



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:59 am GMT

PDB ID : 1K83
Title : Crystal Structure of Yeast RNA Polymerase II Complexed with the Inhibitor Alpha Amanitin
Authors : Bushnell, D.A.; Cramer, P.; Kornberg, R.D.
Deposited on : 2001-10-22
Resolution : 2.80 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 |
| Mogul | : | 1.7.2 (RC1), CSD as538be (2017) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | trunk28620 |
| 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) | : | recalc28949 |

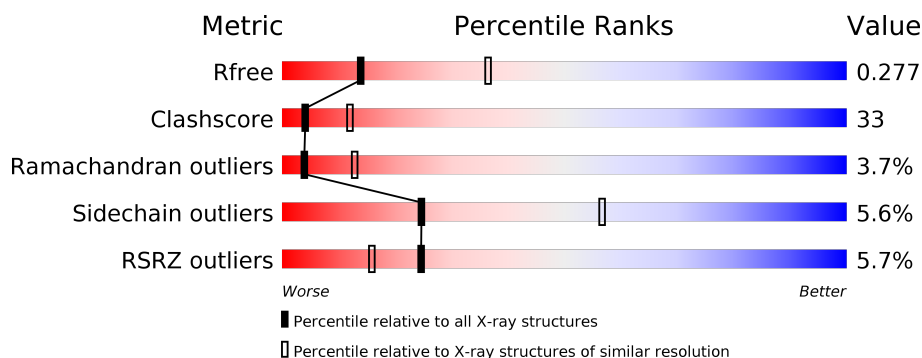
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 | 2583 (2.80-2.80) |
| Clashscore | 112137 | 3033 (2.80-2.80) |
| Ramachandran outliers | 110173 | 2983 (2.80-2.80) |
| Sidechain outliers | 110143 | 2985 (2.80-2.80) |
| RSRZ outliers | 101464 | 2610 (2.80-2.80) |

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 | 1733 | <div> <div>4%</div> <div> <div>40%</div> <div>33%</div> <div>5%</div> <div>21%</div> </div> </div> |
| 2 | B | 1224 | <div> <div>6%</div> <div> <div>47%</div> <div>38%</div> <div>•</div> <div>12%</div> </div> </div> |
| 3 | C | 318 | <div> <div>%</div> <div> <div>36%</div> <div>43%</div> <div>•</div> <div>16%</div> </div> </div> |
| 4 | E | 215 | <div> <div>3%</div> <div> <div>56%</div> <div>39%</div> <div>5%</div> <div>•</div> </div> </div> |
| 5 | F | 155 | <div> <div>%</div> <div> <div>25%</div> <div>27%</div> <div>•</div> <div>46%</div> </div> </div> |
| 6 | H | 146 | <div> <div>21%</div> <div> <div>31%</div> <div>50%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 7 | I | 122 | <div><div></div><div>4%</div><div>48%</div><div>45%</div><div>7%</div></div> |
| 8 | J | 70 | <div><div></div><div>%</div><div>47%</div><div>43%</div><div>7%</div></div> |
| 9 | K | 120 | <div><div></div><div>3%</div><div>43%</div><div>43%</div><div>9%</div><div>5%</div></div> |
| 10 | L | 70 | <div><div></div><div>14%</div><div>13%</div><div>39%</div><div>13%</div><div>36%</div></div> |
| 11 | M | 8 | <div><div></div><div>50%</div><div>38%</div><div>13%</div></div> |

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27902 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 DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1366 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10751 | 6785 | 1871 | 2036 | 59 | | | |

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | B | 1082 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8616 | 5467 | 1503 | 1594 | 52 | | | |

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 266 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2095 | 1317 | 348 | 417 | 13 | | | |

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | E | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1744 | 1107 | 308 | 318 | 11 | | | |

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | F | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 679 | 434 | 115 | 127 | 3 | | | |

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

TIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | H | 133 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1068 | 673 | 180 | 211 | 4 | | | |

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7 | I | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 997 | 613 | 182 | 191 | 11 | | | |

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | J | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 532 | 339 | 93 | 94 | 6 | | | |

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | K | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 919 | 590 | 156 | 171 | 2 | | | |

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | L | 45 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 359 | 221 | 71 | 63 | 4 | | | |

- Molecule 11 is a protein called ALPHA AMANITIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 11 | M | 8 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 64 | 39 | 10 | 14 | 1 | | | |

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 12 | J | 1 | Total 1 | Zn 1 | 0 | 0 |
| 12 | B | 1 | Total 1 | Zn 1 | 0 | 0 |
| 12 | I | 2 | Total 2 | Zn 2 | 0 | 0 |
| 12 | C | 1 | Total 1 | Zn 1 | 0 | 0 |
| 12 | A | 2 | Total 2 | Zn 2 | 0 | 0 |
| 12 | L | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 13 | A | 1 | Total 1 | Mn 1 | 0 | 0 |

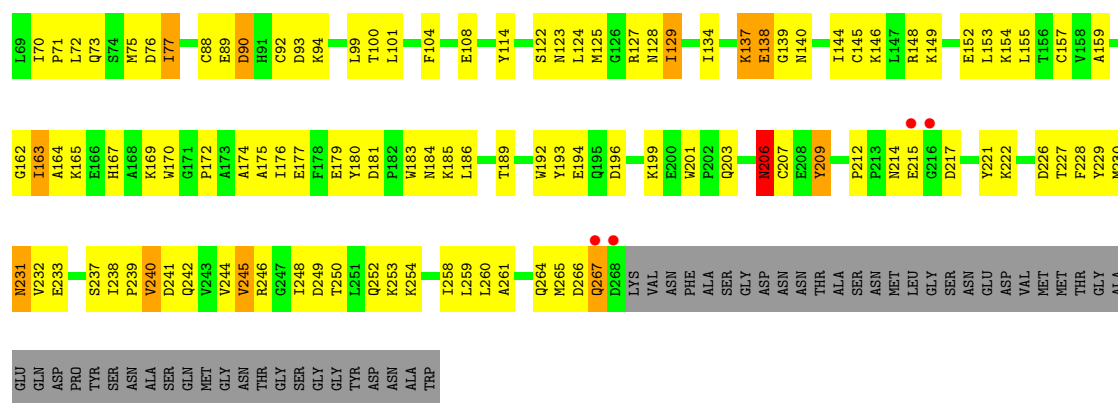
- Molecule 14 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 14 | A | 31 | Total 31 | O 31 | 0 | 0 |
| 14 | B | 23 | Total 23 | O 23 | 0 | 0 |
| 14 | C | 3 | Total 3 | O 3 | 0 | 0 |
| 14 | E | 6 | Total 6 | O 6 | 0 | 0 |
| 14 | F | 4 | Total 4 | O 4 | 0 | 0 |
| 14 | J | 1 | Total 1 | O 1 | 0 | 0 |
| 14 | M | 1 | Total 1 | O 1 | 0 | 0 |

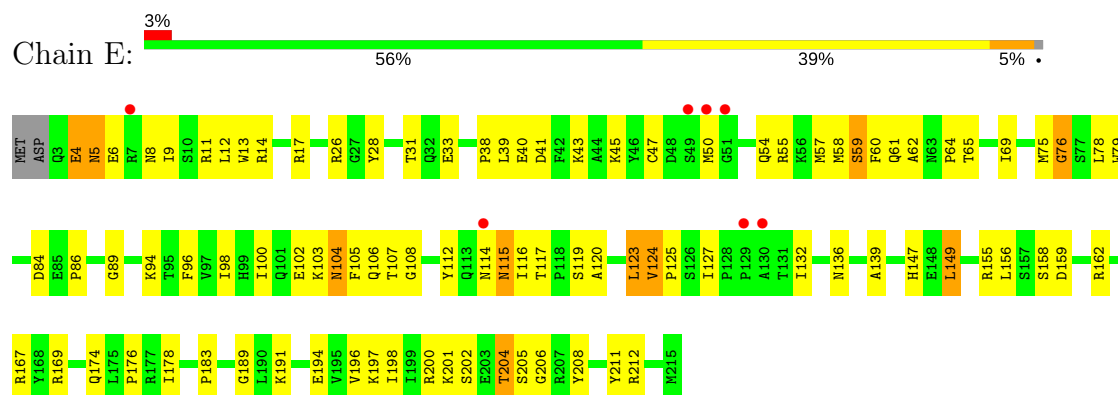


| Frequency | Percentage |
|------------|------------|
| Very often | 6% |
| Often | 47% |
| Sometimes | 38% |
| Never | 12% |

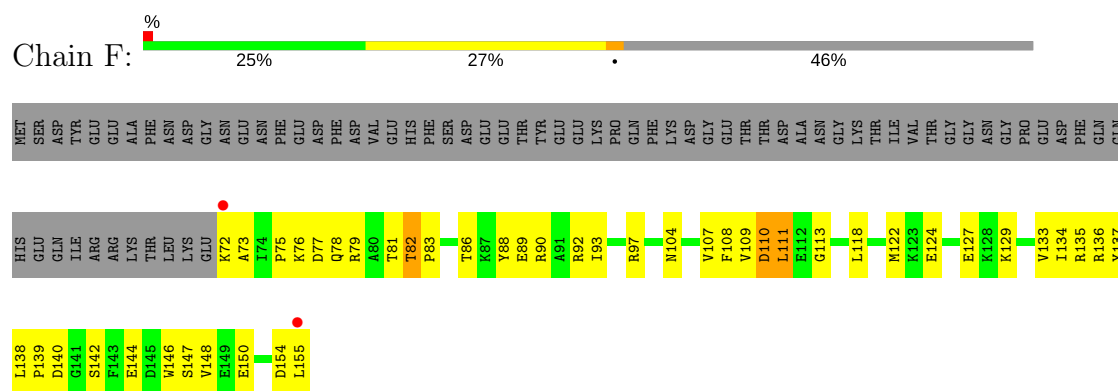




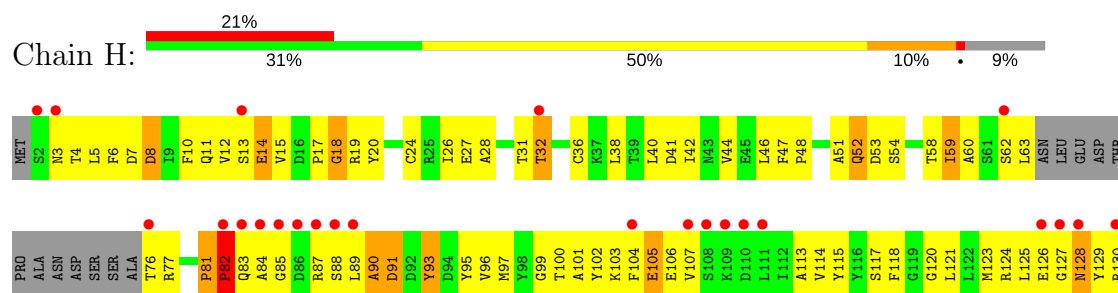
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

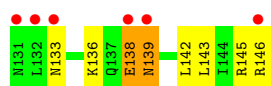


• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE



• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE





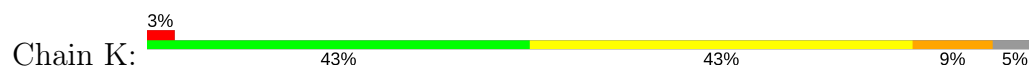
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE



• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE



• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE



• Molecule 11: ALPHA AMANITIN



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | I 2 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 122.51Å 222.48Å 374.23Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 2.80 20.00 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (20.00-2.80) 93.4 (20.00-2.80) | Depositor EDS |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.42 (at 2.79Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.229 , 0.280 0.227 , 0.277 | Depositor DCC |
| R_{free} test set | 3507 reflections (3.01%) | DCC |
| Wilson B-factor (Å ²) | 50.5 | Xtriage |
| Anisotropy | 0.352 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 47.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 27902 | wwPDB-VP |
| Average B, all atoms (Å ²) | 56.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, HYP, TRX, CSX, ILX

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 | 0.42 | 0/10940 | 0.68 | 2/14792 (0.0%) |
| 2 | B | 0.42 | 0/8786 | 0.68 | 1/11847 (0.0%) |
| 3 | C | 0.40 | 0/2133 | 0.66 | 0/2891 |
| 4 | E | 0.40 | 0/1780 | 0.67 | 0/2395 |
| 5 | F | 0.46 | 0/691 | 0.67 | 0/933 |
| 6 | H | 0.36 | 0/1086 | 0.68 | 0/1470 |
| 7 | I | 0.48 | 0/1016 | 0.68 | 0/1365 |
| 8 | J | 0.44 | 0/541 | 0.70 | 0/727 |
| 9 | K | 0.39 | 0/937 | 0.62 | 0/1265 |
| 10 | L | 0.47 | 0/361 | 0.71 | 0/478 |
| 11 | M | 2.39 | 1/22 (4.5%) | 1.63 | 0/26 |
| All | All | 0.42 | 1/28293 (0.0%) | 0.68 | 3/38189 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 11 | M | 7 | ASN | CA-C | 5.26 | 1.66 | 1.52 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 200 | GLY | N-CA-C | 5.82 | 127.64 | 113.10 |
| 1 | A | 798 | GLY | N-CA-C | 5.55 | 126.98 | 113.10 |
| 1 | A | 472 | LEU | CA-CB-CG | -5.01 | 103.78 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

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 | 10751 | 0 | 10819 | 759 | 0 |
| 2 | B | 8616 | 0 | 8645 | 586 | 0 |
| 3 | C | 2095 | 0 | 2051 | 165 | 0 |
| 4 | E | 1744 | 0 | 1772 | 87 | 0 |
| 5 | F | 679 | 0 | 701 | 55 | 0 |
| 6 | H | 1068 | 0 | 1040 | 115 | 0 |
| 7 | I | 997 | 0 | 953 | 75 | 0 |
| 8 | J | 532 | 0 | 542 | 56 | 0 |
| 9 | K | 919 | 0 | 929 | 71 | 0 |
| 10 | L | 359 | 0 | 382 | 61 | 1 |
| 11 | M | 64 | 0 | 51 | 7 | 0 |
| 12 | A | 2 | 0 | 0 | 0 | 0 |
| 12 | B | 1 | 0 | 0 | 0 | 0 |
| 12 | C | 1 | 0 | 0 | 0 | 0 |
| 12 | I | 2 | 0 | 0 | 0 | 0 |
| 12 | J | 1 | 0 | 0 | 0 | 0 |
| 12 | L | 1 | 0 | 0 | 0 | 0 |
| 13 | A | 1 | 0 | 0 | 0 | 0 |
| 14 | A | 31 | 0 | 0 | 1 | 0 |
| 14 | B | 23 | 0 | 0 | 5 | 0 |
| 14 | C | 3 | 0 | 0 | 0 | 0 |
| 14 | E | 6 | 0 | 0 | 1 | 0 |
| 14 | F | 4 | 0 | 0 | 0 | 0 |
| 14 | J | 1 | 0 | 0 | 0 | 0 |
| 14 | M | 1 | 0 | 0 | 0 | 0 |
| All | All | 27902 | 0 | 27885 | 1826 | 1 |

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 33.

