:ALA:O | 1.86 | 0.59 |
| 3:K:135:PHE:CZ | 3:K:192:ILE:CG1 | 2.85 | 0.59 |
| 2:N:41:LYS:O | 2:N:42:ASN:OD1 | 2.20 | 0.59 |
| 1:A:37:ASP:HB3 | 1:A:40:ALA:HB2 | 1.84 | 0.59 |
| 1:G:209:TYR:CD1 | 1:G:210:PRO:HA | 2.37 | 0.59 |
| 1:G:220:ASP:OD2 | 1:G:256:ARG:NH1 | 2.35 | 0.59 |
| 4:J:113:VAL:C | 4:J:114:LEU:CG | 2.69 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:135:PHE:HE1 | 3:K:138:PHE:HB3 | 1.66 | 0.59 |
| 1:M:146:LYS:NZ | 4:P:97:THR:OG1 | 2.31 | 0.59 |
| 1:A:203:CYS:HB2 | 1:A:217:TRP:CZ3 | 2.38 | 0.59 |
| 1:G:259:CYS:HB3 | 1:G:272:LEU:HB2 | 1.84 | 0.59 |
| 1:G:192:HIS:CE1 | 2:H:98:ASP:HB3 | 2.37 | 0.59 |
| 1:M:103:VAL:HB | 1:M:107:TRP:HA | 1.83 | 0.59 |
| 4:J:129:GLU:CD | 4:J:130:PRO:HD3 | 2.23 | 0.59 |
| 4:J:194:LEU:HD21 | 4:J:196:VAL:CG2 | 2.33 | 0.59 |
| 4:L:201:TRP:C | 4:L:204:PRO:HD3 | 2.23 | 0.59 |
| 1:C:35:ARG:HH11 | 2:D:53:ASP:CG | 2.06 | 0.59 |
| 4:F:223:TRP:CE3 | 4:F:230:PRO:HD2 | 2.37 | 0.59 |
| 3:K:136:THR:CG2 | 3:K:171:SER:CB | 2.80 | 0.59 |
| 3:K:192:ILE:CG1 | 3:K:193:PRO:HD2 | 2.29 | 0.59 |
| 1:A:170:ARG:O | 1:A:174:ASN:ND2 | 2.32 | 0.59 |
| 3:I:115:PRO:HB3 | 3:I:137:ASP:OD2 | 2.01 | 0.59 |
| 3:K:21:PHE:HB2 | 3:K:75:LEU:HB3 | 1.85 | 0.59 |
| 1:M:197:HIS:N | 1:M:197:HIS:HD1 | 2.01 | 0.59 |
| 1:M:213:ILE:HG13 | 1:M:263:HIS:HB2 | 1.85 | 0.59 |
| 4:P:66:SER:HG | 4:P:78:THR:HG1 | 1.49 | 0.59 |
| 4:J:69:ARG:HA | 4:J:75:SER:HB2 | 1.84 | 0.59 |
| 3:K:144:VAL:HG23 | 3:K:157:LYS:HZ2 | 1.67 | 0.59 |
| 3:K:20:ASN:HA | 3:K:75:LEU:O | 2.03 | 0.59 |
| 1:M:255:GLN:NE2 | 1:M:255:GLN:O | 2.35 | 0.59 |
| 4:P:23:CYS:SG | 4:P:24:ASP:N | 2.76 | 0.59 |
| 2:B:92:ILE:O | 2:B:92:ILE:HG23 | 2.03 | 0.58 |
| 4:F:110:ARG:HH21 | 4:F:154:HIS:CD2 | 2.20 | 0.58 |
| 1:G:133:TRP:CE3 | 1:G:147:TRP:CE3 | 2.90 | 0.58 |
| 1:M:270:LEU:HD13 | 1:M:272:LEU:CD2 | 2.32 | 0.58 |
| 4:J:26:ILE:HG22 | 4:J:27:SER:N | 2.18 | 0.58 |
| 3:K:136:THR:HG21 | 3:K:171:SER:CB | 2.33 | 0.58 |
| 1:M:197:HIS:O | 1:M:198:GLU:CG | 2.50 | 0.58 |
| 2:H:35:ILE:HG13 | 2:H:83:ASN:O | 2.03 | 0.58 |
| 1:M:198:GLU:HA | 1:M:251:SER:H | 1.67 | 0.58 |
| 1:M:203:CYS:HB2 | 1:M:217:TRP:HE1 | 1.68 | 0.58 |
| 1:C:238:ASP:HB3 | 1:C:240:THR:HG22 | 1.84 | 0.58 |
| 3:K:138:PHE:HZ | 3:K:157:LYS:HG2 | 1.68 | 0.58 |
| 3:O:118:ALA:HB1 | 3:O:120:TYR:CZ | 2.39 | 0.58 |
| 4:P:160:TRP:CH2 | 4:P:211:GLN:HG3 | 2.38 | 0.58 |
| 4:P:47:ILE:HG22 | 4:P:57:LYS:HA | 1.85 | 0.58 |
| 4:J:229:LYS:CB | 4:J:230:PRO:HA | 2.33 | 0.58 |
| 4:L:204:PRO:HG3 | 4:L:241:GLY:CA | 2.25 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:253:GLN:HG3 | 1:M:256:ARG:HE | 1.68 | 0.58 |
| 1:C:216:THR:HG23 | 1:C:260:HIS:HB2 | 1.85 | 0.58 |
| 1:G:178:THR:O | 1:G:181:ARG:HB3 | 2.02 | 0.58 |
| 1:M:13:SER:HB3 | 1:M:78:LEU:HD13 | 1.85 | 0.58 |
| 2:N:81:ARG:CG | 2:N:92:ILE:HG13 | 2.33 | 0.58 |
| 1:C:35:ARG:HD2 | 2:D:53:ASP:OD2 | 2.04 | 0.58 |
| 1:C:72:GLN:CG | 4:F:55:PRO:HB2 | 2.34 | 0.58 |
| 1:G:73:THR:HG23 | 5:U:8:THR:HG22 | 1.85 | 0.58 |
| 4:L:147:ALA:HB2 | 4:L:212:VAL:HG21 | 1.84 | 0.58 |
| 1:A:89:GLU:OE2 | 1:C:86:ASN:ND2 | 2.32 | 0.58 |
| 4:F:153:ASP:O | 4:F:155:VAL:N | 2.37 | 0.58 |
| 4:J:135:ILE:O | 4:J:139:GLN:OE1 | 2.20 | 0.58 |
| 4:J:162:ASN:HA | 4:J:207:HIS:CE1 | 2.39 | 0.58 |
| 3:E:82:PRO:HA | 3:E:108:VAL:CG2 | 2.33 | 0.58 |
| 4:F:97:THR:OG1 | 4:F:98:GLN:N | 2.35 | 0.58 |
| 1:M:10:THR:HG21 | 2:N:54:LEU:CD2 | 2.29 | 0.58 |
| 4:P:14:GLU:CG | 4:P:117:LEU:CG | 2.66 | 0.58 |
| 4:F:50:GLN:NE2 | 4:F:97:THR:O | 2.36 | 0.58 |
| 1:G:133:TRP:CZ3 | 1:G:147:TRP:HZ3 | 2.20 | 0.58 |
| 1:G:35:ARG:HH21 | 1:G:48:ARG:CD | 2.17 | 0.58 |
| 3:K:61:ARG:CB | 3:K:78:LYS:O | 2.51 | 0.58 |
| 3:O:182:ALA:CB | 3:O:185:ASN:HB3 | 2.15 | 0.58 |
| 4:P:211:GLN:HE21 | 4:P:234:ILE:HG13 | 1.68 | 0.58 |
| 3:E:82:PRO:O | 3:E:84:ASP:HA | 2.03 | 0.57 |
| 3:E:134:LEU:HD11 | 4:F:144:VAL:HG21 | 1.86 | 0.57 |
| 1:M:170:ARG:O | 1:M:174:ASN:ND2 | 2.37 | 0.57 |
| 1:G:123:TYR:CE2 | 5:U:9:VAL:HG21 | 2.39 | 0.57 |
| 1:A:66:LYS:HE2 | 3:I:29:ASN:CG | 2.25 | 0.57 |
| 3:E:145:SER:HB2 | 3:E:189:ASN:HB3 | 1.86 | 0.57 |
| 3:E:192:ILE:HG23 | 3:E:193:PRO:HD3 | 1.84 | 0.57 |
| 3:E:84:ASP:CB | 3:E:85:SER:HB2 | 2.34 | 0.57 |
| 4:J:83:GLN:CG | 4:J:84:GLN:H | 2.17 | 0.57 |
| 3:K:175:TRP:HZ2 | 4:L:146:LEU:CB | 2.15 | 0.57 |
| 4:L:147:ALA:CB | 4:L:212:VAL:HG21 | 2.35 | 0.57 |
| 4:L:201:TRP:O | 4:L:204:PRO:CD | 2.52 | 0.57 |
| 2:N:70:PHE:CZ | 2:N:72:PRO:HB3 | 2.39 | 0.57 |
| 3:I:121:GLN:O | 3:I:132:VAL:O | 2.23 | 0.57 |
| 4:J:217:LEU:HD13 | 4:J:221:ASP:CB | 2.34 | 0.57 |
| 1:M:74:HIS:O | 1:M:77:ASP:N | 2.36 | 0.57 |
| 1:A:266:LEU:HD13 | 1:A:270:LEU:HD13 | 1.87 | 0.57 |
| 4:F:143:LEU:HB2 | 4:F:194:LEU:O | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:95:SER:OG | 4:L:103:GLN:HB3 | 2.05 | 0.57 |
| 4:L:121:PHE:O | 4:L:150:PHE:HA | 2.04 | 0.57 |
| 3:O:140:SER:C | 3:O:142:THR:N | 2.56 | 0.57 |
| 3:O:27:SER:HB2 | 3:O:69:LYS:HD2 | 1.86 | 0.57 |
| 1:A:163:THR:HA | 1:A:166:GLU:HB2 | 1.86 | 0.57 |
| 2:D:5:PRO:HB3 | 2:D:30:PHE:HB3 | 1.86 | 0.57 |
| 1:G:35:ARG:HG2 | 1:G:46:GLU:HB3 | 1.86 | 0.57 |
| 3:I:122:LEU:N | 3:I:132:VAL:O | 2.37 | 0.57 |
| 4:J:194:LEU:HD21 | 4:J:196:VAL:HG23 | 1.84 | 0.57 |
| 4:P:226:ASP:N | 4:P:226:ASP:OD1 | 2.36 | 0.57 |
| 4:F:118:LYS:CD | 4:F:217:LEU:HD21 | 2.35 | 0.57 |
| 1:G:220:ASP:OD1 | 1:G:256:ARG:HG3 | 2.05 | 0.57 |
| 3:I:2:LEU:HD21 | 3:I:26:PRO:HB3 | 1.87 | 0.57 |
| 4:J:14:GLU:HB2 | 4:J:114:LEU:O | 2.04 | 0.57 |
| 1:M:139:ALA:O | 1:M:142:THR:OG1 | 2.22 | 0.57 |
| 1:C:113:TYR:N | 1:C:113:TYR:CD2 | 2.73 | 0.57 |
| 1:G:35:ARG:NH2 | 1:G:48:ARG:NE | 2.53 | 0.57 |
| 3:I:2:LEU:HD13 | 3:I:26:PRO:HG3 | 1.87 | 0.57 |
| 4:J:6:GLN:NE2 | 4:J:92:CYS:HB3 | 2.20 | 0.57 |
| 1:M:58:GLU:O | 1:M:62:GLY:N | 2.30 | 0.57 |
| 3:O:187:PHE:N | 3:O:187:PHE:CD2 | 2.73 | 0.57 |
| 3:O:53:ASN:ND2 | 3:O:68:THR:OG1 | 2.38 | 0.57 |
| 1:G:12:VAL:HG11 | 2:H:33:SER:HB3 | 1.86 | 0.56 |
| 1:M:5:MET:HB2 | 1:M:28:VAL:HG12 | 1.87 | 0.56 |
| 4:P:197:SER:HB3 | 4:P:200:PHE:CD2 | 2.40 | 0.56 |
| 2:B:84:HIS:ND1 | 2:B:85:VAL:O | 2.39 | 0.56 |
| 4:F:87:SER:HB3 | 4:F:113:VAL:HG12 | 1.87 | 0.56 |
| 3:K:135:PHE:CE1 | 3:K:138:PHE:CD2 | 2.93 | 0.56 |
| 3:K:35:TRP:O | 3:K:47:LEU:HB3 | 2.05 | 0.56 |
| 1:A:204:TRP:CZ3 | 1:A:244:TRP:HB2 | 2.41 | 0.56 |
| 1:C:73:THR:HG21 | 5:R:6:VAL:HG23 | 1.86 | 0.56 |
| 3:E:157:LYS:NZ | 3:E:170:ASN:HD21 | 2.03 | 0.56 |
| 3:I:146:GLN:NE2 | 3:I:154:ILE:CD1 | 2.69 | 0.56 |
| 4:P:7:SER:OG | 4:P:22:ARG:HD3 | 2.05 | 0.56 |
| 4:P:37:GLN:HG3 | 4:P:41:GLN:OE1 | 2.05 | 0.56 |
| 4:L:170:VAL:CA | 4:L:194:LEU:HD21 | 2.30 | 0.56 |
| 2:B:20:SER:OG | 4:L:18:ASP:OD2 | 2.23 | 0.56 |
| 1:A:96:GLN:NE2 | 2:B:62:PHE:CE1 | 2.67 | 0.56 |
| 1:C:10:THR:HG21 | 2:D:54:LEU:CD2 | 2.35 | 0.56 |
| 1:G:124:ILE:HD12 | 1:G:143:THR:HG23 | 1.87 | 0.56 |
| 1:C:243:LYS:HG2 | 1:C:244:TRP:H | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:145:CYS:SG | 4:L:146:LEU:N | 2.77 | 0.56 |
| 1:C:5:MET:HB2 | 1:C:168:LEU:HD13 | 1.88 | 0.56 |
| 3:I:50:MET:HB3 | 3:I:66:LEU:HD22 | 1.88 | 0.56 |
| 3:K:185:ASN:CB | 3:K:188:ASN:HD22 | 2.18 | 0.56 |
| 1:M:133:TRP:HB2 | 1:M:144:LYS:CG | 2.36 | 0.56 |
| 4:F:150:PHE:CD1 | 4:F:155:VAL:HG11 | 2.40 | 0.56 |
| 1:G:234:ARG:HB3 | 2:H:8:GLN:HE21 | 1.71 | 0.56 |
| 4:P:223:TRP:CZ3 | 4:P:229:LYS:O | 2.57 | 0.56 |
| 3:K:62:ILE:HG22 | 3:K:75:LEU:HD11 | 1.88 | 0.56 |
| 4:F:179:GLU:HB2 | 4:F:187:ARG:O | 2.06 | 0.56 |
| 4:F:230:PRO:O | 4:F:231:VAL:HG22 | 2.06 | 0.56 |
| 1:G:199:ALA:N | 1:G:249:VAL:O | 2.39 | 0.56 |
| 4:J:29:HIS:HD2 | 4:J:94:SER:CA | 2.13 | 0.56 |
| 1:A:89:GLU:HG2 | 1:C:86:ASN:OD1 | 2.05 | 0.55 |
| 1:C:122:ASP:OD1 | 2:D:60:TRP:NE1 | 2.36 | 0.55 |
| 2:D:74:GLU:HA | 2:D:97:ARG:NH2 | 2.21 | 0.55 |
| 1:A:33:PHE:CD1 | 1:A:52:ILE:HD12 | 2.38 | 0.55 |
| 2:D:76:ASP:HB3 | 2:D:78:TYR:CE1 | 2.36 | 0.55 |
| 1:G:133:TRP:CZ3 | 1:G:147:TRP:HE3 | 2.21 | 0.55 |
| 3:K:138:PHE:CZ | 3:K:157:LYS:CE | 2.82 | 0.55 |
| 1:M:256:ARG:HD3 | 6:M:301:HOH:O | 2.05 | 0.55 |
| 1:A:131:ARG:NH2 | 1:A:157:ARG:NH2 | 2.54 | 0.55 |
| 2:H:24:ASN:ND2 | 2:H:65:LEU:HD21 | 2.21 | 0.55 |
| 4:J:160:TRP:CE3 | 4:J:211:GLN:CB | 2.90 | 0.55 |
| 4:J:207:HIS:HB3 | 4:J:240:TRP:CZ3 | 2.41 | 0.55 |
| 3:K:180:ASP:N | 3:K:180:ASP:OD1 | 2.38 | 0.55 |
| 1:M:253:GLN:O | 1:M:256:ARG:HG3 | 2.06 | 0.55 |
| 1:C:131:ARG:HH11 | 1:C:131:ARG:CG | 2.12 | 0.55 |
| 2:D:56:PHE:HA | 2:D:62:PHE:HA | 1.86 | 0.55 |
| 4:J:129:GLU:HG3 | 4:J:130:PRO:CD | 2.34 | 0.55 |
| 1:M:14:ARG:NH2 | 1:M:21:ARG:HB2 | 2.21 | 0.55 |
| 4:F:150:PHE:CE1 | 4:F:155:VAL:CG1 | 2.90 | 0.55 |
| 3:I:42:LYS:NZ | 3:I:43:SER:OG | 2.40 | 0.55 |
| 3:E:93:ILE:HG22 | 5:R:5:MET:HE1 | 1.87 | 0.55 |
| 4:J:157:LEU:HD23 | 4:J:158:SER:N | 2.22 | 0.55 |
| 3:K:136:THR:CB | 3:K:170:ASN:O | 2.51 | 0.55 |
| 4:L:170:VAL:CB | 4:L:194:LEU:HD21 | 2.35 | 0.55 |
| 4:L:82:THR:HG22 | 4:L:83:GLN:N | 2.21 | 0.55 |
| 4:L:88:ALA:HB1 | 4:L:89:VAL:HG12 | 1.89 | 0.55 |
| 2:N:83:ASN:OD1 | 2:N:84:HIS:N | 2.40 | 0.55 |
| 1:M:66:LYS:HE3 | 3:O:29:ASN:ND2 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:37:VAL:CG2 | 2:H:82:VAL:HG12 | 2.36 | 0.55 |
| 4:L:124:GLU:HA | 4:L:235:VAL:HG11 | 1.87 | 0.55 |
| 1:M:219:ARG:O | 1:M:222:GLU:N | 2.40 | 0.55 |
| 3:O:138:PHE:N | 3:O:138:PHE:CD2 | 2.74 | 0.55 |
| 4:P:17:LYS:NZ | 4:P:221:ASP:OD1 | 2.29 | 0.55 |
| 1:G:192:HIS:CB | 1:G:202:ARG:NH2 | 2.70 | 0.55 |
| 3:I:34:HIS:CE1 | 3:I:93:ILE:HD11 | 2.42 | 0.55 |
| 4:J:131:SER:HB2 | 4:J:134:GLU:HB3 | 1.89 | 0.55 |
| 4:J:127:VAL:HG23 | 4:J:237:ALA:HB3 | 1.89 | 0.55 |
| 3:K:122:LEU:HD13 | 4:L:144:VAL:HG23 | 1.88 | 0.55 |
| 4:L:59:GLY:O | 4:L:61:PRO:HD3 | 2.06 | 0.55 |
| 1:C:231:VAL:HG23 | 1:C:232:GLU:O | 2.06 | 0.55 |
| 1:M:133:TRP:CB | 1:M:144:LYS:HG3 | 2.36 | 0.55 |
| 3:O:123:ARG:HG2 | 3:O:124:ASP:N | 2.22 | 0.55 |
| 4:P:83:GLN:O | 4:P:113:VAL:HG11 | 2.06 | 0.55 |
| 2:B:18:GLY:HA2 | 2:B:71:THR:HG22 | 1.88 | 0.55 |
| 2:D:90:PRO:HG2 | 2:D:90:PRO:O | 2.07 | 0.55 |
| 1:G:81:LEU:HG | 5:U:9:VAL:HG11 | 1.88 | 0.54 |
| 3:I:14:GLN:O | 3:I:15:GLU:HB3 | 2.07 | 0.54 |
| 1:M:163:THR:HA | 1:M:166:GLU:HB2 | 1.89 | 0.54 |
| 1:M:268:LYS:HB2 | 1:M:269:PRO:HD2 | 1.89 | 0.54 |
| 5:T:7:ALA:O | 5:T:8:THR:HG23 | 2.06 | 0.54 |
| 1:A:88:SER:OG | 1:A:89:GLU:N | 2.40 | 0.54 |
| 4:F:125:VAL:HG21 | 4:F:212:VAL:HG21 | 1.89 | 0.54 |
| 4:F:36:ARG:HB3 | 4:F:46:LEU:HD11 | 1.89 | 0.54 |
| 1:G:98:MET:CE | 1:G:99:TYR:CA | 2.85 | 0.54 |
| 3:K:185:ASN:CB | 3:K:188:ASN:ND2 | 2.69 | 0.54 |
| 4:L:201:TRP:C | 4:L:204:PRO:HD2 | 2.28 | 0.54 |
| 3:E:136:THR:HG22 | 3:E:171:SER:CB | 2.24 | 0.54 |
| 2:N:83:ASN:HB2 | 2:N:90:PRO:HG3 | 1.89 | 0.54 |
| 4:P:141:ALA:HB2 | 4:P:198:ALA:HA | 1.89 | 0.54 |
| 1:A:103:VAL:HG12 | 1:A:108:ARG:C | 2.28 | 0.54 |
| 3:E:138:PHE:CD1 | 3:E:138:PHE:N | 2.72 | 0.54 |
| 2:H:11:SER:HB2 | 2:H:95:TRP:CZ2 | 2.42 | 0.54 |
| 4:J:221:ASP:CG | 4:J:222:GLU:H | 2.11 | 0.54 |
| 3:K:52:LEU:O | 3:K:52:LEU:HD12 | 2.07 | 0.54 |
| 4:F:54:ALA:CB | 4:F:57:LYS:CE | 2.78 | 0.54 |
| 4:F:98:GLN:HE21 | 4:F:98:GLN:CA | 2.19 | 0.54 |
| 1:G:82:ARG:HH21 | 1:G:88:SER:C | 2.08 | 0.54 |
| 3:K:144:VAL:CG2 | 3:K:157:LYS:HZ1 | 2.15 | 0.54 |
| 3:K:66:LEU:HD23 | 3:K:67:ASN:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:L:7:SER:O | 4:L:22:ARG:HB3 | 2.08 | 0.54 |
| 3:O:87:THR:HA | 3:O:105:SER:HA | 1.89 | 0.54 |
| 4:J:123:PRO:HA | 4:J:150:PHE:HB3 | 1.88 | 0.54 |
| 1:M:128:GLU:OE1 | 1:M:128:GLU:N | 2.36 | 0.54 |
| 1:A:12:VAL:HG22 | 1:A:94:THR:HG22 | 1.90 | 0.54 |
| 4:F:155:VAL:HG12 | 4:F:214:PHE:HD1 | 1.71 | 0.54 |
| 3:K:47:LEU:O | 3:K:48:PHE:HD1 | 1.91 | 0.54 |
| 4:P:223:TRP:CE2 | 4:P:229:LYS:O | 2.61 | 0.54 |
| 1:G:143:THR:CB | 5:U:9:VAL:HG23 | 2.38 | 0.54 |
| 1:G:91:GLY:HA3 | 1:G:93:HIS:CE1 | 2.43 | 0.54 |
| 3:I:160:LEU:HD22 | 4:J:169:GLY:O | 2.07 | 0.54 |
| 1:M:66:LYS:NZ | 3:O:29:ASN:CB | 2.71 | 0.54 |
| 1:C:159:TYR:CD1 | 1:C:163:THR:HB | 2.43 | 0.54 |
| 1:G:218:GLN:CD | 1:G:221:GLY:HA2 | 2.27 | 0.54 |
| 2:H:71:THR:O | 2:H:72:PRO:O | 2.26 | 0.54 |
| 4:L:13:THR:OG1 | 4:L:14:GLU:N | 2.40 | 0.54 |
| 4:L:7:SER:OG | 4:L:8:PRO:HA | 2.08 | 0.54 |
| 2:N:46:ILE:O | 2:N:49:VAL:HG23 | 2.08 | 0.54 |
| 2:H:24:ASN:CG | 2:H:65:LEU:CD2 | 2.77 | 0.53 |
| 1:M:175:GLY:O | 1:M:179:LEU:N | 2.41 | 0.53 |
| 1:C:195:SER:OG | 1:C:196:ASP:N | 2.39 | 0.53 |
| 2:H:70:PHE:HE1 | 2:H:78:TYR:CG | 2.26 | 0.53 |
| 3:I:9:GLN:HA | 3:I:104:THR:HA | 1.90 | 0.53 |
| 4:J:177:LEU:HB3 | 4:J:189:ALA:HB3 | 1.91 | 0.53 |
| 4:J:98:GLN:HA | 4:J:98:GLN:NE2 | 2.23 | 0.53 |
| 2:B:21:ASN:OD1 | 2:B:22:PHE:N | 2.33 | 0.53 |
| 3:E:8:PRO:O | 3:E:104:THR:HB | 2.08 | 0.53 |
| 4:F:160:TRP:CD1 | 4:F:165:GLU:CA | 2.91 | 0.53 |
| 1:G:138:MET:N | 1:G:138:MET:SD | 2.82 | 0.53 |
| 4:L:203:ASN:N | 4:L:204:PRO:HD2 | 2.22 | 0.53 |
| 1:M:219:ARG:O | 1:M:220:ASP:C | 2.46 | 0.53 |
| 2:D:30:PHE:CE1 | 2:D:62:PHE:HB2 | 2.44 | 0.53 |
| 4:J:160:TRP:CH2 | 4:J:211:GLN:CB | 2.91 | 0.53 |
| 1:M:110:LEU:HD23 | 1:M:111:ARG:HG2 | 1.91 | 0.53 |
| 1:G:58:GLU:O | 1:G:61:ASP:N | 2.42 | 0.53 |
| 4:J:122:PRO:HG3 | 4:J:230:PRO:HB2 | 1.90 | 0.53 |
| 1:M:191:HIS:NE2 | 1:M:193:ALA:HB2 | 2.24 | 0.53 |
| 2:B:57:SER:O | 2:B:60:TRP:N | 2.41 | 0.53 |
| 2:B:85:VAL:O | 2:B:86:THR:OG1 | 2.19 | 0.53 |
| 3:E:84:ASP:HB3 | 3:E:85:SER:CB | 2.39 | 0.53 |
| 4:J:130:PRO:HG3 | 4:J:142:THR:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:4:VAL:HG21 | 3:O:99:TYR:O | 2.08 | 0.53 |
| 1:M:154:GLU:HB3 | 3:O:52:LEU:HD11 | 1.90 | 0.53 |
| 4:P:159:TRP:O | 4:P:165:GLU:HB2 | 2.07 | 0.53 |
| 1:A:2:SER:HB3 | 1:A:103:VAL:O | 2.08 | 0.53 |
| 3:E:136:THR:CA | 3:E:138:PHE:CE1 | 2.86 | 0.53 |
| 4:L:191:SER:CB | 4:L:193:ARG:NH2 | 2.70 | 0.53 |
| 2:N:58:LYS:NZ | 6:N:102:HOH:O | 2.40 | 0.53 |
| 1:A:4:SER:CB | 1:A:102:ASP:OD2 | 2.53 | 0.53 |
| 1:C:59:TYR:O | 1:C:63:GLU:HG2 | 2.09 | 0.53 |
| 4:F:26:ILE:HG22 | 4:F:26:ILE:O | 2.09 | 0.53 |
| 3:I:160:LEU:HD23 | 4:J:169:GLY:O | 2.09 | 0.53 |
| 3:K:185:ASN:O | 3:K:188:ASN:CG | 2.46 | 0.53 |
| 3:K:52:LEU:H | 3:K:52:LEU:HD12 | 1.73 | 0.53 |
| 4:F:123:PRO:HB3 | 4:F:150:PHE:CD2 | 2.43 | 0.53 |
| 3:K:59:LYS:CD | 3:K:60:GLY:H | 2.21 | 0.53 |
| 3:O:182:ALA:O | 3:O:186:ALA:N | 2.40 | 0.53 |
| 1:A:131:ARG:NH1 | 6:A:302:HOH:O | 2.31 | 0.53 |
| 3:I:115:PRO:CA | 3:I:137:ASP:OD2 | 2.56 | 0.53 |
| 4:F:118:LYS:HD2 | 4:F:217:LEU:HD21 | 1.91 | 0.52 |
| 4:F:217:LEU:HD12 | 4:F:218:SER:H | 1.73 | 0.52 |
| 1:G:218:GLN:CB | 1:G:223:ASP:HA | 2.37 | 0.52 |
| 3:I:74:TYR:HB3 | 3:I:76:TYR:CE1 | 2.44 | 0.52 |
| 4:L:191:SER:HB2 | 4:L:193:ARG:HH21 | 1.74 | 0.52 |
| 1:M:63:GLU:OE1 | 5:T:2:LEU:HD12 | 2.08 | 0.52 |
| 3:O:29:ASN:HB2 | 5:T:4:PRO:HG3 | 1.91 | 0.52 |
| 1:G:99:TYR:OH | 5:U:3:VAL:HG12 | 2.09 | 0.52 |
| 3:E:157:LYS:HZ2 | 3:E:170:ASN:HD21 | 1.56 | 0.52 |
| 2:H:70:PHE:CZ | 2:H:78:TYR:CD2 | 2.97 | 0.52 |
| 3:K:25:PHE:CE1 | 3:K:71:GLY:HA2 | 2.44 | 0.52 |
| 1:M:67:VAL:O | 1:M:70:HIS:HB2 | 2.09 | 0.52 |
| 4:F:140:LYS:CD | 4:F:197:SER:HA | 2.39 | 0.52 |
| 3:I:117:PRO:O | 3:I:196:THR:C | 2.48 | 0.52 |
| 4:P:11:LYS:HZ3 | 4:P:19:VAL:HB | 1.72 | 0.52 |
| 4:P:70:THR:O | 4:P:74:VAL:HB | 2.09 | 0.52 |
| 4:J:135:ILE:CA | 4:J:140:LYS:O | 2.52 | 0.52 |
| 4:L:203:ASN:N | 4:L:204:PRO:CD | 2.72 | 0.52 |
| 1:M:97:ARG:HH22 | 1:M:147:TRP:HH2 | 1.56 | 0.52 |
| 2:D:37:VAL:HG22 | 2:D:82:VAL:HG12 | 1.90 | 0.52 |
| 3:E:49:VAL:HG21 | 4:F:102:THR:CG2 | 2.36 | 0.52 |
| 4:F:193:ARG:NH1 | 4:F:193:ARG:HG3 | 2.18 | 0.52 |
| 1:G:192:HIS:HD2 | 1:G:202:ARG:HD2 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:44:PRO:O | 3:O:44:PRO:HG2 | 2.10 | 0.52 |
| 4:P:15:LYS:HZ2 | 4:P:83:GLN:HG3 | 1.75 | 0.52 |
| 1:C:74:HIS:CD2 | 1:C:97:ARG:HH21 | 2.27 | 0.52 |
| 2:D:74:GLU:HA | 2:D:97:ARG:HH22 | 1.75 | 0.52 |
| 3:E:89:LEU:HD21 | 3:E:100:PHE:CD1 | 2.43 | 0.52 |
| 4:L:217:LEU:HB2 | 4:L:230:PRO:O | 2.09 | 0.52 |
| 4:L:125:VAL:HG21 | 4:L:236:SER:O | 2.10 | 0.52 |
| 4:P:61:PRO:O | 6:P:301:HOH:O | 2.19 | 0.52 |
| 4:J:11:LYS:NZ | 4:J:217:LEU:CD2 | 2.73 | 0.52 |
| 3:I:155:THR:HG21 | 4:J:191:SER:OG | 2.09 | 0.52 |
| 2:N:60:TRP:CE3 | 2:N:60:TRP:HA | 2.42 | 0.52 |
| 1:G:12:VAL:HA | 1:G:94:THR:HA | 1.92 | 0.52 |
| 2:H:55:SER:OG | 2:H:56:PHE:N | 2.43 | 0.52 |
| 4:J:36:ARG:HB3 | 4:J:46:LEU:HD11 | 1.92 | 0.52 |
| 4:J:96:GLN:O | 4:J:98:GLN:N | 2.40 | 0.52 |
| 3:E:181:PHE:CB | 3:E:182:ALA:CA | 2.86 | 0.52 |
| 4:F:6:GLN:HG3 | 4:F:22:ARG:O | 2.10 | 0.52 |
| 3:I:146:GLN:CG | 3:I:154:ILE:HG12 | 2.40 | 0.52 |
| 1:M:219:ARG:N | 1:M:222:GLU:O | 2.41 | 0.52 |
| 2:N:41:LYS:O | 2:N:77:GLU:O | 2.27 | 0.52 |
| 1:C:155:GLN:HE21 | 3:E:51:THR:HG21 | 1.75 | 0.52 |
| 3:I:182:ALA:O | 3:I:186:ALA:HB2 | 2.10 | 0.52 |
| 3:E:157:LYS:CE | 3:E:170:ASN:OD1 | 2.58 | 0.51 |
| 1:G:131:ARG:NH2 | 6:G:303:HOH:O | 2.27 | 0.51 |
| 2:H:37:VAL:HG21 | 2:H:82:VAL:HG12 | 1.93 | 0.51 |
| 3:I:158:CYS:SG | 4:J:193:ARG:NH1 | 2.83 | 0.51 |
| 4:L:130:PRO:HG2 | 4:L:201:TRP:CE2 | 2.45 | 0.51 |
| 4:L:36:ARG:HD2 | 4:L:90:TYR:CG | 2.45 | 0.51 |
| 1:M:230:LEU:HD12 | 1:M:230:LEU:C | 2.30 | 0.51 |
| 3:O:61:ARG:NH1 | 3:O:81:GLN:HB2 | 2.25 | 0.51 |
| 2:D:73:THR:HG22 | 2:D:74:GLU:H | 1.74 | 0.51 |
| 1:G:168:LEU:O | 1:G:172:LEU:HG | 2.11 | 0.51 |
| 1:G:200:THR:HG21 | 1:G:202:ARG:NH2 | 2.26 | 0.51 |
| 4:J:141:ALA:CB | 4:J:196:VAL:O | 2.45 | 0.51 |
| 4:J:6:GLN:HE21 | 4:J:92:CYS:HB3 | 1.74 | 0.51 |
| 2:N:12:ARG:O | 2:N:12:ARG:HG2 | 2.09 | 0.51 |
| 4:P:97:THR:CG2 | 4:P:98:GLN:N | 2.73 | 0.51 |
| 3:E:30:PHE:CD2 | 3:E:92:PHE:HE2 | 2.23 | 0.51 |
| 3:O:52:LEU:O | 3:O:55:ASP:N | 2.42 | 0.51 |
| 2:D:54:LEU:HD21 | 2:D:62:PHE:HD1 | 1.72 | 0.51 |
| 4:F:37:GLN:NE2 | 4:F:38:ARG:O | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:50:MET:HB3 | 3:K:66:LEU:CD1 | 2.40 | 0.51 |
| 3:O:134:LEU:HD12 | 3:O:135:PHE:H | 1.74 | 0.51 |
| 3:O:140:SER:O | 3:O:142:THR:N | 2.43 | 0.51 |
| 4:F:121:PHE:HE2 | 4:F:187:ARG:NH2 | 1.92 | 0.51 |
| 1:G:249:VAL:HG22 | 1:G:257:TYR:CZ | 2.46 | 0.51 |
| 2:H:24:ASN:OD1 | 2:H:66:TYR:O | 2.28 | 0.51 |
| 3:I:81:GLN:HG2 | 3:I:82:PRO:HD2 | 1.92 | 0.51 |
| 4:J:113:VAL:HG22 | 4:J:114:LEU:N | 2.26 | 0.51 |
| 4:L:62:SER:CA | 4:L:65:PHE:HE2 | 2.24 | 0.51 |
| 2:B:37:VAL:CG2 | 2:B:66:TYR:CZ | 2.94 | 0.51 |
| 3:E:161:ASP:OD1 | 3:E:161:ASP:N | 2.43 | 0.51 |
| 3:E:157:LYS:NZ | 3:E:170:ASN:OD1 | 2.44 | 0.51 |
| 4:F:73:SER:OG | 4:F:74:VAL:N | 2.43 | 0.51 |
| 3:K:152:VAL:HG13 | 3:K:153:TYR:N | 2.26 | 0.51 |
| 3:K:59:LYS:CD | 3:K:60:GLY:N | 2.73 | 0.51 |
| 3:K:21:PHE:HE1 | 3:K:88:TYR:CD2 | 2.28 | 0.51 |