All (1826) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------|--------------------------|-------------------|
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H | 1.09 | 1.15 |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:H | 1.17 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:871:THR:HG22 | 2:B:872:GLU:H | 1.09 | 1.09 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:HE | 1.10 | 1.08 |
| 1:A:445:ASN:HB2 | 1:A:455:MET:HG2 | 1.33 | 1.07 |
| 2:B:705:MET:HE3 | 2:B:742:GLU:HG3 | 1.37 | 1.07 |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:H | 1.10 | 1.06 |
| 2:B:800:GLN:HB3 | 8:J:52:THR:CG2 | 1.86 | 1.05 |
| 2:B:955:THR:HG22 | 2:B:956:THR:H | 1.23 | 1.04 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HE3 | 1.39 | 1.03 |
| 9:K:47:ARG:HB3 | 9:K:47:ARG:HH11 | 1.23 | 1.02 |
| 3:C:56:THR:HG23 | 3:C:58:LEU:H | 1.15 | 1.02 |
| 1:A:672:ASP:HB2 | 1:A:736:ASN:ND2 | 1.73 | 1.02 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:CD1 | 1.88 | 1.02 |
| 1:A:470:LEU:HD11 | 1:A:487:MET:HE1 | 1.40 | 1.02 |
| 1:A:308:ILE:HG22 | 1:A:309:ALA:H | 1.25 | 1.01 |
| 1:A:450:LEU:H | 1:A:450:LEU:HD12 | 1.27 | 0.99 |
| 2:B:103:ASN:HB2 | 2:B:169:ARG:HH22 | 1.28 | 0.99 |
| 1:A:901:LEU:N | 1:A:926:GLN:HE21 | 1.61 | 0.98 |
| 2:B:726:ALA:HB1 | 2:B:1051:THR:HG21 | 1.45 | 0.98 |
| 1:A:55:ASP:H | 1:A:56:PRO:HD2 | 1.28 | 0.97 |
| 1:A:974:ASP:HB2 | 6:H:136:LYS:HZ3 | 1.27 | 0.97 |
| 7:I:111:THR:HG22 | 7:I:113:ASP:H | 1.28 | 0.97 |
| 1:A:351:THR:HG23 | 2:B:1103:ILE:HA | 1.46 | 0.97 |
| 2:B:800:GLN:HB3 | 8:J:52:THR:HG22 | 1.43 | 0.97 |
| 9:K:65:HIS:HD2 | 9:K:67:PHE:H | 1.04 | 0.96 |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:HG2 | 1.80 | 0.96 |
| 1:A:470:LEU:HD11 | 1:A:487:MET:CE | 1.95 | 0.96 |
| 2:B:839:MET:HE3 | 2:B:1010:LEU:HD11 | 1.48 | 0.95 |
| 1:A:80:HIS:O | 1:A:243:PRO:HB3 | 1.66 | 0.95 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:CD | 1.94 | 0.95 |
| 1:A:345:VAL:HG21 | 2:B:1129:ARG:HA | 1.46 | 0.95 |
| 1:A:901:LEU:H | 1:A:926:GLN:NE2 | 1.64 | 0.94 |
| 2:B:392:ARG:NH2 | 7:I:52:ILE:HD11 | 1.81 | 0.94 |
| 5:F:111:LEU:H | 5:F:111:LEU:HD12 | 1.30 | 0.94 |
| 2:B:1153:GLU:HG2 | 2:B:1154:ALA:H | 1.30 | 0.94 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:HD13 | 1.47 | 0.94 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:H | 1.65 | 0.94 |
| 6:H:26:ILE:HD12 | 6:H:42:ILE:HD12 | 1.48 | 0.94 |
| 2:B:244:LEU:HD11 | 2:B:366:GLN:HE21 | 1.29 | 0.94 |
| 2:B:205:ILE:HD13 | 2:B:461:LEU:HB3 | 1.48 | 0.93 |
| 2:B:654:ARG:H | 2:B:657:HIS:HD2 | 1.12 | 0.93 |
| 2:B:542:MET:HG3 | 2:B:747:MET:HE3 | 1.46 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:875:ALA:HB2 | 1:A:1366:ARG:HD2 | 1.51 | 0.93 |
| 1:A:597:LEU:H | 1:A:597:LEU:HD12 | 1.34 | 0.92 |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HH11 | 0.94 | 0.92 |
| 1:A:49:LYS:HD3 | 1:A:55:ASP:HB2 | 1.49 | 0.92 |
| 1:A:399:HIS:O | 1:A:401:GLY:N | 2.02 | 0.92 |
| 8:J:44:TYR:HA | 8:J:47:ARG:HG3 | 1.52 | 0.92 |
| 1:A:903:ASN:HD22 | 1:A:905:ASP:H | 1.14 | 0.91 |
| 8:J:1:MET:HG3 | 8:J:60:PHE:HE2 | 1.32 | 0.91 |
| 1:A:704:ALA:HB2 | 1:A:710:LEU:HD12 | 1.52 | 0.91 |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:HB | 1.50 | 0.91 |
| 1:A:1446:ASP:HB2 | 5:F:133:VAL:HG23 | 1.50 | 0.91 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:HD13 | 1.53 | 0.91 |
| 2:B:103:ASN:HB2 | 2:B:169:ARG:NH2 | 1.86 | 0.90 |
| 8:J:64:ASN:HB3 | 8:J:65:PRO:HD3 | 1.53 | 0.90 |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:HE1 | 1.36 | 0.90 |
| 2:B:365:THR:HG22 | 2:B:367:LEU:H | 1.35 | 0.90 |
| 1:A:672:ASP:HB2 | 1:A:736:ASN:HD21 | 1.31 | 0.90 |
| 1:A:374:LEU:HD23 | 2:B:1107:ALA:HB2 | 1.53 | 0.90 |
| 1:A:902:LEU:HG | 1:A:926:GLN:HG3 | 1.53 | 0.90 |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:NH1 | 1.69 | 0.89 |
| 1:A:567:LYS:HB3 | 6:H:96:VAL:N | 1.88 | 0.89 |
| 2:B:205:ILE:HD11 | 2:B:461:LEU:HD23 | 1.51 | 0.89 |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:HH11 | 1.69 | 0.89 |
| 5:F:93:ILE:HD11 | 5:F:134:ILE:HD11 | 1.55 | 0.88 |
| 1:A:33:ALA:O | 1:A:83:HIS:HB3 | 1.74 | 0.88 |
| 1:A:179:LEU:HD21 | 1:A:308:ILE:HD13 | 1.56 | 0.87 |
| 3:C:148:ARG:NH1 | 8:J:64:ASN:HA | 1.89 | 0.87 |
| 1:A:1151:GLU:HG2 | 7:I:45:ARG:HD2 | 1.56 | 0.87 |
| 2:B:563:MET:CE | 2:B:580:VAL:HB | 2.05 | 0.87 |
| 6:H:100:THR:OG1 | 6:H:138:GLU:HG3 | 1.73 | 0.87 |
| 1:A:407:ARG:HD2 | 1:A:413:ILE:HD11 | 1.54 | 0.87 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N | 1.90 | 0.87 |
| 5:F:81:THR:CG2 | 5:F:136:ARG:HH11 | 1.88 | 0.87 |
| 1:A:112:LYS:NZ | 1:A:165:GLY:H | 1.73 | 0.87 |
| 4:E:78:LEU:HD23 | 4:E:107:THR:HB | 1.56 | 0.87 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:H | 1.39 | 0.86 |
| 6:H:81:PRO:HB2 | 6:H:82:PRO:HD3 | 1.54 | 0.86 |
| 2:B:864:LYS:HG2 | 2:B:871:THR:HG23 | 1.56 | 0.86 |
| 1:A:587:HIS:CE1 | 1:A:969:GLN:HG2 | 2.10 | 0.86 |
| 2:B:130:VAL:HG12 | 2:B:131:ASP:H | 1.41 | 0.86 |
| 2:B:205:ILE:CD1 | 2:B:461:LEU:HB3 | 2.06 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:159:ASP:HA | 4:E:162:ARG:NH1 | 1.91 | 0.86 |
| 1:A:1383:SER:HB3 | 1:A:1387:HIS:NE2 | 1.91 | 0.86 |
| 9:K:113:THR:O | 9:K:114:LEU:HB2 | 1.74 | 0.85 |
| 1:A:305:ASP:HB3 | 1:A:326:ARG:CZ | 2.06 | 0.85 |
| 10:L:61:THR:HB | 10:L:63:ARG:HG2 | 1.58 | 0.85 |
| 2:B:281:PRO:HG2 | 2:B:284:ILE:HD12 | 1.59 | 0.85 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:H | 1.24 | 0.84 |
| 4:E:96:PHE:CZ | 4:E:100:ILE:HD11 | 2.11 | 0.84 |
| 1:A:535:THR:HG23 | 1:A:575:LYS:HG2 | 1.57 | 0.84 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:HG2 | 1.57 | 0.84 |
| 2:B:825:VAL:HG22 | 2:B:1010:LEU:HB3 | 1.58 | 0.84 |
| 2:B:871:THR:HG22 | 2:B:872:GLU:N | 1.92 | 0.84 |
| 2:B:268:THR:HG21 | 2:B:270:LYS:HE3 | 1.60 | 0.83 |
| 1:A:414:ASP:OD1 | 1:A:416:ARG:HG2 | 1.77 | 0.83 |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:N | 1.92 | 0.83 |
| 1:A:500:GLU:OE2 | 1:A:1438:THR:HG21 | 1.77 | 0.83 |
| 2:B:763:GLN:HG2 | 2:B:765:PRO:HD2 | 1.61 | 0.83 |
| 1:A:399:HIS:HB3 | 1:A:400:PRO:HD3 | 1.61 | 0.83 |
| 6:H:130:ARG:HA | 6:H:133:ASN:HD22 | 1.41 | 0.83 |
| 1:A:444:PHE:CE2 | 1:A:470:LEU:HD21 | 2.13 | 0.83 |
| 2:B:651:LEU:HD11 | 2:B:707:PRO:HB3 | 1.59 | 0.83 |
| 3:C:39:ALA:HA | 3:C:164:ALA:HB3 | 1.61 | 0.83 |
| 1:A:132:LYS:HZ1 | 1:A:1411:GLU:HB3 | 1.44 | 0.82 |
| 1:A:901:LEU:H | 1:A:926:GLN:HE21 | 0.85 | 0.82 |
| 2:B:983:ARG:HD2 | 2:B:1091:TYR:HD2 | 1.44 | 0.82 |
| 2:B:324:ILE:HD11 | 2:B:333:PHE:CD1 | 2.15 | 0.82 |
| 1:A:587:HIS:NE2 | 1:A:969:GLN:HG2 | 1.94 | 0.81 |
| 3:C:77:ILE:HA | 3:C:129:ILE:HD11 | 1.62 | 0.81 |
| 6:H:130:ARG:HA | 6:H:133:ASN:ND2 | 1.95 | 0.81 |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:N | 1.92 | 0.81 |
| 1:A:709:THR:HG21 | 7:I:93:LYS:O | 1.79 | 0.81 |
| 7:I:47:GLU:OE1 | 7:I:50:THR:HG23 | 1.79 | 0.81 |
| 1:A:32:VAL:HG11 | 1:A:68:GLN:HE22 | 1.44 | 0.81 |
| 3:C:174:ALA:O | 8:J:10:CYS:HB2 | 1.79 | 0.81 |
| 1:A:982:THR:HG22 | 1:A:984:LYS:H | 1.46 | 0.81 |
| 2:B:914:LYS:HB3 | 2:B:937:ALA:O | 1.81 | 0.81 |
| 1:A:1198:ASP:O | 1:A:1202:MET:HG2 | 1.81 | 0.80 |
| 1:A:38:PRO:HA | 1:A:270:LEU:HD13 | 1.63 | 0.80 |
| 3:C:25:VAL:HG23 | 3:C:228:PHE:HE1 | 1.46 | 0.80 |
| 2:B:999:MET:HG3 | 2:B:1000:PRO:HD2 | 1.61 | 0.80 |
| 1:A:444:PHE:HE2 | 1:A:470:LEU:HD21 | 1.47 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:L:26:THR:HG22 | 10:L:27:LEU:H | 1.47 | 0.80 |
| 1:A:503:GLN:HE21 | 5:F:90:ARG:NH2 | 1.80 | 0.80 |
| 5:F:109:VAL:HG12 | 5:F:110:ASP:N | 1.96 | 0.80 |
| 5:F:109:VAL:HG12 | 5:F:110:ASP:H | 1.46 | 0.80 |
| 1:A:913:LEU:HD11 | 1:A:981:LEU:O | 1.81 | 0.79 |
| 1:A:55:ASP:O | 1:A:57:ARG:N | 2.14 | 0.79 |
| 3:C:51:VAL:HG22 | 3:C:155:LEU:HD12 | 1.64 | 0.79 |
| 9:K:65:HIS:CD2 | 9:K:67:PHE:H | 1.96 | 0.79 |
| 1:A:1336:MET:HE2 | 1:A:1380:GLY:HA2 | 1.64 | 0.79 |
| 1:A:567:LYS:NZ | 6:H:46:LEU:HB2 | 1.98 | 0.79 |
| 2:B:244:LEU:HD11 | 2:B:366:GLN:NE2 | 1.96 | 0.79 |
| 1:A:1151:GLU:CG | 7:I:45:ARG:HD2 | 2.12 | 0.79 |
| 1:A:1364:ASN:HD22 | 1:A:1366:ARG:HG2 | 1.47 | 0.79 |
| 1:A:347:PHE:H | 2:B:1107:ALA:HA | 1.47 | 0.79 |
| 1:A:55:ASP:N | 1:A:56:PRO:HD2 | 1.97 | 0.79 |
| 3:C:56:THR:HG23 | 3:C:58:LEU:N | 1.94 | 0.79 |
| 9:K:29:ASN:HD21 | 9:K:79:GLU:HA | 1.48 | 0.79 |
| 2:B:63:ILE:HB | 2:B:95:ILE:HD11 | 1.65 | 0.79 |
| 2:B:889:THR:HG22 | 2:B:891:ASP:H | 1.44 | 0.78 |
| 1:A:328:ARG:HD3 | 1:A:332:LYS:NZ | 1.97 | 0.78 |
| 1:A:871:ASP:HB3 | 4:E:204:THR:CG2 | 2.13 | 0.78 |
| 6:H:105:GLU:O | 6:H:107:VAL:HG23 | 1.84 | 0.78 |
| 3:C:148:ARG:HH12 | 8:J:64:ASN:HA | 1.45 | 0.78 |
| 2:B:294:ASP:H | 7:I:12:ASN:ND2 | 1.82 | 0.78 |
| 5:F:147:SER:OG | 5:F:150:GLU:HG3 | 1.84 | 0.77 |
| 1:A:112:LYS:HZ2 | 1:A:165:GLY:H | 1.30 | 0.77 |
| 6:H:40:LEU:HD13 | 6:H:123:MET:HB2 | 1.67 | 0.77 |
| 1:A:974:ASP:HB2 | 6:H:136:LYS:NZ | 1.98 | 0.77 |
| 2:B:871:THR:CG2 | 2:B:872:GLU:H | 1.91 | 0.77 |
| 10:L:26:THR:HG22 | 10:L:27:LEU:N | 2.00 | 0.77 |
| 2:B:652:LYS:HE3 | 2:B:688:GLY:O | 1.85 | 0.77 |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:H | 1.49 | 0.77 |
| 7:I:50:THR:H | 7:I:92:ARG:HH12 | 1.33 | 0.76 |
| 3:C:258:ILE:HD13 | 9:K:35:PHE:HE2 | 1.50 | 0.76 |
| 2:B:280:ILE:HD13 | 2:B:334:ILE:HG12 | 1.65 | 0.76 |
| 4:E:100:ILE:HD13 | 4:E:108:GLY:HA3 | 1.66 | 0.76 |
| 3:C:22:LEU:HD21 | 9:K:101:LEU:HD21 | 1.64 | 0.76 |
| 1:A:1400:CYS:HB3 | 1:A:1405:THR:OG1 | 1.85 | 0.76 |
| 1:A:596:THR:HG22 | 1:A:597:LEU:H | 1.51 | 0.76 |
| 1:A:677:ARG:O | 1:A:681:GLU:HG3 | 1.85 | 0.76 |
| 2:B:800:GLN:HB3 | 8:J:52:THR:HG21 | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:523:ILE:HB | 1:A:622:VAL:HG13 | 1.67 | 0.76 |
| 2:B:531:GLN:H | 2:B:531:GLN:CD | 1.87 | 0.76 |
| 1:A:276:LEU:HD13 | 1:A:292:ALA:HB3 | 1.67 | 0.76 |
| 4:E:94:LYS:HG3 | 4:E:123:LEU:HD11 | 1.65 | 0.75 |
| 6:H:15:VAL:HG22 | 6:H:26:ILE:HG12 | 1.68 | 0.75 |
| 6:H:101:ALA:H | 6:H:138:GLU:HA | 1.50 | 0.75 |
| 2:B:616:ILE:HG12 | 2:B:697:GLU:HA | 1.67 | 0.75 |
| 6:H:103:LYS:HZ2 | 6:H:114:VAL:HB | 1.51 | 0.75 |
| 4:E:155:ARG:HD2 | 4:E:194:GLU:OE2 | 1.86 | 0.75 |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:H | 1.51 | 0.75 |
| 1:A:1208:THR:HB | 1:A:1211:GLN:HG3 | 1.67 | 0.75 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:NE | 1.96 | 0.75 |
| 1:A:901:LEU:HA | 1:A:907:THR:HG23 | 1.67 | 0.74 |
| 2:B:639:ILE:HD11 | 2:B:691:GLU:HG3 | 1.68 | 0.74 |
| 3:C:261:ALA:O | 3:C:265:MET:HB2 | 1.86 | 0.74 |
| 7:I:45:ARG:HH11 | 7:I:45:ARG:HG2 | 1.53 | 0.74 |
| 1:A:760:GLN:HE22 | 11:M:1:ILX:HG23 | 1.53 | 0.74 |
| 2:B:345:LYS:HA | 2:B:348:ARG:NH1 | 2.03 | 0.74 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:HD2 | 1.69 | 0.74 |
| 8:J:2:ILE:HD11 | 8:J:57:ILE:CD1 | 2.18 | 0.74 |
| 2:B:169:ARG:HB2 | 2:B:454:THR:HG23 | 1.68 | 0.74 |
| 1:A:567:LYS:HB3 | 6:H:96:VAL:H | 1.52 | 0.73 |
| 8:J:48:ARG:HG2 | 8:J:48:ARG:HH11 | 1.51 | 0.73 |
| 2:B:130:VAL:HG12 | 2:B:131:ASP:N | 2.02 | 0.73 |
| 3:C:47:ASP:HA | 10:L:69:ALA:HB3 | 1.70 | 0.73 |
| 10:L:32:ALA:HB2 | 10:L:55:ILE:HB | 1.70 | 0.73 |
| 1:A:666:ILE:HD12 | 2:B:1030:LEU:HD22 | 1.69 | 0.73 |
| 7:I:98:VAL:HG21 | 7:I:113:ASP:HB2 | 1.69 | 0.73 |
| 1:A:900:ASP:HA | 1:A:926:GLN:NE2 | 2.03 | 0.73 |
| 9:K:47:ARG:HB3 | 9:K:47:ARG:NH1 | 2.01 | 0.73 |
| 3:C:137:LYS:H | 3:C:137:LYS:HD2 | 1.53 | 0.73 |
| 6:H:104:PHE:O | 6:H:106:GLU:N | 2.21 | 0.73 |
| 6:H:81:PRO:HB2 | 6:H:82:PRO:CD | 2.18 | 0.73 |
| 9:K:10:PHE:CD1 | 9:K:11:LEU:HD13 | 2.24 | 0.73 |
| 3:C:241:ASP:HB3 | 9:K:109:TRP:CE2 | 2.24 | 0.73 |
| 1:A:170:THR:HG21 | 1:A:186:LYS:O | 1.89 | 0.73 |
| 1:A:567:LYS:HZ1 | 6:H:46:LEU:HB2 | 1.54 | 0.73 |
| 2:B:654:ARG:H | 2:B:657:HIS:CD2 | 2.03 | 0.73 |
| 6:H:36:CYS:HB2 | 6:H:129:TYR:OH | 1.88 | 0.73 |
| 2:B:709:ASP:HB2 | 2:B:733:HIS:HB3 | 1.71 | 0.73 |
| 1:A:1128:GLN:O | 1:A:1132:LYS:HG3 | 1.87 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:644:GLU:HG3 | 2:B:654:ARG:HH22 | 1.54 | 0.72 |
| 3:C:196:ASP:OD2 | 3:C:199:LYS:HG3 | 1.90 | 0.72 |
| 1:A:329:LEU:O | 1:A:333:GLU:N | 2.22 | 0.72 |
| 2:B:542:MET:HE1 | 2:B:747:MET:HG3 | 1.70 | 0.72 |
| 1:A:492:PRO:HB2 | 1:A:497:THR:HG22 | 1.72 | 0.72 |
| 6:H:11:GLN:NE2 | 6:H:52:GLN:HA | 2.04 | 0.72 |
| 1:A:108:MET:HG2 | 1:A:171:GLN:HE22 | 1.53 | 0.72 |
| 1:A:903:ASN:ND2 | 1:A:905:ASP:H | 1.86 | 0.72 |
| 1:A:353:ILE:HD13 | 1:A:487:MET:HE2 | 1.70 | 0.72 |
| 1:A:567:LYS:HD2 | 1:A:568:PRO:HD2 | 1.72 | 0.72 |
| 2:B:680:THR:HG22 | 2:B:681:TRP:N | 2.05 | 0.71 |
| 1:A:523:ILE:HD12 | 1:A:622:VAL:HG22 | 1.70 | 0.71 |
| 2:B:997:GLU:HG2 | 3:C:39:ALA:HB2 | 1.72 | 0.71 |
| 1:A:526:ASP:HB2 | 2:B:835:GLN:OE1 | 1.91 | 0.71 |
| 3:C:250:THR:O | 3:C:254:LYS:HG3 | 1.90 | 0.71 |
| 5:F:81:THR:HG22 | 5:F:136:ARG:HH11 | 1.54 | 0.71 |
| 1:A:14:VAL:H | 1:A:1432:GLN:HE22 | 1.38 | 0.71 |
| 1:A:132:LYS:NZ | 1:A:1411:GLU:HB3 | 2.04 | 0.71 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CZ2 | 2.25 | 0.71 |
| 1:A:5:GLN:HG2 | 1:A:6:TYR:H | 1.55 | 0.71 |
| 2:B:879:ARG:HB3 | 2:B:883:LEU:CD2 | 2.21 | 0.71 |
| 3:C:66:ARG:NH2 | 8:J:3:VAL:O | 2.23 | 0.71 |
| 1:A:907:THR:HG22 | 1:A:908:LEU:H | 1.56 | 0.71 |
| 2:B:277:LYS:HD2 | 2:B:277:LYS:N | 2.06 | 0.71 |
| 9:K:30:ALA:HB2 | 9:K:76:GLN:HG3 | 1.73 | 0.71 |
| 2:B:243:ALA:HB2 | 2:B:251:ILE:HG12 | 1.73 | 0.71 |
| 2:B:1097:HIS:HB3 | 2:B:1102:LYS:NZ | 2.06 | 0.70 |
| 1:A:1398:MET:HG3 | 1:A:1426:GLU:OE2 | 1.92 | 0.70 |
| 1:A:567:LYS:CD | 1:A:568:PRO:HD2 | 2.21 | 0.70 |
| 3:C:92:CYS:SG | 3:C:94:LYS:HB2 | 2.30 | 0.70 |
| 1:A:567:LYS:CB | 1:A:568:PRO:CD | 2.69 | 0.70 |
| 1:A:308:ILE:HG22 | 1:A:309:ALA:N | 2.04 | 0.70 |
| 1:A:55:ASP:C | 1:A:57:ARG:H | 1.95 | 0.70 |
| 1:A:573:SER:HB3 | 1:A:576:GLN:HG3 | 1.74 | 0.70 |
| 2:B:955:THR:HG23 | 10:L:54:ARG:O | 1.92 | 0.70 |
| 2:B:1159:ARG:HB3 | 2:B:1159:ARG:HH11 | 1.56 | 0.70 |
| 2:B:834:ASN:HB3 | 2:B:840:ILE:HG13 | 1.73 | 0.70 |
| 2:B:705:MET:CE | 2:B:742:GLU:HG3 | 2.17 | 0.70 |
| 10:L:46:VAL:HG13 | 10:L:56:LEU:HD12 | 1.74 | 0.70 |
| 1:A:1004:ASN:ND2 | 4:E:167:ARG:HD2 | 2.07 | 0.70 |
| 7:I:111:THR:HG22 | 7:I:112:SER:N | 2.07 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:329:LEU:HA | 1:A:332:LYS:HB2 | 1.74 | 0.69 |
| 2:B:899:ILE:HG22 | 2:B:900:ALA:N | 2.05 | 0.69 |
| 2:B:952:VAL:HB | 10:L:58:LYS:HB2 | 1.73 | 0.69 |
| 1:A:672:ASP:CB | 1:A:736:ASN:HD21 | 2.03 | 0.69 |
| 2:B:822:ASN:ND2 | 8:J:52:THR:HG21 | 2.07 | 0.69 |
| 1:A:886:ILE:HD12 | 1:A:943:LEU:HB3 | 1.73 | 0.69 |
| 2:B:1181:GLU:HG3 | 2:B:1188:LYS:HE2 | 1.73 | 0.69 |
| 2:B:890:TYR:HB3 | 2:B:893:LEU:HD12 | 1.73 | 0.69 |
| 6:H:130:ARG:HA | 6:H:133:ASN:HB2 | 1.74 | 0.69 |
| 1:A:855:THR:CG2 | 1:A:857:ARG:HE | 1.98 | 0.69 |
| 2:B:954:VAL:O | 10:L:55:ILE:O | 2.11 | 0.69 |
| 3:C:25:VAL:HG23 | 3:C:228:PHE:CE1 | 2.28 | 0.69 |
| 8:J:36:LEU:HB2 | 8:J:47:ARG:HH21 | 1.57 | 0.69 |
| 1:A:1398:MET:HG2 | 1:A:1425:SER:HB2 | 1.73 | 0.69 |
| 1:A:262:LEU:O | 1:A:266:LEU:HG | 1.93 | 0.69 |
| 1:A:56:PRO:O | 1:A:57:ARG:HG3 | 1.93 | 0.69 |
| 2:B:542:MET:CE | 2:B:747:MET:HG3 | 2.23 | 0.69 |
| 2:B:801:LYS:O | 8:J:52:THR:HG23 | 1.93 | 0.69 |
| 10:L:38:LEU:HG | 10:L:39:SER:H | 1.58 | 0.69 |
| 5:F:76:LYS:O | 5:F:79:ARG:HD2 | 1.93 | 0.69 |
| 1:A:1147:THR:HB | 7:I:48:LEU:HD12 | 1.75 | 0.69 |
| 3:C:52:GLU:HA | 10:L:64:LEU:HD22 | 1.74 | 0.68 |
| 1:A:1336:MET:HE1 | 1:A:1381:LEU:H | 1.58 | 0.68 |
| 2:B:1198:TYR:CE1 | 2:B:1201:LYS:HD3 | 2.28 | 0.68 |
| 1:A:1325:THR:HG22 | 1:A:1326:ARG:HG3 | 1.74 | 0.68 |
| 6:H:125:LEU:C | 6:H:130:ARG:HH12 | 1.97 | 0.68 |
| 1:A:900:ASP:HA | 1:A:926:GLN:HE22 | 1.57 | 0.68 |
| 2:B:640:VAL:HG22 | 2:B:651:LEU:HD23 | 1.75 | 0.68 |
| 2:B:737:THR:HG21 | 7:I:66:PRO:HA | 1.76 | 0.68 |
| 1:A:974:ASP:CB | 6:H:136:LYS:HZ3 | 2.05 | 0.68 |
| 2:B:638:PHE:CE1 | 2:B:743:ILE:HA | 2.28 | 0.68 |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:HA2 | 1.76 | 0.68 |
| 1:A:910:PRO:HA | 1:A:916:GLY:HA3 | 1.75 | 0.68 |
| 2:B:120:ARG:NH2 | 10:L:54:ARG:HD2 | 2.09 | 0.68 |
| 2:B:102:VAL:HG22 | 2:B:112:LEU:HD22 | 1.74 | 0.68 |
| 1:A:140:THR:HA | 1:A:143:LYS:HE2 | 1.76 | 0.67 |
| 1:A:725:ALA:HA | 1:A:728:LYS:HE2 | 1.74 | 0.67 |
| 9:K:7:PHE:HB2 | 9:K:11:LEU:HD22 | 1.75 | 0.67 |
| 1:A:445:ASN:CB | 1:A:455:MET:HG2 | 2.19 | 0.67 |
| 3:C:241:ASP:HB3 | 9:K:109:TRP:CZ2 | 2.28 | 0.67 |
| 1:A:1077:THR:HG22 | 1:A:1077:THR:O | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:130:ASP:HB3 | 1:A:133:LYS:HB2 | 1.77 | 0.67 |
| 1:A:465:TYR:HA | 9:K:2:ASN:HB3 | 1.76 | 0.67 |
| 2:B:118:ARG:NH1 | 2:B:204:ILE:HD11 | 2.09 | 0.67 |
| 1:A:567:LYS:CG | 1:A:568:PRO:HD2 | 2.24 | 0.67 |
| 3:C:196:ASP:CG | 3:C:199:LYS:HG3 | 2.14 | 0.67 |
| 6:H:103:LYS:NZ | 6:H:114:VAL:HB | 2.09 | 0.67 |
| 1:A:1341:ILE:HD11 | 1:A:1376:THR:HG23 | 1.77 | 0.67 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:N | 2.41 | 0.67 |
| 10:L:34:CYS:HB3 | 10:L:51:CYS:SG | 2.34 | 0.67 |
| 2:B:1181:GLU:CG | 2:B:1188:LYS:HE2 | 2.25 | 0.67 |
| 6:H:95:TYR:CE2 | 6:H:97:MET:HG3 | 2.30 | 0.67 |
| 3:C:265:MET:HE1 | 9:K:19:LEU:HB2 | 1.77 | 0.67 |
| 1:A:1394:THR:CG2 | 1:A:1395:GLY:H | 1.93 | 0.67 |
| 2:B:130:VAL:CG2 | 2:B:167:ILE:HD12 | 2.25 | 0.67 |
| 1:A:1345:ARG:HG2 | 1:A:1372:VAL:CG1 | 2.25 | 0.67 |
| 5:F:77:ASP:O | 5:F:78:GLN:HB2 | 1.94 | 0.67 |
| 5:F:138:LEU:HD12 | 5:F:142:SER:OG | 1.94 | 0.67 |
| 1:A:567:LYS:CB | 1:A:568:PRO:HD2 | 2.24 | 0.66 |
| 2:B:876:LYS:HE2 | 2:B:893:LEU:O | 1.94 | 0.66 |
| 1:A:1438:THR:HG22 | 2:B:1144:ALA:HB3 | 1.76 | 0.66 |
| 2:B:979:LYS:HE3 | 2:B:987:LYS:HD2 | 1.77 | 0.66 |
| 1:A:67:CYS:O | 1:A:68:GLN:HB2 | 1.93 | 0.66 |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:HG23 | 1.76 | 0.66 |
| 2:B:62:ILE:O | 2:B:65:GLU:HG2 | 1.95 | 0.66 |
| 3:C:22:LEU:HD12 | 3:C:230:MET:CE | 2.26 | 0.66 |
| 2:B:955:THR:HG22 | 2:B:956:THR:N | 2.05 | 0.66 |
| 1:A:49:LYS:HD3 | 1:A:55:ASP:CB | 2.22 | 0.66 |
| 3:C:134:ILE:HG21 | 3:C:139:GLY:HA2 | 1.77 | 0.66 |
| 1:A:1191:TRP:HZ3 | 7:I:43:VAL:HG21 | 1.60 | 0.66 |
| 1:A:597:LEU:HD12 | 1:A:597:LEU:N | 2.07 | 0.66 |
| 5:F:81:THR:HG22 | 5:F:136:ARG:NH1 | 2.10 | 0.66 |
| 1:A:503:GLN:NE2 | 5:F:90:ARG:NH2 | 2.44 | 0.66 |
| 8:J:2:ILE:HD11 | 8:J:57:ILE:HD13 | 1.78 | 0.66 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:HA | 1.78 | 0.66 |
| 1:A:263:THR:HA | 1:A:266:LEU:HD12 | 1.78 | 0.66 |
| 1:A:689:LYS:O | 1:A:693:VAL:HG23 | 1.96 | 0.66 |
| 5:F:81:THR:CG2 | 5:F:136:ARG:NH1 | 2.56 | 0.66 |
| 1:A:1269:GLU:OE2 | 2:B:263:GLY:HA3 | 1.95 | 0.66 |
| 2:B:874:PHE:O | 2:B:875:GLU:HG3 | 1.95 | 0.66 |
| 7:I:50:THR:CG2 | 7:I:52:ILE:HG23 | 2.26 | 0.66 |
| 1:A:464:PRO:O | 1:A:465:TYR:O | 2.14 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1160:VAL:HG12 | 2:B:1161:HIS:N | 2.11 | 0.66 |
| 3:C:148:ARG:HD2 | 8:J:61:LEU:O | 1.96 | 0.66 |
| 9:K:18:LYS:HZ3 | 9:K:38:GLU:HG2 | 1.61 | 0.66 |
| 1:A:23:SER:O | 1:A:27:VAL:HG23 | 1.95 | 0.65 |
| 1:A:768:GLN:NE2 | 1:A:816:HIS:ND1 | 2.44 | 0.65 |
| 3:C:249:ASP:OD1 | 3:C:253:LYS:HE3 | 1.96 | 0.65 |
| 5:F:81:THR:HG21 | 5:F:136:ARG:HH11 | 1.60 | 0.65 |
| 2:B:737:THR:HG21 | 7:I:66:PRO:O | 1.96 | 0.65 |
| 1:A:541:ILE:N | 1:A:541:ILE:HD12 | 2.11 | 0.65 |
| 3:C:5:GLY:C | 3:C:24:ASN:HD22 | 2.00 | 0.65 |
| 8:J:1:MET:HG3 | 8:J:60:PHE:CE2 | 2.24 | 0.65 |
| 1:A:855:THR:CG2 | 1:A:857:ARG:HG3 | 2.26 | 0.65 |
| 1:A:901:LEU:O | 1:A:920:LEU:HD23 | 1.95 | 0.65 |
| 2:B:726:ALA:CB | 2:B:1051:THR:HG21 | 2.23 | 0.65 |
| 2:B:408:LEU:HD11 | 2:B:545:ILE:HD12 | 1.79 | 0.65 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:CD1 | 2.26 | 0.65 |
| 4:E:5:ASN:O | 4:E:9:ILE:HG13 | 1.97 | 0.65 |
| 1:A:1390:ASN:O | 1:A:1391:ARG:HB2 | 1.96 | 0.65 |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:CE1 | 2.26 | 0.65 |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:HD2 | 1.76 | 0.65 |
| 2:B:737:THR:CG2 | 7:I:66:PRO:HA | 2.27 | 0.65 |
| 5:F:81:THR:HB | 5:F:144:GLU:OE1 | 1.95 | 0.65 |
| 1:A:537:ARG:NH1 | 6:H:120:GLY:O | 2.30 | 0.65 |
| 6:H:42:ILE:HG23 | 6:H:95:TYR:CE1 | 2.32 | 0.65 |
| 1:A:65:LEU:O | 1:A:71:GLN:HA | 1.97 | 0.65 |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:H | 1.62 | 0.65 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:N | 2.08 | 0.65 |
| 2:B:957:ASN:OD1 | 2:B:958:GLN:N | 2.28 | 0.65 |
| 1:A:387:ARG:O | 1:A:391:LEU:HG | 1.96 | 0.65 |
| 2:B:1099:VAL:HG12 | 2:B:1103:ILE:HD11 | 1.78 | 0.65 |
| 2:B:731:VAL:HG12 | 2:B:732:SER:N | 2.12 | 0.65 |
| 6:H:44:VAL:HG13 | 6:H:48:PRO:HA | 1.79 | 0.65 |
| 1:A:1140:HIS:CE1 | 1:A:1272:THR:HG23 | 2.32 | 0.65 |
| 2:B:296:GLU:O | 2:B:300:HIS:HD2 | 1.79 | 0.65 |
| 2:B:515:HIS:HD2 | 2:B:517:THR:H | 1.43 | 0.65 |
| 1:A:998:LEU:HD12 | 1:A:1001:ARG:NH1 | 2.11 | 0.64 |
| 1:A:1111:MET:HE1 | 1:A:1331:SER:HB2 | 1.78 | 0.64 |
| 1:A:666:ILE:HG12 | 2:B:1026:LEU:HB3 | 1.77 | 0.64 |
| 1:A:768:GLN:HE21 | 1:A:816:HIS:HA | 1.63 | 0.64 |
| 2:B:680:THR:CG2 | 2:B:681:TRP:N | 2.61 | 0.64 |
| 2:B:864:LYS:CG | 2:B:871:THR:HG23 | 2.25 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:265:MET:CE | 9:K:19:LEU:HB2 | 2.27 | 0.64 |
| 6:H:103:LYS:HB3 | 6:H:105:GLU:OE2 | 1.97 | 0.64 |
| 1:A:754:SER:OG | 1:A:756:ILE:HG22 | 1.97 | 0.64 |
| 6:H:82:PRO:O | 6:H:84:ALA:N | 2.28 | 0.64 |
| 1:A:328:ARG:HD3 | 1:A:332:LYS:HZ1 | 1.61 | 0.64 |
| 1:A:59:GLY:HA2 | 1:A:67:CYS:SG | 2.38 | 0.64 |
| 1:A:826:ASP:O | 1:A:830:LYS:HB2 | 1.97 | 0.64 |
| 6:H:5:LEU:HD22 | 6:H:133:ASN:O | 1.97 | 0.64 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:N | 1.95 | 0.64 |
| 5:F:109:VAL:CG1 | 5:F:110:ASP:H | 2.11 | 0.64 |
| 9:K:24:ASP:OD2 | 9:K:74:ARG:NH1 | 2.29 | 0.64 |
| 2:B:1022:THR:HG23 | 2:B:1022:THR:O | 1.97 | 0.64 |
| 2:B:864:LYS:HB3 | 2:B:871:THR:HA | 1.79 | 0.64 |
| 2:B:898:LEU:HD22 | 2:B:964:VAL:HG11 | 1.79 | 0.64 |
| 3:C:67:LEU:HD13 | 3:C:155:LEU:HD21 | 1.80 | 0.64 |
| 1:A:1376:THR:HG22 | 4:E:212:ARG:HH22 | 1.62 | 0.64 |
| 1:A:1395:GLY:C | 1:A:1397:LEU:H | 2.01 | 0.64 |
| 9:K:10:PHE:HD1 | 9:K:11:LEU:HD13 | 1.63 | 0.64 |
| 10:L:38:LEU:HD22 | 10:L:56:LEU:HD21 | 1.78 | 0.64 |
| 2:B:1159:ARG:CG | 2:B:1193:GLN:HE21 | 2.11 | 0.64 |
| 2:B:239:GLU:HG2 | 2:B:255:GLN:HG2 | 1.79 | 0.64 |
| 1:A:93:VAL:HG13 | 1:A:301:ALA:HB1 | 1.79 | 0.63 |
| 1:A:595:THR:OG1 | 1:A:603:ASN:HB3 | 1.97 | 0.63 |
| 1:A:70:CYS:O | 1:A:72:GLU:HG3 | 1.98 | 0.63 |
| 1:A:469:ARG:NH2 | 2:B:991:GLY:O | 2.31 | 0.63 |
| 2:B:235:SER:HA | 2:B:261:ARG:NH2 | 2.14 | 0.63 |
| 3:C:239:PRO:O | 3:C:242:GLN:HB2 | 1.97 | 0.63 |
| 9:K:103:THR:HG22 | 9:K:104:ASN:N | 2.13 | 0.63 |
| 9:K:38:GLU:OE1 | 9:K:42:LEU:HD22 | 1.98 | 0.63 |
| 1:A:705:LYS:HB2 | 1:A:708:MET:HE3 | 1.80 | 0.63 |
| 2:B:956:THR:HA | 2:B:961:LEU:O | 1.97 | 0.63 |
| 3:C:214:ASN:HB2 | 3:C:217:ASP:OD2 | 1.98 | 0.63 |
| 6:H:11:GLN:HE21 | 6:H:52:GLN:HA | 1.61 | 0.63 |
| 1:A:1138:ILE:HG22 | 1:A:1279:ILE:HG21 | 1.81 | 0.63 |
| 2:B:282:ILE:HD12 | 2:B:382:ILE:HD13 | 1.80 | 0.63 |
| 6:H:85:GLY:O | 6:H:89:LEU:HD21 | 1.98 | 0.63 |
| 1:A:203:SER:OG | 1:A:206:GLU:HG3 | 1.98 | 0.63 |
| 2:B:606:LYS:HD2 | 2:B:608:ASP:OD2 | 1.98 | 0.63 |
| 1:A:1155:ASP:OD1 | 1:A:1162:VAL:HG23 | 1.99 | 0.63 |
| 1:A:79:GLY:HA3 | 1:A:245:PRO:HG3 | 1.81 | 0.63 |
| 1:A:869:GLY:O | 4:E:204:THR:HG21 | 1.97 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:E:204:THR:HG22 | 4:E:205:SER:N | 2.11 | 0.63 |
| 1:A:535:THR:O | 1:A:535:THR:HG22 | 1.98 | 0.63 |
| 4:E:4:GLU:O | 4:E:6:GLU:N | 2.32 | 0.63 |
| 1:A:1447:GLU:HA | 1:A:1447:GLU:OE1 | 1.97 | 0.63 |
| 1:A:596:THR:HG22 | 1:A:597:LEU:N | 2.13 | 0.63 |
| 2:B:284:ILE:HG12 | 2:B:324:ILE:HD12 | 1.81 | 0.63 |
| 2:B:339:THR:HG21 | 2:B:348:ARG:HG2 | 1.80 | 0.63 |
| 2:B:995:ARG:HD3 | 9:K:6:ARG:HH12 | 1.63 | 0.63 |
| 3:C:52:GLU:HA | 10:L:64:LEU:CD2 | 2.29 | 0.63 |
| 1:A:697:ALA:HB2 | 1:A:702:LEU:HD12 | 1.79 | 0.62 |
| 2:B:103:ASN:CB | 2:B:169:ARG:HH22 | 2.10 | 0.62 |
| 2:B:25:ILE:HG23 | 2:B:29:ASP:HB2 | 1.81 | 0.62 |
| 1:A:901:LEU:HB2 | 1:A:926:GLN:HG2 | 1.80 | 0.62 |
| 2:B:43:LEU:HD11 | 2:B:811:TYR:O | 1.98 | 0.62 |
| 2:B:872:GLU:CD | 2:B:914:LYS:HE2 | 2.19 | 0.62 |
| 2:B:969:ARG:HH11 | 2:B:969:ARG:HB3 | 1.64 | 0.62 |
| 4:E:120:ALA:O | 4:E:123:LEU:HB2 | 2.00 | 0.62 |
| 1:A:208:LEU:HD22 | 1:A:212:LYS:HE3 | 1.81 | 0.62 |
| 1:A:929:LEU:HD11 | 1:A:983:ILE:HD13 | 1.80 | 0.62 |
| 1:A:58:LEU:HD22 | 1:A:80:HIS:O | 2.00 | 0.62 |
| 10:L:51:CYS:O | 10:L:53:HIS:N | 2.31 | 0.62 |
| 1:A:565:ILE:HG23 | 1:A:567:LYS:HG3 | 1.82 | 0.62 |
| 2:B:796:LEU:HB3 | 2:B:799:PRO:HG3 | 1.82 | 0.62 |
| 9:K:56:VAL:HA | 9:K:77:THR:HG22 | 1.81 | 0.62 |
| 1:A:682:THR:HG21 | 1:A:728:LYS:HG3 | 1.80 | 0.62 |
| 1:A:858:ASN:HD22 | 1:A:858:ASN:C | 2.02 | 0.62 |
| 1:A:878:ILE:CG2 | 1:A:955:PRO:HB2 | 2.29 | 0.62 |
| 2:B:25:ILE:HD13 | 2:B:658:ILE:HD11 | 1.81 | 0.62 |
| 10:L:26:THR:CG2 | 10:L:27:LEU:H | 2.11 | 0.62 |
| 10:L:38:LEU:O | 10:L:39:SER:HB2 | 2.00 | 0.62 |
| 1:A:994:GLN:HE22 | 1:A:1023:ARG:HE | 1.46 | 0.62 |
| 2:B:680:THR:HG22 | 2:B:682:SER:H | 1.63 | 0.62 |
| 1:A:871:ASP:HB3 | 4:E:204:THR:HG22 | 1.80 | 0.62 |
| 1:A:14:VAL:N | 1:A:1432:GLN:HE22 | 1.97 | 0.62 |
| 1:A:446:ARG:HB2 | 1:A:487:MET:SD | 2.39 | 0.62 |
| 4:E:28:TYR:CZ | 4:E:78:LEU:HG | 2.35 | 0.62 |