| 4:L:161:VAL:O | 4:L:162:ASN:CB | 2.59 | 0.51 |
| 2:N:11:SER:C | 2:N:13:HIS:H | 2.13 | 0.51 |
| 3:O:181:PHE:O | 3:O:182:ALA:HB3 | 2.11 | 0.51 |
| 1:C:226:GLN:OE1 | 1:C:227:ASP:HB2 | 2.10 | 0.51 |
| 1:G:101:CYS:N | 1:G:164:CYS:SG | 2.84 | 0.51 |
| 3:I:34:HIS:O | 3:I:90:CYS:HA | 2.10 | 0.51 |
| 3:K:185:ASN:HB2 | 3:K:188:ASN:HB3 | 1.92 | 0.51 |
| 1:M:188:HIS:HD2 | 1:M:204:TRP:HE3 | 1.59 | 0.51 |
| 2:B:1:ILE:HG13 | 2:B:2:GLN:N | 2.26 | 0.51 |
| 1:C:6:ARG:HA | 1:C:100:GLY:HA3 | 1.92 | 0.51 |
| 2:D:70:PHE:HE1 | 2:D:72:PRO:HB3 | 1.75 | 0.51 |
| 3:E:21:PHE:N | 3:E:21:PHE:CD2 | 2.79 | 0.51 |
| 3:O:134:LEU:HD12 | 3:O:135:PHE:N | 2.26 | 0.51 |
| 4:F:29:HIS:ND1 | 4:F:96:GLN:HG2 | 2.26 | 0.51 |
| 3:I:113:GLN:OE1 | 3:I:113:GLN:N | 2.24 | 0.51 |
| 1:M:9:PHE:HE2 | 1:M:99:TYR:CE2 | 2.28 | 0.51 |
| 4:P:135:ILE:HG13 | 4:P:141:ALA:HA | 1.92 | 0.51 |
| 1:A:143:THR:HG21 | 5:Q:9:VAL:HG12 | 1.92 | 0.51 |
| 3:E:187:PHE:O | 3:E:192:ILE:HD12 | 2.11 | 0.51 |
| 3:E:83:GLU:OE1 | 3:E:162:MET:CE | 2.58 | 0.51 |
| 3:I:81:GLN:N | 3:I:84:ASP:OD2 | 2.40 | 0.51 |
| 4:L:123:PRO:CG | 4:L:150:PHE:HD2 | 2.18 | 0.51 |
| 4:L:215:TYR:HA | 4:L:232:THR:OG1 | 2.11 | 0.51 |
| 4:F:35:TYR:OH | 4:F:103:GLN:OE1 | 2.20 | 0.50 |
| 4:F:47:ILE:CG2 | 4:F:48:TYR:N | 2.73 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:44:PRO:HG2 | 4:J:105:PHE:CD2 | 2.47 | 0.50 |
| 1:A:207:SER:O | 1:A:207:SER:OG | 2.22 | 0.50 |
| 2:B:1:ILE:HG13 | 2:B:2:GLN:H | 1.75 | 0.50 |
| 4:F:135:ILE:CD1 | 4:F:201:TRP:HZ3 | 2.24 | 0.50 |
| 4:F:83:GLN:HA | 4:F:113:VAL:HG21 | 1.93 | 0.50 |
| 4:P:160:TRP:HA | 4:P:165:GLU:HB3 | 1.92 | 0.50 |
| 4:F:123:PRO:HA | 4:F:149:GLY:HA3 | 1.92 | 0.50 |
| 4:F:170:VAL:HA | 4:F:194:LEU:CD1 | 2.40 | 0.50 |
| 1:G:37:ASP:HB3 | 1:G:40:ALA:HB2 | 1.93 | 0.50 |
| 3:I:2:LEU:HD23 | 3:I:3:ASN:H | 1.77 | 0.50 |
| 4:L:150:PHE:CD1 | 4:L:150:PHE:C | 2.85 | 0.50 |
| 2:N:33:SER:O | 2:N:35:ILE:HD12 | 2.11 | 0.50 |
| 2:N:38:ASP:OD2 | 2:N:45:ARG:HB3 | 2.12 | 0.50 |
| 2:N:2:GLN:HE22 | 2:N:85:VAL:HB | 1.76 | 0.50 |
| 3:O:96:ASN:H | 5:T:5:MET:HE2 | 1.75 | 0.50 |
| 1:G:98:MET:CE | 1:G:99:TYR:HA | 2.41 | 0.50 |
| 3:K:30:PHE:HD1 | 3:K:92:PHE:HE1 | 1.57 | 0.50 |
| 4:L:46:LEU:O | 4:L:47:ILE:HG22 | 2.12 | 0.50 |
| 4:P:130:PRO:HB3 | 4:P:142:THR:O | 2.11 | 0.50 |
| 1:C:13:SER:HB3 | 1:C:78:LEU:HD13 | 1.93 | 0.50 |
| 4:F:203:ASN:N | 4:F:204:PRO:CD | 2.75 | 0.50 |
| 1:G:102:ASP:HB2 | 1:G:111:ARG:HG3 | 1.93 | 0.50 |
| 3:I:154:ILE:HD12 | 3:I:155:THR:N | 2.26 | 0.50 |
| 1:M:249:VAL:HG22 | 1:M:257:TYR:CD1 | 2.46 | 0.50 |
| 1:M:66:LYS:NZ | 3:O:29:ASN:HB2 | 2.25 | 0.50 |
| 4:P:64:ARG:NH1 | 4:P:64:ARG:CG | 2.73 | 0.50 |
| 3:E:84:ASP:HA | 3:E:85:SER:HG | 1.76 | 0.50 |
| 4:F:170:VAL:CA | 4:F:194:LEU:CD1 | 2.90 | 0.50 |
| 4:J:29:HIS:CD2 | 4:J:94:SER:O | 2.64 | 0.50 |
| 3:K:144:VAL:CG2 | 3:K:157:LYS:HZ2 | 2.23 | 0.50 |
| 3:K:161:ASP:HA | 3:K:168:LYS:HB3 | 1.93 | 0.50 |
| 4:L:10:ASN:OD1 | 4:L:109:THR:HA | 2.12 | 0.50 |
| 4:L:89:VAL:CG1 | 4:L:110:ARG:CG | 2.83 | 0.50 |
| 4:L:204:PRO:HB2 | 4:L:205:ARG:HA | 1.93 | 0.50 |
| 4:F:110:ARG:HH21 | 4:F:154:HIS:HA | 1.77 | 0.50 |
| 4:L:67:ALA:HB2 | 4:L:77:LEU:HD13 | 1.93 | 0.50 |
| 2:N:20:SER:HB3 | 4:F:18:ASP:CG | 2.32 | 0.50 |
| 1:A:131:ARG:NH2 | 6:A:302:HOH:O | 2.19 | 0.50 |
| 1:G:189:MET:CE | 1:G:274:TRP:N | 2.75 | 0.50 |
| 1:C:188:HIS:ND1 | 1:C:188:HIS:N | 2.60 | 0.50 |
| 2:H:70:PHE:CE1 | 2:H:78:TYR:CZ | 3.00 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:J:150:PHE:O | 4:J:187:ARG:HB2 | 2.12 | 0.50 |
| 4:L:146:LEU:O | 4:L:146:LEU:HD12 | 2.12 | 0.50 |
| 4:P:37:GLN:HG3 | 4:P:41:GLN:CD | 2.32 | 0.50 |
| 1:A:147:TRP:HB3 | 1:A:152:VAL:HB | 1.92 | 0.49 |
| 2:B:18:GLY:N | 2:B:72:PRO:O | 2.37 | 0.49 |
| 2:H:96:ASP:HB3 | 2:H:99:MET:HB2 | 1.94 | 0.49 |
| 3:I:36:TYR:O | 3:I:88:TYR:HA | 2.12 | 0.49 |
| 3:K:135:PHE:CZ | 3:K:192:ILE:HD11 | 2.44 | 0.49 |
| 4:L:150:PHE:CD1 | 4:L:188:TYR:O | 2.65 | 0.49 |
| 1:M:227:ASP:OD1 | 1:M:248:VAL:HG12 | 2.12 | 0.49 |
| 1:G:97:ARG:HH22 | 5:U:8:THR:HA | 1.77 | 0.49 |
| 3:K:61:ARG:HH21 | 3:K:84:ASP:CG | 2.15 | 0.49 |
| 4:P:11:LYS:O | 4:P:111:LEU:HD12 | 2.13 | 0.49 |
| 1:A:98:MET:C | 1:A:98:MET:HE2 | 2.33 | 0.49 |
| 1:G:195:SER:HB2 | 1:G:196:ASP:HA | 1.93 | 0.49 |
| 3:K:135:PHE:CD1 | 3:K:135:PHE:C | 2.85 | 0.49 |
| 2:B:89:GLN:CB | 2:B:90:PRO:HD2 | 2.42 | 0.49 |
| 1:C:202:ARG:HG3 | 1:C:244:TRP:NE1 | 2.26 | 0.49 |
| 3:E:6:GLN:OE1 | 3:E:103:GLY:HA2 | 2.11 | 0.49 |
| 4:F:162:ASN:O | 4:F:164:LYS:HG3 | 2.13 | 0.49 |
| 4:F:69:ARG:HB2 | 4:F:75:SER:HB2 | 1.94 | 0.49 |
| 3:K:48:PHE:HD2 | 3:K:64:ALA:HB2 | 1.77 | 0.49 |
| 1:C:99:TYR:OH | 5:R:3:VAL:HG12 | 2.12 | 0.49 |
| 1:A:203:CYS:HB2 | 1:A:217:TRP:HZ3 | 1.75 | 0.49 |
| 2:B:52:SER:OG | 2:B:65:LEU:N | 2.43 | 0.49 |
| 1:C:25:VAL:HG21 | 1:C:32:GLN:HE21 | 1.77 | 0.49 |
| 1:G:185:PRO:HB3 | 1:G:208:PHE:HB3 | 1.93 | 0.49 |
| 4:J:131:SER:HB2 | 4:J:134:GLU:CB | 2.42 | 0.49 |
| 3:K:35:TRP:C | 3:K:36:TYR:HD1 | 2.16 | 0.49 |
| 4:L:202:GLN:N | 4:L:204:PRO:HD2 | 2.27 | 0.49 |
| 1:M:8:PHE:HB2 | 1:M:25:VAL:HG13 | 1.92 | 0.49 |
| 1:G:142:THR:O | 1:G:146:LYS:HG3 | 2.13 | 0.49 |
| 4:J:162:ASN:HB2 | 4:J:164:LYS:NZ | 2.28 | 0.49 |
| 3:K:119:VAL:HA | 3:K:134:LEU:O | 2.13 | 0.49 |
| 3:K:72:TYR:C | 3:K:72:TYR:CD1 | 2.85 | 0.49 |
| 4:L:170:VAL:CG2 | 4:L:194:LEU:CD2 | 2.87 | 0.49 |
| 4:P:129:GLU:HG3 | 4:P:201:TRP:CZ2 | 2.48 | 0.49 |
| 4:P:21:LEU:HD22 | 4:P:109:THR:HG21 | 1.95 | 0.49 |
| 4:P:38:ARG:O | 4:P:40:GLY:HA2 | 2.12 | 0.49 |
| 4:L:150:PHE:C | 4:L:150:PHE:HD1 | 2.16 | 0.49 |
| 4:L:36:ARG:HD2 | 4:L:90:TYR:HA | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:9:PHE:HB2 | 1:A:97:ARG:HB3 | 1.95 | 0.49 |
| 2:H:54:LEU:HA | 2:H:64:LEU:HD21 | 1.93 | 0.49 |
| 4:L:11:LYS:O | 4:L:111:LEU:HA | 2.13 | 0.49 |
| 1:M:49:ALA:HB3 | 1:M:52:ILE:HG22 | 1.94 | 0.49 |
| 1:M:73:THR:HG22 | 5:T:8:THR:HG21 | 1.95 | 0.49 |
| 1:G:142:THR:OG1 | 6:G:302:HOH:O | 2.20 | 0.49 |
| 4:J:113:VAL:O | 4:J:114:LEU:CB | 2.60 | 0.49 |
| 3:K:133:CYS:SG | 3:K:183:CYS:N | 2.86 | 0.49 |
| 3:K:159:VAL:N | 4:L:171:CYS:SG | 2.85 | 0.49 |
| 1:M:21:ARG:NH2 | 1:M:37:ASP:OD2 | 2.38 | 0.49 |
| 1:A:219:ARG:HD2 | 1:A:257:TYR:CZ | 2.47 | 0.49 |
| 4:F:218:SER:HG | 4:F:221:ASP:CB | 2.22 | 0.49 |
| 4:J:154:HIS:N | 4:J:154:HIS:CD2 | 2.80 | 0.49 |
| 4:J:49:PHE:CE1 | 4:J:54:ALA:HB2 | 2.47 | 0.49 |
| 4:F:217:LEU:CD1 | 4:F:218:SER:N | 2.72 | 0.48 |
| 4:F:35:TYR:CD1 | 4:F:43:LEU:HD21 | 2.48 | 0.48 |
| 1:G:98:MET:HE3 | 1:G:99:TYR:CA | 2.40 | 0.48 |
| 4:J:153:ASP:OD2 | 4:J:176:PRO:HG3 | 2.12 | 0.48 |
| 3:K:2:LEU:CB | 3:K:3:ASN:HA | 2.39 | 0.48 |
| 3:K:175:TRP:CZ2 | 4:L:146:LEU:CB | 2.95 | 0.48 |
| 4:L:125:VAL:HG22 | 4:L:235:VAL:HG12 | 1.95 | 0.48 |
| 1:M:37:ASP:OD1 | 1:M:38:SER:N | 2.46 | 0.48 |
| 2:N:3:ARG:O | 2:N:30:PHE:HA | 2.13 | 0.48 |
| 4:P:196:VAL:CG2 | 4:P:197:SER:H | 2.06 | 0.48 |
| 2:D:89:GLN:HG3 | 2:D:90:PRO:N | 2.28 | 0.48 |
| 3:E:31:TYR:C | 3:E:31:TYR:CD2 | 2.86 | 0.48 |
| 2:H:7:ILE:HG23 | 2:H:93:VAL:HG21 | 1.95 | 0.48 |
| 3:K:63:SER:O | 3:K:75:LEU:HA | 2.12 | 0.48 |
| 1:M:197:HIS:N | 1:M:197:HIS:ND1 | 2.60 | 0.48 |
| 1:C:102:ASP:OD2 | 1:C:113:TYR:OH | 2.29 | 0.48 |
| 3:I:134:LEU:HB3 | 3:I:173:VAL:HA | 1.94 | 0.48 |
| 3:I:7:SER:HB2 | 3:I:8:PRO:HD3 | 1.96 | 0.48 |
| 3:K:48:PHE:HE2 | 3:K:63:SER:HA | 1.77 | 0.48 |
| 4:L:141:ALA:H | 4:L:198:ALA:H | 1.61 | 0.48 |
| 1:M:259:CYS:HB3 | 1:M:272:LEU:CB | 2.43 | 0.48 |
| 1:M:270:LEU:HD13 | 1:M:272:LEU:HD21 | 1.95 | 0.48 |
| 2:N:12:ARG:O | 2:N:13:HIS:CE1 | 2.67 | 0.48 |
| 1:C:145:HIS:HD2 | 6:C:305:HOH:O | 1.95 | 0.48 |
| 1:C:24:ALA:HB3 | 1:C:36:PHE:HB3 | 1.96 | 0.48 |
| 3:E:178:LYS:HG2 | 3:E:179:SER:OG | 2.13 | 0.48 |
| 1:G:192:HIS:CB | 1:G:202:ARG:HH22 | 2.23 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:35:ARG:NH2 | 1:G:48:ARG:CD | 2.76 | 0.48 |
| 2:H:24:ASN:ND2 | 2:H:65:LEU:CD2 | 2.76 | 0.48 |
| 4:L:62:SER:CA | 4:L:65:PHE:CD2 | 2.97 | 0.48 |
| 1:M:203:CYS:HB2 | 1:M:217:TRP:NE1 | 2.28 | 0.48 |
| 1:M:225:THR:OG1 | 1:M:226:GLN:N | 2.47 | 0.48 |
| 1:M:73:THR:HG22 | 5:T:8:THR:CG2 | 2.43 | 0.48 |
| 2:B:10:TYR:HE2 | 2:B:26:TYR:HB3 | 1.79 | 0.48 |
| 2:B:37:VAL:HG21 | 2:B:66:TYR:CD1 | 2.49 | 0.48 |
| 4:F:160:TRP:H | 4:F:209:ARG:HG3 | 1.78 | 0.48 |
| 3:K:136:THR:HG21 | 3:K:171:SER:HB3 | 1.95 | 0.48 |
| 4:L:88:ALA:CB | 4:L:110:ARG:HA | 2.42 | 0.48 |
| 2:N:54:LEU:HD23 | 2:N:54:LEU:C | 2.34 | 0.48 |
| 2:N:63:TYR:C | 2:N:63:TYR:CD1 | 2.87 | 0.48 |
| 4:P:14:GLU:OE2 | 4:P:117:LEU:HD11 | 2.13 | 0.48 |
| 1:A:70:HIS:HD2 | 5:Q:6:VAL:HG22 | 1.77 | 0.48 |
| 3:E:87:THR:HA | 3:E:105:SER:HA | 1.96 | 0.48 |
| 2:H:70:PHE:HZ | 2:H:78:TYR:CD2 | 2.31 | 0.48 |
| 3:I:152:VAL:HA | 3:I:176:SER:OG | 2.13 | 0.48 |
| 3:O:120:TYR:HB3 | 4:P:131:SER:OG | 2.14 | 0.48 |
| 3:O:123:ARG:HB2 | 3:O:131:SER:HB3 | 1.95 | 0.48 |
| 1:A:225:THR:OG1 | 1:A:226:GLN:HB2 | 2.14 | 0.48 |
| 1:A:59:TYR:OH | 1:A:171:TYR:OH | 2.16 | 0.48 |
| 1:G:163:THR:HA | 1:G:166:GLU:HG2 | 1.95 | 0.48 |
| 3:I:121:GLN:HG3 | 4:J:131:SER:HA | 1.95 | 0.48 |
| 3:K:138:PHE:HD2 | 3:K:138:PHE:H | 1.61 | 0.48 |
| 1:M:102:ASP:HB2 | 1:M:111:ARG:HG2 | 1.95 | 0.48 |
| 3:O:79:GLY:C | 3:O:81:GLN:OE1 | 2.51 | 0.48 |
| 1:C:22:PHE:H | 1:C:38:SER:HB3 | 1.78 | 0.48 |
| 3:E:84:ASP:CA | 3:E:85:SER:CB | 2.91 | 0.48 |
| 4:F:123:PRO:HA | 4:F:149:GLY:CA | 2.44 | 0.48 |
| 4:F:201:TRP:O | 4:F:204:PRO:CG | 2.62 | 0.48 |
| 1:G:10:THR:HG22 | 2:H:56:PHE:CE2 | 2.48 | 0.48 |
| 4:J:45:PHE:HZ | 4:J:48:TYR:HB3 | 1.78 | 0.48 |
| 4:L:130:PRO:HD2 | 4:L:201:TRP:CZ2 | 2.49 | 0.48 |
| 4:L:82:THR:CG2 | 4:L:83:GLN:N | 2.77 | 0.48 |
| 2:N:30:PHE:CE1 | 2:N:35:ILE:HD11 | 2.48 | 0.48 |
| 4:P:160:TRP:HH2 | 4:P:234:ILE:HD11 | 1.78 | 0.48 |
| 1:A:177:GLU:CG | 1:A:178:THR:N | 2.77 | 0.48 |
| 2:D:74:GLU:N | 2:D:74:GLU:OE1 | 2.47 | 0.48 |
| 4:F:130:PRO:HB3 | 4:F:142:THR:O | 2.14 | 0.48 |
| 4:F:33:TYR:O | 4:F:92:CYS:HA | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:118:ALA:HB2 | 3:K:197:PHE:HB3 | 1.96 | 0.48 |
| 3:O:131:SER:OG | 3:O:181:PHE:HE2 | 1.97 | 0.48 |
| 1:C:103:VAL:HG12 | 1:C:109:PHE:HA | 1.96 | 0.47 |
| 3:I:33:LEU:O | 3:I:50:MET:N | 2.41 | 0.47 |
| 4:L:150:PHE:HE1 | 4:L:188:TYR:C | 2.15 | 0.47 |
| 4:L:161:VAL:HG12 | 4:L:162:ASN:H | 1.78 | 0.47 |
| 1:C:159:TYR:HD1 | 1:C:163:THR:HB | 1.78 | 0.47 |
| 1:G:234:ARG:CG | 1:G:242:GLN:HB2 | 2.43 | 0.47 |
| 2:H:3:ARG:HH21 | 2:H:61:SER:HB2 | 1.78 | 0.47 |
| 4:J:14:GLU:HA | 4:J:114:LEU:O | 2.14 | 0.47 |
| 3:K:124:ASP:CA | 4:L:128:PHE:HA | 2.45 | 0.47 |
| 4:L:150:PHE:CZ | 4:L:155:VAL:HG11 | 2.49 | 0.47 |
| 1:M:11:SER:HA | 1:M:21:ARG:O | 2.14 | 0.47 |
| 1:M:217:TRP:HZ3 | 1:M:247:VAL:HG22 | 1.79 | 0.47 |
| 2:B:49:VAL:HG12 | 2:B:50:GLU:O | 2.15 | 0.47 |
| 1:C:66:LYS:HE3 | 5:R:2:LEU:HB2 | 1.95 | 0.47 |
| 4:F:201:TRP:O | 4:F:204:PRO:HG3 | 2.14 | 0.47 |
| 4:F:60:LEU:HD22 | 4:F:65:PHE:HB3 | 1.94 | 0.47 |
| 1:G:98:MET:SD | 1:G:99:TYR:N | 2.87 | 0.47 |
| 4:P:173:ASP:N | 4:P:173:ASP:OD1 | 2.47 | 0.47 |
| 3:O:155:THR:CG2 | 4:P:173:ASP:OD2 | 2.60 | 0.47 |
| 1:C:27:TYR:CD2 | 1:C:32:GLN:HB2 | 2.49 | 0.47 |
| 1:A:66:LYS:HE2 | 3:I:29:ASN:OD1 | 2.14 | 0.47 |
| 4:L:103:GLN:N | 4:L:103:GLN:OE1 | 2.48 | 0.47 |
| 4:L:131:SER:HB2 | 4:L:135:ILE:HG21 | 1.96 | 0.47 |
| 1:G:66:LYS:NZ | 5:U:2:LEU:O | 2.45 | 0.47 |
| 1:A:202:ARG:HG3 | 1:A:244:TRP:NE1 | 2.26 | 0.47 |
| 2:D:55:SER:O | 2:D:63:TYR:N | 2.46 | 0.47 |
| 4:F:84:GLN:CG | 4:F:85:GLU:H | 2.27 | 0.47 |
| 1:G:68:LYS:O | 1:G:72:GLN:HG2 | 2.15 | 0.47 |
| 1:M:14:ARG:HH21 | 1:M:21:ARG:HB2 | 1.78 | 0.47 |
| 2:B:40:LEU:HD23 | 2:B:43:GLY:HA2 | 1.96 | 0.47 |
| 1:C:155:GLN:HG2 | 3:E:51:THR:HG21 | 1.96 | 0.47 |
| 4:J:191:SER:OG | 4:J:191:SER:O | 2.33 | 0.47 |
| 3:K:135:PHE:HZ | 3:K:192:ILE:HG12 | 1.67 | 0.47 |
| 4:L:140:LYS:HA | 4:L:197:SER:HA | 1.95 | 0.47 |
| 1:M:203:CYS:HB2 | 1:M:217:TRP:CZ2 | 2.50 | 0.47 |
| 1:M:213:ILE:HD11 | 1:M:261:VAL:CG1 | 2.44 | 0.47 |
| 1:G:117:ALA:HB2 | 2:H:60:TRP:CE2 | 2.50 | 0.47 |
| 1:G:42:SER:HB3 | 1:G:44:ARG:HG3 | 1.97 | 0.47 |
| 1:G:98:MET:C | 1:G:98:MET:SD | 2.93 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:89:LEU:HD22 | 3:I:100:PHE:HD2 | 1.79 | 0.47 |
| 4:J:86:ASP:N | 4:J:86:ASP:OD1 | 2.48 | 0.47 |
| 3:O:118:ALA:CB | 3:O:120:TYR:CZ | 2.98 | 0.47 |
| 4:P:118:LYS:O | 4:P:120:VAL:N | 2.48 | 0.47 |
| 3:O:153:TYR:HB3 | 4:P:177:LEU:HD21 | 1.97 | 0.47 |
| 1:A:49:ALA:O | 1:A:52:ILE:HG22 | 2.15 | 0.47 |
| 1:C:9:PHE:HE2 | 1:C:99:TYR:CE2 | 2.33 | 0.47 |
| 3:E:138:PHE:CE1 | 3:E:170:ASN:O | 2.68 | 0.47 |
| 1:G:218:GLN:HB2 | 1:G:222:GLU:C | 2.35 | 0.47 |
| 3:I:61:ARG:NH1 | 3:I:84:ASP:OD2 | 2.48 | 0.47 |
| 4:J:223:TRP:NE1 | 4:J:228:ALA:O | 2.47 | 0.47 |
| 4:L:36:ARG:HB2 | 4:L:44:GLU:OE2 | 2.15 | 0.47 |
| 4:P:154:HIS:N | 4:P:154:HIS:ND1 | 2.60 | 0.47 |
| 4:P:172:THR:HG22 | 4:P:173:ASP:H | 1.80 | 0.47 |
| 4:F:83:GLN:CA | 4:F:113:VAL:HG21 | 2.45 | 0.47 |
| 4:J:175:GLN:HG3 | 4:J:176:PRO:HD2 | 1.96 | 0.47 |
| 3:K:115:PRO:HG3 | 3:K:139:ASP:OD2 | 2.14 | 0.47 |
| 4:L:224:THR:OG1 | 4:L:225:GLN:N | 2.48 | 0.47 |
| 3:O:137:ASP:HB3 | 3:O:169:SER:HA | 1.97 | 0.47 |
| 3:O:168:LYS:HE2 | 3:O:168:LYS:HB3 | 1.67 | 0.47 |
| 4:P:84:GLN:HA | 4:P:113:VAL:HG13 | 1.96 | 0.47 |
| 4:P:190:LEU:HD12 | 4:P:191:SER:H | 1.80 | 0.47 |
| 4:P:223:TRP:CZ2 | 4:P:225:GLN:CG | 2.97 | 0.47 |
| 1:A:35:ARG:HD3 | 1:A:48:ARG:NE | 2.14 | 0.47 |
| 1:C:172:LEU:HD23 | 1:C:179:LEU:HD13 | 1.97 | 0.47 |
| 1:C:231:VAL:CG1 | 1:C:244:TRP:HE3 | 2.17 | 0.47 |
| 1:C:22:PHE:H | 1:C:38:SER:CB | 2.27 | 0.47 |
| 4:F:155:VAL:HG12 | 4:F:214:PHE:CD1 | 2.50 | 0.47 |
| 4:F:201:TRP:HA | 4:F:204:PRO:HG3 | 1.96 | 0.47 |
| 3:I:42:LYS:HG2 | 3:I:43:SER:N | 2.30 | 0.47 |
| 4:J:123:PRO:CA | 4:J:150:PHE:HB3 | 2.45 | 0.47 |
| 3:K:33:LEU:HD23 | 3:K:91:ALA:O | 2.15 | 0.47 |
| 3:O:112:ILE:HG22 | 3:O:114:ASN:H | 1.80 | 0.47 |
| 3:E:13:VAL:O | 3:E:108:VAL:HA | 2.15 | 0.47 |
| 1:G:125:ALA:C | 1:G:134:THR:HG22 | 2.34 | 0.47 |
| 3:K:137:ASP:N | 3:K:137:ASP:OD1 | 2.47 | 0.47 |
| 3:K:175:TRP:NE1 | 4:L:146:LEU:HD22 | 2.12 | 0.47 |
| 4:P:33:TYR:OH | 4:P:95:SER:OG | 2.13 | 0.47 |
| 2:B:26:TYR:CE2 | 2:B:28:SER:HB2 | 2.51 | 0.46 |
| 3:E:138:PHE:O | 3:E:139:ASP:O | 2.33 | 0.46 |
| 3:E:84:ASP:HB3 | 3:E:85:SER:C | 2.35 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:187:THR:HB | 1:G:272:LEU:CD2 | 2.32 | 0.46 |
| 1:C:147:TRP:N | 1:C:147:TRP:CD1 | 2.83 | 0.46 |
| 4:F:56:ASP:OD1 | 4:F:57:LYS:N | 2.48 | 0.46 |
| 1:G:163:THR:HA | 1:G:166:GLU:CG | 2.45 | 0.46 |
| 1:G:159:TYR:CE1 | 1:G:163:THR:OG1 | 2.68 | 0.46 |
| 4:L:150:PHE:CE2 | 4:L:155:VAL:HG11 | 2.50 | 0.46 |
| 2:N:22:PHE:HD2 | 2:N:67:TYR:HB2 | 1.80 | 0.46 |
| 3:E:114:ASN:HA | 3:E:115:PRO:HD2 | 1.57 | 0.46 |
| 4:F:15:LYS:NZ | 4:F:83:GLN:HE21 | 2.14 | 0.46 |
| 4:F:36:ARG:HE | 4:F:38:ARG:NH1 | 2.13 | 0.46 |
| 2:H:7:ILE:HD11 | 2:H:25:CYS:SG | 2.56 | 0.46 |
| 3:K:151:ASP:OD2 | 3:K:181:PHE:HB3 | 2.15 | 0.46 |
| 3:K:38:TRP:CZ3 | 3:K:44:PRO:HG3 | 2.38 | 0.46 |
| 4:L:89:VAL:HG11 | 4:L:110:ARG:HB2 | 1.91 | 0.46 |
| 4:P:196:VAL:CG2 | 4:P:197:SER:N | 2.73 | 0.46 |
| 1:C:243:LYS:CG | 1:C:244:TRP:H | 2.28 | 0.46 |
| 2:H:3:ARG:NH2 | 2:H:59:ASP:O | 2.43 | 0.46 |
| 1:M:266:LEU:HD12 | 1:M:266:LEU:N | 2.31 | 0.46 |
| 1:C:136:ALA:O | 1:C:137:ASP:HB3 | 2.16 | 0.46 |
| 4:J:11:LYS:HZ1 | 4:J:217:LEU:CD2 | 2.29 | 0.46 |
| 3:O:7:SER:HB3 | 3:O:22:THR:HB | 1.98 | 0.46 |
| 1:A:93:HIS:CG | 1:A:119:ASP:OD1 | 2.68 | 0.46 |
| 2:D:96:ASP:HB3 | 2:D:99:MET:HB3 | 1.97 | 0.46 |
| 1:G:97:ARG:HH12 | 5:U:6:VAL:HG12 | 1.74 | 0.46 |
| 1:G:234:ARG:HB3 | 2:H:8:GLN:NE2 | 2.31 | 0.46 |
| 4:J:217:LEU:CD1 | 4:J:221:ASP:HB3 | 2.41 | 0.46 |
| 4:L:159:TRP:CE3 | 4:L:170:VAL:HG13 | 2.50 | 0.46 |
| 1:M:188:HIS:CD2 | 1:M:204:TRP:HE3 | 2.33 | 0.46 |
| 3:O:53:ASN:CA | 3:O:68:THR:HG23 | 2.46 | 0.46 |
| 4:P:24:ASP:HA | 4:P:25:PRO:HD2 | 1.76 | 0.46 |
| 1:A:84:TYR:OH | 1:A:146:LYS:NZ | 2.26 | 0.46 |
| 1:C:33:PHE:O | 1:C:52:ILE:HG21 | 2.15 | 0.46 |
| 4:F:176:PRO:HB2 | 4:F:188:TYR:HB3 | 1.97 | 0.46 |
| 3:I:15:GLU:OE1 | 3:I:110:PRO:HA | 2.15 | 0.46 |
| 1:M:187:THR:HB | 1:M:272:LEU:HD11 | 1.98 | 0.46 |
| 4:P:130:PRO:HD2 | 4:P:201:TRP:CZ2 | 2.51 | 0.46 |
| 1:A:106:ASP:OD1 | 1:A:106:ASP:N | 2.48 | 0.46 |
| 1:C:106:ASP:N | 1:C:106:ASP:OD1 | 2.47 | 0.46 |
| 1:C:189:MET:HG3 | 1:C:202:ARG:O | 2.16 | 0.46 |
| 4:F:165:GLU:C | 4:F:166:VAL:HG23 | 2.36 | 0.46 |
| 1:G:97:ARG:CD | 1:G:116:TYR:CE1 | 2.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:154:GLU:O | 1:G:157:ARG:HG2 | 2.16 | 0.46 |
| 4:J:202:GLN:O | 4:J:205:ARG:N | 2.49 | 0.46 |
| 1:M:129:ASP:N | 1:M:129:ASP:OD1 | 2.46 | 0.46 |
| 1:A:217:TRP:CD1 | 1:A:247:VAL:HG11 | 2.51 | 0.46 |
| 2:B:3:ARG:NH1 | 2:B:59:ASP:O | 2.29 | 0.46 |
| 4:F:202:GLN:C | 4:F:204:PRO:HD3 | 2.36 | 0.46 |
| 3:I:137:ASP:CG | 3:I:138:PHE:H | 2.19 | 0.46 |
| 3:I:159:VAL:HA | 3:I:169:SER:O | 2.15 | 0.46 |
| 1:M:135:ALA:HB1 | 1:M:140:ALA:HB1 | 1.97 | 0.46 |
| 1:M:198:GLU:HB3 | 1:M:249:VAL:O | 2.16 | 0.46 |
| 1:M:78:LEU:CD2 | 1:M:95:VAL:CG2 | 2.74 | 0.46 |
| 3:E:11:LEU:HD13 | 3:E:19:THR:HG21 | 1.97 | 0.46 |
| 3:K:81:GLN:O | 3:K:108:VAL:HG21 | 2.16 | 0.46 |
| 1:G:99:TYR:CE2 | 5:U:3:VAL:HG12 | 2.51 | 0.46 |
| 2:B:5:PRO:HA | 2:B:30:PHE:HB3 | 1.97 | 0.45 |
| 1:C:35:ARG:HD3 | 1:C:48:ARG:HD3 | 1.98 | 0.45 |
| 4:F:180:GLN:CA | 4:F:186:SER:OG | 2.63 | 0.45 |
| 4:F:195:ARG:CG | 4:F:195:ARG:NH1 | 2.73 | 0.45 |
| 2:H:21:ASN:OD1 | 2:H:22:PHE:O | 2.34 | 0.45 |
| 2:H:70:PHE:CE1 | 2:H:78:TYR:CG | 3.04 | 0.45 |
| 4:J:84:GLN:O | 4:J:87:SER:OG | 2.33 | 0.45 |
| 3:K:158:CYS:SG | 4:L:172:THR:N | 2.84 | 0.45 |
| 1:M:14:ARG:HB3 | 1:M:17:ARG:HB2 | 1.98 | 0.45 |
| 1:M:96:GLN:HE22 | 2:N:31:HIS:HE1 | 1.62 | 0.45 |
| 3:O:50:MET:HB3 | 3:O:66:LEU:HD22 | 1.98 | 0.45 |
| 4:P:14:GLU:OE2 | 4:P:117:LEU:CD1 | 2.63 | 0.45 |
| 3:E:154:ILE:HG22 | 3:E:155:THR:N | 2.31 | 0.45 |
| 1:G:98:MET:HE3 | 1:G:113:TYR:HD1 | 1.73 | 0.45 |
| 1:G:6:ARG:CB | 1:G:8:PHE:HE2 | 2.27 | 0.45 |
| 2:H:40:LEU:HD12 | 2:H:79:ALA:HB3 | 1.98 | 0.45 |
| 2:H:7:ILE:HD12 | 2:H:82:VAL:HG11 | 1.97 | 0.45 |
| 4:J:180:GLN:HA | 4:J:181:PRO:HA | 1.72 | 0.45 |
| 2:N:59:ASP:O | 2:N:60:TRP:HB2 | 2.17 | 0.45 |
| 4:P:38:ARG:HH11 | 4:P:38:ARG:HG2 | 1.81 | 0.45 |
| 3:E:157:LYS:HE2 | 3:E:170:ASN:OD1 | 2.16 | 0.45 |
| 3:E:82:PRO:HG3 | 3:E:110:PRO:HB3 | 1.98 | 0.45 |
| 1:G:59:TYR:O | 1:G:63:GLU:HG2 | 2.17 | 0.45 |
| 3:I:138:PHE:O | 3:I:138:PHE:CD1 | 2.70 | 0.45 |
| 3:I:21:PHE:CE2 | 3:I:77:ILE:HD11 | 2.51 | 0.45 |