| 10:L:55:ILE:O | 10:L:56:LEU:HB2 | 1.99 | 0.62 |
| 1:A:704:ALA:HB2 | 1:A:710:LEU:CD1 | 2.27 | 0.61 |
| 4:E:40:GLU:OE1 | 4:E:43:LYS:HD2 | 2.00 | 0.61 |
| 3:C:258:ILE:CD1 | 9:K:42:LEU:HD21 | 2.30 | 0.61 |
| 1:A:1394:THR:CG2 | 1:A:1398:MET:HB2 | 2.29 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:332:LYS:HD3 | 2:B:1206:GLU:OE2 | 2.00 | 0.61 |
| 2:B:1159:ARG:HG3 | 2:B:1193:GLN:HE21 | 1.65 | 0.61 |
| 2:B:705:MET:HE1 | 2:B:745:PRO:HB3 | 1.82 | 0.61 |
| 6:H:95:TYR:HE2 | 6:H:97:MET:HG3 | 1.65 | 0.61 |
| 3:C:67:LEU:HA | 3:C:70:ILE:HD12 | 1.82 | 0.61 |
| 6:H:130:ARG:CA | 6:H:133:ASN:HD22 | 2.12 | 0.61 |
| 9:K:18:LYS:NZ | 9:K:38:GLU:HG2 | 2.15 | 0.61 |
| 1:A:1116:LEU:HD12 | 1:A:1329:THR:HB | 1.82 | 0.61 |
| 1:A:912:LEU:HD22 | 1:A:1033:GLN:HA | 1.82 | 0.61 |
| 2:B:788:ARG:NH1 | 2:B:790:ASP:OD1 | 2.32 | 0.61 |
| 1:A:1264:GLU:HG3 | 1:A:1265:ASN:N | 2.15 | 0.61 |
| 2:B:886:LYS:NZ | 2:B:886:LYS:HB3 | 2.16 | 0.61 |
| 1:A:693:VAL:CG2 | 1:A:721:PHE:HE1 | 2.10 | 0.61 |
| 1:A:1409:LEU:HD13 | 2:B:1207:LEU:HD21 | 1.83 | 0.61 |
| 6:H:89:LEU:C | 6:H:91:ASP:H | 2.03 | 0.61 |
| 1:A:503:GLN:HE21 | 5:F:90:ARG:HH21 | 1.49 | 0.61 |
| 1:A:597:LEU:CD1 | 1:A:597:LEU:H | 2.11 | 0.61 |
| 1:A:825:ILE:CD1 | 2:B:512:ARG:HG3 | 2.30 | 0.61 |
| 2:B:63:ILE:O | 2:B:67:SER:HB3 | 2.01 | 0.61 |
| 2:B:879:ARG:HB3 | 2:B:883:LEU:HD22 | 1.81 | 0.61 |
| 3:C:67:LEU:CD1 | 3:C:155:LEU:HD21 | 2.31 | 0.61 |
| 7:I:51:ASN:O | 7:I:54:GLU:HG3 | 2.00 | 0.61 |
| 1:A:152:VAL:HG13 | 1:A:153:PRO:HD2 | 1.83 | 0.61 |
| 2:B:164:LYS:O | 2:B:165:VAL:HB | 2.01 | 0.61 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:HB2 | 1.83 | 0.61 |
| 3:C:51:VAL:HG22 | 3:C:155:LEU:CD1 | 2.30 | 0.61 |
| 7:I:50:THR:HG22 | 7:I:52:ILE:HG23 | 1.82 | 0.61 |
| 1:A:724:GLU:O | 1:A:728:LYS:HG2 | 2.01 | 0.60 |
| 5:F:79:ARG:HH22 | 5:F:150:GLU:CD | 2.03 | 0.60 |
| 1:A:1111:MET:CE | 1:A:1331:SER:HB2 | 2.31 | 0.60 |
| 1:A:32:VAL:HG11 | 1:A:68:GLN:NE2 | 2.16 | 0.60 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:CA | 2.30 | 0.60 |
| 2:B:1097:HIS:HB3 | 2:B:1102:LYS:HZ2 | 1.64 | 0.60 |
| 7:I:95:THR:HG22 | 7:I:96:SER:N | 2.15 | 0.60 |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:HB3 | 1.83 | 0.60 |
| 2:B:579:ARG:HB2 | 2:B:586:TRP:NE1 | 2.16 | 0.60 |
| 1:A:873:MET:HB3 | 1:A:878:ILE:HD11 | 1.82 | 0.60 |
| 10:L:58:LYS:O | 10:L:58:LYS:HD3 | 2.01 | 0.60 |
| 1:A:903:ASN:HD22 | 1:A:905:ASP:N | 1.94 | 0.60 |
| 1:A:825:ILE:HD13 | 2:B:512:ARG:HG3 | 1.83 | 0.60 |
| 2:B:731:VAL:HG12 | 2:B:732:SER:H | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:63:GLY:O | 7:I:70:ARG:NH2 | 2.35 | 0.60 |
| 1:A:1139:GLU:HG3 | 1:A:1280:GLU:O | 2.02 | 0.60 |
| 1:A:556:TRP:CZ3 | 1:A:558:GLY:HA2 | 2.37 | 0.60 |
| 1:A:760:GLN:HB2 | 2:B:1021:MET:CE | 2.31 | 0.60 |
| 2:B:274:PRO:CG | 2:B:359:GLU:HB3 | 2.31 | 0.60 |
| 2:B:544:CYS:HB2 | 2:B:634:TYR:CE1 | 2.37 | 0.60 |
| 5:F:154:ASP:O | 5:F:155:LEU:HD23 | 2.01 | 0.60 |
| 2:B:798:TYR:CD2 | 8:J:4:PRO:HG3 | 2.37 | 0.60 |
| 2:B:800:GLN:CB | 8:J:52:THR:HG22 | 2.26 | 0.60 |
| 7:I:98:VAL:HG21 | 7:I:113:ASP:CB | 2.31 | 0.60 |
| 9:K:46:ILE:O | 9:K:50:LEU:HB2 | 2.01 | 0.60 |
| 1:A:1144:LYS:HB2 | 1:A:1268:LEU:O | 2.01 | 0.60 |
| 2:B:103:ASN:HB2 | 2:B:169:ARG:CZ | 2.30 | 0.60 |
| 10:L:33:GLU:HB2 | 10:L:53:HIS:CD2 | 2.37 | 0.60 |
| 1:A:1259:MET:O | 1:A:1263:ILE:HG13 | 2.02 | 0.60 |
| 1:A:1277:GLU:O | 1:A:1278:ASN:HB2 | 2.01 | 0.60 |
| 1:A:673:GLY:N | 1:A:674:PRO:HD2 | 2.17 | 0.60 |
| 1:A:1113:THR:HG22 | 1:A:1113:THR:O | 2.02 | 0.60 |
| 1:A:283:GLY:O | 1:A:284:ALA:HB2 | 2.02 | 0.60 |
| 1:A:303:TYR:CZ | 1:A:325:ILE:HD11 | 2.37 | 0.60 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:HB2 | 2.01 | 0.60 |
| 2:B:120:ARG:HG3 | 2:B:955:THR:HG21 | 1.84 | 0.60 |
| 4:E:124:VAL:HB | 4:E:125:PRO:CD | 2.32 | 0.60 |
| 1:A:831:THR:HG22 | 1:A:832:ALA:N | 2.17 | 0.59 |
| 2:B:1103:ILE:O | 2:B:1103:ILE:HG22 | 2.02 | 0.59 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:N | 2.16 | 0.59 |
| 4:E:127:ILE:HD11 | 4:E:132:ILE:HD11 | 1.83 | 0.59 |
| 6:H:130:ARG:CA | 6:H:133:ASN:HB2 | 2.32 | 0.59 |
| 1:A:378:GLU:CD | 1:A:387:ARG:HH22 | 2.05 | 0.59 |
| 6:H:76:THR:HG22 | 6:H:76:THR:O | 2.02 | 0.59 |
| 2:B:915:THR:HG21 | 2:B:934:LYS:HG2 | 1.84 | 0.59 |
| 1:A:276:LEU:HD13 | 1:A:292:ALA:CB | 2.33 | 0.59 |
| 1:A:523:ILE:HD13 | 1:A:649:ILE:HG21 | 1.83 | 0.59 |
| 1:A:879:GLU:OE2 | 1:A:962:ARG:NH2 | 2.36 | 0.59 |
| 1:A:849:MET:CE | 1:A:1436:ILE:HA | 2.31 | 0.59 |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:N | 2.18 | 0.59 |
| 1:A:565:ILE:HG23 | 1:A:567:LYS:CG | 2.32 | 0.59 |
| 1:A:57:ARG:HB3 | 1:A:68:GLN:NE2 | 2.18 | 0.59 |
| 1:A:840:ARG:HG3 | 1:A:1385:THR:HG22 | 1.85 | 0.59 |
| 5:F:81:THR:HG21 | 5:F:136:ARG:CD | 2.32 | 0.59 |
| 6:H:103:LYS:CD | 6:H:114:VAL:HB | 2.31 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:N | 2.17 | 0.59 |
| 2:B:98:THR:HG22 | 2:B:99:LYS:N | 2.17 | 0.59 |
| 10:L:48:CYS:SG | 10:L:49:LYS:N | 2.75 | 0.59 |
| 2:B:102:VAL:CG2 | 2:B:112:LEU:HB2 | 2.33 | 0.59 |
| 1:A:741:ASN:HD22 | 1:A:744:LYS:H | 1.50 | 0.59 |
| 8:J:2:ILE:HD11 | 8:J:57:ILE:HD12 | 1.84 | 0.59 |
| 3:C:6:PRO:HB2 | 9:K:101:LEU:HB2 | 1.85 | 0.59 |
| 2:B:134:LYS:NZ | 2:B:446:LEU:HD13 | 2.17 | 0.59 |
| 3:C:31:ASN:O | 3:C:35:ARG:HG3 | 2.03 | 0.59 |
| 1:A:108:MET:HG2 | 1:A:171:GLN:NE2 | 2.16 | 0.58 |
| 1:A:608:ILE:HD12 | 1:A:613:ILE:HD12 | 1.84 | 0.58 |
| 1:A:1080:THR:O | 1:A:1081:LEU:HG | 2.03 | 0.58 |
| 1:A:526:ASP:HB2 | 2:B:835:GLN:CD | 2.24 | 0.58 |
| 1:A:63:ARG:HA | 1:A:74:MET:HE2 | 1.83 | 0.58 |
| 2:B:167:ILE:HG22 | 2:B:453:ILE:HD12 | 1.85 | 0.58 |
| 2:B:526:GLU:HG2 | 2:B:538:ASN:ND2 | 2.18 | 0.58 |
| 10:L:51:CYS:HB3 | 10:L:53:HIS:CD2 | 2.38 | 0.58 |
| 1:A:1265:ASN:HD21 | 2:B:263:GLY:C | 2.06 | 0.58 |
| 2:B:35:SER:O | 2:B:39:ARG:HG3 | 2.02 | 0.58 |
| 3:C:93:ASP:O | 3:C:127:ARG:NH2 | 2.37 | 0.58 |
| 9:K:12:LEU:HD11 | 9:K:18:LYS:HE2 | 1.86 | 0.58 |
| 10:L:34:CYS:O | 10:L:36:SER:N | 2.36 | 0.58 |
| 1:A:381:THR:CG2 | 1:A:383:TYR:H | 2.16 | 0.58 |
| 1:A:763:ALA:O | 1:A:803:SER:HB3 | 2.04 | 0.58 |
| 1:A:1041:ALA:O | 1:A:1045:VAL:HG23 | 2.03 | 0.58 |
| 1:A:208:LEU:CD2 | 1:A:212:LYS:HE3 | 2.33 | 0.58 |
| 3:C:39:ALA:O | 3:C:163:ILE:HG23 | 2.03 | 0.58 |
| 6:H:87:ARG:O | 6:H:89:LEU:HG | 2.04 | 0.58 |
| 2:B:515:HIS:CD2 | 2:B:517:THR:H | 2.22 | 0.58 |
| 2:B:563:MET:HE2 | 2:B:580:VAL:HB | 1.81 | 0.58 |
| 4:E:158:SER:O | 4:E:162:ARG:HG3 | 2.04 | 0.58 |
| 6:H:40:LEU:HD12 | 6:H:41:ASP:H | 1.69 | 0.58 |
| 8:J:14:VAL:CG1 | 8:J:50:ILE:HD11 | 2.33 | 0.58 |
| 1:A:494:SER:OG | 1:A:497:THR:HB | 2.04 | 0.58 |
| 2:B:983:ARG:HH11 | 2:B:1091:TYR:HB3 | 1.68 | 0.58 |
| 2:B:1153:GLU:CG | 2:B:1154:ALA:H | 2.07 | 0.58 |
| 10:L:30:ILE:HG22 | 10:L:31:CYS:N | 2.19 | 0.58 |
| 1:A:1015:VAL:HG13 | 1:A:1019:CYS:SG | 2.44 | 0.58 |
| 1:A:975:HIS:ND1 | 1:A:1036:ARG:HG3 | 2.19 | 0.58 |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:CA | 2.34 | 0.58 |
| 2:B:879:ARG:HB3 | 2:B:883:LEU:HD23 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:H:87:ARG:O | 6:H:89:LEU:N | 2.37 | 0.58 |
| 9:K:29:ASN:ND2 | 9:K:79:GLU:HA | 2.18 | 0.58 |
| 1:A:666:ILE:HD11 | 2:B:1030:LEU:HB2 | 1.85 | 0.58 |
| 2:B:25:ILE:CD1 | 2:B:653:VAL:HB | 2.34 | 0.58 |
| 2:B:889:THR:HG21 | 2:B:891:ASP:OD2 | 2.04 | 0.58 |
| 10:L:27:LEU:HD13 | 10:L:37:LYS:HG2 | 1.85 | 0.58 |
| 1:A:760:GLN:HB2 | 2:B:1021:MET:HE1 | 1.85 | 0.57 |
| 2:B:229:ALA:C | 2:B:231:PRO:HD2 | 2.23 | 0.57 |
| 2:B:25:ILE:HD12 | 2:B:653:VAL:HB | 1.85 | 0.57 |
| 3:C:49:VAL:CG1 | 3:C:155:LEU:HD11 | 2.34 | 0.57 |
| 4:E:117:THR:HG22 | 4:E:119:SER:H | 1.69 | 0.57 |
| 8:J:12:LYS:NZ | 8:J:17:LYS:NZ | 2.52 | 0.57 |
| 1:A:1155:ASP:OD2 | 1:A:1161:THR:HG23 | 2.04 | 0.57 |
| 1:A:184:SER:HA | 1:A:198:GLU:O | 2.04 | 0.57 |
| 1:A:682:THR:HG23 | 1:A:728:LYS:HE3 | 1.86 | 0.57 |
| 2:B:1153:GLU:HG2 | 2:B:1154:ALA:N | 2.12 | 0.57 |
| 2:B:98:THR:O | 2:B:126:SER:HB3 | 2.04 | 0.57 |
| 2:B:200:GLY:HA2 | 2:B:202:TYR:CE2 | 2.39 | 0.57 |
| 2:B:341:LEU:HG | 2:B:341:LEU:O | 2.04 | 0.57 |
| 2:B:826:ALA:HB2 | 2:B:1087:PHE:CD1 | 2.39 | 0.57 |
| 2:B:860:MET:HG2 | 2:B:861:ASP:H | 1.68 | 0.57 |
| 9:K:47:ARG:CB | 9:K:47:ARG:HH11 | 2.06 | 0.57 |
| 4:E:38:PRO:HG2 | 4:E:41:ASP:OD2 | 2.04 | 0.57 |
| 5:F:107:VAL:HG12 | 5:F:109:VAL:H | 1.69 | 0.57 |
| 1:A:567:LYS:CB | 6:H:96:VAL:H | 2.16 | 0.57 |
| 2:B:822:ASN:HD22 | 8:J:52:THR:HG21 | 1.69 | 0.57 |
| 8:J:64:ASN:HB3 | 8:J:65:PRO:CD | 2.29 | 0.57 |
| 1:A:244:PRO:N | 1:A:245:PRO:HD2 | 2.19 | 0.57 |
| 2:B:1174:LYS:HB2 | 2:B:1179:GLN:HB2 | 1.86 | 0.57 |
| 3:C:54:ASN:OD1 | 3:C:56:THR:HG22 | 2.05 | 0.57 |
| 1:A:1101:LEU:HB2 | 1:A:1355:VAL:HG11 | 1.86 | 0.57 |
| 1:A:381:THR:HG23 | 1:A:383:TYR:H | 1.70 | 0.57 |
| 2:B:130:VAL:CG1 | 2:B:131:ASP:H | 2.15 | 0.57 |
| 2:B:521:LEU:HD22 | 2:B:633:VAL:HG12 | 1.86 | 0.57 |
| 8:J:3:VAL:HG21 | 8:J:18:TRP:CB | 2.34 | 0.57 |
| 1:A:329:LEU:HB3 | 1:A:333:GLU:HB3 | 1.87 | 0.57 |
| 1:A:522:GLY:HA2 | 1:A:630:ILE:CD1 | 2.35 | 0.57 |
| 1:A:32:VAL:CG2 | 1:A:58:LEU:HD23 | 2.34 | 0.57 |
| 2:B:274:PRO:HG2 | 2:B:359:GLU:HB3 | 1.86 | 0.57 |
| 2:B:616:ILE:HD13 | 2:B:696:GLU:HG3 | 1.86 | 0.57 |
| 1:A:345:VAL:HG11 | 2:B:1128:LEU:O | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:556:TRP:CH2 | 1:A:558:GLY:HA2 | 2.40 | 0.57 |
| 4:E:116:ILE:HG22 | 4:E:117:THR:N | 2.20 | 0.57 |
| 4:E:58:MET:O | 4:E:59:SER:O | 2.23 | 0.57 |
| 6:H:103:LYS:HG2 | 6:H:115:TYR:N | 2.19 | 0.57 |
| 6:H:7:ASP:O | 6:H:8:ASP:HB2 | 2.05 | 0.57 |
| 1:A:172:PRO:HB3 | 1:A:185:TRP:CE2 | 2.40 | 0.56 |
| 1:A:682:THR:CG2 | 1:A:728:LYS:HG3 | 2.34 | 0.56 |
| 1:A:862:ASN:OD1 | 4:E:174:GLN:HA | 2.05 | 0.56 |
| 2:B:1072:MET:CE | 2:B:1085:ILE:HB | 2.30 | 0.56 |
| 2:B:737:THR:O | 2:B:737:THR:HG22 | 2.04 | 0.56 |
| 3:C:242:GLN:HE21 | 3:C:246:ARG:HE | 1.53 | 0.56 |
| 1:A:1150:SER:OG | 7:I:46:HIS:HB3 | 2.05 | 0.56 |
| 2:B:103:ASN:CB | 2:B:169:ARG:HH12 | 2.18 | 0.56 |
| 2:B:955:THR:CG2 | 2:B:956:THR:H | 2.03 | 0.56 |
| 1:A:32:VAL:HB | 1:A:57:ARG:HB3 | 1.85 | 0.56 |
| 1:A:598:LEU:HG | 6:H:115:TYR:HE2 | 1.69 | 0.56 |
| 2:B:284:ILE:CG1 | 2:B:324:ILE:HD12 | 2.35 | 0.56 |
| 2:B:654:ARG:N | 2:B:657:HIS:HD2 | 1.93 | 0.56 |
| 2:B:957:ASN:CG | 2:B:958:GLN:H | 2.08 | 0.56 |
| 1:A:1390:ASN:O | 1:A:1391:ARG:CB | 2.52 | 0.56 |
| 1:A:613:ILE:HD13 | 6:H:102:TYR:HB3 | 1.87 | 0.56 |
| 2:B:114:PRO:HD3 | 2:B:124:TYR:CE1 | 2.40 | 0.56 |
| 2:B:172:ILE:CD1 | 2:B:178:ASN:HD22 | 2.18 | 0.56 |
| 2:B:365:THR:HG22 | 2:B:366:GLN:N | 2.20 | 0.56 |
| 1:A:537:ARG:HD2 | 6:H:20:TYR:CE1 | 2.41 | 0.56 |
| 7:I:2:THR:O | 7:I:3:THR:C | 2.43 | 0.56 |
| 1:A:112:LYS:NZ | 1:A:164:ARG:HB2 | 2.20 | 0.56 |
| 1:A:1435:PRO:HA | 1:A:1439:GLY:O | 2.05 | 0.56 |
| 1:A:451:HIS:CD2 | 1:A:1074:GLU:HG3 | 2.40 | 0.56 |
| 1:A:1295:THR:HB | 1:A:1297:GLU:OE1 | 2.06 | 0.56 |
| 1:A:1383:SER:HB3 | 1:A:1387:HIS:CD2 | 2.40 | 0.56 |
| 1:A:38:PRO:HB3 | 1:A:270:LEU:HB3 | 1.87 | 0.56 |
| 1:A:768:GLN:HG3 | 1:A:816:HIS:HA | 1.87 | 0.56 |
| 1:A:92:HIS:CD2 | 1:A:94:GLY:H | 2.23 | 0.56 |
| 2:B:234:ILE:HD13 | 2:B:257:LYS:HD3 | 1.85 | 0.56 |
| 4:E:114:ASN:O | 4:E:115:ASN:HB3 | 2.05 | 0.56 |
| 1:A:1376:THR:CG2 | 4:E:212:ARG:HH22 | 2.19 | 0.56 |
| 1:A:567:LYS:HB2 | 1:A:568:PRO:HD3 | 1.84 | 0.56 |
| 1:A:636:GLU:OE1 | 1:A:966:ASN:ND2 | 2.38 | 0.56 |
| 2:B:899:ILE:HG22 | 2:B:900:ALA:H | 1.70 | 0.56 |
| 4:E:31:THR:C | 4:E:33:GLU:N | 2.58 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:22:ASP:O | 9:K:31:VAL:HG13 | 2.06 | 0.56 |
| 1:A:534:LEU:O | 1:A:574:GLY:HA3 | 2.05 | 0.56 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:H | 1.70 | 0.56 |
| 1:A:774:ARG:HB2 | 1:A:797:LYS:HG2 | 1.87 | 0.56 |
| 2:B:860:MET:HG2 | 2:B:861:ASP:N | 2.21 | 0.56 |
| 2:B:864:LYS:CB | 2:B:871:THR:HA | 2.36 | 0.56 |
| 2:B:884:ARG:O | 2:B:936:ASP:HB2 | 2.06 | 0.56 |
| 6:H:103:LYS:HZ1 | 6:H:114:VAL:CG2 | 2.18 | 0.56 |
| 3:C:57:VAL:HG11 | 8:J:60:PHE:HB2 | 1.86 | 0.56 |
| 1:A:1015:VAL:CG1 | 1:A:1019:CYS:SG | 2.94 | 0.56 |
| 2:B:102:VAL:HG23 | 2:B:112:LEU:HB2 | 1.88 | 0.56 |
| 2:B:648:HIS:N | 2:B:648:HIS:CD2 | 2.72 | 0.56 |
| 1:A:382:PRO:HD2 | 5:F:104:ASN:OD1 | 2.06 | 0.56 |
| 5:F:93:ILE:HD13 | 5:F:148:VAL:HG22 | 1.88 | 0.56 |
| 6:H:138:GLU:HG2 | 6:H:139:ASN:N | 2.21 | 0.56 |
| 1:A:1118:VAL:HG22 | 1:A:1306:LEU:HB2 | 1.87 | 0.56 |
| 2:B:104:GLU:OE2 | 10:L:54:ARG:HD3 | 2.06 | 0.56 |
| 2:B:35:SER:HA | 2:B:811:TYR:HE2 | 1.70 | 0.56 |
| 1:A:465:TYR:CA | 9:K:2:ASN:HB3 | 2.36 | 0.56 |
| 1:A:35:ILE:HG23 | 1:A:52:GLY:O | 2.06 | 0.55 |
| 1:A:388:LEU:HD23 | 1:A:391:LEU:HD12 | 1.88 | 0.55 |
| 1:A:694:THR:O | 1:A:698:GLN:HG3 | 2.06 | 0.55 |
| 2:B:839:MET:CE | 2:B:1010:LEU:HD11 | 2.29 | 0.55 |
| 1:A:329:LEU:HD21 | 2:B:1203:LEU:HD13 | 1.87 | 0.55 |
| 2:B:953:LEU:HD21 | 2:B:955:THR:OG1 | 2.06 | 0.55 |
| 1:A:889:SER:HB3 | 1:A:1297:GLU:HG3 | 1.87 | 0.55 |
| 1:A:540:PHE:C | 1:A:541:ILE:HD12 | 2.26 | 0.55 |
| 1:A:69:THR:O | 1:A:71:GLN:HG3 | 2.06 | 0.55 |
| 1:A:725:ALA:HA | 1:A:728:LYS:CE | 2.36 | 0.55 |
| 3:C:22:LEU:HD12 | 3:C:230:MET:HE3 | 1.87 | 0.55 |
| 7:I:111:THR:HG22 | 7:I:112:SER:H | 1.70 | 0.55 |
| 2:B:604:ARG:NH1 | 2:B:691:GLU:OE2 | 2.38 | 0.55 |
| 2:B:726:ALA:HB1 | 2:B:1051:THR:CG2 | 2.29 | 0.55 |
| 2:B:119:LEU:HD22 | 2:B:953:LEU:CD1 | 2.37 | 0.55 |
| 3:C:123:ASN:ND2 | 3:C:125:MET:HG2 | 2.20 | 0.55 |
| 5:F:81:THR:HG21 | 5:F:136:ARG:HD3 | 1.89 | 0.55 |
| 7:I:103:CYS:O | 7:I:107:SER:HA | 2.07 | 0.55 |
| 1:A:399:HIS:HB3 | 1:A:400:PRO:CD | 2.33 | 0.55 |
| 2:B:181:LEU:HD22 | 2:B:189:LEU:HD23 | 1.87 | 0.55 |
| 1:A:1216:ILE:O | 1:A:1219:THR:HB | 2.07 | 0.55 |
| 1:A:500:GLU:O | 1:A:504:LEU:HB2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:629:LEU:O | 1:A:633:VAL:HG23 | 2.07 | 0.55 |
| 5:F:93:ILE:CD1 | 5:F:134:ILE:HD11 | 2.31 | 0.55 |
| 2:B:651:LEU:HD11 | 2:B:707:PRO:CB | 2.32 | 0.55 |
| 1:A:1169:ILE:O | 1:A:1173:HIS:HD2 | 1.89 | 0.55 |
| 2:B:293:PRO:HG2 | 2:B:296:GLU:HB2 | 1.89 | 0.55 |
| 4:E:13:TRP:CE3 | 4:E:39:LEU:HD13 | 2.42 | 0.55 |
| 4:E:156:LEU:HD21 | 4:E:197:LYS:HB2 | 1.89 | 0.55 |
| 1:A:1167:GLU:O | 1:A:1171:GLN:HG3 | 2.07 | 0.55 |
| 1:A:1265:ASN:HD21 | 2:B:263:GLY:HA2 | 1.71 | 0.55 |
| 1:A:1146:VAL:HG11 | 1:A:1202:MET:SD | 2.47 | 0.55 |
| 1:A:418:SER:O | 1:A:420:ARG:N | 2.40 | 0.55 |
| 6:H:13:SER:O | 6:H:14:GLU:HB2 | 2.05 | 0.55 |
| 1:A:108:MET:HA | 1:A:210:ILE:HD13 | 1.87 | 0.55 |
| 1:A:849:MET:HE3 | 1:A:1436:ILE:HA | 1.87 | 0.55 |
| 2:B:824:ILE:HG12 | 8:J:48:ARG:NH1 | 2.22 | 0.55 |
| 2:B:847:ASP:OD2 | 9:K:6:ARG:NH2 | 2.39 | 0.55 |
| 3:C:93:ASP:OD1 | 3:C:122:SER:HB2 | 2.06 | 0.55 |
| 7:I:111:THR:HG22 | 7:I:113:ASP:N | 2.11 | 0.54 |
| 1:A:1277:GLU:CD | 1:A:1277:GLU:H | 2.10 | 0.54 |
| 1:A:157:ASP:C | 1:A:159:THR:H | 2.09 | 0.54 |
| 1:A:595:THR:HG23 | 1:A:599:SER:HB3 | 1.88 | 0.54 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:CG1 | 2.36 | 0.54 |
| 1:A:381:THR:HG21 | 1:A:383:TYR:CD1 | 2.42 | 0.54 |
| 1:A:82:GLY:HA3 | 1:A:241:VAL:HB | 1.89 | 0.54 |
| 1:A:919:ILE:HG12 | 1:A:925:LEU:HD12 | 1.89 | 0.54 |
| 2:B:1003:ALA:O | 3:C:177:GLU:HA | 2.06 | 0.54 |
| 2:B:121:ASN:HA | 2:B:207:GLY:HA3 | 1.89 | 0.54 |
| 2:B:514:LEU:HD12 | 2:B:518:HIS:HD2 | 1.72 | 0.54 |
| 10:L:39:SER:O | 10:L:40:LEU:HD23 | 2.07 | 0.54 |
| 1:A:1128:GLN:O | 1:A:1128:GLN:HG3 | 2.07 | 0.54 |
| 2:B:971:THR:OG1 | 3:C:61:GLU:HG3 | 2.08 | 0.54 |
| 1:A:551:TYR:CE2 | 9:K:62:LYS:HE2 | 2.42 | 0.54 |
| 1:A:1147:THR:HB | 7:I:48:LEU:CD1 | 2.37 | 0.54 |
| 1:A:1194:ARG:NH2 | 1:A:1237:ILE:HD13 | 2.23 | 0.54 |
| 1:A:579:SER:OG | 1:A:612:ILE:HG23 | 2.07 | 0.54 |
| 1:A:267:ALA:O | 1:A:270:LEU:HB2 | 2.07 | 0.54 |
| 2:B:843:GLN:N | 2:B:994:TYR:O | 2.35 | 0.54 |
| 5:F:93:ILE:HD11 | 5:F:134:ILE:CD1 | 2.32 | 0.54 |
| 6:H:103:LYS:HD3 | 6:H:114:VAL:HB | 1.88 | 0.54 |
| 1:A:450:LEU:N | 1:A:450:LEU:HD12 | 2.08 | 0.54 |
| 1:A:767:GLN:O | 11:M:3:GLY:HA2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:1148:LYS:HG3 | 2:B:1152:MET:CE | 2.38 | 0.54 |
| 2:B:861:ASP:OD2 | 2:B:914:LYS:HD2 | 2.08 | 0.54 |
| 8:J:3:VAL:HG21 | 8:J:18:TRP:HB2 | 1.89 | 0.54 |
| 9:K:20:LYS:HB2 | 9:K:34:THR:HB | 1.88 | 0.54 |
| 1:A:1098:VAL:N | 1:A:1099:PRO:HD2 | 2.23 | 0.54 |
| 1:A:269:ILE:HG12 | 1:A:299:HIS:HB3 | 1.88 | 0.54 |
| 1:A:470:LEU:HD11 | 1:A:487:MET:HE2 | 1.84 | 0.54 |
| 1:A:57:ARG:C | 1:A:68:GLN:HE21 | 2.11 | 0.54 |
| 2:B:103:ASN:HB2 | 2:B:169:ARG:NH1 | 2.23 | 0.54 |
| 2:B:89:GLU:N | 2:B:135:ARG:O | 2.40 | 0.54 |
| 2:B:313:MET:CE | 2:B:386:LEU:HD22 | 2.37 | 0.54 |
| 3:C:258:ILE:HD11 | 9:K:42:LEU:HD21 | 1.90 | 0.54 |
| 3:C:55:THR:O | 3:C:55:THR:HG22 | 2.08 | 0.54 |
| 6:H:107:VAL:HG12 | 6:H:107:VAL:O | 2.08 | 0.54 |
| 1:A:683:ILE:HG21 | 1:A:801:GLU:HG3 | 1.88 | 0.54 |
| 1:A:994:GLN:NE2 | 1:A:1023:ARG:HE | 2.06 | 0.54 |
| 2:B:272:THR:O | 2:B:272:THR:HG22 | 2.08 | 0.54 |
| 1:A:761:MET:O | 1:A:803:SER:HB2 | 2.08 | 0.54 |
| 2:B:1008:PRO:HB3 | 2:B:1087:PHE:HE1 | 1.72 | 0.54 |
| 2:B:63:ILE:CB | 2:B:95:ILE:HD11 | 2.38 | 0.54 |
| 1:A:1265:ASN:HD21 | 2:B:263:GLY:CA | 2.20 | 0.53 |
| 1:A:112:LYS:HZ1 | 1:A:165:GLY:H | 1.54 | 0.53 |
| 1:A:239:LEU:HD23 | 1:A:240:PRO:N | 2.22 | 0.53 |
| 5:F:75:PRO:O | 5:F:77:ASP:O | 2.25 | 0.53 |
| 1:A:134:ARG:HD2 | 1:A:221:SER:O | 2.09 | 0.53 |
| 1:A:327:ALA:HA | 1:A:330:LYS:HD2 | 1.89 | 0.53 |
| 2:B:1099:VAL:C | 2:B:1101:ASP:H | 2.12 | 0.53 |
| 2:B:899:ILE:CG2 | 2:B:900:ALA:N | 2.71 | 0.53 |
| 1:A:1318:THR:HG21 | 4:E:11:ARG:HH12 | 1.72 | 0.53 |
| 1:A:1336:MET:HE1 | 1:A:1381:LEU:N | 2.22 | 0.53 |
| 1:A:1336:MET:CE | 1:A:1381:LEU:HG | 2.38 | 0.53 |
| 1:A:93:VAL:HG22 | 1:A:301:ALA:HA | 1.91 | 0.53 |
| 1:A:399:HIS:O | 1:A:400:PRO:C | 2.44 | 0.53 |
| 1:A:736:ASN:O | 1:A:737:LEU:C | 2.46 | 0.53 |
| 1:A:911:SER:O | 1:A:978:PRO:HG3 | 2.09 | 0.53 |
| 2:B:1127:GLY:O | 2:B:1128:LEU:HB3 | 2.08 | 0.53 |
| 2:B:230:ALA:N | 2:B:231:PRO:HD2 | 2.24 | 0.53 |
| 2:B:952:VAL:HB | 10:L:58:LYS:CB | 2.36 | 0.53 |
| 4:E:5:ASN:HA | 4:E:8:ASN:HB3 | 1.90 | 0.53 |
| 6:H:59:ILE:O | 6:H:60:ALA:HB3 | 2.09 | 0.53 |
| 1:A:1328:TYR:CG | 1:A:1329:THR:N | 2.75 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:313:MET:HE2 | 2:B:386:LEU:HD22 | 1.90 | 0.53 |
| 3:C:162:GLY:HA3 | 3:C:170:TRP:CE2 | 2.44 | 0.53 |
| 4:E:89:GLY:HA2 | 4:E:117:THR:OG1 | 2.08 | 0.53 |
| 1:A:709:THR:HG23 | 7:I:94:ASP:HA | 1.90 | 0.53 |
| 1:A:518:LYS:HB2 | 1:A:519:PRO:HD2 | 1.90 | 0.53 |
| 1:A:575:LYS:HD3 | 1:A:612:ILE:HD11 | 1.90 | 0.53 |
| 6:H:89:LEU:O | 6:H:91:ASP:N | 2.39 | 0.53 |
| 1:A:567:LYS:CG | 6:H:96:VAL:H | 2.21 | 0.53 |
| 2:B:311:LEU:HB3 | 7:I:4:PHE:CE2 | 2.44 | 0.53 |
| 1:A:146:MET:HA | 1:A:171:GLN:HB3 | 1.91 | 0.53 |
| 1:A:23:SER:HB3 | 1:A:233:TRP:CE2 | 2.44 | 0.53 |
| 1:A:243:PRO:C | 1:A:245:PRO:HD2 | 2.29 | 0.53 |
| 1:A:605:MET:HE2 | 1:A:607:ILE:CG1 | 2.39 | 0.53 |
| 1:A:907:THR:HG22 | 1:A:908:LEU:N | 2.21 | 0.53 |
| 1:A:345:VAL:CG1 | 2:B:1150:ARG:HH22 | 2.21 | 0.53 |
| 2:B:496:ARG:NH2 | 2:B:541:LEU:HA | 2.23 | 0.53 |
| 1:A:399:HIS:CB | 1:A:400:PRO:HD3 | 2.34 | 0.53 |
| 2:B:69:LEU:HD21 | 2:B:425:THR:HG23 | 1.91 | 0.53 |
| 3:C:124:LEU:O | 3:C:127:ARG:HG2 | 2.09 | 0.53 |
| 3:C:167:HIS:HD2 | 3:C:169:LYS:H | 1.57 | 0.53 |
| 3:C:22:LEU:HD12 | 3:C:230:MET:HE1 | 1.91 | 0.53 |
| 9:K:47:ARG:HD3 | 9:K:59:ALA:O | 2.08 | 0.53 |
| 1:A:1392:SER:O | 1:A:1393:ASN:HB2 | 2.09 | 0.53 |
| 1:A:579:SER:HB3 | 1:A:611:GLN:HA | 1.91 | 0.53 |
| 1:A:683:ILE:HD13 | 1:A:801:GLU:HG3 | 1.90 | 0.53 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:H | 1.50 | 0.53 |
| 2:B:1084:GLN:NE2 | 3:C:192:TRP:H | 2.07 | 0.53 |
| 5:F:111:LEU:N | 5:F:111:LEU:HD12 | 2.11 | 0.53 |
| 1:A:1199:ARG:O | 1:A:1202:MET:HB2 | 2.09 | 0.53 |
| 1:A:531:ILE:HD11 | 1:A:578:LEU:HD21 | 1.89 | 0.53 |
| 1:A:630:ILE:HD13 | 1:A:646:PHE:CZ | 2.44 | 0.53 |
| 3:C:181:ASP:CG | 3:C:186:LEU:HD13 | 2.29 | 0.53 |
| 1:A:503:GLN:NE2 | 5:F:90:ARG:HH22 | 2.06 | 0.53 |
| 7:I:45:ARG:NH1 | 7:I:45:ARG:HG2 | 2.20 | 0.53 |
| 8:J:32:GLU:CD | 8:J:32:GLU:H | 2.13 | 0.53 |
| 1:A:1405:THR:HG23 | 1:A:1408:ILE:HD12 | 1.89 | 0.53 |
| 1:A:705:LYS:HD2 | 1:A:708:MET:HE1 | 1.91 | 0.53 |
| 1:A:738:LYS:HZ1 | 3:C:194:GLU:C | 2.13 | 0.53 |
| 3:C:242:GLN:NE2 | 3:C:246:ARG:HE | 2.07 | 0.53 |
| 4:E:112:TYR:CE1 | 4:E:115:ASN:HA | 2.44 | 0.53 |
| 6:H:97:MET:CE | 6:H:142:LEU:HD23 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:606:LEU:HD11 | 1:A:608:ILE:HD11 | 1.91 | 0.52 |
| 1:A:901:LEU:N | 1:A:926:GLN:NE2 | 2.37 | 0.52 |
| 1:A:10:PRO:HG2 | 2:B:1192:TYR:HD2 | 1.74 | 0.52 |
| 2:B:273:LEU:HD12 | 2:B:280:ILE:HD12 | 1.91 | 0.52 |
| 2:B:563:MET:HE3 | 2:B:580:VAL:HB | 1.89 | 0.52 |
| 6:H:123:MET:HE1 | 6:H:142:LEU:HD13 | 1.90 | 0.52 |
| 10:L:27:LEU:HD22 | 10:L:37:LYS:HD3 | 1.91 | 0.52 |
| 1:A:1336:MET:CE | 1:A:1380:GLY:HA2 | 2.37 | 0.52 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:CD | 2.28 | 0.52 |
| 1:A:406:ILE:HA | 1:A:411:ASP:O | 2.10 | 0.52 |
| 1:A:855:THR:HG23 | 1:A:857:ARG:HG3 | 1.91 | 0.52 |
| 2:B:1065:GLN:HE22 | 2:B:1067:ARG:HB2 | 1.74 | 0.52 |
| 1:A:17:VAL:HA | 2:B:1215:ARG:O | 2.09 | 0.52 |
| 2:B:284:ILE:CD1 | 2:B:324:ILE:HD12 | 2.39 | 0.52 |
| 3:C:49:VAL:HG11 | 3:C:155:LEU:HD11 | 1.90 | 0.52 |
| 1:A:1206:ASP:HB2 | 1:A:1274:ARG:HH12 | 1.73 | 0.52 |
| 1:A:1341:ILE:CD1 | 1:A:1376:THR:HG23 | 2.40 | 0.52 |
| 1:A:834:THR:CG2 | 1:A:1077:THR:OG1 | 2.57 | 0.52 |
| 2:B:1002:THR:CG2 | 2:B:1006:ILE:HB | 2.40 | 0.52 |
| 2:B:1099:VAL:O | 2:B:1103:ILE:HG13 | 2.09 | 0.52 |
| 2:B:164:LYS:O | 2:B:165:VAL:CB | 2.57 | 0.52 |
| 2:B:65:GLU:HG3 | 2:B:65:GLU:O | 2.10 | 0.52 |
| 2:B:735:ALA:HB3 | 2:B:738:PHE:CE1 | 2.44 | 0.52 |
| 2:B:884:ARG:O | 2:B:936:ASP:CB | 2.57 | 0.52 |
| 2:B:997:GLU:CG | 3:C:39:ALA:HB2 | 2.39 | 0.52 |
| 1:A:1161:THR:HG22 | 1:A:1162:VAL:N | 2.23 | 0.52 |
| 1:A:345:VAL:HG13 | 2:B:1150:ARG:HH12 | 1.74 | 0.52 |
| 1:A:68:GLN:C | 1:A:70:CYS:H | 2.13 | 0.52 |
| 2:B:167:ILE:O | 2:B:167:ILE:HG22 | 2.09 | 0.52 |
| 4:E:176:PRO:O | 4:E:212:ARG:HA | 2.10 | 0.52 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:CE | 2.26 | 0.52 |
| 1:A:472:LEU:HD13 | 2:B:835:GLN:NE2 | 2.24 | 0.52 |
| 2:B:105:SER:O | 2:B:106:ASP:HB2 | 2.10 | 0.52 |
| 3:C:237:SER:O | 3:C:238:ILE:HG13 | 2.10 | 0.52 |
| 6:H:125:LEU:HB3 | 6:H:130:ARG:CZ | 2.40 | 0.52 |
| 8:J:48:ARG:O | 8:J:52:THR:HB | 2.10 | 0.52 |
| 1:A:1386:ARG:HG3 | 1:A:1386:ARG:O | 2.10 | 0.52 |
| 2:B:1165:ILE:HG13 | 2:B:1187:ASN:HD21 | 1.75 | 0.52 |
| 2:B:344:LYS:H | 2:B:347:LYS:HZ1 | 1.57 | 0.52 |
| 2:B:906:SER:O | 2:B:907:GLY:C | 2.47 | 0.52 |
| 1:A:899:VAL:HG12 | 1:A:929:LEU:HD13 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:137:LYS:H | 3:C:137:LYS:CD | 2.21 | 0.52 |
| 6:H:103:LYS:HG2 | 6:H:115:TYR:H | 1.74 | 0.52 |
| 2:B:824:ILE:CG1 | 8:J:48:ARG:HH12 | 2.23 | 0.52 |
| 1:A:1146:VAL:O | 1:A:1146:VAL:CG1 | 2.57 | 0.52 |
| 2:B:130:VAL:CG1 | 2:B:131:ASP:N | 2.73 | 0.52 |
| 2:B:484:ASN:ND2 | 2:B:486:TYR:HE1 | 2.08 | 0.52 |
| 2:B:98:THR:HG22 | 2:B:99:LYS:H | 1.74 | 0.52 |
| 5:F:77:ASP:O | 5:F:78:GLN:CB | 2.57 | 0.52 |
| 1:A:262:LEU:HD11 | 1:A:328:ARG:HD2 | 1.92 | 0.52 |
| 2:B:272:THR:OG1 | 2:B:279:ASP:OD1 | 2.26 | 0.52 |
| 6:H:18:GLY:O | 6:H:20:TYR:N | 2.42 | 0.52 |
| 1:A:479:ASN:HD22 | 1:A:479:ASN:C | 2.12 | 0.52 |
| 1:A:72:GLU:HB3 | 1:A:76:GLU:HB2 | 1.90 | 0.52 |
| 1:A:768:GLN:NE2 | 1:A:816:HIS:HA | 2.23 | 0.52 |
| 2:B:416:LEU:HD11 | 2:B:466:TRP:CZ2 | 2.45 | 0.52 |
| 3:C:77:ILE:CA | 3:C:129:ILE:HD11 | 2.38 | 0.52 |
| 9:K:111:LEU:N | 9:K:111:LEU:HD23 | 2.24 | 0.52 |
| 10:L:26:THR:CG2 | 10:L:27:LEU:N | 2.67 | 0.52 |
| 10:L:68:GLU:CD | 10:L:68:GLU:H | 2.12 | 0.52 |
| 1:A:1195:LEU:HD11 | 1:A:1267:MET:HE3 | 1.91 | 0.51 |
| 1:A:606:LEU:HG | 1:A:613:ILE:HB | 1.92 | 0.51 |
| 1:A:971:PHE:O | 1:A:972:HIS:C | 2.46 | 0.51 |
| 2:B:130:VAL:HG21 | 2:B:167:ILE:HD12 | 1.92 | 0.51 |
| 3:C:18:VAL:O | 3:C:20:PHE:HD2 | 1.93 | 0.51 |
| 4:E:59:SER:O | 4:E:60:PHE:HB3 | 2.09 | 0.51 |
| 10:L:51:CYS:C | 10:L:53:HIS:H | 2.10 | 0.51 |
| 1:A:1410:PHE:HD2 | 2:B:1212:ILE:HD11 | 1.74 | 0.51 |
| 1:A:32:VAL:HB | 1:A:57:ARG:CB | 2.40 | 0.51 |
| 1:A:533:LYS:HE3 | 1:A:745:GLN:HE22 | 1.75 | 0.51 |
| 1:A:751:SER:O | 1:A:752:LYS:O | 2.29 | 0.51 |
| 1:A:901:LEU:HD23 | 1:A:907:THR:HG23 | 1.92 | 0.51 |
| 1:A:998:LEU:HD12 | 1:A:1001:ARG:HH12 | 1.74 | 0.51 |
| 2:B:830:TYR:CE1 | 2:B:1000:PRO:HB3 | 2.46 | 0.51 |
| 2:B:911:ILE:HG22 | 2:B:912:ILE:HG13 | 1.92 | 0.51 |
| 3:C:73:GLN:NE2 | 3:C:75:MET:HB2 | 2.26 | 0.51 |
| 4:E:61:GLN:HG2 | 4:E:62:ALA:N | 2.25 | 0.51 |
| 6:H:113:ALA:HB1 | 6:H:124:ARG:HE | 1.74 | 0.51 |
| 6:H:125:LEU:HB3 | 6:H:130:ARG:NH1 | 2.24 | 0.51 |
| 7:I:72:ASP:O | 7:I:81:ARG:HD2 | 2.10 | 0.51 |
| 1:A:1336:MET:HG2 | 1:A:1336:MET:O | 2.09 | 0.51 |
| 2:B:227:LYS:NZ | 2:B:236:HIS:HE1 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:640:VAL:HG22 | 2:B:651:LEU:CD2 | 2.39 | 0.51 |
| 1:A:1318:THR:CG2 | 4:E:11:ARG:HH12 | 2.24 | 0.51 |
| 6:H:62:SER:O | 6:H:63:LEU:C | 2.48 | 0.51 |
| 2:B:737:THR:HG21 | 7:I:66:PRO:CA | 2.41 | 0.51 |
| 1:A:1191:TRP:CE2 | 1:A:1257:ASP:OD1 | 2.64 | 0.51 |
| 1:A:328:ARG:HB3 | 1:A:332:LYS:NZ | 2.25 | 0.51 |
| 1:A:540:PHE:HB3 | 1:A:571:LEU:HG | 1.93 | 0.51 |