| 3:K:124:ASP:H | 3:K:131:SER:CB | 2.29 | 0.45 |
| 4:F:202:GLN:C | 4:F:204:PRO:CD | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:69:ALA:O | 1:G:73:THR:OG1 | 2.26 | 0.45 |
| 4:J:151:TYR:HB2 | 4:J:187:ARG:HB3 | 1.97 | 0.45 |
| 3:K:190:SER:O | 3:K:190:SER:OG | 2.34 | 0.45 |
| 1:M:97:ARG:NH2 | 1:M:147:TRP:HH2 | 2.13 | 0.45 |
| 3:O:112:ILE:HB | 3:O:115:PRO:HG3 | 1.98 | 0.45 |
| 3:K:31:TYR:CD1 | 5:U:4:PRO:HB2 | 2.42 | 0.45 |
| 1:A:22:PHE:H | 1:A:38:SER:CB | 2.29 | 0.45 |
| 1:A:98:MET:C | 1:A:98:MET:CE | 2.85 | 0.45 |
| 2:B:89:GLN:HB2 | 2:B:90:PRO:CD | 2.44 | 0.45 |
| 1:C:67:VAL:HA | 1:C:70:HIS:HD2 | 1.82 | 0.45 |
| 1:G:102:ASP:HB2 | 1:G:111:ARG:CG | 2.47 | 0.45 |
| 1:M:220:ASP:HB3 | 1:M:221:GLY:H | 1.64 | 0.45 |
| 4:P:160:TRP:HA | 4:P:165:GLU:CB | 2.46 | 0.45 |
| 1:A:9:PHE:HZ | 5:Q:2:LEU:HD23 | 1.82 | 0.45 |
| 4:F:138:THR:O | 4:F:139:GLN:HB2 | 2.16 | 0.45 |
| 1:G:124:ILE:HG12 | 1:G:135:ALA:HA | 1.99 | 0.45 |
| 4:L:46:LEU:C | 4:L:47:ILE:CG2 | 2.85 | 0.45 |
| 2:N:2:GLN:HE21 | 2:N:85:VAL:CB | 2.27 | 0.45 |
| 3:O:102:THR:HA | 3:O:103:GLY:HA3 | 1.74 | 0.45 |
| 1:C:99:TYR:CZ | 5:R:3:VAL:HG12 | 2.52 | 0.45 |
| 2:H:7:ILE:HB | 2:H:27:VAL:HG12 | 1.99 | 0.45 |
| 3:I:53:ASN:HA | 3:I:54:GLY:HA2 | 1.57 | 0.45 |
| 2:B:3:ARG:NH1 | 2:B:60:TRP:O | 2.50 | 0.45 |
| 3:E:84:ASP:HA | 3:E:85:SER:CB | 2.47 | 0.45 |
| 1:G:179:LEU:HD12 | 1:G:179:LEU:N | 2.31 | 0.45 |
| 1:G:235:PRO:HA | 1:G:241:PHE:HA | 1.98 | 0.45 |
| 4:P:159:TRP:HD1 | 4:P:209:ARG:O | 1.99 | 0.45 |
| 2:D:13:HIS:HB2 | 2:D:21:ASN:OD1 | 2.17 | 0.45 |
| 1:G:179:LEU:CD1 | 1:G:179:LEU:N | 2.80 | 0.45 |
| 1:G:81:LEU:HG | 5:U:9:VAL:CG1 | 2.47 | 0.45 |
| 4:J:194:LEU:HD23 | 4:J:195:ARG:C | 2.37 | 0.45 |
| 4:J:29:HIS:HD2 | 4:J:94:SER:C | 2.13 | 0.45 |
| 3:K:136:THR:CG2 | 3:K:171:SER:CA | 2.83 | 0.45 |
| 3:K:38:TRP:CE3 | 3:K:42:LYS:O | 2.69 | 0.45 |
| 4:L:169:GLY:C | 4:L:194:LEU:HD22 | 2.37 | 0.45 |
| 2:N:5:PRO:HD3 | 2:N:84:HIS:CD2 | 2.51 | 0.45 |
| 1:A:103:VAL:HG12 | 1:A:108:ARG:O | 2.17 | 0.45 |
| 1:C:8:PHE:HB2 | 1:C:25:VAL:HG13 | 1.99 | 0.45 |
| 2:D:70:PHE:CE1 | 2:D:72:PRO:HB3 | 2.52 | 0.45 |
| 1:G:234:ARG:NH2 | 1:G:244:TRP:HE1 | 2.15 | 0.45 |
| 1:G:81:LEU:CG | 5:U:9:VAL:HG11 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:48:PHE:CE1 | 3:I:59:LYS:HG3 | 2.41 | 0.45 |
| 4:J:120:VAL:O | 4:J:121:PHE:CG | 2.70 | 0.45 |
| 3:K:72:TYR:O | 3:K:72:TYR:CD1 | 2.70 | 0.45 |
| 3:O:161:ASP:O | 3:O:162:MET:HB3 | 2.16 | 0.45 |
| 1:A:259:CYS:HB3 | 1:A:272:LEU:HB2 | 2.00 | 0.44 |
| 2:B:46:ILE:HG13 | 2:B:47:GLU:N | 2.31 | 0.44 |
| 4:F:26:ILE:HB | 4:F:29:HIS:CD2 | 2.52 | 0.44 |
| 4:J:84:GLN:CD | 1:G:177:GLU:OE1 | 2.56 | 0.44 |
| 1:G:185:PRO:CA | 1:G:208:PHE:HB3 | 2.46 | 0.44 |
| 1:G:188:HIS:HB3 | 1:G:204:TRP:CB | 2.41 | 0.44 |
| 3:I:138:PHE:HD1 | 3:I:142:THR:OG1 | 1.95 | 0.44 |
| 4:L:154:HIS:CD2 | 4:L:215:TYR:CB | 3.01 | 0.44 |
| 4:L:70:THR:N | 4:L:75:SER:OG | 2.44 | 0.44 |
| 2:N:39:LEU:HD23 | 2:N:39:LEU:HA | 1.80 | 0.44 |
| 2:N:75:LYS:O | 2:N:76:ASP:C | 2.54 | 0.44 |
| 2:N:2:GLN:HE21 | 2:N:85:VAL:CG2 | 2.30 | 0.44 |
| 4:P:97:THR:HG22 | 4:P:98:GLN:N | 2.32 | 0.44 |
| 1:A:223:ASP:O | 1:A:225:THR:HG22 | 2.16 | 0.44 |
| 4:F:29:HIS:CE1 | 4:F:96:GLN:HG2 | 2.52 | 0.44 |
| 2:H:3:ARG:NH2 | 2:H:61:SER:HB2 | 2.32 | 0.44 |
| 2:H:72:PRO:HB2 | 2:H:78:TYR:HH | 1.81 | 0.44 |
| 4:J:48:TYR:CD1 | 4:J:99:LEU:HD11 | 2.52 | 0.44 |
| 3:K:175:TRP:CZ2 | 4:L:146:LEU:HB2 | 2.52 | 0.44 |
| 4:L:83:GLN:CG | 4:L:84:GLN:N | 2.54 | 0.44 |
| 3:O:1:ILE:HG13 | 3:O:1:ILE:O | 2.17 | 0.44 |
| 1:C:66:LYS:CD | 5:R:4:PRO:HA | 2.42 | 0.44 |
| 4:F:41:GLN:O | 4:F:42:GLY:C | 2.55 | 0.44 |
| 2:N:22:PHE:CE1 | 4:F:80:GLN:NE2 | 2.85 | 0.44 |
| 1:G:157:ARG:HG3 | 1:G:158:ALA:N | 2.31 | 0.44 |
| 1:G:82:ARG:NH2 | 1:G:89:GLU:N | 2.46 | 0.44 |
| 3:I:146:GLN:OE1 | 3:I:154:ILE:HG12 | 2.14 | 0.44 |
| 4:J:119:ASN:N | 4:J:119:ASN:OD1 | 2.50 | 0.44 |
| 4:J:177:LEU:CD1 | 4:J:177:LEU:C | 2.86 | 0.44 |
| 3:K:47:LEU:O | 3:K:48:PHE:CD1 | 2.70 | 0.44 |
| 4:L:130:PRO:HB3 | 4:L:142:THR:O | 2.16 | 0.44 |
| 1:M:66:LYS:HZ1 | 3:O:29:ASN:ND2 | 2.14 | 0.44 |
| 4:P:211:GLN:HE22 | 4:P:213:GLN:HB2 | 1.83 | 0.44 |
| 1:A:274:TRP:CE3 | 1:A:275:GLU:HB2 | 2.53 | 0.44 |
| 2:H:24:ASN:ND2 | 2:H:65:LEU:CG | 2.77 | 0.44 |
| 4:L:10:ASN:HB3 | 4:L:110:ARG:O | 2.17 | 0.44 |
| 2:N:51:HIS:HB3 | 2:N:66:TYR:CE1 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:58:SER:HA | 4:P:59:GLY:HA2 | 1.42 | 0.44 |
| 5:T:3:VAL:O | 5:T:4:PRO:C | 2.55 | 0.44 |
| 3:E:102:THR:OG1 | 3:E:102:THR:O | 2.34 | 0.44 |
| 3:E:49:VAL:HG23 | 4:F:102:THR:HG22 | 1.97 | 0.44 |
| 1:G:156:LEU:HA | 1:G:156:LEU:HD23 | 1.77 | 0.44 |
| 1:G:204:TRP:CE3 | 1:G:244:TRP:HB3 | 2.51 | 0.44 |
| 2:H:9:VAL:CG2 | 2:H:80:CYS:HB2 | 2.47 | 0.44 |
| 3:I:115:PRO:HA | 3:I:137:ASP:CG | 2.38 | 0.44 |
| 4:L:171:CYS:HB2 | 4:L:193:ARG:O | 2.17 | 0.44 |
| 1:M:189:MET:SD | 1:M:274:TRP:CZ3 | 3.10 | 0.44 |
| 1:A:49:ALA:HA | 1:A:50:PRO:HD2 | 1.77 | 0.44 |
| 1:A:98:MET:HB3 | 1:A:98:MET:HE2 | 1.49 | 0.44 |
| 1:G:116:TYR:C | 1:G:116:TYR:CD2 | 2.85 | 0.44 |
| 3:I:66:LEU:HD12 | 3:I:67:ASN:N | 2.32 | 0.44 |
| 4:J:125:VAL:O | 4:J:237:ALA:HB2 | 2.17 | 0.44 |
| 3:K:113:GLN:O | 3:K:114:ASN:C | 2.53 | 0.44 |
| 3:K:135:PHE:CZ | 3:K:192:ILE:HD13 | 2.51 | 0.44 |
| 3:K:192:ILE:O | 3:K:193:PRO:C | 2.56 | 0.44 |
| 2:B:86:THR:O | 2:B:87:LEU:HD23 | 2.18 | 0.44 |
| 4:F:230:PRO:C | 4:F:231:VAL:HG23 | 2.37 | 0.44 |
| 3:I:137:ASP:O | 3:I:138:PHE:CD2 | 2.70 | 0.44 |
| 4:L:37:GLN:HG2 | 4:L:89:VAL:H | 1.82 | 0.44 |
| 1:M:195:SER:O | 1:M:197:HIS:CE1 | 2.70 | 0.44 |
| 1:M:231:VAL:HG13 | 1:M:244:TRP:HE3 | 1.83 | 0.44 |
| 1:A:47:PRO:HB3 | 1:A:60:TRP:CH2 | 2.53 | 0.44 |
| 4:J:39:LEU:HA | 4:J:40:GLY:HA2 | 1.68 | 0.44 |
| 1:C:37:ASP:HB3 | 1:C:40:ALA:HB2 | 2.00 | 0.44 |
| 3:E:160:LEU:HD23 | 4:F:169:GLY:O | 2.18 | 0.44 |
| 4:F:172:THR:HG22 | 4:F:192:SER:HB2 | 2.00 | 0.44 |
| 4:J:196:VAL:HG12 | 4:J:197:SER:N | 2.33 | 0.44 |
| 3:O:31:TYR:HB2 | 5:T:4:PRO:HB2 | 2.00 | 0.44 |
| 4:P:45:PHE:HZ | 4:P:48:TYR:HB3 | 1.83 | 0.44 |
| 1:C:25:VAL:CG2 | 1:C:32:GLN:HE21 | 2.31 | 0.43 |
| 1:C:117:ALA:HB2 | 2:D:60:TRP:CE2 | 2.53 | 0.43 |
| 4:F:220:ASN:N | 4:F:220:ASN:OD1 | 2.51 | 0.43 |
| 1:G:133:TRP:HZ3 | 1:G:147:TRP:HZ3 | 1.65 | 0.43 |
| 1:G:16:GLY:CA | 1:G:17:ARG:CB | 2.77 | 0.43 |
| 1:G:189:MET:HE3 | 1:G:274:TRP:N | 2.33 | 0.43 |
| 4:J:120:VAL:C | 4:J:121:PHE:CG | 2.91 | 0.43 |
| 3:K:136:THR:O | 3:K:137:ASP:HB2 | 2.18 | 0.43 |
| 3:K:21:PHE:O | 3:K:74:TYR:HA | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:14:GLU:HG2 | 4:P:117:LEU:CD1 | 2.45 | 0.43 |
| 1:A:247:VAL:HG23 | 1:A:249:VAL:HG23 | 1.99 | 0.43 |
| 3:E:124:ASP:CG | 3:E:125:SER:HA | 2.37 | 0.43 |
| 4:F:135:ILE:HD13 | 4:F:201:TRP:HZ3 | 1.83 | 0.43 |
| 4:J:11:LYS:HZ1 | 4:J:217:LEU:HD22 | 1.83 | 0.43 |
| 4:J:49:PHE:CE2 | 4:J:69:ARG:HB2 | 2.53 | 0.43 |
| 4:J:84:GLN:O | 4:J:113:VAL:HG11 | 2.18 | 0.43 |
| 3:K:160:LEU:O | 3:K:168:LYS:HB3 | 2.18 | 0.43 |
| 3:K:131:SER:HA | 4:L:128:PHE:HE1 | 1.83 | 0.43 |
| 4:L:130:PRO:HG2 | 4:L:201:TRP:NE1 | 2.32 | 0.43 |
| 1:M:59:TYR:O | 1:M:63:GLU:HG2 | 2.18 | 0.43 |
| 2:D:40:LEU:HD13 | 2:D:81:ARG:H | 1.83 | 0.43 |
| 4:F:33:TYR:OH | 4:F:99:LEU:HA | 2.19 | 0.43 |
| 1:G:127:LYS:HA | 1:G:127:LYS:HD2 | 1.66 | 0.43 |
| 1:G:228:THR:HG23 | 1:G:228:THR:O | 2.18 | 0.43 |
| 4:J:120:VAL:O | 4:J:121:PHE:CD1 | 2.70 | 0.43 |
| 2:N:63:TYR:CD1 | 2:N:63:TYR:O | 2.70 | 0.43 |
| 2:N:81:ARG:CD | 2:N:92:ILE:CG1 | 2.96 | 0.43 |
| 3:O:123:ARG:O | 4:P:129:GLU:HB3 | 2.19 | 0.43 |
| 3:O:176:SER:CB | 3:O:181:PHE:O | 2.66 | 0.43 |
| 1:A:73:THR:HB | 5:Q:8:THR:HG22 | 2.01 | 0.43 |
| 1:C:188:HIS:O | 1:C:204:TRP:N | 2.42 | 0.43 |
| 3:E:53:ASN:HA | 3:E:54:GLY:HA2 | 1.63 | 0.43 |
| 4:F:149:GLY:CA | 4:F:150:PHE:HB3 | 2.35 | 0.43 |
| 1:G:191:HIS:C | 1:G:191:HIS:ND1 | 2.72 | 0.43 |
| 4:J:131:SER:O | 4:J:135:ILE:HG23 | 2.19 | 0.43 |
| 3:K:63:SER:O | 3:K:75:LEU:HD12 | 2.19 | 0.43 |
| 4:L:160:TRP:C | 4:L:161:VAL:CG2 | 2.85 | 0.43 |
| 4:L:39:LEU:HD12 | 4:L:39:LEU:HA | 1.76 | 0.43 |
| 1:M:162:GLY:O | 1:M:166:GLU:HG3 | 2.17 | 0.43 |
| 1:M:177:GLU:OE1 | 1:M:177:GLU:N | 2.51 | 0.43 |
| 4:P:64:ARG:HH11 | 4:P:64:ARG:HG2 | 1.80 | 0.43 |
| 1:A:124:ILE:HG13 | 1:A:134:THR:O | 2.19 | 0.43 |
| 4:F:218:SER:CB | 4:F:221:ASP:HB2 | 2.44 | 0.43 |
| 4:J:223:TRP:CE2 | 4:J:228:ALA:O | 2.72 | 0.43 |
| 3:O:131:SER:OG | 3:O:181:PHE:CE2 | 2.72 | 0.43 |
| 4:P:223:TRP:CE2 | 4:P:225:GLN:HG2 | 2.52 | 0.43 |
| 2:H:23:LEU:HD13 | 2:H:70:PHE:CE1 | 2.53 | 0.43 |
| 3:K:11:LEU:O | 3:K:12:HIS:ND1 | 2.51 | 0.43 |
| 4:L:120:VAL:O | 4:L:230:PRO:HG3 | 2.19 | 0.43 |
| 4:L:34:TRP:CZ3 | 4:L:92:CYS:HB2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:231:VAL:HG22 | 1:M:244:TRP:H | 1.84 | 0.43 |
| 3:O:123:ARG:HG3 | 3:O:130:LYS:O | 2.18 | 0.43 |
| 4:P:11:LYS:HG3 | 4:P:12:VAL:N | 2.33 | 0.43 |
| 4:P:160:TRP:CH2 | 4:P:234:ILE:HD11 | 2.53 | 0.43 |
| 1:C:160:LEU:O | 1:C:165:VAL:HG23 | 2.18 | 0.43 |
| 3:E:157:LYS:HB3 | 3:E:157:LYS:HE2 | 1.75 | 0.43 |
| 3:E:163:ARG:HA | 3:E:163:ARG:HD3 | 1.63 | 0.43 |
| 4:F:22:ARG:HG2 | 4:F:76:THR:HG22 | 2.01 | 0.43 |
| 1:G:214:THR:O | 1:G:214:THR:CG2 | 2.60 | 0.43 |
| 1:G:58:GLU:HA | 1:G:61:ASP:HB2 | 2.00 | 0.43 |
| 3:I:20:ASN:HA | 3:I:75:LEU:O | 2.19 | 0.43 |
| 4:J:164:LYS:HE2 | 4:J:164:LYS:HB2 | 1.87 | 0.43 |
| 3:K:21:PHE:HZ | 3:K:106:LEU:HD22 | 1.84 | 0.43 |
| 3:K:29:ASN:O | 3:K:94:THR:OG1 | 2.21 | 0.43 |
| 4:L:88:ALA:CB | 4:L:110:ARG:HG2 | 2.39 | 0.43 |
| 1:A:237:GLY:C | 1:A:239:GLY:H | 2.22 | 0.43 |
| 3:E:37:ARG:HB2 | 3:E:47:LEU:HD11 | 2.01 | 0.43 |
| 1:G:17:ARG:HH11 | 1:G:17:ARG:CG | 2.14 | 0.43 |
| 1:G:97:ARG:HE | 1:G:116:TYR:HE1 | 0.61 | 0.43 |
| 4:J:84:GLN:OE1 | 1:G:177:GLU:OE1 | 2.37 | 0.43 |
| 3:K:47:LEU:HD12 | 3:K:47:LEU:HA | 1.77 | 0.43 |
| 1:M:92:SER:OG | 1:M:92:SER:O | 2.25 | 0.43 |
| 2:N:89:GLN:O | 2:N:90:PRO:C | 2.56 | 0.43 |
| 1:A:66:LYS:CD | 5:Q:4:PRO:HA | 2.48 | 0.43 |
| 2:D:82:VAL:O | 2:D:90:PRO:CB | 2.65 | 0.43 |
| 4:F:153:ASP:CG | 4:F:176:PRO:HG3 | 2.39 | 0.43 |
| 4:F:194:LEU:HA | 4:F:194:LEU:HD12 | 1.81 | 0.43 |
| 3:I:25:PHE:HB2 | 3:I:26:PRO:HD2 | 2.01 | 0.43 |
| 3:I:2:LEU:HD23 | 3:I:3:ASN:N | 2.33 | 0.43 |
| 3:I:34:HIS:ND1 | 3:I:93:ILE:HD11 | 2.34 | 0.43 |
| 4:L:159:TRP:CE2 | 4:L:194:LEU:HG | 2.54 | 0.43 |
| 1:M:53:GLU:HA | 1:M:60:TRP:HZ2 | 1.84 | 0.43 |
| 3:O:34:HIS:NE2 | 3:O:93:ILE:HD11 | 2.33 | 0.43 |
| 1:G:97:ARG:NH1 | 5:U:7:ALA:O | 2.46 | 0.43 |
| 1:A:172:LEU:HD23 | 1:A:179:LEU:HD13 | 2.01 | 0.43 |
| 1:A:231:VAL:O | 1:A:232:GLU:C | 2.57 | 0.43 |
| 4:F:193:ARG:CG | 4:F:193:ARG:NH1 | 2.72 | 0.43 |
| 4:F:32:LEU:O | 4:F:49:PHE:N | 2.46 | 0.43 |
| 3:K:4:VAL:HG11 | 3:K:92:PHE:HB3 | 2.00 | 0.43 |
| 4:L:82:THR:HG21 | 4:L:113:VAL:HG22 | 2.00 | 0.43 |
| 1:M:256:ARG:HB3 | 6:M:301:HOH:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:53:ASN:HA | 3:O:54:GLY:HA2 | 1.66 | 0.43 |
| 1:A:228:THR:HA | 1:A:247:VAL:HG12 | 2.01 | 0.42 |
| 2:B:25:CYS:HB2 | 2:B:39:LEU:HD21 | 1.99 | 0.42 |
| 1:C:154:GLU:HB3 | 3:E:52:LEU:HD11 | 2.01 | 0.42 |
| 4:J:211:GLN:HA | 4:J:236:SER:HB3 | 2.00 | 0.42 |
| 4:J:217:LEU:O | 4:J:231:VAL:HG12 | 2.19 | 0.42 |
| 3:K:122:LEU:HG | 4:L:130:PRO:HA | 2.00 | 0.42 |
| 3:K:134:LEU:CD2 | 4:L:142:THR:HG21 | 2.49 | 0.42 |
| 1:M:59:TYR:HH | 1:M:171:TYR:HH | 1.36 | 0.42 |
| 1:M:233:THR:HG22 | 1:M:243:LYS:HD3 | 2.00 | 0.42 |
| 1:M:78:LEU:HB3 | 1:M:82:ARG:NH2 | 2.33 | 0.42 |
| 3:O:111:ASN:OD1 | 3:O:112:ILE:N | 2.43 | 0.42 |
| 3:O:63:SER:O | 3:O:75:LEU:HD12 | 2.19 | 0.42 |
| 1:A:46:GLU:HG3 | 1:A:47:PRO:HD2 | 2.00 | 0.42 |
| 3:K:111:ASN:OD1 | 3:K:112:ILE:N | 2.52 | 0.42 |
| 4:L:88:ALA:HB1 | 4:L:89:VAL:CG1 | 2.49 | 0.42 |
| 4:P:6:GLN:OE1 | 4:P:108:GLY:N | 2.52 | 0.42 |
| 1:A:77:ASP:OD1 | 5:Q:9:VAL:HG22 | 2.18 | 0.42 |
| 1:A:69:ALA:HB1 | 3:I:96:ASN:ND2 | 2.34 | 0.42 |
| 1:C:31:THR:HG23 | 1:C:209:TYR:CE1 | 2.54 | 0.42 |
| 1:C:63:GLU:OE2 | 1:C:66:LYS:NZ | 2.49 | 0.42 |
| 4:F:217:LEU:HD12 | 4:F:218:SER:N | 2.34 | 0.42 |
| 1:G:162:GLY:C | 1:G:166:GLU:OE2 | 2.58 | 0.42 |
| 1:G:162:GLY:O | 1:G:166:GLU:CD | 2.58 | 0.42 |
| 1:G:218:GLN:CB | 1:G:222:GLU:O | 2.62 | 0.42 |
| 1:G:49:ALA:HB1 | 1:G:51:TRP:NE1 | 2.35 | 0.42 |
| 4:J:231:VAL:O | 4:J:232:THR:C | 2.57 | 0.42 |
| 4:J:58:SER:OG | 4:J:58:SER:O | 2.32 | 0.42 |
| 4:L:175:GLN:HG2 | 4:L:175:GLN:H | 1.59 | 0.42 |
| 3:K:96:ASN:ND2 | 4:L:48:TYR:OH | 2.52 | 0.42 |
| 1:C:201:LEU:O | 1:C:246:ALA:HA | 2.19 | 0.42 |
| 1:G:32:GLN:O | 1:G:49:ALA:HB2 | 2.19 | 0.42 |
| 4:J:4:VAL:HG11 | 4:J:105:PHE:O | 2.19 | 0.42 |
| 4:J:151:TYR:HA | 4:J:152:PRO:HA | 1.84 | 0.42 |
| 1:M:25:VAL:HG11 | 2:N:55:SER:OG | 2.20 | 0.42 |
| 2:N:57:SER:C | 2:N:59:ASP:H | 2.15 | 0.42 |
| 1:A:128:GLU:HG2 | 1:A:128:GLU:H | 1.39 | 0.42 |
| 1:A:107:TRP:CZ2 | 1:A:172:LEU:HD13 | 2.54 | 0.42 |
| 3:E:11:LEU:HD12 | 3:E:106:LEU:HD13 | 2.01 | 0.42 |
| 3:I:146:GLN:HB3 | 3:I:147:SER:H | 1.39 | 0.42 |
| 3:I:177:ASN:OD1 | 3:I:178:LYS:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:I:11:LEU:HD12 | 3:I:21:PHE:CE1 | 2.55 | 0.42 |
| 3:I:36:TYR:N | 3:I:89:LEU:O | 2.48 | 0.42 |
| 4:L:170:VAL:CB | 4:L:194:LEU:CD2 | 2.95 | 0.42 |
| 4:L:83:GLN:O | 4:L:84:GLN:C | 2.57 | 0.42 |
| 1:M:225:THR:O | 1:M:228:THR:HG22 | 2.20 | 0.42 |
| 1:M:4:SER:OG | 1:M:6:ARG:NH1 | 2.52 | 0.42 |
| 1:A:209:TYR:CD1 | 1:A:210:PRO:HA | 2.54 | 0.42 |
| 1:A:76:VAL:O | 1:A:80:THR:HG22 | 2.20 | 0.42 |
| 3:E:167:PHE:HD2 | 3:E:168:LYS:H | 0.61 | 0.42 |
| 1:G:70:HIS:O | 1:G:74:HIS:N | 2.49 | 0.42 |
| 4:J:43:LEU:HD23 | 4:J:44:GLU:N | 2.34 | 0.42 |
| 1:M:73:THR:HG21 | 5:T:6:VAL:CG2 | 2.32 | 0.42 |
| 2:N:30:PHE:CE2 | 2:N:63:TYR:HA | 2.55 | 0.42 |
| 3:O:187:PHE:HD2 | 3:O:187:PHE:H | 1.66 | 0.42 |
| 4:P:26:ILE:HB | 4:P:29:HIS:HD2 | 1.82 | 0.42 |
| 1:A:150:ALA:HB3 | 1:A:152:VAL:HG23 | 2.01 | 0.42 |
| 1:A:75:ARG:HB2 | 1:A:75:ARG:HE | 1.74 | 0.42 |
| 1:C:192:HIS:CE1 | 1:C:202:ARG:NH1 | 2.78 | 0.42 |
| 1:C:259:CYS:HB3 | 1:C:272:LEU:HB2 | 2.00 | 0.42 |
| 1:C:35:ARG:HD2 | 2:D:53:ASP:OD1 | 2.19 | 0.42 |
| 1:G:64:THR:O | 1:G:68:LYS:HG3 | 2.20 | 0.42 |
| 4:J:15:LYS:HA | 4:J:82:THR:O | 2.19 | 0.42 |
| 3:K:115:PRO:CG | 3:K:139:ASP:OD2 | 2.68 | 0.42 |
| 3:K:193:PRO:C | 3:K:195:ASP:N | 2.72 | 0.42 |
| 3:K:94:THR:HG23 | 3:K:95:GLY:N | 2.35 | 0.42 |
| 1:C:73:THR:HG23 | 5:R:8:THR:CG2 | 2.49 | 0.42 |
| 1:A:152:VAL:HA | 1:A:155:GLN:OE1 | 2.19 | 0.42 |
| 2:B:17:ASN:HD22 | 2:B:74:GLU:CD | 2.23 | 0.42 |
| 1:C:217:TRP:HZ3 | 1:C:257:TYR:HB3 | 1.85 | 0.42 |
| 3:K:61:ARG:CG | 3:K:78:LYS:O | 2.65 | 0.42 |
| 1:M:114:HIS:HB3 | 1:M:126:LEU:HB3 | 2.02 | 0.42 |
| 2:N:11:SER:O | 2:N:13:HIS:N | 2.53 | 0.42 |
| 2:N:40:LEU:HB3 | 2:N:43:GLY:CA | 2.49 | 0.42 |
| 4:P:38:ARG:O | 4:P:41:GLN:NE2 | 2.52 | 0.42 |
| 4:P:64:ARG:HB3 | 4:P:80:GLN:O | 2.20 | 0.42 |
| 1:A:66:LYS:HD3 | 5:Q:4:PRO:HA | 2.02 | 0.42 |
| 1:A:173:GLU:HA | 1:A:176:LYS:HD3 | 2.02 | 0.42 |
| 3:E:117:PRO:HB2 | 3:E:196:THR:HA | 2.02 | 0.42 |
| 1:G:61:ASP:O | 1:G:65:ARG:HG3 | 2.20 | 0.42 |
| 3:I:47:LEU:HD12 | 3:I:47:LEU:HA | 1.90 | 0.42 |
| 4:J:238:GLU:HG3 | 4:J:239:ALA:H | 1.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:47:ILE:CD1 | 4:J:60:LEU:HD21 | 2.05 | 0.42 |
| 3:O:52:LEU:HD23 | 3:O:52:LEU:HA | 1.85 | 0.42 |
| 3:O:80:SER:N | 3:O:81:GLN:NE2 | 2.68 | 0.42 |
| 2:B:55:SER:OG | 2:B:56:PHE:N | 2.52 | 0.42 |
| 4:F:45:PHE:HZ | 4:F:48:TYR:HD2 | 1.67 | 0.42 |
| 1:G:218:GLN:HB3 | 1:G:223:ASP:OD1 | 2.20 | 0.42 |
| 3:I:63:SER:OG | 3:I:76:TYR:HB2 | 2.19 | 0.42 |
| 4:J:46:LEU:HD22 | 4:J:60:LEU:HA | 2.02 | 0.42 |
| 3:K:152:VAL:CG1 | 3:K:153:TYR:N | 2.83 | 0.42 |
| 4:L:122:PRO:HA | 4:L:123:PRO:HD3 | 1.87 | 0.42 |
| 4:L:218:SER:O | 4:L:219:GLU:HB2 | 2.20 | 0.42 |
| 1:M:142:THR:O | 1:M:146:LYS:HG3 | 2.19 | 0.42 |
| 1:M:69:ALA:O | 1:M:73:THR:OG1 | 2.29 | 0.42 |
| 3:O:176:SER:HB2 | 3:O:181:PHE:O | 2.20 | 0.42 |
| 4:P:121:PHE:HA | 4:P:122:PRO:HD3 | 1.81 | 0.42 |
| 1:C:202:ARG:HG2 | 1:C:244:TRP:NE1 | 2.28 | 0.41 |
| 2:D:84:HIS:CG | 2:D:85:VAL:H | 2.38 | 0.41 |
| 1:G:200:THR:HG21 | 1:G:202:ARG:CZ | 2.49 | 0.41 |
| 1:G:8:PHE:HB2 | 1:G:25:VAL:HG13 | 2.01 | 0.41 |
| 4:J:143:LEU:HB3 | 4:J:194:LEU:HB3 | 2.02 | 0.41 |
| 3:K:131:SER:OG | 3:K:132:VAL:N | 2.47 | 0.41 |
| 3:K:115:PRO:CB | 3:K:139:ASP:OD2 | 2.67 | 0.41 |
| 3:K:158:CYS:SG | 3:K:159:VAL:N | 2.93 | 0.41 |
| 4:L:141:ALA:N | 4:L:198:ALA:H | 2.18 | 0.41 |
| 4:L:6:GLN:HE21 | 4:L:6:GLN:HB2 | 1.64 | 0.41 |
| 1:M:219:ARG:CD | 1:M:224:GLN:NE2 | 2.70 | 0.41 |
| 2:B:74:GLU:HA | 2:B:74:GLU:OE1 | 2.20 | 0.41 |
| 2:D:28:SER:OG | 2:D:29:GLY:N | 2.53 | 0.41 |
| 4:F:203:ASN:N | 4:F:204:PRO:HD3 | 2.35 | 0.41 |
| 4:F:230:PRO:O | 4:F:231:VAL:HG23 | 2.19 | 0.41 |
| 3:I:132:VAL:HG12 | 3:I:173:VAL:HG13 | 2.01 | 0.41 |
| 4:L:88:ALA:HB1 | 4:L:110:ARG:CA | 2.46 | 0.41 |
| 1:M:197:HIS:C | 1:M:198:GLU:CG | 2.89 | 0.41 |
| 4:P:119:ASN:HB3 | 4:P:151:TYR:CE2 | 2.55 | 0.41 |
| 1:G:70:HIS:CD2 | 5:U:2:LEU:HD23 | 2.55 | 0.41 |
| 1:A:11:SER:HA | 1:A:22:PHE:HA | 2.02 | 0.41 |
| 1:A:73:THR:HG23 | 3:I:96:ASN:ND2 | 2.35 | 0.41 |
| 1:C:52:ILE:HD12 | 1:C:52:ILE:HA | 1.89 | 0.41 |
| 1:G:72:GLN:HG2 | 1:G:72:GLN:H | 1.57 | 0.41 |
| 4:J:112:LEU:HG | 4:J:113:VAL:O | 2.20 | 0.41 |
| 3:K:135:PHE:HD1 | 3:K:135:PHE:C | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:175:GLN:HA | 4:L:176:PRO:HD3 | 1.83 | 0.41 |
| 4:P:125:VAL:HG12 | 4:P:237:ALA:HB2 | 2.01 | 0.41 |
| 4:P:36:ARG:O | 4:P:44:GLU:HB2 | 2.21 | 0.41 |
| 1:A:13:SER:HB3 | 1:A:93:HIS:H | 1.85 | 0.41 |
| 1:C:218:GLN:HG2 | 1:C:260:HIS:HD2 | 1.79 | 0.41 |
| 1:C:243:LYS:HG2 | 1:C:244:TRP:N | 2.33 | 0.41 |
| 1:G:211:ALA:HB2 | 1:G:241:PHE:HE2 | 1.84 | 0.41 |
| 1:G:98:MET:CE | 1:G:99:TYR:N | 2.84 | 0.41 |
| 3:K:135:PHE:CE1 | 3:K:138:PHE:CG | 3.08 | 0.41 |
| 3:K:188:ASN:O | 3:K:189:ASN:HB2 | 2.19 | 0.41 |
| 4:L:21:LEU:HD12 | 4:L:21:LEU:N | 2.35 | 0.41 |
| 1:M:99:TYR:OH | 5:T:3:VAL:HG12 | 2.20 | 0.41 |
| 2:N:10:TYR:HE2 | 2:N:26:TYR:HB3 | 1.85 | 0.41 |
| 4:P:160:TRP:HD1 | 4:P:165:GLU:CG | 2.23 | 0.41 |
| 3:E:144:VAL:HG21 | 3:E:155:THR:O | 2.19 | 0.41 |
| 4:F:230:PRO:C | 4:F:231:VAL:CG2 | 2.88 | 0.41 |
| 4:F:51:GLY:O | 4:F:69:ARG:NH1 | 2.52 | 0.41 |
| 4:F:96:GLN:C | 4:F:97:THR:HG1 | 2.11 | 0.41 |
| 1:G:11:SER:O | 1:G:95:VAL:N | 2.53 | 0.41 |
| 1:G:266:LEU:HD23 | 1:G:266:LEU:HA | 1.77 | 0.41 |
| 1:G:268:LYS:O | 1:G:269:PRO:C | 2.58 | 0.41 |
| 4:J:134:GLU:HA | 4:J:137:HIS:HB2 | 2.01 | 0.41 |