| 2:B:757:PRO:HG2 | 2:B:984:HIS:CE1 | 2.44 | 0.51 |
| 2:B:794:ASN:C | 2:B:795:ILE:HD12 | 2.30 | 0.51 |
| 6:H:130:ARG:HA | 6:H:133:ASN:CB | 2.40 | 0.51 |
| 7:I:51:ASN:HB2 | 7:I:118:ARG:NH1 | 2.26 | 0.51 |
| 10:L:34:CYS:C | 10:L:36:SER:H | 2.12 | 0.51 |
| 1:A:775:ILE:O | 1:A:797:LYS:HE3 | 2.10 | 0.51 |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:HB | 1.93 | 0.51 |
| 2:B:1006:ILE:HD12 | 14:B:2021:HOH:O | 2.09 | 0.51 |
| 2:B:210:LYS:HE3 | 2:B:480:SER:OG | 2.11 | 0.51 |
| 2:B:763:GLN:HB2 | 2:B:1021:MET:HB2 | 1.91 | 0.51 |
| 2:B:776:GLN:O | 2:B:1095:LEU:HA | 2.10 | 0.51 |
| 2:B:859:TYR:OH | 2:B:941:LEU:HD12 | 2.10 | 0.51 |
| 1:A:1107:VAL:O | 1:A:1107:VAL:HG12 | 2.09 | 0.51 |
| 1:A:1395:GLY:C | 1:A:1397:LEU:N | 2.64 | 0.51 |
| 2:B:46:GLN:HE22 | 2:B:496:ARG:HA | 1.76 | 0.51 |
| 4:E:55:ARG:HH11 | 4:E:55:ARG:HG3 | 1.75 | 0.51 |
| 4:E:65:THR:O | 4:E:69:ILE:HG13 | 2.09 | 0.51 |
| 1:A:1356:ILE:HD12 | 1:A:1368:MET:SD | 2.51 | 0.51 |
| 1:A:857:ARG:HD3 | 1:A:861:GLY:O | 2.11 | 0.51 |
| 2:B:1034:VAL:CG2 | 2:B:1059:LEU:HB2 | 2.41 | 0.51 |
| 9:K:21:ILE:CG2 | 9:K:31:VAL:HG11 | 2.40 | 0.51 |
| 9:K:43:GLY:O | 9:K:47:ARG:HB2 | 2.11 | 0.51 |
| 1:A:549:MET:SD | 1:A:577:ILE:HD12 | 2.51 | 0.51 |
| 1:A:756:ILE:HD13 | 1:A:756:ILE:O | 2.11 | 0.51 |
| 2:B:54:PHE:HA | 2:B:58:THR:HB | 1.92 | 0.51 |
| 10:L:46:VAL:O | 10:L:54:ARG:HA | 2.11 | 0.51 |
| 1:A:1336:MET:HE1 | 1:A:1381:LEU:HG | 1.92 | 0.51 |
| 1:A:871:ASP:OD2 | 4:E:204:THR:HG23 | 2.10 | 0.51 |
| 1:A:961:ARG:O | 1:A:965:GLN:HG3 | 2.10 | 0.51 |
| 2:B:1002:THR:CG2 | 2:B:1006:ILE:H | 2.23 | 0.51 |
| 2:B:759:PRO:HG2 | 2:B:1046:PRO:HB3 | 1.92 | 0.51 |
| 2:B:174:LEU:HD22 | 2:B:202:TYR:CZ | 2.46 | 0.51 |
| 2:B:847:ASP:O | 3:C:65:HIS:HE1 | 1.93 | 0.51 |
| 9:K:45:LEU:HG | 9:K:94:ILE:HD13 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1197:LEU:HD11 | 1:A:1238:ILE:HD11 | 1.92 | 0.51 |
| 1:A:329:LEU:C | 1:A:331:GLY:H | 2.13 | 0.51 |
| 1:A:78:PRO:HA | 2:B:1201:LYS:NZ | 2.26 | 0.51 |
| 2:B:1051:THR:HG22 | 2:B:1052:VAL:N | 2.25 | 0.51 |
| 2:B:1148:LYS:HG3 | 2:B:1152:MET:HE3 | 1.93 | 0.51 |
| 2:B:1165:ILE:HD12 | 2:B:1187:ASN:ND2 | 2.26 | 0.51 |
| 6:H:93:TYR:CD1 | 6:H:93:TYR:N | 2.79 | 0.51 |
| 10:L:38:LEU:O | 10:L:39:SER:CB | 2.59 | 0.51 |
| 1:A:157:ASP:C | 1:A:159:THR:N | 2.64 | 0.50 |
| 1:A:61:ILE:O | 1:A:62:ASP:HB2 | 2.11 | 0.50 |
| 1:A:754:SER:H | 1:A:757:ASN:HD22 | 1.59 | 0.50 |
| 1:A:869:GLY:O | 1:A:870:GLU:HB2 | 2.12 | 0.50 |
| 3:C:89:GLU:O | 3:C:90:ASP:HB3 | 2.10 | 0.50 |
| 4:E:45:LYS:HG2 | 4:E:45:LYS:O | 2.11 | 0.50 |
| 1:A:327:ALA:HA | 1:A:330:LYS:CD | 2.41 | 0.50 |
| 1:A:858:ASN:ND2 | 1:A:858:ASN:C | 2.65 | 0.50 |
| 6:H:10:PHE:O | 6:H:54:SER:HA | 2.11 | 0.50 |
| 6:H:118:PHE:HB2 | 6:H:121:LEU:HB2 | 1.92 | 0.50 |
| 2:B:737:THR:CG2 | 7:I:66:PRO:CA | 2.89 | 0.50 |
| 8:J:25:LEU:O | 8:J:29:GLU:HA | 2.12 | 0.50 |
| 1:A:1187:GLN:CG | 1:A:1188:GLN:H | 2.24 | 0.50 |
| 1:A:1285:MET:HG3 | 1:A:1307:GLU:OE1 | 2.11 | 0.50 |
| 1:A:1394:THR:HG23 | 1:A:1398:MET:CE | 2.41 | 0.50 |
| 1:A:606:LEU:HD23 | 1:A:614:PHE:CE2 | 2.47 | 0.50 |
| 1:A:73:GLY:C | 1:A:75:ASN:H | 2.15 | 0.50 |
| 1:A:848:ILE:HG12 | 1:A:864:ILE:CD1 | 2.41 | 0.50 |
| 2:B:1056:SER:HB3 | 2:B:1066:SER:HB2 | 1.93 | 0.50 |
| 2:B:824:ILE:HG12 | 8:J:48:ARG:HH12 | 1.77 | 0.50 |
| 3:C:175:ALA:O | 3:C:176:ILE:HG12 | 2.12 | 0.50 |
| 5:F:81:THR:CG2 | 5:F:82:THR:N | 2.75 | 0.50 |
| 1:A:1096:SER:O | 1:A:1099:PRO:HG2 | 2.11 | 0.50 |
| 2:B:1185:CYS:O | 2:B:1186:ASP:HB2 | 2.12 | 0.50 |
| 2:B:18:PHE:N | 2:B:18:PHE:CD2 | 2.80 | 0.50 |
| 2:B:733:HIS:O | 2:B:735:ALA:N | 2.38 | 0.50 |
| 2:B:999:MET:HA | 2:B:999:MET:CE | 2.41 | 0.50 |
| 3:C:258:ILE:HD13 | 9:K:35:PHE:CE2 | 2.38 | 0.50 |
| 6:H:47:PHE:CB | 6:H:95:TYR:HD1 | 2.25 | 0.50 |
| 3:C:57:VAL:HG11 | 8:J:60:PHE:CB | 2.41 | 0.50 |
| 3:C:7:GLN:HG2 | 9:K:104:ASN:ND2 | 2.26 | 0.50 |
| 2:B:900:ALA:HB2 | 10:L:58:LYS:NZ | 2.26 | 0.50 |
| 1:A:557:ASP:N | 1:A:557:ASP:OD1 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:294:ASP:H | 7:I:12:ASN:HD22 | 1.57 | 0.50 |
| 2:B:969:ARG:NH1 | 2:B:969:ARG:HB3 | 2.25 | 0.50 |
| 3:C:137:LYS:C | 3:C:138:GLU:HG2 | 2.32 | 0.50 |
| 3:C:148:ARG:HH12 | 8:J:64:ASN:CA | 2.20 | 0.50 |
| 7:I:55:THR:O | 7:I:58:VAL:HG23 | 2.11 | 0.50 |
| 1:A:128:ILE:HG22 | 1:A:130:ASP:H | 1.77 | 0.50 |
| 1:A:1395:GLY:O | 1:A:1397:LEU:N | 2.45 | 0.50 |
| 2:B:976:ILE:O | 2:B:1099:VAL:HG21 | 2.11 | 0.50 |
| 2:B:357:GLN:OE1 | 2:B:358:LYS:HE3 | 2.11 | 0.50 |
| 3:C:179:GLU:CG | 3:C:180:TYR:N | 2.74 | 0.50 |
| 5:F:109:VAL:HG13 | 5:F:127:GLU:OE1 | 2.11 | 0.50 |
| 8:J:24:LEU:O | 8:J:30:LEU:HB2 | 2.11 | 0.50 |
| 8:J:57:ILE:HA | 8:J:60:PHE:CD2 | 2.47 | 0.50 |
| 1:A:535:THR:O | 1:A:575:LYS:HE3 | 2.12 | 0.50 |
| 2:B:834:ASN:O | 2:B:1013:ASN:HB2 | 2.10 | 0.50 |
| 2:B:1163:CYS:SG | 2:B:1165:ILE:HB | 2.52 | 0.50 |
| 2:B:46:GLN:OE1 | 2:B:47:GLN:HG2 | 2.12 | 0.50 |
| 2:B:680:THR:CG2 | 2:B:681:TRP:H | 2.24 | 0.50 |
| 8:J:12:LYS:HZ1 | 8:J:17:LYS:HZ1 | 1.60 | 0.50 |
| 1:A:523:ILE:HD12 | 1:A:622:VAL:CG2 | 2.42 | 0.50 |
| 2:B:29:ASP:CB | 2:B:658:ILE:HD13 | 2.31 | 0.50 |
| 2:B:879:ARG:HE | 2:B:885:MET:HE2 | 1.77 | 0.50 |
| 2:B:998:ASP:OD1 | 3:C:35:ARG:NH2 | 2.42 | 0.50 |
| 1:A:246:VAL:C | 1:A:328:ARG:HH12 | 2.14 | 0.50 |
| 1:A:705:LYS:O | 1:A:708:MET:HB2 | 2.11 | 0.50 |
| 2:B:235:SER:OG | 2:B:236:HIS:HD2 | 1.95 | 0.50 |
| 2:B:284:ILE:HD13 | 2:B:324:ILE:HD12 | 1.93 | 0.50 |
| 6:H:100:THR:HG23 | 6:H:138:GLU:CB | 2.42 | 0.50 |
| 8:J:12:LYS:NZ | 8:J:17:LYS:HZ1 | 2.10 | 0.50 |
| 8:J:2:ILE:HG22 | 8:J:3:VAL:N | 2.26 | 0.50 |
| 1:A:714:PHE:HB2 | 7:I:97:MET:CE | 2.42 | 0.49 |
| 2:B:542:MET:HG3 | 2:B:747:MET:CE | 2.29 | 0.49 |
| 2:B:621:GLU:O | 2:B:623:GLU:HG3 | 2.12 | 0.49 |
| 2:B:969:ARG:HE | 3:C:59:ALA:HB1 | 1.77 | 0.49 |
| 2:B:773:MET:HE3 | 2:B:985:GLY:HA2 | 1.93 | 0.49 |
| 1:A:1101:LEU:O | 1:A:1105:LEU:HG | 2.11 | 0.49 |
| 1:A:106:VAL:HG22 | 1:A:111:GLY:HA2 | 1.93 | 0.49 |
| 1:A:472:LEU:O | 1:A:475:THR:HB | 2.12 | 0.49 |
| 2:B:126:SER:OG | 2:B:172:ILE:HD12 | 2.12 | 0.49 |
| 3:C:203:GLN:HG2 | 3:C:207:CYS:SG | 2.51 | 0.49 |
| 9:K:31:VAL:HG12 | 9:K:32:VAL:N | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:L:30:ILE:HG22 | 10:L:31:CYS:H | 1.77 | 0.49 |
| 10:L:32:ALA:HB2 | 10:L:55:ILE:CB | 2.42 | 0.49 |
| 1:A:185:TRP:O | 1:A:186:LYS:HB2 | 2.12 | 0.49 |
| 2:B:134:LYS:HZ1 | 2:B:446:LEU:HD13 | 1.77 | 0.49 |
| 3:C:162:GLY:HA3 | 3:C:170:TRP:CD2 | 2.47 | 0.49 |
| 3:C:56:THR:HG23 | 3:C:57:VAL:N | 2.26 | 0.49 |
| 2:B:195:CYS:SG | 2:B:197:PHE:HB2 | 2.52 | 0.49 |
| 2:B:983:ARG:HD3 | 14:B:2018:HOH:O | 2.12 | 0.49 |
| 3:C:128:ASN:O | 3:C:129:ILE:HG13 | 2.12 | 0.49 |
| 3:C:196:ASP:HB3 | 3:C:199:LYS:HB2 | 1.94 | 0.49 |
| 1:A:1277:GLU:O | 1:A:1278:ASN:CB | 2.61 | 0.49 |
| 1:A:784:LEU:HB3 | 1:A:786:HIS:HD2 | 1.76 | 0.49 |
| 2:B:305:VAL:O | 2:B:305:VAL:HG12 | 2.12 | 0.49 |
| 2:B:735:ALA:HB3 | 2:B:738:PHE:CZ | 2.47 | 0.49 |
| 1:A:767:GLN:HG2 | 11:M:4:ILE:CD1 | 2.42 | 0.49 |
| 1:A:1192:LEU:HD11 | 1:A:1239:ARG:HB3 | 1.94 | 0.49 |
| 1:A:457:ALA:HB3 | 1:A:506:ALA:HA | 1.95 | 0.49 |
| 2:B:241:ARG:HG2 | 2:B:251:ILE:CG2 | 2.41 | 0.49 |
| 2:B:809:MET:HG2 | 2:B:814:PHE:HB3 | 1.93 | 0.49 |
| 2:B:979:LYS:CE | 2:B:987:LYS:HD2 | 2.41 | 0.49 |
| 3:C:244:VAL:HG12 | 3:C:248:ILE:HD11 | 1.94 | 0.49 |
| 4:E:4:GLU:O | 4:E:5:ASN:C | 2.51 | 0.49 |
| 6:H:126:GLU:N | 6:H:130:ARG:HH12 | 2.11 | 0.49 |
| 1:A:964:ILE:HD13 | 1:A:1035:TYR:CE1 | 2.46 | 0.49 |
| 1:A:492:PRO:HB2 | 1:A:497:THR:CG2 | 2.39 | 0.49 |
| 1:A:598:LEU:O | 1:A:599:SER:C | 2.50 | 0.49 |
| 1:A:606:LEU:HD11 | 1:A:608:ILE:CD1 | 2.43 | 0.49 |
| 2:B:1020:ARG:O | 2:B:1021:MET:HB2 | 2.12 | 0.49 |
| 2:B:103:ASN:HB2 | 2:B:169:ARG:HH12 | 1.77 | 0.49 |
| 7:I:111:THR:HG1 | 7:I:121:PHE:HE2 | 1.60 | 0.49 |
| 3:C:165:LYS:O | 9:K:6:ARG:NH1 | 2.46 | 0.49 |
| 10:L:43:THR:O | 10:L:43:THR:HG22 | 2.12 | 0.49 |
| 1:A:329:LEU:HD23 | 1:A:332:LYS:HB2 | 1.94 | 0.49 |
| 1:A:786:HIS:CD2 | 1:A:786:HIS:N | 2.81 | 0.49 |
| 3:C:183:TRP:O | 3:C:185:LYS:N | 2.41 | 0.49 |
| 6:H:103:LYS:NZ | 6:H:114:VAL:CG2 | 2.76 | 0.49 |
| 11:M:4:ILE:H | 11:M:4:ILE:HD12 | 1.78 | 0.49 |
| 1:A:1263:ILE:O | 1:A:1267:MET:HG3 | 2.13 | 0.49 |
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:N | 2.28 | 0.49 |
| 1:A:220:THR:O | 1:A:222:LEU:O | 2.31 | 0.49 |
| 1:A:705:LYS:HB2 | 1:A:708:MET:CE | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:5:GLN:OE1 | 2:B:1175:LEU:HD12 | 2.13 | 0.49 |
| 2:B:705:MET:CE | 2:B:745:PRO:HB3 | 2.42 | 0.49 |
| 2:B:784:ASN:OD1 | 2:B:788:ARG:HD2 | 2.12 | 0.49 |
| 3:C:27:LEU:HA | 3:C:228:PHE:CZ | 2.48 | 0.49 |
| 1:A:1030:ARG:HD3 | 1:A:1034:GLU:OE1 | 2.12 | 0.48 |
| 1:A:332:LYS:O | 1:A:336:ILE:HD12 | 2.13 | 0.48 |
| 1:A:541:ILE:HG21 | 1:A:549:MET:HE3 | 1.94 | 0.48 |
| 1:A:982:THR:HG22 | 1:A:984:LYS:N | 2.22 | 0.48 |
| 2:B:241:ARG:HG2 | 2:B:251:ILE:HG23 | 1.93 | 0.48 |
| 2:B:258:LEU:HB2 | 2:B:385:LEU:HD21 | 1.95 | 0.48 |
| 2:B:787:VAL:O | 2:B:787:VAL:HG12 | 2.12 | 0.48 |
| 5:F:109:VAL:CG1 | 5:F:110:ASP:N | 2.64 | 0.48 |
| 6:H:81:PRO:CB | 6:H:82:PRO:CD | 2.91 | 0.48 |
| 1:A:1190:PRO:HG3 | 7:I:18:GLU:OE2 | 2.13 | 0.48 |
| 7:I:95:THR:HG22 | 7:I:96:SER:O | 2.13 | 0.48 |
| 9:K:82:ASP:OD1 | 9:K:84:LYS:N | 2.44 | 0.48 |
| 1:A:1225:PHE:O | 1:A:1240:CYS:HA | 2.13 | 0.48 |
| 1:A:1348:LEU:HD21 | 1:A:1375:MET:SD | 2.52 | 0.48 |
| 1:A:1384:VAL:O | 1:A:1386:ARG:N | 2.46 | 0.48 |
| 2:B:1162:ILE:HD11 | 2:B:1216:LEU:HD12 | 1.94 | 0.48 |
| 2:B:185:THR:HG23 | 2:B:188:ASP:OD2 | 2.13 | 0.48 |
| 2:B:234:ILE:CD1 | 2:B:257:LYS:HD3 | 2.43 | 0.48 |
| 2:B:40:GLU:OE1 | 2:B:680:THR:CG2 | 2.60 | 0.48 |
| 2:B:35:SER:HA | 2:B:811:TYR:CE2 | 2.47 | 0.48 |
| 3:C:227:THR:HG22 | 3:C:229:TYR:CE1 | 2.47 | 0.48 |
| 4:E:147:HIS:CD2 | 4:E:149:LEU:H | 2.31 | 0.48 |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:N | 2.23 | 0.48 |
| 1:A:407:ARG:HG2 | 1:A:430:TRP:CZ2 | 2.48 | 0.48 |
| 1:A:55:ASP:N | 1:A:56:PRO:CD | 2.74 | 0.48 |
| 1:A:697:ALA:HB2 | 1:A:702:LEU:CD1 | 2.43 | 0.48 |
| 2:B:181:LEU:HD22 | 2:B:189:LEU:CD2 | 2.43 | 0.48 |
| 2:B:756:ILE:HG12 | 2:B:770:GLN:HG2 | 1.96 | 0.48 |
| 3:C:209:TYR:N | 3:C:209:TYR:CD1 | 2.80 | 0.48 |
| 4:E:98:ILE:O | 4:E:102:GLU:HG3 | 2.13 | 0.48 |
| 1:A:1111:MET:HE3 | 1:A:1114:PRO:HA | 1.94 | 0.48 |
| 1:A:849:MET:CE | 1:A:1437:GLY:H | 2.27 | 0.48 |
| 1:A:535:THR:HG22 | 1:A:575:LYS:HE2 | 1.94 | 0.48 |
| 1:A:982:THR:HG22 | 1:A:983:ILE:N | 2.28 | 0.48 |
| 2:B:1099:VAL:O | 2:B:1101:ASP:N | 2.45 | 0.48 |
| 2:B:365:THR:HG22 | 2:B:367:LEU:N | 2.16 | 0.48 |
| 3:C:258:ILE:HD12 | 9:K:42:LEU:HD21 | 1.93 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:31:ASN:O | 3:C:34:ARG:HB3 | 2.13 | 0.48 |
| 10:L:60:ARG:HG2 | 10:L:61:THR:N | 2.27 | 0.48 |
| 1:A:1129:GLU:O | 1:A:1133:LEU:HG | 2.14 | 0.48 |
| 1:A:1152:ILE:HA | 1:A:1192:LEU:O | 2.14 | 0.48 |
| 1:A:367:PRO:HG2 | 1:A:370:ILE:HD12 | 1.94 | 0.48 |
| 1:A:767:GLN:HG3 | 1:A:768:GLN:O | 2.12 | 0.48 |
| 2:B:758:PHE:CE1 | 2:B:1027:ILE:HG22 | 2.48 | 0.48 |
| 3:C:148:ARG:HG2 | 3:C:149:LYS:N | 2.29 | 0.48 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:H | 1.78 | 0.48 |
| 1:A:1016:THR:CG2 | 4:E:206:GLY:HA3 | 2.43 | 0.48 |
| 7:I:69:PRO:HG2 | 7:I:85:PHE:O | 2.14 | 0.48 |
| 1:A:884:ASP:OD2 | 1:A:1030:ARG:NH2 | 2.46 | 0.48 |
| 5:F:127:GLU:O | 5:F:129:LYS:HG3 | 2.13 | 0.48 |
| 7:I:84:VAL:HG12 | 7:I:102:VAL:HB | 1.94 | 0.48 |
| 7:I:111:THR:CG2 | 7:I:112:SER:N | 2.75 | 0.48 |
| 9:K:96:ASN:O | 9:K:99:GLY:N | 2.46 | 0.48 |
| 1:A:1159:ARG:O | 1:A:1170:ILE:HG21 | 2.12 | 0.48 |
| 1:A:528:LEU:HD23 | 1:A:751:SER:N | 2.29 | 0.48 |
| 1:A:55:ASP:C | 1:A:57:ARG:N | 2.63 | 0.48 |
| 2:B:514:LEU:HD12 | 2:B:518:HIS:CD2 | 2.49 | 0.48 |
| 2:B:552:MET:N | 2:B:553:PRO:HD2 | 2.28 | 0.48 |
| 2:B:859:TYR:CD1 | 2:B:859:TYR:N | 2.82 | 0.48 |
| 2:B:882:THR:C | 2:B:884:ARG:H | 2.17 | 0.48 |
| 2:B:898:LEU:CD2 | 2:B:964:VAL:HG11 | 2.41 | 0.48 |
| 2:B:969:ARG:HH11 | 2:B:969:ARG:CB | 2.26 | 0.48 |
| 3:C:145:CYS:SG | 3:C:146:LYS:N | 2.86 | 0.48 |
| 3:C:152:GLU:OE2 | 3:C:154:LYS:HE3 | 2.12 | 0.48 |
| 6:H:63:LEU:C | 6:H:90:ALA:CB | 2.82 | 0.48 |
| 9:K:70:ARG:O | 9:K:70:ARG:HG3 | 2.12 | 0.48 |
| 1:A:384:ASN:ND2 | 1:A:388:LEU:HD11 | 2.29 | 0.48 |
| 2:B:339:THR:CG2 | 2:B:343:ILE:HB | 2.44 | 0.48 |
| 2:B:566:LEU:HD13 | 2:B:588:GLY:HA2 | 1.96 | 0.48 |
| 2:B:731:VAL:CG1 | 2:B:732:SER:H | 2.27 | 0.48 |
| 4:E:64:PRO:HG2 | 4:E:75:MET:O | 2.14 | 0.48 |
| 1:A:179:LEU:HG | 1:A:308:ILE:HG21 | 1.96 | 0.48 |
| 1:A:438:ASP:O | 1:A:439:ASN:HB2 | 2.14 | 0.48 |
| 1:A:567:LYS:HD3 | 6:H:95:TYR:CG | 2.49 | 0.48 |
| 2:B:1160:VAL:HG12 | 2:B:1161:HIS:H | 1.79 | 0.48 |
| 2:B:644:GLU:HG3 | 2:B:654:ARG:NH2 | 2.26 | 0.48 |
| 2:B:652:LYS:CE | 2:B:688:GLY:O | 2.61 | 0.48 |
| 2:B:842:ASN:OD1 | 2:B:844:SER:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:871:ASP:CB | 4:E:204:THR:CG2 | 2.90 | 0.48 |
| 1:A:32:VAL:HB | 1:A:57:ARG:HD2 | 1.96 | 0.48 |
| 2:B:326:ASP:C | 2:B:326:ASP:OD2 | 2.52 | 0.48 |
| 2:B:38:PHE:HZ | 2:B:541:LEU:HB3 | 1.79 | 0.48 |
| 1:A:482:PHE:CD1 | 2:B:836:GLU:HB2 | 2.49 | 0.48 |
| 4:E:31:THR:C | 4:E:33:GLU:H | 2.16 | 0.48 |
| 7:I:103:CYS:HB3 | 7:I:108:HIS:H | 1.79 | 0.48 |
| 1:A:78:PRO:O | 1:A:79:GLY:C | 2.52 | 0.47 |
| 1:A:899:VAL:CG1 | 1:A:929:LEU:HD13 | 2.44 | 0.47 |
| 1:A:867:ILE:HD11 | 1:A:999:VAL:HG11 | 1.95 | 0.47 |
| 2:B:999:MET:HB3 | 2:B:1007:VAL:CG2 | 2.44 | 0.47 |
| 3:C:186:LEU:HD12 | 3:C:186:LEU:N | 2.28 | 0.47 |
| 4:E:12:LEU:HD21 | 4:E:58:MET:SD | 2.54 | 0.47 |
| 1:A:968:GLN:NE2 | 1:A:1035:TYR:O | 2.47 | 0.47 |
| 1:A:1127:ASP:C | 1:A:1129:GLU:N | 2.67 | 0.47 |
| 1:A:528:LEU:O | 1:A:531:ILE:HG22 | 2.14 | 0.47 |
| 1:A:550:LEU:HD13 | 1:A:556:TRP:CZ2 | 2.48 | 0.47 |
| 2:B:332:ASP:OD2 | 2:B:345:LYS:HG3 | 2.14 | 0.47 |
| 4:E:197:LYS:HG3 | 4:E:211:TYR:CE2 | 2.48 | 0.47 |
| 1:A:1198:ASP:OD1 | 1:A:1200:ALA:HB3 | 2.14 | 0.47 |
| 2:B:221:ASN:O | 2:B:222:ILE:HG13 | 2.14 | 0.47 |
| 2:B:235:SER:HA | 2:B:261:ARG:HH21 | 1.79 | 0.47 |
| 3:C:206:ASN:ND2 | 3:C:229:TYR:CB | 2.78 | 0.47 |
| 4:E:202:SER:O | 4:E:205:SER:O | 2.33 | 0.47 |
| 9:K:49:GLU:HG3 | 9:K:94:ILE:CG1 | 2.44 | 0.47 |
| 1:A:95:PHE:CE2 | 1:A:1414:ALA:HB2 | 2.49 | 0.47 |
| 1:A:38:PRO:HA | 1:A:270:LEU:CD1 | 2.40 | 0.47 |
| 1:A:399:HIS:CB | 1:A:400:PRO:CD | 2.92 | 0.47 |
| 2:B:254:LEU:HD23 | 2:B:381:MET:CE | 2.45 | 0.47 |
| 2:B:123:THR:OG1 | 2:B:458:LYS:HE3 | 2.14 | 0.47 |
| 2:B:64:CYS:HA | 2:B:67:SER:HB3 | 1.95 | 0.47 |
| 2:B:89:GLU:O | 2:B:90:ILE:HB | 2.14 | 0.47 |
| 4:E:96:PHE:CE1 | 4:E:100:ILE:HD11 | 2.48 | 0.47 |
| 2:B:824:ILE:CG1 | 8:J:48:ARG:NH1 | 2.77 | 0.47 |
| 1:A:1315:GLU:O | 1:A:1318:THR:HG22 | 2.14 | 0.47 |
| 1:A:523:ILE:CD1 | 1:A:649:ILE:HG21 | 2.43 | 0.47 |
| 2:B:1065:GLN:O | 2:B:1065:GLN:HG3 | 2.14 | 0.47 |
| 2:B:254:LEU:HD23 | 2:B:381:MET:HE1 | 1.96 | 0.47 |
| 2:B:46:GLN:HG3 | 2:B:46:GLN:H | 1.30 | 0.47 |
| 2:B:557:PHE:HZ | 2:B:599:THR:HG21 | 1.79 | 0.47 |
| 8:J:12:LYS:HZ1 | 8:J:17:LYS:NZ | 2.11 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:252:GLN:HE22 | 9:K:99:GLY:HA2 | 1.79 | 0.47 |
| 1:A:1220:PHE:O | 1:A:1221:LYS:C | 2.53 | 0.47 |
| 2:B:1051:THR:CG2 | 2:B:1052:VAL:N | 2.77 | 0.47 |
| 3:C:68:GLY:O | 3:C:169:LYS:HB2 | 2.14 | 0.47 |
| 3:C:44:LEU:HG | 3:C:159:ALA:HB1 | 1.96 | 0.47 |
| 1:A:1169:ILE:O | 1:A:1173:HIS:CD2 | 2.68 | 0.47 |
| 1:A:21:LEU:HD11 | 1:A:1414:ALA:HA | 1.97 | 0.47 |
| 1:A:264:PHE:O | 1:A:267:ALA:HB3 | 2.15 | 0.47 |
| 1:A:537:ARG:HG2 | 1:A:537:ARG:HH11 | 1.80 | 0.47 |
| 2:B:915:THR:HG22 | 2:B:916:THR:N | 2.29 | 0.47 |
| 3:C:8:VAL:HG21 | 9:K:105:PHE:HB2 | 1.97 | 0.47 |
| 9:K:7:PHE:HB2 | 9:K:11:LEU:CD2 | 2.44 | 0.47 |
| 1:A:10:PRO:HG2 | 2:B:1192:TYR:CD2 | 2.49 | 0.47 |
| 1:A:1295:THR:O | 1:A:1295:THR:HG22 | 2.14 | 0.47 |
| 1:A:532:ARG:NH2 | 1:A:748:MET:HE3 | 2.30 | 0.47 |
| 2:B:268:THR:CG2 | 2:B:270:LYS:HE3 | 2.36 | 0.47 |
| 2:B:274:PRO:HG3 | 2:B:359:GLU:HB3 | 1.96 | 0.47 |
| 2:B:581:PHE:HA | 2:B:585:VAL:O | 2.15 | 0.47 |
| 2:B:863:GLU:O | 2:B:864:LYS:O | 2.33 | 0.47 |
| 2:B:997:GLU:H | 2:B:997:GLU:HG3 | 1.52 | 0.47 |
| 8:J:48:ARG:NH1 | 8:J:48:ARG:HG2 | 2.26 | 0.47 |
| 1:A:946:VAL:HG22 | 4:E:201:LYS:HD2 | 1.96 | 0.47 |
| 1:A:1431:GLY:O | 2:B:1148:LYS:HE3 | 2.15 | 0.47 |
| 2:B:169:ARG:N | 2:B:454:THR:OG1 | 2.48 | 0.47 |
| 2:B:351:TYR:O | 2:B:355:ILE:HG13 | 2.15 | 0.47 |
| 2:B:983:ARG:HD2 | 2:B:1091:TYR:CD2 | 2.36 | 0.47 |
| 3:C:206:ASN:ND2 | 3:C:229:TYR:HB2 | 2.30 | 0.47 |
| 1:A:112:LYS:NZ | 1:A:165:GLY:N | 2.54 | 0.47 |
| 1:A:602:ASP:O | 1:A:615:GLY:HA2 | 2.14 | 0.47 |
| 2:B:315:LYS:N | 2:B:316:PRO:HD2 | 2.29 | 0.47 |
| 2:B:882:THR:HG21 | 2:B:935:ARG:HA | 1.97 | 0.47 |
| 2:B:392:ARG:HH22 | 7:I:52:ILE:HD11 | 1.75 | 0.47 |
| 7:I:95:THR:CG2 | 7:I:96:SER:N | 2.78 | 0.47 |
| 1:A:1400:CYS:SG | 1:A:1405:THR:HG21 | 2.55 | 0.47 |
| 1:A:517:ASN:HD22 | 1:A:1364:ASN:HB2 | 1.80 | 0.47 |
| 1:A:54:ASN:O | 1:A:55:ASP:HB2 | 2.15 | 0.47 |
| 2:B:1000:PRO:O | 2:B:1007:VAL:HG23 | 2.14 | 0.47 |
| 2:B:114:PRO:HD3 | 2:B:124:TYR:CZ | 2.49 | 0.47 |
| 2:B:579:ARG:HG3 | 2:B:581:PHE:HE1 | 1.80 | 0.47 |
| 1:A:740:LEU:HD21 | 3:C:193:TYR:CE2 | 2.51 | 0.47 |
| 4:E:79:TRP:HB2 | 4:E:105:PHE:CD1 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:H:31:THR:O | 6:H:32:THR:CB | 2.62 | 0.47 |
| 1:A:626:ASN:O | 1:A:631:HIS:CD2 | 2.69 | 0.46 |
| 2:B:46:GLN:NE2 | 2:B:496:ARG:HD2 | 2.30 | 0.46 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:H | 1.80 | 0.46 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:HG12 | 1.96 | 0.46 |
| 5:F:111:LEU:O | 5:F:113:GLY:N | 2.39 | 0.46 |
| 5:F:79:ARG:NH2 | 5:F:150:GLU:OE2 | 2.44 | 0.46 |
| 7:I:26:LEU:HD23 | 7:I:37:GLU:HA | 1.95 | 0.46 |
| 1:A:1206:ASP:HB2 | 1:A:1274:ARG:NH1 | 2.30 | 0.46 |
| 1:A:840:ARG:HG3 | 1:A:1385:THR:CG2 | 2.45 | 0.46 |
| 2:B:296:GLU:O | 2:B:300:HIS:CD2 | 2.66 | 0.46 |
| 2:B:705:MET:HB3 | 2:B:706:GLN:HE21 | 1.81 | 0.46 |
| 3:C:41:ILE:HB | 3:C:172:PRO:HG3 | 1.97 | 0.46 |
| 6:H:27:GLU:HA | 6:H:38:LEU:O | 2.15 | 0.46 |
| 6:H:6:PHE:O | 6:H:58:THR:HG23 | 2.14 | 0.46 |
| 6:H:97:MET:HE2 | 6:H:142:LEU:HD23 | 1.97 | 0.46 |
| 1:A:465:TYR:CE2 | 9:K:4:PRO:HD2 | 2.50 | 0.46 |
| 10:L:60:ARG:HG2 | 10:L:61:THR:H | 1.80 | 0.46 |
| 1:A:65:LEU:HD22 | 1:A:72:GLU:O | 2.16 | 0.46 |
| 1:A:741:ASN:HD21 | 1:A:743:VAL:HB | 1.79 | 0.46 |
| 2:B:121:ASN:HA | 2:B:207:GLY:CA | 2.45 | 0.46 |
| 2:B:899:ILE:CG2 | 2:B:900:ALA:H | 2.28 | 0.46 |
| 1:A:567:LYS:HZ2 | 6:H:46:LEU:HB2 | 1.75 | 0.46 |
| 1:A:417:TYR:O | 1:A:418:SER:HB2 | 2.15 | 0.46 |
| 2:B:229:ALA:HB1 | 2:B:231:PRO:HD2 | 1.96 | 0.46 |
| 2:B:324:ILE:HD11 | 2:B:333:PHE:CG | 2.50 | 0.46 |
| 2:B:122:LEU:HD22 | 2:B:958:GLN:CG | 2.45 | 0.46 |
| 2:B:757:PRO:HG2 | 2:B:984:HIS:HE1 | 1.81 | 0.46 |
| 3:C:229:TYR:CD1 | 3:C:229:TYR:N | 2.83 | 0.46 |
| 3:C:266:ASP:O | 3:C:267:GLN:HB2 | 2.15 | 0.46 |
| 6:H:63:LEU:C | 6:H:90:ALA:HB3 | 2.35 | 0.46 |
| 1:A:418:SER:C | 1:A:420:ARG:H | 2.18 | 0.46 |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:HD22 | 1.79 | 0.46 |
| 2:B:404:LYS:O | 2:B:405:ARG:NH1 | 2.37 | 0.46 |
| 3:C:179:GLU:HG3 | 3:C:180:TYR:H | 1.79 | 0.46 |
| 7:I:40:SER:HB2 | 7:I:41:PRO:HD2 | 1.97 | 0.46 |
| 7:I:74:GLU:HB2 | 7:I:81:ARG:NH1 | 2.30 | 0.46 |
| 9:K:49:GLU:HG3 | 9:K:94:ILE:HG13 | 1.97 | 0.46 |
| 1:A:353:ILE:HD13 | 1:A:487:MET:CE | 2.42 | 0.46 |
| 1:A:416:ARG:HG3 | 1:A:417:TYR:CD1 | 2.51 | 0.46 |
| 1:A:939:ASP:OD1 | 1:A:1023:ARG:NH1 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:854:ASN:ND2 | 1:A:999:VAL:O | 2.48 | 0.46 |
| 2:B:215:GLN:HE22 | 2:B:499:ASN:HD22 | 1.64 | 0.46 |
| 2:B:731:VAL:CG1 | 2:B:732:SER:N | 2.77 | 0.46 |
| 4:E:100:ILE:HG23 | 4:E:105:PHE:HB2 | 1.96 | 0.46 |
| 6:H:99:GLY:N | 6:H:118:PHE:CD2 | 2.84 | 0.46 |
| 6:H:127:GLY:O | 6:H:128:ASN:HB2 | 2.15 | 0.46 |
| 1:A:567:LYS:NZ | 6:H:95:TYR:CE1 | 2.72 | 0.46 |
| 7:I:59:VAL:HG12 | 7:I:61:ASP:H | 1.81 | 0.46 |
| 3:C:259:LEU:HD21 | 9:K:91:CYS:HB2 | 1.97 | 0.46 |
| 10:L:27:LEU:HD13 | 10:L:37:LYS:CG | 2.45 | 0.46 |
| 10:L:33:GLU:C | 10:L:35:SER:H | 2.18 | 0.46 |
| 1:A:243:PRO:HB2 | 1:A:245:PRO:HD2 | 1.98 | 0.46 |
| 1:A:345:VAL:HG12 | 2:B:1150:ARG:HH22 | 1.80 | 0.46 |
| 2:B:651:LEU:HD23 | 2:B:710:LEU:HD11 | 1.96 | 0.46 |
| 3:C:248:ILE:H | 3:C:248:ILE:HG13 | 1.40 | 0.46 |
| 6:H:100:THR:CB | 6:H:138:GLU:HG3 | 2.46 | 0.46 |
| 1:A:265:LYS:O | 1:A:269:ILE:HG13 | 2.15 | 0.46 |
| 1:A:345:VAL:HG13 | 2:B:1150:ARG:NH1 | 2.31 | 0.46 |
| 2:B:1008:PRO:HB3 | 2:B:1087:PHE:CE1 | 2.50 | 0.46 |
| 2:B:25:ILE:HG23 | 2:B:29:ASP:CB | 2.46 | 0.46 |
| 2:B:484:ASN:O | 2:B:485:ARG:HD2 | 2.15 | 0.46 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:CG | 2.38 | 0.46 |
| 1:A:1340:GLY:HA2 | 4:E:183:PRO:HD2 | 1.98 | 0.46 |
| 1:A:53:LEU:HB3 | 1:A:54:ASN:OD1 | 2.16 | 0.46 |
| 1:A:5:GLN:CG | 1:A:6:TYR:H | 2.21 | 0.46 |
| 1:A:786:HIS:CD2 | 1:A:786:HIS:H | 2.34 | 0.46 |
| 1:A:79:GLY:HA3 | 1:A:245:PRO:CG | 2.46 | 0.46 |
| 1:A:834:THR:HG22 | 1:A:1077:THR:OG1 | 2.16 | 0.46 |
| 2:B:1082:MET:HA | 3:C:189:THR:HA | 1.98 | 0.46 |
| 2:B:101:MET:SD | 2:B:109:THR:HG21 | 2.55 | 0.46 |
| 2:B:564:GLU:HB2 | 2:B:589:VAL:HG12 | 1.96 | 0.46 |
| 2:B:979:LYS:HE2 | 2:B:979:LYS:HB3 | 1.81 | 0.46 |
| 3:C:20:PHE:HE1 | 3:C:22:LEU:HG | 1.80 | 0.46 |
| 6:H:113:ALA:CB | 6:H:124:ARG:HH21 | 2.29 | 0.46 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:OG1 | 2.16 | 0.46 |
| 1:A:307:ASP:C | 1:A:308:ILE:HG13 | 2.36 | 0.46 |
| 1:A:35:ILE:HB | 1:A:83:HIS:O | 2.16 | 0.46 |
| 2:B:47:GLN:HA | 2:B:47:GLN:OE1 | 2.15 | 0.46 |
| 2:B:821:GLN:OE1 | 2:B:850:LEU:HD12 | 2.15 | 0.46 |
| 2:B:996:ARG:HD3 | 14:B:2017:HOH:O | 2.16 | 0.46 |
| 3:C:60:ASP:OD2 | 10:L:60:ARG:NH2 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:H:105:GLU:H | 6:H:105:GLU:CD | 2.19 | 0.46 |
| 2:B:120:ARG:NH2 | 10:L:54:ARG:HH11 | 2.14 | 0.46 |
| 1:A:1148:ILE:HD12 | 1:A:1196:GLU:HG2 | 1.99 | 0.45 |
| 1:A:1391:ARG:O | 1:A:1392:SER:HB3 | 2.16 | 0.45 |
| 1:A:368:LYS:HB2 | 1:A:368:LYS:HE3 | 1.68 | 0.45 |
| 1:A:84:ILE:HG22 | 1:A:239:LEU:O | 2.15 | 0.45 |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:CG2 | 2.46 | 0.45 |
| 1:A:973:ILE:HD11 | 1:A:1041:ALA:CB | 2.47 | 0.45 |
| 2:B:484:ASN:ND2 | 2:B:486:TYR:CE1 | 2.83 | 0.45 |
| 2:B:904:ARG:HH21 | 2:B:948:ILE:HD11 | 1.81 | 0.45 |
| 4:E:124:VAL:HG13 | 4:E:132:ILE:HB | 1.98 | 0.45 |
| 1:A:870:GLU:HG2 | 4:E:208:TYR:CD2 | 2.51 | 0.45 |
| 2:B:295:GLY:HA3 | 7:I:11:ASN:ND2 | 2.32 | 0.45 |
| 7:I:15:TYR:N | 7:I:15:TYR:CD1 | 2.85 | 0.45 |
| 1:A:148:CYS:O | 1:A:167:CYS:O | 2.35 | 0.45 |
| 1:A:261:ASP:O | 1:A:264:PHE:HB2 | 2.17 | 0.45 |
| 1:A:722:LEU:HD22 | 1:A:799:PHE:CD1 | 2.51 | 0.45 |
| 1:A:69:THR:HB | 2:B:1174:LYS:HE2 | 1.98 | 0.45 |
| 2:B:25:ILE:HD12 | 2:B:653:VAL:CB | 2.46 | 0.45 |
| 2:B:339:THR:HG23 | 2:B:343:ILE:HB | 1.98 | 0.45 |
| 2:B:351:TYR:CE2 | 2:B:355:ILE:HD11 | 2.51 | 0.45 |
| 2:B:416:LEU:HD11 | 2:B:466:TRP:CE2 | 2.52 | 0.45 |
| 1:A:738:LYS:NZ | 3:C:194:GLU:O | 2.42 | 0.45 |
| 3:C:221:TYR:CD1 | 3:C:222:LYS:HG3 | 2.51 | 0.45 |
| 1:A:857:ARG:CZ | 5:F:139:PRO:HG3 | 2.46 | 0.45 |
| 7:I:59:VAL:HG12 | 7:I:60:GLN:N | 2.31 | 0.45 |
| 8:J:7:CYS:HA | 8:J:49:MET:HG2 | 1.98 | 0.45 |
| 9:K:108:GLU:O | 9:K:112:GLN:HG2 | 2.17 | 0.45 |
| 1:A:265:LYS:NZ | 1:A:302:THR:HB | 2.30 | 0.45 |
| 1:A:329:LEU:C | 1:A:331:GLY:N | 2.70 | 0.45 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CE2 | 2.51 | 0.45 |
| 2:B:115:GLN:HG2 | 2:B:193:LYS:HB2 | 1.97 | 0.45 |
| 2:B:957:ASN:CG | 2:B:958:GLN:N | 2.70 | 0.45 |
| 3:C:186:LEU:CD1 | 3:C:186:LEU:N | 2.79 | 0.45 |
| 4:E:75:MET:O | 4:E:76:GLY:O | 2.34 | 0.45 |
| 6:H:103:LYS:HA | 6:H:115:TYR:HB2 | 1.98 | 0.45 |
| 6:H:4:THR:HA | 6:H:60:ALA:HA | 1.98 | 0.45 |
| 1:A:1431:GLY:HA2 | 2:B:1152:MET:HE2 | 1.99 | 0.45 |
| 1:A:381:THR:HG21 | 1:A:383:TYR:HD1 | 1.82 | 0.45 |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:O | 2.16 | 0.45 |
| 3:C:179:GLU:HG3 | 3:C:180:TYR:N | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:231:ASN:C | 3:C:231:ASN:OD1 | 2.54 | 0.45 |
| 6:H:95:TYR:HE2 | 6:H:97:MET:CG | 2.29 | 0.45 |
| 10:L:46:VAL:CG1 | 10:L:56:LEU:HD12 | 2.43 | 0.45 |
| 1:A:1111:MET:CE | 1:A:1114:PRO:HA | 2.46 | 0.45 |
| 1:A:130:ASP:OD2 | 1:A:133:LYS:HG3 | 2.16 | 0.45 |
| 1:A:156:ASP:HB2 | 1:A:157:ASP:H | 1.55 | 0.45 |
| 1:A:541:ILE:HG12 | 1:A:549:MET:HE1 | 1.98 | 0.45 |
| 1:A:577:ILE:HG12 | 1:A:577:ILE:H | 1.57 | 0.45 |
| 1:A:78:PRO:O | 1:A:79:GLY:O | 2.35 | 0.45 |
| 1:A:90:VAL:HG12 | 1:A:91:PHE:O | 2.17 | 0.45 |
| 4:E:43:LYS:O | 4:E:47:CYS:HB2 | 2.16 | 0.45 |
| 6:H:81:PRO:HD2 | 6:H:82:PRO:HD2 | 1.98 | 0.45 |
| 1:A:982:THR:O | 1:A:985:ASP:HB2 | 2.16 | 0.45 |
| 2:B:341:LEU:CG | 2:B:341:LEU:O | 2.64 | 0.45 |
| 3:C:100:THR:HG22 | 3:C:101:LEU:N | 2.30 | 0.45 |
| 3:C:70:ILE:HD11 | 3:C:144:ILE:HG12 | 1.98 | 0.45 |
| 4:E:28:TYR:CE2 | 4:E:78:LEU:HG | 2.51 | 0.45 |
| 6:H:96:VAL:HG22 | 6:H:143:LEU:HD22 | 1.97 | 0.45 |
| 1:A:1392:SER:O | 1:A:1393:ASN:CB | 2.65 | 0.45 |
| 2:B:863:GLU:OE1 | 2:B:962:LYS:HD2 | 2.17 | 0.45 |
| 5:F:140:ASP:C | 5:F:140:ASP:OD1 | 2.56 | 0.45 |