| 3:K:193:PRO:C | 3:K:195:ASP:H | 2.23 | 0.41 |
| 4:L:33:TYR:O | 4:L:92:CYS:HA | 2.21 | 0.41 |
| 1:M:128:GLU:H | 1:M:128:GLU:CD | 2.15 | 0.41 |
| 1:M:203:CYS:CB | 1:M:217:TRP:HE1 | 2.31 | 0.41 |
| 1:M:234:ARG:HE | 1:M:234:ARG:HB2 | 1.62 | 0.41 |
| 3:O:30:PHE:CD2 | 3:O:68:THR:HG22 | 2.55 | 0.41 |
| 3:O:80:SER:C | 3:O:81:GLN:NE2 | 2.73 | 0.41 |
| 3:O:85:SER:OG | 3:O:108:VAL:HG22 | 2.20 | 0.41 |
| 1:A:52:ILE:HD13 | 1:A:60:TRP:CH2 | 2.55 | 0.41 |
| 1:A:242:GLN:NE2 | 2:B:12:ARG:O | 2.46 | 0.41 |
| 1:C:185:PRO:HD2 | 1:C:266:LEU:HG | 2.03 | 0.41 |
| 3:E:125:SER:HB3 | 3:E:126:LYS:HD2 | 2.03 | 0.41 |
| 3:E:136:THR:N | 3:E:138:PHE:HE1 | 2.18 | 0.41 |
| 4:F:140:LYS:HD3 | 4:F:197:SER:HA | 2.02 | 0.41 |
| 1:G:157:ARG:CG | 1:G:158:ALA:N | 2.83 | 0.41 |
| 1:G:262:GLN:HA | 1:G:269:PRO:HB3 | 2.01 | 0.41 |
| 1:G:64:THR:HG22 | 1:G:68:LYS:CE | 2.51 | 0.41 |
| 4:L:154:HIS:O | 4:L:215:TYR:HD2 | 2.02 | 0.41 |
| 1:M:96:GLN:HE21 | 2:N:31:HIS:HE1 | 1.66 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:3:ARG:O | 2:H:30:PHE:HA | 2.20 | 0.41 |
| 3:K:155:THR:O | 3:K:172:ALA:HB1 | 2.20 | 0.41 |
| 3:K:95:GLY:O | 3:K:96:ASN:HB3 | 2.20 | 0.41 |
| 1:M:102:ASP:HB2 | 1:M:111:ARG:CG | 2.51 | 0.41 |
| 1:M:95:VAL:HG22 | 1:M:118:TYR:HD1 | 1.84 | 0.41 |
| 2:N:7:ILE:HA | 2:N:27:VAL:HG12 | 2.03 | 0.41 |
| 4:P:13:THR:HB | 4:P:17:LYS:HZ2 | 1.85 | 0.41 |
| 4:P:29:HIS:ND1 | 4:P:96:GLN:HA | 2.36 | 0.41 |
| 1:C:82:ARG:HD3 | 1:C:89:GLU:HA | 2.03 | 0.41 |
| 1:C:92:SER:O | 1:C:93:HIS:HD2 | 2.04 | 0.41 |
| 4:F:124:GLU:N | 4:F:148:THR:O | 2.48 | 0.41 |
| 4:F:60:LEU:HA | 4:F:61:PRO:HD3 | 1.97 | 0.41 |
| 1:G:33:PHE:CD1 | 1:G:34:VAL:HG13 | 2.56 | 0.41 |
| 3:I:188:ASN:ND2 | 3:I:192:ILE:CD1 | 2.83 | 0.41 |
| 3:I:76:TYR:CD1 | 3:I:76:TYR:N | 2.88 | 0.41 |
| 3:K:11:LEU:HG | 3:K:21:PHE:HE2 | 1.85 | 0.41 |
| 3:K:136:THR:HA | 3:K:138:PHE:CE2 | 2.55 | 0.41 |
| 4:L:225:GLN:HB3 | 4:L:226:ASP:H | 1.67 | 0.41 |
| 1:A:248:VAL:HG21 | 6:A:303:HOH:O | 2.21 | 0.41 |
| 1:C:200:THR:HA | 1:C:247:VAL:O | 2.21 | 0.41 |
| 1:G:230:LEU:HA | 1:G:230:LEU:HD12 | 1.83 | 0.41 |
| 1:G:259:CYS:C | 1:G:260:HIS:HD1 | 2.23 | 0.41 |
| 1:G:82:ARG:HH21 | 1:G:89:GLU:CA | 2.31 | 0.41 |
| 3:I:121:GLN:C | 3:I:132:VAL:O | 2.59 | 0.41 |
| 4:J:4:VAL:CG1 | 4:J:106:GLY:HA2 | 2.51 | 0.41 |
| 3:K:116:ASP:OD1 | 3:K:137:ASP:OD2 | 2.39 | 0.41 |
| 3:K:79:GLY:O | 3:K:81:GLN:HG2 | 2.21 | 0.41 |
| 1:M:49:ALA:HB1 | 1:M:51:TRP:NE1 | 2.36 | 0.41 |
| 1:A:23:ILE:HD12 | 2:B:54:LEU:HB3 | 2.02 | 0.41 |
| 4:F:154:HIS:CD2 | 4:F:154:HIS:N | 2.88 | 0.41 |
| 1:G:97:ARG:CZ | 1:G:116:TYR:HE1 | 2.21 | 0.41 |
| 1:G:134:THR:HG23 | 1:G:134:THR:O | 2.20 | 0.41 |
| 1:G:192:HIS:HD2 | 1:G:202:ARG:CD | 2.34 | 0.41 |
| 3:K:35:TRP:O | 3:K:47:LEU:CB | 2.69 | 0.41 |
| 4:L:90:TYR:HB2 | 4:L:109:THR:CG2 | 2.49 | 0.41 |
| 2:N:22:PHE:HE1 | 4:F:80:GLN:NE2 | 2.19 | 0.41 |
| 4:P:45:PHE:CZ | 4:P:48:TYR:HB3 | 2.56 | 0.41 |
| 5:R:2:LEU:N | 5:R:2:LEU:HD12 | 2.36 | 0.41 |
| 1:A:45:MET:HG2 | 1:A:67:VAL:HG11 | 2.03 | 0.41 |
| 1:A:93:HIS:CB | 1:A:119:ASP:OD1 | 2.67 | 0.41 |
| 4:F:8:PRO:O | 4:F:109:THR:HG22 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:F:35:TYR:HB3 | 4:F:43:LEU:HD21 | 2.02 | 0.41 |
| 1:G:235:PRO:HG2 | 2:H:65:LEU:HD12 | 2.03 | 0.41 |
| 3:I:133:CYS:SG | 3:I:182:ALA:O | 2.79 | 0.41 |
| 1:M:222:GLU:H | 1:M:222:GLU:HG3 | 1.70 | 0.41 |
| 1:M:22:PHE:CD1 | 1:M:71:SER:HA | 2.56 | 0.41 |
| 1:M:66:LYS:CE | 3:O:29:ASN:CG | 2.88 | 0.41 |
| 4:P:200:PHE:HA | 4:P:200:PHE:HD1 | 1.74 | 0.41 |
| 4:P:206:ASN:HD22 | 4:P:240:TRP:C | 2.24 | 0.41 |
| 1:A:31:THR:HG23 | 1:A:209:TYR:CE1 | 2.56 | 0.40 |
| 1:C:231:VAL:O | 1:C:243:LYS:HE2 | 2.22 | 0.40 |
| 2:D:27:VAL:HG23 | 2:D:30:PHE:HE2 | 1.86 | 0.40 |
| 4:F:87:SER:HA | 4:F:111:LEU:O | 2.21 | 0.40 |
| 1:G:35:ARG:HH21 | 1:G:48:ARG:NE | 2.18 | 0.40 |
| 2:H:65:LEU:HD23 | 2:H:66:TYR:N | 2.36 | 0.40 |
| 2:H:7:ILE:HD12 | 2:H:82:VAL:CG1 | 2.51 | 0.40 |
| 4:J:129:GLU:HA | 4:J:130:PRO:HD3 | 1.89 | 0.40 |
| 4:J:69:ARG:NH1 | 4:J:73:SER:O | 2.55 | 0.40 |
| 4:J:50:GLN:NE2 | 4:J:97:THR:O | 2.54 | 0.40 |
| 3:K:185:ASN:HB2 | 3:K:188:ASN:CB | 2.50 | 0.40 |
| 4:L:97:THR:CB | 4:L:98:GLN:NE2 | 2.84 | 0.40 |
| 1:M:167:TRP:CZ3 | 1:M:170:ARG:HD3 | 2.56 | 0.40 |
| 2:N:37:VAL:HG21 | 2:N:66:TYR:CD2 | 2.56 | 0.40 |
| 3:O:121:GLN:HA | 3:O:132:VAL:O | 2.21 | 0.40 |
| 1:A:177:GLU:HG2 | 1:A:178:THR:N | 2.36 | 0.40 |
| 1:C:121:LYS:HD2 | 1:C:121:LYS:HA | 1.73 | 0.40 |
| 1:C:202:ARG:HG2 | 1:C:244:TRP:CD1 | 2.56 | 0.40 |
| 1:C:35:ARG:NH1 | 2:D:53:ASP:OD1 | 2.45 | 0.40 |
| 3:I:146:GLN:NE2 | 3:I:154:ILE:HG21 | 2.37 | 0.40 |
| 3:K:161:ASP:OD1 | 3:K:168:LYS:HB3 | 2.21 | 0.40 |
| 3:K:87:THR:HA | 3:K:105:SER:HA | 2.03 | 0.40 |
| 4:L:124:GLU:O | 4:L:147:ALA:HA | 2.20 | 0.40 |
| 4:L:88:ALA:HB2 | 4:L:111:LEU:N | 2.37 | 0.40 |
| 3:O:166:ASP:O | 3:O:167:PHE:C | 2.58 | 0.40 |
| 1:A:9:PHE:N | 1:A:97:ARG:O | 2.48 | 0.40 |
| 1:C:73:THR:HG23 | 5:R:8:THR:HG22 | 2.03 | 0.40 |
| 2:D:54:LEU:C | 2:D:54:LEU:HD23 | 2.41 | 0.40 |
| 1:G:2:SER:HA | 1:G:103:VAL:O | 2.21 | 0.40 |
| 2:H:71:THR:OG1 | 2:H:72:PRO:CD | 2.66 | 0.40 |
| 3:K:187:PHE:O | 3:K:190:SER:OG | 2.37 | 0.40 |
| 4:L:161:VAL:CG1 | 4:L:162:ASN:N | 2.84 | 0.40 |
| 1:M:79:GLY:O | 1:M:82:ARG:HB2 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:11:SER:HB3 | 2:N:95:TRP:CZ2 | 2.56 | 0.40 |
| 3:O:53:ASN:HB2 | 3:O:68:THR:H | 1.87 | 0.40 |
| 1:A:70:HIS:NE2 | 5:Q:6:VAL:HG13 | 2.35 | 0.40 |
| 1:A:216:THR:OG1 | 1:A:217:TRP:N | 2.54 | 0.40 |
| 1:A:29:ASP:HB3 | 1:A:30:ASP:H | 1.61 | 0.40 |
| 1:A:13:SER:HB3 | 1:A:93:HIS:N | 2.36 | 0.40 |
| 2:B:33:SER:HB3 | 2:B:62:PHE:CD2 | 2.56 | 0.40 |
| 3:E:136:THR:C | 3:E:138:PHE:CD1 | 2.95 | 0.40 |
| 3:E:61:ARG:HH12 | 3:E:81:GLN:HB3 | 1.86 | 0.40 |
| 2:H:57:SER:O | 2:H:58:LYS:C | 2.60 | 0.40 |
| 1:A:69:ALA:O | 3:I:96:ASN:ND2 | 2.54 | 0.40 |
| 4:J:98:GLN:NE2 | 4:J:98:GLN:CA | 2.82 | 0.40 |
| 3:K:136:THR:HG22 | 3:K:171:SER:CB | 2.43 | 0.40 |
| 3:K:35:TRP:O | 3:K:36:TYR:HD1 | 2.04 | 0.40 |
| 1:M:185:PRO:HD2 | 1:M:266:LEU:HD11 | 2.03 | 0.40 |
| 1:M:217:TRP:CZ3 | 1:M:247:VAL:HG22 | 2.56 | 0.40 |
| 1:C:231:VAL:CG1 | 1:C:244:TRP:CE3 | 3.00 | 0.40 |
| 3:E:66:LEU:HD23 | 3:E:67:ASN:N | 2.36 | 0.40 |
| 4:F:36:ARG:HD2 | 4:F:90:TYR:CZ | 2.56 | 0.40 |
| 4:F:36:ARG:HH11 | 4:F:46:LEU:HD21 | 1.87 | 0.40 |
| 1:G:187:THR:CB | 1:G:272:LEU:HD21 | 2.35 | 0.40 |
| 1:G:4:SER:O | 1:G:29:ASP:N | 2.42 | 0.40 |
| 1:G:27:TYR:HE2 | 2:H:55:SER:HG | 1.64 | 0.40 |
| 3:K:136:THR:CG2 | 3:K:171:SER:HB3 | 2.50 | 0.40 |
| 4:P:151:TYR:CD1 | 4:P:152:PRO:HA | 2.57 | 0.40 |

All (5) 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 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 3:K:12:HIS:ND1 | 3:O:10:SER:OG[1_556] | 1.92 | 0.28 |
| 3:K:12:HIS:CG | 3:O:10:SER:OG[1_556] | 2.00 | 0.20 |
| 3:K:189:ASN:OD1 | 4:P:181:PRO:CG[1_556] | 2.09 | 0.11 |
| 3:I:10:SER:OG | 3:I:12:HIS:ND1[3_655] | 2.14 | 0.06 |
| 3:K:189:ASN:OD1 | 4:P:181:PRO:CD[1_556] | 2.17 | 0.03 |

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 | A | 272/276 (99%) | 255 (94%) | 17 (6%) | 0 | 100 | 100 |
| 1 | C | 272/276 (99%) | 248 (91%) | 23 (8%) | 1 (0%) | 38 | 77 |
| 1 | G | 264/276 (96%) | 239 (90%) | 25 (10%) | 0 | 100 | 100 |
| 1 | M | 271/276 (98%) | 242 (89%) | 29 (11%) | 0 | 100 | 100 |
| 2 | B | 97/100 (97%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 2 | D | 98/100 (98%) | 85 (87%) | 13 (13%) | 0 | 100 | 100 |
| 2 | H | 92/100 (92%) | 82 (89%) | 9 (10%) | 1 (1%) | 17 | 58 |
| 2 | N | 98/100 (98%) | 85 (87%) | 13 (13%) | 0 | 100 | 100 |
| 3 | E | 179/205 (87%) | 152 (85%) | 26 (14%) | 1 (1%) | 28 | 70 |
| 3 | I | 175/205 (85%) | 137 (78%) | 37 (21%) | 1 (1%) | 28 | 70 |
| 3 | K | 188/205 (92%) | 158 (84%) | 26 (14%) | 4 (2%) | 8 | 45 |
| 3 | O | 181/205 (88%) | 160 (88%) | 20 (11%) | 1 (1%) | 28 | 70 |
| 4 | F | 234/245 (96%) | 197 (84%) | 34 (14%) | 3 (1%) | 14 | 55 |
| 4 | J | 214/245 (87%) | 185 (86%) | 28 (13%) | 1 (0%) | 32 | 73 |
| 4 | L | 214/245 (87%) | 183 (86%) | 29 (14%) | 2 (1%) | 20 | 63 |
| 4 | P | 227/245 (93%) | 192 (85%) | 32 (14%) | 3 (1%) | 14 | 55 |
| 5 | Q | 7/9 (78%) | 5 (71%) | 2 (29%) | 0 | 100 | 100 |
| 5 | R | 7/9 (78%) | 6 (86%) | 1 (14%) | 0 | 100 | 100 |
| 5 | T | 7/9 (78%) | 6 (86%) | 1 (14%) | 0 | 100 | 100 |
| 5 | U | 7/9 (78%) | 6 (86%) | 1 (14%) | 0 | 100 | 100 |
| All | All | 3104/3340 (93%) | 2707 (87%) | 379 (12%) | 18 (1%) | 28 | 70 |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 122 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | J | 114 | LEU |
| 3 | K | 147 | SER |
| 3 | K | 150 | SER |
| 4 | L | 174 | PRO |
| 4 | P | 229 | LYS |
| 4 | F | 181 | PRO |
| 3 | K | 153 | TYR |
| 3 | O | 178 | LYS |
| 3 | E | 190 | SER |
| 4 | P | 139 | GLN |
| 2 | H | 71 | THR |
| 3 | K | 115 | PRO |
| 4 | P | 119 | ASN |
| 4 | L | 203 | ASN |
| 1 | C | 235 | PRO |
| 4 | F | 203 | ASN |
| 4 | F | 180 | GLN |

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 | A | 231/232 (100%) | 226 (98%) | 5 (2%) | 57 | 83 |
| 1 | C | 231/232 (100%) | 221 (96%) | 10 (4%) | 33 | 70 |
| 1 | G | 226/232 (97%) | 216 (96%) | 10 (4%) | 33 | 69 |