| 8:J:48:ARG:CG | 8:J:48:ARG:HH11 | 2.24 | 0.45 |
| 1:A:1293:SER:HB2 | 1:A:1294:PRO:HD2 | 1.99 | 0.45 |
| 1:A:407:ARG:O | 1:A:408:ASP:C | 2.56 | 0.45 |
| 1:A:896:ARG:HD3 | 1:A:897:TYR:CE1 | 2.52 | 0.45 |
| 3:C:14:SER:O | 3:C:240:VAL:HG21 | 2.16 | 0.45 |
| 5:F:72:LYS:N | 5:F:142:SER:HA | 2.31 | 0.45 |
| 5:F:90:ARG:HD3 | 5:F:155:LEU:HD12 | 1.98 | 0.45 |
| 6:H:100:THR:HG23 | 6:H:138:GLU:HB2 | 1.99 | 0.45 |
| 9:K:110:ASN:C | 9:K:112:GLN:H | 2.20 | 0.45 |
| 9:K:63:VAL:O | 9:K:63:VAL:HG22 | 2.17 | 0.45 |
| 2:B:315:LYS:HB2 | 2:B:315:LYS:HE3 | 1.72 | 0.45 |
| 2:B:771:SER:O | 2:B:775:LYS:HE3 | 2.17 | 0.45 |
| 2:B:950:ASP:O | 2:B:951:GLN:HG3 | 2.17 | 0.45 |
| 2:B:766:ARG:NH1 | 2:B:985:GLY:O | 2.44 | 0.45 |
| 2:B:99:LYS:HB3 | 2:B:180:TYR:CZ | 2.52 | 0.45 |
| 3:C:22:LEU:O | 3:C:227:THR:HA | 2.17 | 0.45 |
| 1:A:1391:ARG:HH21 | 1:A:1417:GLU:CD | 2.20 | 0.45 |
| 1:A:327:ALA:O | 1:A:330:LYS:N | 2.50 | 0.45 |
| 1:A:92:HIS:C | 1:A:92:HIS:CD2 | 2.91 | 0.45 |
| 2:B:977:GLY:HA3 | 2:B:1099:VAL:CG2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:169:ARG:HB2 | 2:B:454:THR:CG2 | 2.43 | 0.45 |
| 3:C:260:LEU:O | 3:C:260:LEU:HD12 | 2.16 | 0.45 |
| 1:A:164:ARG:HB2 | 1:A:165:GLY:H | 1.60 | 0.44 |
| 1:A:329:LEU:O | 1:A:333:GLU:HG2 | 2.18 | 0.44 |
| 1:A:78:PRO:O | 1:A:78:PRO:HG2 | 2.17 | 0.44 |
| 1:A:774:ARG:CB | 1:A:797:LYS:HG2 | 2.47 | 0.44 |
| 2:B:193:LYS:HD3 | 2:B:787:VAL:HG11 | 1.99 | 0.44 |
| 2:B:25:ILE:HD12 | 2:B:653:VAL:CG2 | 2.47 | 0.44 |
| 2:B:69:LEU:HD21 | 2:B:425:THR:CG2 | 2.47 | 0.44 |
| 2:B:913:GLY:HA2 | 2:B:938:SER:HB3 | 2.00 | 0.44 |
| 8:J:11:GLY:O | 8:J:12:LYS:C | 2.55 | 0.44 |
| 1:A:476:SER:N | 1:A:477:PRO:HD2 | 2.33 | 0.44 |
| 2:B:805:THR:HB | 2:B:809:MET:SD | 2.57 | 0.44 |
| 3:C:175:ALA:O | 3:C:176:ILE:CG1 | 2.65 | 0.44 |
| 4:E:114:ASN:OD1 | 4:E:115:ASN:N | 2.50 | 0.44 |
| 1:A:32:VAL:HG23 | 1:A:33:ALA:N | 2.32 | 0.44 |
| 1:A:740:LEU:N | 1:A:740:LEU:CD1 | 2.80 | 0.44 |
| 1:A:757:ASN:HA | 2:B:1021:MET:HE1 | 1.99 | 0.44 |
| 2:B:1084:GLN:HG2 | 3:C:201:TRP:CH2 | 2.52 | 0.44 |
| 2:B:188:ASP:O | 2:B:192:LEU:HD12 | 2.17 | 0.44 |
| 2:B:590:HIS:HD2 | 2:B:593:PRO:HA | 1.83 | 0.44 |
| 3:C:71:PRO:O | 3:C:72:LEU:HD23 | 2.18 | 0.44 |
| 1:A:31:SER:OG | 1:A:83:HIS:HB2 | 2.18 | 0.44 |
| 2:B:1096:ARG:HA | 2:B:1098:MET:HE2 | 1.99 | 0.44 |
| 2:B:276:ILE:HG21 | 2:B:280:ILE:HD11 | 2.00 | 0.44 |
| 2:B:956:THR:CG2 | 2:B:960:GLY:HA2 | 2.47 | 0.44 |
| 3:C:226:ASP:O | 3:C:227:THR:HB | 2.18 | 0.44 |
| 1:A:38:PRO:HB3 | 1:A:270:LEU:CB | 2.48 | 0.44 |
| 1:A:278:THR:O | 1:A:278:THR:HG22 | 2.18 | 0.44 |
| 1:A:871:ASP:CG | 4:E:204:THR:HG23 | 2.38 | 0.44 |
| 2:B:1100:ASP:HA | 2:B:1103:ILE:CD1 | 2.48 | 0.44 |
| 2:B:995:ARG:NH1 | 2:B:997:GLU:OE1 | 2.51 | 0.44 |
| 3:C:66:ARG:NH1 | 3:C:144:ILE:O | 2.47 | 0.44 |
| 3:C:221:TYR:HE1 | 3:C:222:LYS:HE3 | 1.82 | 0.44 |
| 6:H:31:THR:O | 6:H:32:THR:HB | 2.17 | 0.44 |
| 1:A:154:SER:HB3 | 1:A:162:VAL:CG2 | 2.48 | 0.44 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:OE1 | 2.18 | 0.44 |
| 1:A:499:ALA:O | 1:A:503:GLN:HB2 | 2.18 | 0.44 |
| 1:A:741:ASN:ND2 | 1:A:743:VAL:HB | 2.33 | 0.44 |
| 2:B:692:TYR:O | 2:B:693:ILE:HG13 | 2.18 | 0.44 |
| 2:B:876:LYS:HE2 | 2:B:893:LEU:C | 2.37 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:103:LYS:HZ1 | 6:H:114:VAL:HG21 | 1.81 | 0.44 |
| 6:H:42:ILE:HG23 | 6:H:95:TYR:CZ | 2.53 | 0.44 |
| 7:I:50:THR:HG22 | 7:I:51:ASN:H | 1.82 | 0.44 |
| 8:J:12:LYS:NZ | 8:J:17:LYS:HZ2 | 2.16 | 0.44 |
| 1:A:1102:LYS:HG2 | 1:A:1106:ASN:ND2 | 2.31 | 0.44 |
| 1:A:1204:ASP:C | 1:A:1206:ASP:H | 2.20 | 0.44 |
| 1:A:1295:THR:O | 1:A:1295:THR:CG2 | 2.66 | 0.44 |
| 1:A:642:CYS:O | 1:A:645:LEU:HB3 | 2.18 | 0.44 |
| 1:A:829:VAL:O | 1:A:830:LYS:C | 2.54 | 0.44 |
| 1:A:973:ILE:HD11 | 1:A:1041:ALA:HB2 | 1.99 | 0.44 |
| 2:B:259:TYR:OH | 2:B:279:ASP:OD2 | 2.36 | 0.44 |
| 2:B:826:ALA:HB2 | 2:B:1087:PHE:CE1 | 2.53 | 0.44 |
| 2:B:860:MET:O | 2:B:861:ASP:HB2 | 2.18 | 0.44 |
| 4:E:26:ARG:NH1 | 4:E:189:GLY:HA3 | 2.33 | 0.44 |
| 7:I:2:THR:HG22 | 7:I:2:THR:O | 2.17 | 0.44 |
| 2:B:311:LEU:HB3 | 7:I:4:PHE:CZ | 2.53 | 0.44 |
| 1:A:666:ILE:CD1 | 2:B:1030:LEU:HB2 | 2.47 | 0.44 |
| 2:B:650:GLU:HG3 | 2:B:651:LEU:N | 2.33 | 0.44 |
| 3:C:114:TYR:HB3 | 3:C:140:ASN:O | 2.18 | 0.44 |
| 7:I:68:LEU:HB3 | 7:I:84:VAL:HG22 | 1.99 | 0.44 |
| 10:L:33:GLU:O | 10:L:35:SER:N | 2.51 | 0.44 |
| 1:A:756:ILE:HD13 | 1:A:756:ILE:C | 2.37 | 0.44 |
| 1:A:1438:THR:HG22 | 2:B:1144:ALA:H | 1.83 | 0.44 |
| 2:B:653:VAL:HG13 | 2:B:689:LEU:HB3 | 1.99 | 0.44 |
| 2:B:778:MET:SD | 2:B:1094:ARG:HD3 | 2.57 | 0.44 |
| 9:K:61:TYR:HA | 9:K:72:LYS:O | 2.18 | 0.44 |
| 1:A:1217:LYS:C | 1:A:1219:THR:H | 2.21 | 0.43 |
| 1:A:360:GLU:OE2 | 1:A:651:LYS:NZ | 2.51 | 0.43 |
| 1:A:67:CYS:O | 1:A:68:GLN:CB | 2.66 | 0.43 |
| 1:A:752:LYS:HD2 | 2:B:1015:HIS:O | 2.18 | 0.43 |
| 2:B:864:LYS:HD3 | 2:B:871:THR:OG1 | 2.17 | 0.43 |
| 2:B:912:ILE:O | 2:B:938:SER:HB2 | 2.18 | 0.43 |
| 7:I:55:THR:HG23 | 7:I:58:VAL:HG21 | 2.00 | 0.43 |
| 2:B:104:GLU:CG | 10:L:54:ARG:NH1 | 2.80 | 0.43 |
| 1:A:1348:LEU:HG | 1:A:1372:VAL:HG22 | 2.00 | 0.43 |
| 1:A:230:ARG:HB3 | 1:A:232:GLU:HG2 | 1.99 | 0.43 |
| 1:A:709:THR:HB | 1:A:712:GLU:HG3 | 1.99 | 0.43 |
| 1:A:1431:GLY:HA2 | 2:B:1152:MET:CE | 2.48 | 0.43 |
| 2:B:513:GLN:HG3 | 14:B:2008:HOH:O | 2.17 | 0.43 |
| 3:C:137:LYS:N | 3:C:137:LYS:HD2 | 2.27 | 0.43 |
| 3:C:17:ASN:N | 3:C:17:ASN:HD22 | 2.16 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:E:106:GLN:O | 4:E:106:GLN:HG2 | 2.17 | 0.43 |
| 4:E:124:VAL:HB | 4:E:125:PRO:HD3 | 2.00 | 0.43 |
| 8:J:44:TYR:HA | 8:J:47:ARG:CG | 2.35 | 0.43 |
| 10:L:49:LYS:HD3 | 10:L:49:LYS:HA | 1.67 | 0.43 |
| 1:A:1035:TYR:O | 1:A:1036:ARG:HB2 | 2.19 | 0.43 |
| 1:A:1127:ASP:C | 1:A:1129:GLU:H | 2.22 | 0.43 |
| 1:A:1422:ARG:HA | 1:A:1435:PRO:CG | 2.48 | 0.43 |
| 1:A:367:PRO:CG | 1:A:370:ILE:HD12 | 2.48 | 0.43 |
| 1:A:492:PRO:CB | 1:A:497:THR:CG2 | 2.96 | 0.43 |
| 1:A:622:VAL:HG13 | 1:A:622:VAL:O | 2.17 | 0.43 |
| 1:A:709:THR:HG22 | 1:A:710:LEU:N | 2.33 | 0.43 |
| 2:B:1034:VAL:HG22 | 2:B:1059:LEU:HB2 | 2.00 | 0.43 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:N | 2.09 | 0.43 |
| 2:B:108:VAL:HG12 | 2:B:109:THR:N | 2.34 | 0.43 |
| 2:B:872:GLU:HA | 2:B:915:THR:O | 2.18 | 0.43 |
| 5:F:111:LEU:C | 5:F:113:GLY:H | 2.21 | 0.43 |
| 6:H:12:VAL:HA | 6:H:28:ALA:HB2 | 2.00 | 0.43 |
| 1:A:1187:GLN:HG3 | 1:A:1188:GLN:N | 2.33 | 0.43 |
| 1:A:1258:HIS:O | 1:A:1259:MET:C | 2.56 | 0.43 |
| 1:A:1398:MET:O | 1:A:1399:ARG:C | 2.56 | 0.43 |
| 1:A:666:ILE:HD11 | 2:B:1026:LEU:O | 2.17 | 0.43 |
| 1:A:699:ALA:O | 1:A:700:ASN:HB3 | 2.19 | 0.43 |
| 1:A:903:ASN:C | 1:A:903:ASN:HD22 | 2.22 | 0.43 |
| 2:B:113:TYR:CD2 | 2:B:192:LEU:HD22 | 2.53 | 0.43 |
| 2:B:485:ARG:HG3 | 2:B:485:ARG:HH11 | 1.84 | 0.43 |
| 3:C:241:ASP:O | 3:C:245:VAL:HG23 | 2.19 | 0.43 |
| 1:A:1279:ILE:HD12 | 1:A:1279:ILE:N | 2.32 | 0.43 |
| 1:A:849:MET:HE1 | 1:A:1436:ILE:HA | 2.00 | 0.43 |
| 1:A:367:PRO:HB3 | 1:A:466:SER:HA | 2.01 | 0.43 |
| 2:B:642:ASP:C | 2:B:644:GLU:H | 2.20 | 0.43 |
| 4:E:94:LYS:O | 4:E:98:ILE:HG13 | 2.18 | 0.43 |
| 8:J:36:LEU:HD11 | 8:J:51:LEU:HB2 | 2.00 | 0.43 |
| 9:K:68:PHE:N | 9:K:68:PHE:CD1 | 2.87 | 0.43 |
| 11:M:1:ILX:HB | 11:M:7:ASN:OD1 | 2.17 | 0.43 |
| 1:A:1402:PHE:C | 1:A:1404:GLU:H | 2.20 | 0.43 |
| 1:A:682:THR:CG2 | 1:A:728:LYS:HE3 | 2.48 | 0.43 |
| 2:B:172:ILE:CD1 | 2:B:178:ASN:ND2 | 2.82 | 0.43 |
| 2:B:397:ASP:OD2 | 2:B:515:HIS:HE1 | 2.02 | 0.43 |
| 2:B:792:MET:SD | 2:B:857:ARG:NH2 | 2.91 | 0.43 |
| 2:B:1084:GLN:HE22 | 3:C:192:TRP:H | 1.67 | 0.43 |
| 3:C:75:MET:CE | 3:C:239:PRO:HG2 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:89:GLU:HB3 | 5:F:134:ILE:CD1 | 2.49 | 0.43 |
| 1:A:324:SER:O | 1:A:327:ALA:HB3 | 2.19 | 0.43 |
| 2:B:1002:THR:HG21 | 14:B:2021:HOH:O | 2.18 | 0.43 |
| 2:B:119:LEU:HD22 | 2:B:953:LEU:HD13 | 2.01 | 0.43 |
| 2:B:120:ARG:HG3 | 2:B:955:THR:CG2 | 2.47 | 0.43 |
| 2:B:221:ASN:OD1 | 2:B:242:SER:HA | 2.19 | 0.43 |
| 2:B:324:ILE:HG21 | 2:B:330:ALA:HA | 2.00 | 0.43 |
| 2:B:205:ILE:HD11 | 2:B:461:LEU:HB3 | 1.97 | 0.43 |
| 2:B:397:ASP:OD2 | 2:B:515:HIS:CE1 | 2.72 | 0.43 |
| 4:E:102:GLU:C | 4:E:104:ASN:H | 2.22 | 0.43 |
| 5:F:107:VAL:HG12 | 5:F:108:PHE:N | 2.34 | 0.43 |
| 7:I:50:THR:HG22 | 7:I:51:ASN:N | 2.34 | 0.43 |
| 1:A:73:GLY:O | 1:A:75:ASN:N | 2.51 | 0.43 |
| 1:A:987:VAL:O | 1:A:991:LYS:HB2 | 2.19 | 0.43 |
| 2:B:1160:VAL:CG1 | 2:B:1161:HIS:N | 2.78 | 0.43 |
| 1:A:18:GLN:HB3 | 2:B:1215:ARG:HB2 | 2.00 | 0.43 |
| 2:B:175:ARG:HB3 | 2:B:175:ARG:HH11 | 1.84 | 0.43 |
| 3:C:114:TYR:CD2 | 3:C:140:ASN:HB3 | 2.53 | 0.43 |
| 1:A:1339:LEU:HD13 | 4:E:147:HIS:CD2 | 2.52 | 0.43 |
| 5:F:83:PRO:HA | 5:F:146:TRP:CZ3 | 2.53 | 0.43 |
| 6:H:103:LYS:HD3 | 6:H:114:VAL:CG1 | 2.48 | 0.43 |
| 10:L:46:VAL:HG12 | 10:L:46:VAL:O | 2.19 | 0.43 |
| 1:A:115:LEU:HD22 | 1:A:119:ASN:HD22 | 1.84 | 0.43 |
| 1:A:673:GLY:N | 1:A:674:PRO:CD | 2.82 | 0.43 |
| 4:E:31:THR:O | 4:E:33:GLU:N | 2.52 | 0.43 |
| 8:J:6:ARG:HD3 | 8:J:11:GLY:O | 2.18 | 0.43 |
| 9:K:103:THR:CG2 | 9:K:104:ASN:N | 2.82 | 0.43 |
| 9:K:113:THR:O | 9:K:114:LEU:CB | 2.55 | 0.43 |
| 1:A:1015:VAL:HG13 | 1:A:1015:VAL:O | 2.18 | 0.43 |
| 1:A:1059:HIS:CD2 | 1:A:1059:HIS:N | 2.87 | 0.43 |
| 1:A:1161:THR:CG2 | 1:A:1162:VAL:N | 2.81 | 0.43 |
| 1:A:1236:LEU:C | 1:A:1237:ILE:HG13 | 2.39 | 0.43 |
| 1:A:329:LEU:HD21 | 2:B:1203:LEU:CD1 | 2.48 | 0.43 |
| 1:A:535:THR:HG23 | 1:A:575:LYS:CG | 2.40 | 0.43 |
| 1:A:915:SER:O | 1:A:919:ILE:HB | 2.18 | 0.43 |
| 2:B:1191:ILE:CG2 | 2:B:1192:TYR:N | 2.82 | 0.43 |
| 1:A:1410:PHE:CD2 | 2:B:1212:ILE:HD11 | 2.53 | 0.43 |
| 2:B:544:CYS:HB2 | 2:B:634:TYR:CZ | 2.54 | 0.43 |
| 2:B:887:HIS:O | 2:B:888:GLY:C | 2.58 | 0.43 |
| 2:B:889:THR:HG22 | 2:B:890:TYR:N | 2.34 | 0.43 |
| 10:L:32:ALA:CB | 10:L:55:ILE:HB | 2.44 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:169:LYS:NZ | 10:L:69:ALA:HB3 | 2.34 | 0.43 |
| 1:A:1424:VAL:O | 1:A:1428:VAL:HG23 | 2.19 | 0.42 |
| 1:A:16:GLU:HG3 | 2:B:1220:ARG:HA | 2.01 | 0.42 |
| 4:E:117:THR:C | 4:E:119:SER:N | 2.72 | 0.42 |
| 6:H:40:LEU:HD12 | 6:H:41:ASP:N | 2.33 | 0.42 |
| 1:A:1059:HIS:HB3 | 5:F:86:THR:HB | 2.00 | 0.42 |
| 1:A:13:THR:CA | 1:A:1432:GLN:HE22 | 2.32 | 0.42 |
| 1:A:179:LEU:CG | 1:A:308:ILE:HG21 | 2.48 | 0.42 |
| 1:A:407:ARG:HG2 | 1:A:430:TRP:CH2 | 2.54 | 0.42 |
| 1:A:605:MET:HE2 | 1:A:607:ILE:HD11 | 2.01 | 0.42 |
| 1:A:618:GLU:HB2 | 1:A:619:LYS:H | 1.72 | 0.42 |
| 1:A:69:THR:C | 1:A:71:GLN:H | 2.21 | 0.42 |
| 2:B:841:MET:O | 2:B:993:THR:HA | 2.19 | 0.42 |
| 2:B:122:LEU:CD2 | 2:B:958:GLN:HG3 | 2.49 | 0.42 |
| 3:C:183:TRP:CZ2 | 3:C:212:PRO:HG3 | 2.54 | 0.42 |
| 1:A:870:GLU:HG2 | 4:E:208:TYR:CG | 2.54 | 0.42 |
| 7:I:90:GLN:O | 7:I:91:ARG:HD3 | 2.18 | 0.42 |
| 8:J:7:CYS:SG | 8:J:49:MET:HE3 | 2.59 | 0.42 |
| 9:K:55:LYS:HB3 | 9:K:81:TYR:HD1 | 1.84 | 0.42 |
| 1:A:142:CYS:C | 1:A:144:THR:N | 2.73 | 0.42 |
| 1:A:500:GLU:OE2 | 2:B:1145:SER:OG | 2.36 | 0.42 |
| 1:A:878:ILE:HG21 | 1:A:955:PRO:HB2 | 2.01 | 0.42 |
| 2:B:1165:ILE:CD1 | 2:B:1187:ASN:HD21 | 2.32 | 0.42 |
| 2:B:34:ILE:O | 2:B:37:PHE:HB3 | 2.18 | 0.42 |
| 2:B:995:ARG:HB3 | 2:B:997:GLU:OE2 | 2.19 | 0.42 |
| 5:F:76:LYS:C | 5:F:79:ARG:HD2 | 2.39 | 0.42 |
| 7:I:19:ASP:OD1 | 7:I:22:ASN:HB2 | 2.18 | 0.42 |
| 10:L:68:GLU:C | 10:L:70:ARG:H | 2.22 | 0.42 |
| 1:A:1061:GLY:O | 1:A:1437:GLY:HA2 | 2.19 | 0.42 |
| 1:A:1260:LEU:HA | 1:A:1260:LEU:HD12 | 1.89 | 0.42 |
| 1:A:412:ARG:NH2 | 1:A:433:GLU:OE2 | 2.52 | 0.42 |
| 1:A:714:PHE:HB2 | 7:I:97:MET:HE2 | 2.00 | 0.42 |
| 2:B:872:GLU:OE1 | 2:B:914:LYS:HE2 | 2.19 | 0.42 |
| 2:B:900:ALA:HA | 10:L:58:LYS:HD2 | 2.02 | 0.42 |
| 1:A:1015:VAL:O | 1:A:1015:VAL:CG1 | 2.67 | 0.42 |
| 1:A:980:ASP:OD2 | 1:A:1039:LYS:HB3 | 2.19 | 0.42 |
| 1:A:1336:MET:CE | 1:A:1381:LEU:H | 2.31 | 0.42 |
| 1:A:1394:THR:HG23 | 1:A:1398:MET:HE3 | 2.02 | 0.42 |
| 1:A:1426:GLU:H | 1:A:1426:GLU:HG2 | 1.41 | 0.42 |
| 1:A:464:PRO:HB2 | 1:A:465:TYR:H | 1.67 | 0.42 |
| 1:A:677:ARG:HB2 | 1:A:677:ARG:HE | 1.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:15:TYR:CE1 | 7:I:30:ARG:HG3 | 2.55 | 0.42 |
| 10:L:63:ARG:O | 10:L:64:LEU:C | 2.57 | 0.42 |
| 1:A:1201:ALA:O | 1:A:1205:LYS:HG3 | 2.20 | 0.42 |
| 1:A:523:ILE:HG23 | 1:A:527:THR:HB | 2.02 | 0.42 |
| 3:C:64:ALA:HA | 3:C:67:LEU:HD12 | 2.01 | 0.42 |
| 7:I:45:ARG:NH1 | 7:I:47:GLU:OE2 | 2.52 | 0.42 |
| 8:J:48:ARG:HG3 | 8:J:49:MET:N | 2.34 | 0.42 |
| 3:C:146:LYS:HB2 | 8:J:57:ILE:CD1 | 2.49 | 0.42 |
| 1:A:418:SER:C | 1:A:420:ARG:N | 2.73 | 0.42 |
| 1:A:613:ILE:HG23 | 6:H:117:SER:HB2 | 2.01 | 0.42 |
| 1:A:633:VAL:HG21 | 1:A:645:LEU:HD22 | 2.02 | 0.42 |
| 1:A:705:LYS:O | 1:A:706:HIS:C | 2.57 | 0.42 |
| 1:A:994:GLN:HG2 | 1:A:1019:CYS:SG | 2.60 | 0.42 |
| 2:B:593:PRO:HG2 | 2:B:617:ARG:NH2 | 2.34 | 0.42 |
| 2:B:763:GLN:HB2 | 2:B:1021:MET:CB | 2.50 | 0.42 |
| 2:B:906:SER:CB | 2:B:946:ASN:HB2 | 2.50 | 0.42 |
| 3:C:209:TYR:HD1 | 3:C:209:TYR:H | 1.68 | 0.42 |
| 3:C:258:ILE:HD11 | 9:K:42:LEU:CD2 | 2.49 | 0.42 |
| 3:C:39:ALA:O | 3:C:164:ALA:HB3 | 2.20 | 0.42 |
| 5:F:118:LEU:O | 5:F:122:MET:HG3 | 2.19 | 0.42 |
| 1:A:537:ARG:HD2 | 6:H:20:TYR:CZ | 2.55 | 0.42 |
| 9:K:65:HIS:HD2 | 9:K:67:PHE:N | 1.89 | 0.42 |
| 1:A:1143:LEU:HD13 | 1:A:1273:LEU:HD11 | 2.00 | 0.42 |
| 1:A:324:SER:O | 1:A:328:ARG:HG3 | 2.20 | 0.42 |
| 1:A:351:THR:O | 1:A:486:GLU:HA | 2.20 | 0.42 |
| 1:A:463:ILE:HD12 | 1:A:469:ARG:HD2 | 2.02 | 0.42 |
| 2:B:824:ILE:HD13 | 2:B:1089:PRO:HB3 | 2.01 | 0.42 |
| 2:B:287:ARG:HG2 | 2:B:292:ILE:HA | 2.01 | 0.42 |
| 2:B:550:ASP:OD1 | 2:B:552:MET:HG3 | 2.20 | 0.42 |
| 4:E:61:GLN:HB2 | 4:E:79:TRP:CZ3 | 2.54 | 0.42 |
| 6:H:96:VAL:HG13 | 6:H:143:LEU:CD2 | 2.50 | 0.42 |
| 7:I:14:LEU:HB3 | 7:I:27:PHE:HB3 | 2.02 | 0.42 |
| 1:A:1157:ASP:O | 1:A:1159:ARG:N | 2.53 | 0.42 |
| 1:A:1438:THR:HG22 | 2:B:1144:ALA:CB | 2.48 | 0.42 |
| 1:A:452:LYS:HG2 | 14:A:2026:HOH:O | 2.18 | 0.42 |
| 1:A:606:LEU:HD12 | 1:A:607:ILE:N | 2.35 | 0.42 |
| 1:A:849:MET:HE1 | 1:A:1437:GLY:H | 1.85 | 0.42 |
| 1:A:93:VAL:HB | 1:A:305:ASP:OD2 | 2.19 | 0.42 |
| 2:B:1165:ILE:CD1 | 2:B:1187:ASN:ND2 | 2.83 | 0.42 |
| 2:B:864:LYS:HD3 | 2:B:871:THR:HA | 2.01 | 0.42 |
| 4:E:191:LYS:N | 4:E:194:GLU:OE1 | 2.43 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:H:17:PRO:HA | 6:H:24:CYS:SG | 2.59 | 0.42 |
| 10:L:38:LEU:HD13 | 10:L:48:CYS:HA | 2.01 | 0.42 |
| 10:L:49:LYS:O | 10:L:50:ASP:HB2 | 2.19 | 0.42 |
| 1:A:106:VAL:CG2 | 1:A:111:GLY:HA2 | 2.50 | 0.42 |
| 1:A:1187:GLN:HG3 | 1:A:1188:GLN:H | 1.83 | 0.42 |
| 1:A:1195:LEU:HD11 | 1:A:1267:MET:CE | 2.50 | 0.42 |
| 1:A:903:ASN:O | 1:A:907:THR:OG1 | 2.37 | 0.42 |
| 1:A:977:LYS:HA | 1:A:978:PRO:HD3 | 1.95 | 0.42 |
| 2:B:1022:THR:CG2 | 2:B:1022:THR:O | 2.67 | 0.42 |
| 2:B:175:ARG:HB3 | 2:B:175:ARG:NH1 | 2.35 | 0.42 |
| 2:B:793:ALA:HB3 | 2:B:856:PHE:HB2 | 2.01 | 0.42 |
| 3:C:17:ASN:HA | 3:C:232:VAL:O | 2.20 | 0.42 |
| 3:C:264:GLN:C | 3:C:266:ASP:H | 2.24 | 0.42 |
| 4:E:124:VAL:CB | 4:E:125:PRO:CD | 2.98 | 0.42 |
| 6:H:62:SER:O | 6:H:63:LEU:O | 2.37 | 0.42 |
| 7:I:98:VAL:CG2 | 7:I:113:ASP:HB2 | 2.45 | 0.42 |
| 2:B:120:ARG:CZ | 10:L:54:ARG:HD2 | 2.49 | 0.42 |
| 10:L:61:THR:HG21 | 10:L:63:ARG:HD3 | 2.02 | 0.42 |
| 1:A:1111:MET:HE3 | 1:A:1114:PRO:CA | 2.50 | 0.41 |
| 1:A:1155:ASP:HA | 1:A:1156:PRO:HD2 | 1.87 | 0.41 |
| 1:A:23:SER:CB | 1:A:233:TRP:CE2 | 3.03 | 0.41 |
| 1:A:34:LYS:HA | 1:A:83:HIS:CD2 | 2.55 | 0.41 |
| 1:A:878:ILE:HG22 | 1:A:955:PRO:HB2 | 2.00 | 0.41 |
| 2:B:314:LEU:O | 2:B:315:LYS:C | 2.58 | 0.41 |
| 1:A:829:VAL:O | 1:A:832:ALA:N | 2.53 | 0.41 |
| 1:A:31:SER:CB | 1:A:83:HIS:HB2 | 2.50 | 0.41 |
| 2:B:335:GLY:O | 2:B:339:THR:HB | 2.19 | 0.41 |
| 2:B:566:LEU:HD11 | 2:B:586:TRP:CE2 | 2.55 | 0.41 |
| 3:C:22:LEU:HA | 3:C:22:LEU:HD23 | 1.87 | 0.41 |
| 4:E:54:GLN:HB3 | 4:E:57:MET:HE3 | 2.01 | 0.41 |
| 1:A:140:THR:O | 1:A:140:THR:HG22 | 2.20 | 0.41 |
| 1:A:1391:ARG:NH2 | 1:A:1417:GLU:HG3 | 2.34 | 0.41 |
| 2:B:826:ALA:HB2 | 2:B:1087:PHE:HD1 | 1.83 | 0.41 |
| 2:B:840:ILE:HB | 2:B:1011:ILE:HB | 2.02 | 0.41 |
| 6:H:103:LYS:NZ | 6:H:114:VAL:CB | 2.79 | 0.41 |
| 1:A:1191:TRP:CZ3 | 7:I:43:VAL:HG21 | 2.48 | 0.41 |
| 7:I:59:VAL:CG1 | 7:I:60:GLN:N | 2.83 | 0.41 |
| 1:A:440:ASP:OD1 | 1:A:498:ARG:NH2 | 2.48 | 0.41 |
| 1:A:760:GLN:HB2 | 2:B:1021:MET:HE3 | 2.00 | 0.41 |
| 1:A:883:LEU:O | 1:A:886:ILE:HG22 | 2.21 | 0.41 |
| 1:A:529:CYS:HB2 | 2:B:1015:HIS:CE1 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:344:LYS:H | 2:B:347:LYS:NZ | 2.18 | 0.41 |
| 2:B:461:LEU:HD12 | 2:B:466:TRP:HH2 | 1.85 | 0.41 |
| 2:B:642:ASP:C | 2:B:644:GLU:N | 2.74 | 0.41 |
| 9:K:7:PHE:HA | 9:K:10:PHE:CZ | 2.56 | 0.41 |
| 1:A:1001:ARG:O | 1:A:1002:GLY:C | 2.59 | 0.41 |
| 1:A:1125:ALA:HB1 | 1:A:1303:GLU:HB2 | 2.03 | 0.41 |
| 1:A:1223:ASP:O | 1:A:1224:LEU:HB2 | 2.21 | 0.41 |
| 1:A:1319:VAL:HG12 | 1:A:1320:PRO:O | 2.20 | 0.41 |
| 1:A:372:LYS:HA | 1:A:435:HIS:CD2 | 2.55 | 0.41 |
| 1:A:778:GLY:HA3 | 2:B:516:ASN:ND2 | 2.36 | 0.41 |
| 1:A:858:ASN:ND2 | 1:A:862:ASN:H | 2.18 | 0.41 |
| 2:B:322:PHE:CZ | 7:I:30:ARG:HB2 | 2.55 | 0.41 |
| 2:B:610:ASN:HA | 2:B:611:PRO:HD3 | 1.92 | 0.41 |
| 2:B:65:GLU:O | 2:B:66:ASP:HB2 | 2.20 | 0.41 |
| 2:B:60:GLN:HA | 2:B:95:ILE:HD12 | 2.02 | 0.41 |
| 3:C:167:HIS:CD2 | 3:C:169:LYS:H | 2.36 | 0.41 |
| 3:C:76:ASP:OD2 | 3:C:128:ASN:N | 2.49 | 0.41 |
| 7:I:32:CYS:SG | 7:I:33:SER:N | 2.92 | 0.41 |
| 7:I:4:PHE:H | 7:I:4:PHE:HD2 | 1.68 | 0.41 |
| 1:A:1277:GLU:CD | 1:A:1277:GLU:N | 2.73 | 0.41 |
| 1:A:351:THR:CG2 | 2:B:1103:ILE:HG12 | 2.50 | 0.41 |
| 1:A:364:VAL:O | 1:A:364:VAL:HG13 | 2.21 | 0.41 |
| 1:A:583:PRO:O | 1:A:586:ILE:HG12 | 2.20 | 0.41 |
| 2:B:1158:PHE:CE2 | 2:B:1160:VAL:HG22 | 2.55 | 0.41 |
| 2:B:1163:CYS:SG | 2:B:1165:ILE:N | 2.90 | 0.41 |
| 2:B:876:LYS:HE3 | 2:B:894:ASP:C | 2.40 | 0.41 |
| 4:E:14:ARG:O | 4:E:17:ARG:HB3 | 2.20 | 0.41 |
| 7:I:111:THR:OG1 | 7:I:121:PHE:HE2 | 2.04 | 0.41 |
| 3:C:7:GLN:HG2 | 9:K:104:ASN:HD22 | 1.85 | 0.41 |
| 1:A:547:LEU:HD22 | 9:K:58:PHE:CD1 | 2.56 | 0.41 |
| 1:A:122:MET:CE | 1:A:138:ILE:HG23 | 2.51 | 0.41 |
| 1:A:1336:MET:CE | 1:A:1381:LEU:N | 2.83 | 0.41 |
| 1:A:211:PHE:HA | 1:A:214:ILE:CD1 | 2.50 | 0.41 |
| 1:A:571:LEU:HD22 | 6:H:46:LEU:HD11 | 2.02 | 0.41 |
| 1:A:596:THR:C | 1:A:598:LEU:H | 2.24 | 0.41 |
| 2:B:616:ILE:O | 2:B:624:LEU:HD12 | 2.21 | 0.41 |
| 2:B:549:THR:HG22 | 2:B:628:THR:CG2 | 2.50 | 0.41 |
| 9:K:31:VAL:CG1 | 9:K:32:VAL:N | 2.83 | 0.41 |
| 1:A:130:ASP:OD1 | 1:A:132:LYS:HB2 | 2.21 | 0.41 |
| 1:A:592:ASP:HB2 | 1:A:603:ASN:OD1 | 2.21 | 0.41 |
| 2:B:853:SER:OG | 2:B:1094:ARG:NH1 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1438:THR:CG2 | 2:B:1144:ALA:HB3 | 2.49 | 0.41 |
| 2:B:737:THR:CG2 | 2:B:737:THR:O | 2.69 | 0.41 |
| 2:B:813:LYS:HA | 2:B:816:GLU:OE1 | 2.21 | 0.41 |
| 3:C:206:ASN:N | 3:C:206:ASN:OD1 | 2.54 | 0.41 |
| 6:H:100:THR:HG23 | 6:H:138:GLU:HA | 2.03 | 0.41 |
| 6:H:145:ARG:O | 6:H:146:ARG:OXT | 2.39 | 0.41 |
| 9:K:24:ASP:OD1 | 9:K:26:LYS:N | 2.54 | 0.41 |
| 1:A:719:VAL:HG22 | 11:M:4:ILE:HD13 | 2.03 | 0.41 |
| 1:A:846:GLU:HA | 1:A:1066:VAL:HG23 | 2.03 | 0.41 |
| 1:A:1166:ASP:O | 1:A:1169:ILE:HG22 | 2.21 | 0.41 |
| 1:A:1214:GLU:HA | 1:A:1214:GLU:OE1 | 2.21 | 0.41 |
| 1:A:13:THR:HB | 1:A:1432:GLN:NE2 | 2.36 | 0.41 |
| 1:A:778:GLY:HA3 | 2:B:516:ASN:HB2 | 2.03 | 0.41 |
| 2:B:1017:ILE:HB | 2:B:1018:PRO:HD3 | 2.03 | 0.41 |
| 2:B:571:PRO:C | 2:B:573:GLN:N | 2.73 | 0.41 |
| 4:E:198:ILE:CD1 | 4:E:212:ARG:HG3 | 2.51 | 0.41 |
| 1:A:1438:THR:O | 5:F:92:ARG:HD2 | 2.20 | 0.41 |
| 6:H:126:GLU:N | 6:H:130:ARG:HH22 | 2.18 | 0.41 |
| 10:L:31:CYS:SG | 10:L:34:CYS:SG | 3.19 | 0.41 |
| 1:A:1111:MET:HB2 | 1:A:1114:PRO:HG3 | 2.02 | 0.41 |
| 1:A:1212:VAL:O | 1:A:1216:ILE:HG13 | 2.21 | 0.41 |
| 1:A:1254:ALA:HB3 | 1:A:1256:GLU:HG2 | 2.02 | 0.41 |
| 1:A:381:THR:CG2 | 1:A:383:TYR:CD1 | 3.04 | 0.41 |
| 1:A:70:CYS:SG | 1:A:70:CYS:O | 2.79 | 0.41 |
| 2:B:1221:SER:O | 2:B:1222:ARG:O | 2.39 | 0.41 |
| 2:B:243:ALA:CB | 2:B:251:ILE:HG12 | 2.46 | 0.41 |
| 2:B:883:LEU:O | 2:B:885:MET:HG3 | 2.21 | 0.41 |
| 3:C:46:ILE:HG23 | 3:C:157:CYS:HB3 | 2.03 | 0.41 |
| 1:A:1401:SER:O | 1:A:1402:PHE:HB2 | 2.21 | 0.41 |
| 1:A:84:ILE:CG2 | 1:A:239:LEU:O | 2.69 | 0.41 |
| 1:A:505:CYS:O | 1:A:506:ALA:C | 2.59 | 0.41 |
| 1:A:825:ILE:O | 1:A:828:ALA:HB3 | 2.21 | 0.41 |
| 2:B:361:LEU:HD21 | 2:B:381:MET:HE1 | 2.02 | 0.41 |
| 2:B:387:LEU:HA | 2:B:387:LEU:HD12 | 1.76 | 0.41 |
| 2:B:915:THR:CG2 | 2:B:916:THR:N | 2.84 | 0.41 |
| 3:C:33:LEU:O | 3:C:33:LEU:HD12 | 2.21 | 0.41 |
| 4:E:200:ARG:HD2 | 14:E:2004:HOH:O | 2.20 | 0.41 |
| 5:F:97:ARG:NE | 5:F:124:GLU:OE1 | 2.38 | 0.41 |
| 7:I:120:GLN:O | 7:I:121:PHE:HB2 | 2.21 | 0.41 |
| 7:I:2:THR:HG21 | 7:I:43:VAL:O | 2.21 | 0.41 |
| 1:A:1168:GLU:O | 1:A:1172:LEU:HG | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:260:ASP:OD1 | 1:A:261:ASP:N | 2.53 | 0.40 |
| 1:A:265:LYS:HZ1 | 1:A:302:THR:HB | 1.86 | 0.40 |
| 1:A:584:ASN:O | 1:A:637:LYS:HE3 | 2.21 | 0.40 |
| 1:A:596:THR:CG2 | 1:A:597:LEU:H | 2.28 | 0.40 |
| 1:A:596:THR:HG22 | 1:A:597:LEU:HD12 | 2.03 | 0.40 |
| 2:B:25:ILE:HD13 | 2:B:658:ILE:CD1 | 2.50 | 0.40 |
| 2:B:281:PRO:HB3 | 2:B:320:ASP:OD2 | 2.21 | 0.40 |
| 2:B:882:THR:HB | 2:B:934:LYS:O | 2.21 | 0.40 |
| 4:E:84:ASP:O | 4:E:86:PRO:HD3 | 2.21 | 0.40 |
| 5:F:111:LEU:H | 5:F:111:LEU:CD1 | 2.06 | 0.40 |
| 4:E:169:ARG:NE | 5:F:140:ASP:OD2 | 2.54 | 0.40 |
| 1:A:1438:THR:HA | 5:F:88:TYR:HB3 | 2.02 | 0.40 |
| 6:H:89:LEU:C | 6:H:91:ASP:N | 2.72 | 0.40 |
| 8:J:52:THR:O | 8:J:52:THR:HG22 | 2.20 | 0.40 |
| 1:A:1341:ILE:HD11 | 1:A:1376:THR:O | 2.21 | 0.40 |
| 1:A:835:GLY:O | 1:A:839:ARG:HG3 | 2.21 | 0.40 |
| 1:A:587:HIS:HE2 | 1:A:969:GLN:HG2 | 1.76 | 0.40 |
| 2:B:1065:GLN:HE22 | 2:B:1067:ARG:CB | 2.35 | 0.40 |
| 2:B:879:ARG:HE | 2:B:885:MET:CE | 2.33 | 0.40 |
| 2:B:874:PHE:HA | 2:B:913:GLY:O | 2.21 | 0.40 |
| 3:C:108:GLU:HG2 | 3:C:149:LYS:HD2 | 2.01 | 0.40 |
| 3:C:209:TYR:N | 3:C:209:TYR:HD1 | 2.19 | 0.40 |
| 4:E:116:ILE:HG22 | 4:E:117:THR:H | 1.85 | 0.40 |
| 4:E:198:ILE:HD12 | 4:E:212:ARG:HG3 | 2.03 | 0.40 |
| 1:A:867:ILE:HG22 | 4:E:208:TYR:HE1 | 1.86 | 0.40 |
| 6:H:12:VAL:HG13 | 6:H:26:ILE:HG23 | 2.04 | 0.40 |
| 6:H:36:CYS:HB2 | 6:H:129:TYR:HH | 1.85 | 0.40 |
| 6:H:51:ALA:O | 6:H:53:ASP:N | 2.54 | 0.40 |
| 1:A:1079:MET:HG2 | 1:A:1359:ASP:OD2 | 2.21 | 0.40 |
| 1:A:112:LYS:HD2 | 1:A:165:GLY:HA3 | 2.03 | 0.40 |
| 1:A:326:ARG:HG3 | 1:A:1406:VAL:HG21 | 2.03 | 0.40 |
| 1:A:378:GLU:OE2 | 1:A:387:ARG:NH2 | 2.52 | 0.40 |
| 1:A:535:THR:O | 1:A:535:THR:CG2 | 2.66 | 0.40 |
| 2:B:240:ILE:CG2 | 2:B:254:LEU:HB3 | 2.51 | 0.40 |
| 2:B:590:HIS:CD2 | 2:B:591:ARG:O | 2.74 | 0.40 |
| 2:B:610:ASN:OD1 | 2:B:611:PRO:HD2 | 2.22 | 0.40 |
| 2:B:788:ARG:CB | 2:B:788:ARG:HH11 | 2.34 | 0.40 |
| 3:C:63:ILE:HD13 | 3:C:153:LEU:HD11 | 2.04 | 0.40 |
| 6:H:10:PHE:HB3 | 6:H:28:ALA:HB1 | 2.04 | 0.40 |
| 1:A:1434:ALA:C | 1:A:1436:ILE:H | 2.22 | 0.40 |
| 1:A:997:LEU:HD13 | 1:A:1018:PHE:CE2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:1035:ALA:HB1 | 2:B:1040:ASN:O | 2.21 | 0.40 |
| 2:B:1153:GLU:CG | 2:B:1154:ALA:N | 2.77 | 0.40 |
| 2:B:51:PHE:O | 2:B:54:PHE:HB3 | 2.22 | 0.40 |
| 3:C:104:PHE:HD1 | 3:C:152:GLU:HG3 | 1.87 | 0.40 |
| 3:C:39:ALA:HA | 3:C:164:ALA:CB | 2.41 | 0.40 |
| 3:C:73:GLN:NE2 | 3:C:75:MET:CB | 2.84 | 0.40 |
| 4:E:136:ASN:O | 4:E:139:ALA:N | 2.53 | 0.40 |
| 4:E:178:ILE:O | 4:E:178:ILE:HG23 | 2.22 | 0.40 |
| 5:F:135:ARG:HG2 | 5:F:137:TYR:CE1 | 2.56 | 0.40 |
| 6:H:123:MET:HE1 | 6:H:142:LEU:CD1 | 2.51 | 0.40 |
| 8:J:23:ASN:C | 8:J:25:LEU:N | 2.74 | 0.40 |
| 1:A:1394:THR:HG23 | 1:A:1398:MET:SD | 2.62 | 0.40 |
| 1:A:787:PHE:CZ | 1:A:796:SER:HA | 2.56 | 0.40 |
| 1:A:84:ILE:HG23 | 1:A:84:ILE:O | 2.22 | 0.40 |
| 2:B:118:ARG:NH2 | 2:B:194:GLU:CD | 2.74 | 0.40 |
| 2:B:167:ILE:HG22 | 2:B:453:ILE:CD1 | 2.49 | 0.40 |
| 2:B:242:SER:OG | 2:B:362:PRO:HD2 | 2.22 | 0.40 |
| 2:B:864:LYS:HB3 | 2:B:871:THR:CA | 2.50 | 0.40 |
| 3:C:99:LEU:HD12 | 3:C:99:LEU:N | 2.36 | 0.40 |
| 1:A:767:GLN:HG2 | 11:M:4:ILE:HD12 | 2.03 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 10:L:28:LYS:NZ | 10:L:28:LYS:NZ[3_655] | 2.05 | 0.15 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 1348/1733 (78%) | 1160 (86%) | 134 (10%) | 54 (4%) | 3 11 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 2 | B | 1062/1224 (87%) | 931 (88%) | 107 (10%) | 24 (2%) | 7 | 25 |
| 3 | C | 264/318 (83%) | 223 (84%) | 30 (11%) | 11 (4%) | 3 | 10 |
| 4 | E | 211/215 (98%) | 180 (85%) | 23 (11%) | 8 (4%) | 4 | 12 |
| 5 | F | 82/155 (53%) | 71 (87%) | 10 (12%) | 1 (1%) | 15 | 44 |
| 6 | H | 129/146 (88%) | 88 (68%) | 23 (18%) | 18 (14%) | 0 | 1 |
| 7 | I | 120/122 (98%) | 102 (85%) | 16 (13%) | 2 (2%) | 11 | 34 |
| 8 | J | 63/70 (90%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 9 | K | 112/120 (93%) | 98 (88%) | 13 (12%) | 1 (1%) | 20 | 52 |
| 10 | L | 43/70 (61%) | 23 (54%) | 13 (30%) | 7 (16%) | 0 | 0 |
| 11 | M | 4/8 (50%) | 4 (100%) | 0 | 0 | 100 | 100 |
| All | All | 3438/4181 (82%) | 2938 (86%) | 374 (11%) | 126 (4%) | 4 | 13 |

All (126) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 55 | ASP |
| 1 | A | 56 | PRO |
| 1 | A | 399 | HIS |
| 1 | A | 464 | PRO |
| 1 | A | 465 | TYR |
| 1 | A | 466 | SER |
| 1 | A | 567 | LYS |
| 1 | A | 752 | LYS |
| 1 | A | 1385 | THR |
| 1 | A | 1386 | ARG |
| 1 | A | 1391 | ARG |
| 1 | A | 1392 | SER |
| 1 | A | 1393 | ASN |
| 2 | B | 864 | LYS |
| 2 | B | 879 | ARG |
| 2 | B | 1100 | ASP |
| 2 | B | 1222 | ARG |
| 3 | C | 4 | GLU |
| 3 | C | 206 | ASN |
| 4 | E | 4 | GLU |
| 4 | E | 5 | ASN |
| 4 | E | 59 | SER |
| 6 | H | 19 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | H | 52 | GLN |
| 6 | H | 81 | PRO |
| 6 | H | 88 | SER |
| 6 | H | 105 | GLU |
| 6 | H | 128 | ASN |
| 6 | H | 138 | GLU |
| 10 | L | 39 | SER |
| 10 | L | 64 | LEU |
| 1 | A | 35 | ILE |
| 1 | A | 57 | ARG |
| 1 | A | 58 | LEU |
| 1 | A | 67 | CYS |
| 1 | A | 71 | GLN |
| 1 | A | 74 | MET |
| 1 | A | 79 | GLY |
| 1 | A | 84 | ILE |
| 1 | A | 400 | PRO |
| 1 | A | 419 | LYS |
| 1 | A | 626 | ASN |
| 1 | A | 628 | GLY |
| 1 | A | 846 | GLU |
| 1 | A | 885 | THR |
| 1 | A | 1202 | MET |
| 1 | A | 1221 | LYS |
| 1 | A | 1396 | ALA |
| 1 | A | 1399 | ARG |
| 1 | A | 1400 | CYS |
| 2 | B | 165 | VAL |
| 2 | B | 266 | ALA |
| 2 | B | 367 | LEU |
| 2 | B | 646 | LEU |
| 2 | B | 648 | HIS |
| 2 | B | 1066 | SER |
| 3 | C | 137 | LYS |
| 3 | C | 184 | ASN |
| 3 | C | 215 | GLU |
| 3 | C | 231 | ASN |
| 3 | C | 245 | VAL |
| 4 | E | 50 | MET |
| 4 | E | 76 | GLY |
| 6 | H | 18 | GLY |
| 6 | H | 90 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | L | 34 | CYS |
| 10 | L | 35 | SER |
| 10 | L | 52 | GLY |
| 10 | L | 59 | ALA |
| 1 | A | 68 | GLN |
| 1 | A | 72 | GLU |
| 1 | A | 308 | ILE |
| 1 | A | 408 | ASP |
| 1 | A | 409 | SER |
| 1 | A | 418 | SER |
| 1 | A | 467 | THR |
| 1 | A | 1278 | ASN |
| 2 | B | 666 | TYR |
| 2 | B | 734 | HIS |
| 2 | B | 906 | SER |
| 2 | B | 907 | GLY |
| 2 | B | 1099 | VAL |
| 3 | C | 90 | ASP |
| 4 | E | 115 | ASN |
| 5 | F | 73 | ALA |
| 6 | H | 32 | THR |
| 6 | H | 77 | ARG |
| 6 | H | 82 | PRO |
| 6 | H | 83 | GLN |
| 6 | H | 139 | ASN |
| 7 | I | 3 | THR |
| 9 | K | 111 | LEU |
| 1 | A | 599 | SER |
| 1 | A | 829 | VAL |
| 2 | B | 124 | TYR |
| 2 | B | 323 | VAL |
| 2 | B | 369 | GLY |
| 2 | B | 883 | LEU |
| 3 | C | 9 | LYS |
| 3 | C | 10 | ILE |
| 3 | C | 267 | GLN |
| 6 | H | 3 | ASN |
| 6 | H | 8 | ASP |
| 1 | A | 307 | ASP |
| 1 | A | 538 | ASP |
| 1 | A | 904 | THR |
| 1 | A | 958 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1200 | ALA |
| 2 | B | 90 | ILE |
| 2 | B | 909 | ASP |
| 4 | E | 103 | LYS |
| 4 | E | 124 | VAL |
| 6 | H | 14 | GLU |
| 10 | L | 56 | LEU |
| 1 | A | 283 | GLY |
| 1 | A | 737 | LEU |
| 1 | A | 1172 | LEU |
| 1 | A | 1257 | ASP |
| 2 | B | 464 | GLY |
| 2 | B | 1103 | ILE |
| 7 | I | 76 | PRO |
| 1 | A | 166 | GLY |
| 1 | A | 1002 | GLY |
| 1 | A | 246 | VAL |
| 2 | B | 647 | GLY |
| 6 | H | 59 | ILE |