| 1 | M | 225/232 (97%) | 216 (96%) | 9 (4%) | 36 | 71 |
| 2 | B | 93/95 (98%) | 92 (99%) | 1 (1%) | 78 | 91 |
| 2 | D | 93/95 (98%) | 88 (95%) | 5 (5%) | 26 | 63 |
| 2 | H | 86/95 (90%) | 83 (96%) | 3 (4%) | 41 | 75 |
| 2 | N | 92/95 (97%) | 90 (98%) | 2 (2%) | 57 | 83 |
| 3 | E | 158/185 (85%) | 145 (92%) | 13 (8%) | 13 | 47 |
| 3 | I | 155/185 (84%) | 145 (94%) | 10 (6%) | 20 | 58 |
| 3 | K | 158/185 (85%) | 140 (89%) | 18 (11%) | 7 | 31 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 3 | O | 159/185 (86%) | 145 (91%) | 14 (9%) | 12 | 44 |
| 4 | F | 198/212 (93%) | 184 (93%) | 14 (7%) | 17 | 54 |
| 4 | J | 189/212 (89%) | 176 (93%) | 13 (7%) | 18 | 55 |
| 4 | L | 174/212 (82%) | 162 (93%) | 12 (7%) | 18 | 55 |
| 4 | P | 189/212 (89%) | 178 (94%) | 11 (6%) | 23 | 61 |
| 5 | Q | 8/8 (100%) | 7 (88%) | 1 (12%) | 5 | 27 |
| 5 | R | 8/8 (100%) | 8 (100%) | 0 | 100 | 100 |
| 5 | T | 8/8 (100%) | 7 (88%) | 1 (12%) | 5 | 27 |
| 5 | U | 8/8 (100%) | 8 (100%) | 0 | 100 | 100 |
| All | All | 2689/2928 (92%) | 2537 (94%) | 152 (6%) | 24 | 61 |

All (152) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | ARG |
| 1 | A | 98 | MET |
| 1 | A | 113 | TYR |
| 1 | A | 119 | ASP |
| 1 | A | 230 | LEU |
| 2 | B | 54 | LEU |
| 3 | I | 14 | GLN |
| 3 | I | 15 | GLU |
| 3 | I | 39 | GLU |
| 3 | I | 78 | LYS |
| 3 | I | 80 | SER |
| 3 | I | 81 | GLN |
| 3 | I | 131 | SER |
| 3 | I | 133 | CYS |
| 3 | I | 138 | PHE |
| 3 | I | 179 | SER |
| 4 | J | 29 | HIS |
| 4 | J | 60 | LEU |
| 4 | J | 84 | GLN |
| 4 | J | 97 | THR |
| 4 | J | 114 | LEU |
| 4 | J | 120 | VAL |
| 4 | J | 167 | HIS |
| 4 | J | 177 | LEU |
| 4 | J | 201 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | J | 205 | ARG |
| 4 | J | 223 | TRP |
| 4 | J | 229 | LYS |
| 4 | J | 230 | PRO |
| 5 | Q | 5 | MET |
| 1 | G | 29 | ASP |
| 1 | G | 48 | ARG |
| 1 | G | 58 | GLU |
| 1 | G | 98 | MET |
| 1 | G | 116 | TYR |
| 1 | G | 160 | LEU |
| 1 | G | 161 | GLU |
| 1 | G | 186 | LYS |
| 1 | G | 191 | HIS |
| 1 | G | 268 | LYS |
| 2 | H | 23 | LEU |
| 2 | H | 80 | CYS |
| 2 | H | 81 | ARG |
| 3 | K | 43 | SER |
| 3 | K | 52 | LEU |
| 3 | K | 61 | ARG |
| 3 | K | 70 | GLU |
| 3 | K | 80 | SER |
| 3 | K | 102 | THR |
| 3 | K | 112 | ILE |
| 3 | K | 135 | PHE |
| 3 | K | 137 | ASP |
| 3 | K | 145 | SER |
| 3 | K | 148 | LYS |
| 3 | K | 149 | ASP |
| 3 | K | 155 | THR |
| 3 | K | 157 | LYS |
| 3 | K | 168 | LYS |
| 3 | K | 169 | SER |
| 3 | K | 178 | LYS |
| 3 | K | 180 | ASP |
| 4 | L | 6 | GLN |
| 4 | L | 9 | SER |
| 4 | L | 85 | GLU |
| 4 | L | 118 | LYS |
| 4 | L | 143 | LEU |
| 4 | L | 145 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | L | 148 | THR |
| 4 | L | 150 | PHE |
| 4 | L | 159 | TRP |
| 4 | L | 193 | ARG |
| 4 | L | 217 | LEU |
| 4 | L | 238 | GLU |
| 1 | M | 17 | ARG |
| 1 | M | 88 | SER |
| 1 | M | 155 | GLN |
| 1 | M | 196 | ASP |
| 1 | M | 197 | HIS |
| 1 | M | 222 | GLU |
| 1 | M | 266 | LEU |
| 1 | M | 272 | LEU |
| 1 | M | 274 | TRP |
| 2 | N | 59 | ASP |
| 2 | N | 70 | PHE |
| 3 | O | 69 | LYS |
| 3 | O | 80 | SER |
| 3 | O | 116 | ASP |
| 3 | O | 134 | LEU |
| 3 | O | 138 | PHE |
| 3 | O | 140 | SER |
| 3 | O | 156 | ASP |
| 3 | O | 164 | SER |
| 3 | O | 166 | ASP |
| 3 | O | 168 | LYS |
| 3 | O | 170 | ASN |
| 3 | O | 179 | SER |
| 3 | O | 187 | PHE |
| 3 | O | 188 | ASN |
| 4 | P | 5 | SER |
| 4 | P | 64 | ARG |
| 4 | P | 68 | GLU |
| 4 | P | 97 | THR |
| 4 | P | 154 | HIS |
| 4 | P | 167 | HIS |
| 4 | P | 171 | CYS |
| 4 | P | 179 | GLU |
| 4 | P | 191 | SER |
| 4 | P | 226 | ASP |
| 4 | P | 227 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | T | 2 | LEU |
| 1 | C | 35 | ARG |
| 1 | C | 48 | ARG |
| 1 | C | 61 | ASP |
| 1 | C | 113 | TYR |
| 1 | C | 119 | ASP |
| 1 | C | 131 | ARG |
| 1 | C | 188 | HIS |
| 1 | C | 192 | HIS |
| 1 | C | 226 | GLN |
| 1 | C | 227 | ASP |
| 2 | D | 45 | ARG |
| 2 | D | 53 | ASP |
| 2 | D | 89 | GLN |
| 2 | D | 90 | PRO |
| 2 | D | 91 | LYS |
| 3 | E | 21 | PHE |
| 3 | E | 40 | THR |
| 3 | E | 83 | GLU |
| 3 | E | 85 | SER |
| 3 | E | 136 | THR |
| 3 | E | 137 | ASP |
| 3 | E | 138 | PHE |
| 3 | E | 161 | ASP |
| 3 | E | 167 | PHE |
| 3 | E | 178 | LYS |
| 3 | E | 179 | SER |
| 3 | E | 180 | ASP |
| 3 | E | 183 | CYS |
| 4 | F | 39 | LEU |
| 4 | F | 49 | PHE |
| 4 | F | 160 | TRP |
| 4 | F | 170 | VAL |
| 4 | F | 185 | ASP |
| 4 | F | 193 | ARG |
| 4 | F | 195 | ARG |
| 4 | F | 201 | TRP |
| 4 | F | 217 | LEU |
| 4 | F | 220 | ASN |
| 4 | F | 222 | GLU |
| 4 | F | 225 | GLN |
| 4 | F | 238 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | F | 240 | TRP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 96 | ASN |
| 3 | I | 188 | ASN |
| 4 | J | 29 | HIS |
| 4 | J | 119 | ASN |
| 4 | J | 154 | HIS |
| 1 | G | 93 | HIS |
| 1 | G | 192 | HIS |
| 3 | K | 188 | ASN |
| 4 | L | 220 | ASN |
| 1 | M | 93 | HIS |
| 1 | M | 96 | GLN |
| 2 | N | 2 | GLN |
| 2 | N | 13 | HIS |
| 2 | N | 31 | HIS |
| 4 | P | 83 | GLN |
| 4 | P | 225 | GLN |
| 1 | C | 70 | HIS |
| 3 | E | 97 | GLN |
| 4 | F | 29 | HIS |
| 4 | F | 83 | GLN |
| 4 | F | 98 | GLN |
| 4 | F | 154 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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 | A | 274/276 (99%) | -0.18 | 0 100 100 | 33, 56, 82, 107 | 0 |
| 1 | C | 274/276 (99%) | -0.21 | 1 (0%) 92 89 | 35, 51, 83, 100 | 0 |
| 1 | G | 270/276 (97%) | 0.06 | 6 (2%) 62 53 | 57, 80, 102, 122 | 0 |
| 1 | M | 273/276 (98%) | 0.05 | 4 (1%) 74 66 | 51, 77, 111, 119 | 0 |
| 2 | B | 99/100 (99%) | 0.05 | 3 (3%) 51 42 | 45, 72, 108, 123 | 0 |
| 2 | D | 100/100 (100%) | -0.07 | 0 100 100 | 40, 66, 90, 113 | 0 |
| 2 | H | 96/100 (96%) | 0.19 | 2 (2%) 64 56 | 59, 88, 110, 115 | 0 |
| 2 | N | 100/100 (100%) | 0.17 | 2 (2%) 65 57 | 57, 87, 107, 116 | 0 |
| 3 | E | 187/205 (91%) | -0.06 | 3 (1%) 72 64 | 36, 63, 114, 131 | 0 |
| 3 | I | 185/205 (90%) | -0.05 | 3 (1%) 72 64 | 41, 72, 115, 126 | 0 |
| 3 | K | 192/205 (93%) | 0.35 | 16 (8%) 12 12 | 55, 89, 129, 140 | 0 |
| 3 | O | 187/205 (91%) | 0.13 | 8 (4%) 36 29 | 58, 91, 134, 151 | 0 |
| 4 | F | 238/245 (97%) | 0.05 | 2 (0%) 86 79 | 38, 80, 125, 132 | 0 |
| 4 | J | 226/245 (92%) | 0.16 | 7 (3%) 49 41 | 25, 88, 129, 141 | 0 |
| 4 | L | 226/245 (92%) | 0.30 | 2 (0%) 84 77 | 74, 106, 127, 136 | 0 |
| 4 | P | 235/245 (95%) | 0.32 | 19 (8%) 13 12 | 50, 95, 133, 154 | 0 |
| 5 | Q | 9/9 (100%) | 0.09 | 0 100 100 | 43, 48, 51, 53 | 0 |
| 5 | R | 9/9 (100%) | -0.18 | 0 100 100 | 40, 41, 44, 46 | 0 |
| 5 | T | 9/9 (100%) | 0.03 | 0 100 100 | 59, 63, 71, 72 | 0 |
| 5 | U | 9/9 (100%) | 0.16 | 0 100 100 | 63, 67, 72, 73 | 0 |
| All | All | 3198/3340 (95%) | 0.07 | 78 (2%) 59 50 | 25, 79, 122, 154 | 0 |

All (78) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | K | 134 | LEU | 6.4 |
| 3 | K | 127 | SER | 6.1 |
| 3 | K | 128 | SER | 5.0 |
| 4 | P | 190 | LEU | 5.0 |
| 3 | K | 172 | ALA | 4.7 |
| 3 | K | 129 | ASP | 4.3 |
| 4 | P | 144 | VAL | 4.0 |
| 4 | P | 206 | ASN | 3.8 |
| 4 | L | 194 | LEU | 3.7 |
| 3 | O | 136 | THR | 3.7 |
| 4 | P | 215 | TYR | 3.7 |
| 3 | K | 135 | PHE | 3.6 |
| 4 | J | 239 | ALA | 3.5 |
| 3 | K | 133 | CYS | 3.5 |
| 3 | K | 143 | ASN | 3.4 |
| 3 | E | 190 | SER | 3.4 |
| 4 | J | 144 | VAL | 3.3 |
| 3 | O | 173 | VAL | 3.3 |
| 3 | K | 173 | VAL | 3.2 |
| 3 | O | 134 | LEU | 3.2 |
| 4 | P | 169 | GLY | 3.2 |
| 1 | M | 188 | HIS | 3.1 |
| 3 | O | 114 | ASN | 3.1 |
| 4 | J | 162 | ASN | 3.1 |
| 4 | P | 126 | ALA | 3.0 |
| 2 | H | 71 | THR | 3.0 |
| 3 | I | 118 | ALA | 2.9 |
| 4 | P | 142 | THR | 2.9 |
| 4 | J | 208 | PHE | 2.9 |
| 3 | K | 118 | ALA | 2.8 |
| 3 | K | 174 | ALA | 2.8 |
| 3 | K | 126 | LYS | 2.7 |
| 4 | P | 208 | PHE | 2.7 |
| 2 | B | 40 | LEU | 2.7 |
| 3 | E | 134 | LEU | 2.7 |
| 1 | G | 190 | THR | 2.6 |
| 3 | O | 121 | GLN | 2.5 |
| 4 | P | 131 | SER | 2.5 |
| 4 | F | 194 | LEU | 2.5 |
| 4 | P | 132 | GLU | 2.5 |
| 1 | M | 270 | LEU | 2.5 |
| 3 | I | 134 | LEU | 2.5 |
| 4 | J | 195 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 205 | ALA | 2.4 |
| 3 | I | 172 | ALA | 2.4 |
| 1 | G | 274 | TRP | 2.4 |
| 4 | P | 37 | GLN | 2.4 |
| 4 | P | 104 | TYR | 2.3 |
| 1 | G | 92 | SER | 2.3 |
| 3 | O | 133 | CYS | 2.3 |
| 4 | P | 189 | ALA | 2.3 |
| 4 | P | 145 | CYS | 2.3 |
| 1 | M | 224 | GLN | 2.3 |
| 2 | N | 83 | ASN | 2.3 |
| 4 | P | 214 | PHE | 2.3 |
| 3 | O | 170 | ASN | 2.2 |
| 4 | J | 152 | PRO | 2.2 |
| 4 | F | 143 | LEU | 2.2 |
| 4 | L | 209 | ARG | 2.2 |
| 4 | P | 210 | CYS | 2.2 |
| 3 | E | 170 | ASN | 2.2 |
| 2 | B | 16 | GLU | 2.2 |
| 3 | K | 91 | ALA | 2.2 |
| 2 | H | 66 | TYR | 2.2 |
| 1 | G | 272 | LEU | 2.2 |
| 4 | J | 177 | LEU | 2.1 |
| 4 | P | 105 | PHE | 2.1 |
| 2 | N | 2 | GLN | 2.1 |
| 4 | P | 125 | VAL | 2.1 |
| 2 | B | 15 | ALA | 2.1 |
| 1 | M | 187 | THR | 2.0 |
| 1 | G | 185 | PRO | 2.0 |
| 3 | K | 180 | ASP | 2.0 |
| 1 | C | 17 | ARG | 2.0 |
| 3 | K | 192 | ILE | 2.0 |
| 3 | K | 175 | TRP | 2.0 |
| 3 | O | 175 | TRP | 2.0 |
| 4 | P | 143 | LEU | 2.0 |

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.