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 | 1196/1520 (79%) | 1116 (93%) | 80 (7%) | 19 | 48 |
| 2 | B | 940/1061 (89%) | 899 (96%) | 41 (4%) | 33 | 67 |
| 3 | C | 234/274 (85%) | 221 (94%) | 13 (6%) | 25 | 57 |
| 4 | E | 195/197 (99%) | 190 (97%) | 5 (3%) | 51 | 83 |
| 5 | F | 74/137 (54%) | 71 (96%) | 3 (4%) | 35 | 69 |
| 6 | H | 117/128 (91%) | 114 (97%) | 3 (3%) | 51 | 83 |
| 7 | I | 116/116 (100%) | 108 (93%) | 8 (7%) | 18 | 46 |
| 8 | J | 60/65 (92%) | 57 (95%) | 3 (5%) | 28 | 62 |
| 9 | K | 99/102 (97%) | 88 (89%) | 11 (11%) | 7 | 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 10 | L | 40/57 (70%) | 34 (85%) | 6 (15%) | 3 | 10 |
| 11 | M | 2/2 (100%) | 2 (100%) | 0 | 100 | 100 |
| All | All | 3073/3659 (84%) | 2900 (94%) | 173 (6%) | 25 | 57 |

All (173) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 22 | PHE |
| 1 | A | 70 | CYS |
| 1 | A | 71 | GLN |
| 1 | A | 93 | VAL |
| 1 | A | 116 | ASP |
| 1 | A | 117 | GLU |
| 1 | A | 156 | ASP |
| 1 | A | 159 | THR |
| 1 | A | 164 | ARG |
| 1 | A | 208 | LEU |
| 1 | A | 226 | GLU |
| 1 | A | 247 | ARG |
| 1 | A | 351 | THR |
| 1 | A | 373 | THR |
| 1 | A | 381 | THR |
| 1 | A | 385 | ILE |
| 1 | A | 389 | THR |
| 1 | A | 434 | ARG |
| 1 | A | 445 | ASN |
| 1 | A | 450 | LEU |
| 1 | A | 451 | HIS |
| 1 | A | 465 | TYR |
| 1 | A | 467 | THR |
| 1 | A | 469 | ARG |
| 1 | A | 472 | LEU |
| 1 | A | 474 | VAL |
| 1 | A | 475 | THR |
| 1 | A | 476 | SER |
| 1 | A | 479 | ASN |
| 1 | A | 493 | GLN |
| 1 | A | 497 | THR |
| 1 | A | 503 | GLN |
| 1 | A | 504 | LEU |
| 1 | A | 515 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 544 | ASP |
| 1 | A | 557 | ASP |
| 1 | A | 597 | LEU |
| 1 | A | 603 | ASN |
| 1 | A | 612 | ILE |
| 1 | A | 618 | GLU |
| 1 | A | 622 | VAL |
| 1 | A | 672 | ASP |
| 1 | A | 703 | THR |
| 1 | A | 710 | LEU |
| 1 | A | 741 | ASN |
| 1 | A | 756 | ILE |
| 1 | A | 821 | ARG |
| 1 | A | 822 | GLU |
| 1 | A | 831 | THR |
| 1 | A | 855 | THR |
| 1 | A | 858 | ASN |
| 1 | A | 873 | MET |
| 1 | A | 882 | SER |
| 1 | A | 885 | THR |
| 1 | A | 903 | ASN |
| 1 | A | 919 | ILE |
| 1 | A | 920 | LEU |
| 1 | A | 969 | GLN |
| 1 | A | 1015 | VAL |
| 1 | A | 1030 | ARG |
| 1 | A | 1048 | ASN |
| 1 | A | 1060 | PRO |
| 1 | A | 1118 | VAL |
| 1 | A | 1122 | PRO |
| 1 | A | 1128 | GLN |
| 1 | A | 1240 | CYS |
| 1 | A | 1255 | GLU |
| 1 | A | 1257 | ASP |
| 1 | A | 1264 | GLU |
| 1 | A | 1297 | GLU |
| 1 | A | 1308 | THR |
| 1 | A | 1318 | THR |
| 1 | A | 1325 | THR |
| 1 | A | 1336 | MET |
| 1 | A | 1366 | ARG |
| 1 | A | 1385 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1387 | HIS |
| 1 | A | 1419 | ASP |
| 1 | A | 1426 | GLU |
| 1 | A | 1438 | THR |
| 2 | B | 18 | PHE |
| 2 | B | 20 | ASP |
| 2 | B | 46 | GLN |
| 2 | B | 131 | ASP |
| 2 | B | 183 | GLU |
| 2 | B | 194 | GLU |
| 2 | B | 217 | ARG |
| 2 | B | 261 | ARG |
| 2 | B | 268 | THR |
| 2 | B | 277 | LYS |
| 2 | B | 337 | ARG |
| 2 | B | 339 | THR |
| 2 | B | 424 | LEU |
| 2 | B | 466 | TRP |
| 2 | B | 485 | ARG |
| 2 | B | 490 | SER |
| 2 | B | 513 | GLN |
| 2 | B | 531 | GLN |
| 2 | B | 540 | SER |
| 2 | B | 547 | VAL |
| 2 | B | 567 | GLU |
| 2 | B | 589 | VAL |
| 2 | B | 644 | GLU |
| 2 | B | 648 | HIS |
| 2 | B | 653 | VAL |
| 2 | B | 736 | THR |
| 2 | B | 886 | LYS |
| 2 | B | 939 | THR |
| 2 | B | 951 | GLN |
| 2 | B | 963 | PHE |
| 2 | B | 974 | PRO |
| 2 | B | 997 | GLU |
| 2 | B | 999 | MET |
| 2 | B | 1007 | VAL |
| 2 | B | 1060 | ARG |
| 2 | B | 1065 | GLN |
| 2 | B | 1150 | ARG |
| 2 | B | 1159 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1189 | ILE |
| 2 | B | 1211 | ASN |
| 2 | B | 1222 | ARG |
| 3 | C | 26 | ASP |
| 3 | C | 50 | GLU |
| 3 | C | 52 | GLU |
| 3 | C | 57 | VAL |
| 3 | C | 77 | ILE |
| 3 | C | 88 | CYS |
| 3 | C | 129 | ILE |
| 3 | C | 138 | GLU |
| 3 | C | 163 | ILE |
| 3 | C | 206 | ASN |
| 3 | C | 209 | TYR |
| 3 | C | 233 | GLU |
| 3 | C | 240 | VAL |
| 4 | E | 104 | ASN |
| 4 | E | 123 | LEU |
| 4 | E | 149 | LEU |
| 4 | E | 196 | VAL |
| 4 | E | 204 | THR |
| 5 | F | 82 | THR |
| 5 | F | 110 | ASP |
| 5 | F | 111 | LEU |
| 6 | H | 82 | PRO |
| 6 | H | 91 | ASP |
| 6 | H | 93 | TYR |
| 7 | I | 4 | PHE |
| 7 | I | 30 | ARG |
| 7 | I | 45 | ARG |
| 7 | I | 50 | THR |
| 7 | I | 52 | ILE |
| 7 | I | 70 | ARG |
| 7 | I | 87 | GLN |
| 7 | I | 98 | VAL |
| 8 | J | 1 | MET |
| 8 | J | 28 | ASP |
| 8 | J | 48 | ARG |
| 9 | K | 11 | LEU |
| 9 | K | 29 | ASN |
| 9 | K | 47 | ARG |
| 9 | K | 50 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | K | 63 | VAL |
| 9 | K | 68 | PHE |
| 9 | K | 73 | LEU |
| 9 | K | 76 | GLN |
| 9 | K | 81 | TYR |
| 9 | K | 103 | THR |
| 9 | K | 114 | LEU |
| 10 | L | 27 | LEU |
| 10 | L | 42 | ARG |
| 10 | L | 50 | ASP |
| 10 | L | 61 | THR |
| 10 | L | 65 | VAL |
| 10 | L | 68 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 64 | ASN |
| 1 | A | 68 | GLN |
| 1 | A | 71 | GLN |
| 1 | A | 92 | HIS |
| 1 | A | 118 | HIS |
| 1 | A | 171 | GLN |
| 1 | A | 299 | HIS |
| 1 | A | 358 | ASN |
| 1 | A | 390 | GLN |
| 1 | A | 394 | ASN |
| 1 | A | 397 | ASN |
| 1 | A | 479 | ASN |
| 1 | A | 493 | GLN |
| 1 | A | 503 | GLN |
| 1 | A | 517 | ASN |
| 1 | A | 631 | HIS |
| 1 | A | 736 | ASN |
| 1 | A | 741 | ASN |
| 1 | A | 745 | GLN |
| 1 | A | 757 | ASN |
| 1 | A | 768 | GLN |
| 1 | A | 786 | HIS |
| 1 | A | 854 | ASN |
| 1 | A | 858 | ASN |
| 1 | A | 903 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 926 | GLN |
| 1 | A | 935 | GLN |
| 1 | A | 994 | GLN |
| 1 | A | 1048 | ASN |
| 1 | A | 1124 | HIS |
| 1 | A | 1173 | HIS |
| 1 | A | 1218 | GLN |
| 1 | A | 1265 | ASN |
| 1 | A | 1364 | ASN |
| 1 | A | 1432 | GLN |
| 2 | B | 46 | GLN |
| 2 | B | 115 | GLN |
| 2 | B | 178 | ASN |
| 2 | B | 215 | GLN |
| 2 | B | 236 | HIS |
| 2 | B | 255 | GLN |
| 2 | B | 300 | HIS |
| 2 | B | 325 | GLN |
| 2 | B | 366 | GLN |
| 2 | B | 465 | ASN |
| 2 | B | 484 | ASN |
| 2 | B | 513 | GLN |
| 2 | B | 515 | HIS |
| 2 | B | 516 | ASN |
| 2 | B | 518 | HIS |
| 2 | B | 538 | ASN |
| 2 | B | 587 | HIS |
| 2 | B | 648 | HIS |
| 2 | B | 657 | HIS |
| 2 | B | 706 | GLN |
| 2 | B | 734 | HIS |
| 2 | B | 744 | HIS |
| 2 | B | 786 | ASN |
| 2 | B | 958 | GLN |
| 2 | B | 1015 | HIS |
| 2 | B | 1062 | HIS |
| 2 | B | 1065 | GLN |
| 2 | B | 1076 | HIS |
| 2 | B | 1084 | GLN |
| 2 | B | 1176 | ASN |
| 2 | B | 1177 | HIS |
| 2 | B | 1187 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1193 | GLN |
| 2 | B | 1211 | ASN |
| 3 | C | 17 | ASN |
| 3 | C | 24 | ASN |
| 3 | C | 65 | HIS |
| 3 | C | 73 | GLN |
| 3 | C | 112 | ASN |
| 3 | C | 123 | ASN |
| 3 | C | 131 | HIS |
| 3 | C | 140 | ASN |
| 3 | C | 167 | HIS |
| 3 | C | 203 | GLN |
| 3 | C | 242 | GLN |
| 3 | C | 252 | GLN |
| 4 | E | 101 | GLN |
| 4 | E | 104 | ASN |
| 4 | E | 147 | HIS |
| 6 | H | 11 | GLN |
| 6 | H | 128 | ASN |
| 6 | H | 133 | ASN |
| 7 | I | 11 | ASN |
| 7 | I | 12 | ASN |
| 7 | I | 114 | GLN |
| 9 | K | 29 | ASN |
| 9 | K | 65 | HIS |
| 9 | K | 76 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 11 | ILX | M | 1 | 11 | 9,9,10 | 2.89 | 4 (44%) | 9,11,13 | 2.14 | 4 (44%) |
| 11 | TRX | M | 2 | 11 | 15,16,17 | 2.79 | 7 (46%) | 15,22,24 | 2.04 | 7 (46%) |
| 11 | CSX | M | 6 | 11 | 4,6,7 | 3.62 | 3 (75%) | 2,6,8 | 1.46 | 0 |
| 11 | HYP | M | 8 | 11 | 7,8,9 | 2.72 | 1 (14%) | 5,10,12 | 1.55 | 2 (40%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 11 | ILX | M | 1 | 11 | - | 0/11/12/14 | 0/0/0/0 |
| 11 | TRX | M | 2 | 11 | - | 0/3/6/8 | 0/2/2/2 |
| 11 | CSX | M | 6 | 11 | - | 0/1/5/7 | 0/0/0/0 |
| 11 | HYP | M | 8 | 11 | - | 0/0/11/13 | 0/1/1/1 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11 | M | 2 | TRX | OH2-CH2 | 2.05 | 1.41 | 1.37 |
| 11 | M | 2 | TRX | CD1-CG | 2.20 | 1.43 | 1.37 |
| 11 | M | 6 | CSX | O-C | 2.55 | 1.30 | 1.19 |
| 11 | M | 1 | ILX | CA-N | 2.58 | 1.56 | 1.47 |
| 11 | M | 2 | TRX | CD1-NE1 | 2.93 | 1.42 | 1.36 |
| 11 | M | 2 | TRX | CZ3-CH2 | 2.93 | 1.44 | 1.38 |
| 11 | M | 1 | ILX | OG1-CG1 | 2.99 | 1.49 | 1.43 |
| 11 | M | 1 | ILX | CA-C | 3.90 | 1.55 | 1.50 |
| 11 | M | 6 | CSX | CB-CA | 3.94 | 1.63 | 1.53 |
| 11 | M | 2 | TRX | CA-C | 4.84 | 1.56 | 1.50 |
| 11 | M | 2 | TRX | CZ2-CE2 | 4.91 | 1.49 | 1.41 |
| 11 | M | 6 | CSX | CA-C | 5.42 | 1.57 | 1.50 |
| 11 | M | 2 | TRX | CZ2-CH2 | 5.56 | 1.47 | 1.37 |
| 11 | M | 1 | ILX | CB-CA | 6.34 | 1.60 | 1.54 |
| 11 | M | 8 | HYP | CA-C | 6.87 | 1.59 | 1.50 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11 | M | 2 | TRX | CH2-CZ2-CE2 | -4.22 | 116.37 | 119.17 |
| 11 | M | 1 | ILX | CG2-CB-CG1 | -4.00 | 105.72 | 111.36 |
| 11 | M | 1 | ILX | CB-CA-C | -3.61 | 108.02 | 112.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11 | M | 2 | TRX | OH2-CH2-CZ3 | -2.92 | 111.82 | 120.04 |
| 11 | M | 2 | TRX | CB-CA-N | -2.55 | 102.49 | 112.54 |
| 11 | M | 2 | TRX | O-C-CA | -2.36 | 118.50 | 125.02 |
| 11 | M | 8 | HYP | O-C-CA | -2.18 | 120.06 | 125.15 |
| 11 | M | 1 | ILX | O-C-CA | -2.07 | 120.33 | 125.15 |
| 11 | M | 2 | TRX | OH2-CH2-CZ2 | 2.08 | 127.15 | 121.05 |
| 11 | M | 8 | HYP | CG-CB-CA | 2.34 | 107.01 | 103.93 |
| 11 | M | 1 | ILX | OD1-CD1-CG1 | 2.36 | 116.32 | 111.11 |
| 11 | M | 2 | TRX | CB-CG-CD1 | 2.39 | 130.92 | 127.97 |
| 11 | M | 2 | TRX | CB-CA-C | 3.13 | 117.45 | 111.41 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11 | M | 1 | ILX | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 | 1366/1733 (78%) | -0.05 | 66 (4%) 31 21 | 18, 48, 107, 137 | 0 |
| 2 | B | 1082/1224 (88%) | -0.03 | 72 (6%) 19 11 | 20, 46, 105, 128 | 0 |
| 3 | C | 266/318 (83%) | -0.11 | 4 (1%) 74 67 | 30, 53, 83, 124 | 0 |
| 4 | E | 213/215 (99%) | -0.00 | 7 (3%) 47 36 | 22, 59, 99, 109 | 0 |
| 5 | F | 84/155 (54%) | -0.26 | 2 (2%) 59 49 | 24, 44, 67, 82 | 0 |
| 6 | H | 133/146 (91%) | 1.12 | 30 (22%) 1 1 | 64, 94, 122, 125 | 0 |
| 7 | I | 122/122 (100%) | -0.01 | 5 (4%) 38 27 | 30, 51, 89, 106 | 0 |
| 8 | J | 65/70 (92%) | -0.42 | 1 (1%) 74 67 | 26, 47, 76, 85 | 0 |
| 9 | K | 114/120 (95%) | -0.17 | 3 (2%) 56 45 | 31, 60, 79, 97 | 0 |
| 10 | L | 45/70 (64%) | 1.00 | 10 (22%) 1 1 | 49, 86, 108, 110 | 0 |
| 11 | M | 4/8 (50%) | 0.86 | 0 100 100 | 73, 80, 83, 84 | 0 |
| All | All | 3494/4181 (83%) | -0.00 | 200 (5%) 24 16 | 18, 50, 105, 137 | 0 |

All (200) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 69 | THR | 14.7 |
| 1 | A | 1390 | ASN | 11.0 |
| 2 | B | 882 | THR | 9.0 |
| 2 | B | 866 | TYR | 8.3 |
| 1 | A | 1389 | PHE | 8.1 |
| 2 | B | 137 | TYR | 8.0 |
| 3 | C | 268 | ASP | 7.2 |
| 2 | B | 247 | GLY | 7.0 |
| 1 | A | 1402 | PHE | 6.8 |
| 2 | B | 643 | ASP | 6.8 |
| 1 | A | 1391 | ARG | 6.8 |
| 6 | H | 131 | ASN | 6.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1092 | LYS | 6.4 |
| 1 | A | 1388 | GLY | 6.2 |
| 1 | A | 1393 | ASN | 6.2 |
| 3 | C | 267 | GLN | 6.1 |
| 1 | A | 62 | ASP | 6.1 |
| 2 | B | 1156 | ASP | 5.8 |
| 6 | H | 104 | PHE | 5.8 |
| 2 | B | 1221 | SER | 5.8 |
| 6 | H | 139 | ASN | 5.8 |
| 2 | B | 1223 | ASP | 5.7 |
| 2 | B | 869 | SER | 5.7 |
| 2 | B | 883 | LEU | 5.5 |
| 2 | B | 1155 | SER | 5.4 |
| 2 | B | 734 | HIS | 5.4 |
| 1 | A | 66 | LYS | 5.3 |
| 1 | A | 1404 | GLU | 5.3 |
| 1 | A | 166 | GLY | 5.2 |
| 2 | B | 246 | LYS | 5.2 |
| 1 | A | 49 | LYS | 5.1 |
| 2 | B | 1184 | GLY | 5.0 |
| 7 | I | 1 | MET | 5.0 |
| 2 | B | 870 | ILE | 4.9 |
| 1 | A | 186 | LYS | 4.8 |
| 2 | B | 722 | ASP | 4.7 |
| 1 | A | 68 | GLN | 4.7 |
| 2 | B | 1100 | ASP | 4.7 |
| 1 | A | 65 | LEU | 4.7 |
| 1 | A | 1081 | LEU | 4.6 |
| 2 | B | 733 | HIS | 4.6 |
| 2 | B | 1109 | GLY | 4.6 |
| 2 | B | 868 | MET | 4.5 |
| 10 | L | 43 | THR | 4.5 |
| 1 | A | 1450 | LEU | 4.5 |
| 2 | B | 249 | ARG | 4.5 |
| 1 | A | 1386 | ARG | 4.5 |
| 6 | H | 87 | ARG | 4.5 |
| 1 | A | 311 | GLN | 4.4 |
| 6 | H | 146 | ARG | 4.4 |
| 2 | B | 248 | SER | 4.3 |
| 6 | H | 88 | SER | 4.3 |
| 2 | B | 1105 | ALA | 4.3 |
| 1 | A | 1387 | HIS | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 64 | ASN | 4.2 |
| 1 | A | 1392 | SER | 4.2 |
| 4 | E | 50 | MET | 4.2 |
| 2 | B | 1104 | HIS | 4.2 |
| 2 | B | 265 | SER | 4.2 |
| 6 | H | 132 | LEU | 4.1 |
| 1 | A | 1403 | GLU | 4.0 |
| 10 | L | 26 | THR | 4.0 |
| 1 | A | 1175 | SER | 4.0 |
| 1 | A | 334 | GLY | 4.0 |
| 2 | B | 250 | PHE | 4.0 |
| 1 | A | 281 | HIS | 3.9 |
| 2 | B | 1102 | LYS | 3.9 |
| 1 | A | 1399 | ARG | 3.9 |
| 6 | H | 84 | ALA | 3.9 |
| 6 | H | 107 | VAL | 3.9 |
| 1 | A | 310 | GLY | 3.8 |
| 1 | A | 1080 | THR | 3.8 |
| 10 | L | 50 | ASP | 3.8 |
| 2 | B | 18 | PHE | 3.8 |
| 1 | A | 260 | ASP | 3.8 |
| 2 | B | 1101 | ASP | 3.7 |
| 2 | B | 865 | LYS | 3.7 |
| 6 | H | 85 | GLY | 3.7 |
| 6 | H | 2 | SER | 3.7 |
| 2 | B | 1103 | ILE | 3.7 |
| 1 | A | 61 | ILE | 3.7 |
| 10 | L | 27 | LEU | 3.7 |
| 4 | E | 129 | PRO | 3.7 |
| 2 | B | 1110 | PRO | 3.6 |
| 2 | B | 136 | THR | 3.6 |
| 1 | A | 309 | ALA | 3.5 |
| 4 | E | 49 | SER | 3.5 |
| 1 | A | 1448 | GLU | 3.5 |
| 7 | I | 119 | THR | 3.5 |
| 2 | B | 1224 | PHE | 3.5 |
| 6 | H | 82 | PRO | 3.5 |
| 2 | B | 884 | ARG | 3.5 |
| 6 | H | 3 | ASN | 3.4 |
| 1 | A | 63 | ARG | 3.4 |
| 1 | A | 330 | LYS | 3.4 |
| 2 | B | 1106 | ARG | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | J | 65 | PRO | 3.3 |
| 2 | B | 1108 | ARG | 3.3 |
| 1 | A | 75 | ASN | 3.3 |
| 2 | B | 933 | SER | 3.3 |
| 7 | I | 122 | SER | 3.3 |
| 1 | A | 57 | ARG | 3.2 |
| 9 | K | 1 | MET | 3.2 |
| 6 | H | 83 | GLN | 3.2 |
| 2 | B | 70 | ILE | 3.1 |
| 2 | B | 1154 | ALA | 3.1 |
| 2 | B | 1153 | GLU | 3.1 |
| 1 | A | 328 | ARG | 3.1 |
| 1 | A | 37 | PHE | 3.1 |
| 1 | A | 308 | ILE | 3.1 |
| 1 | A | 157 | ASP | 3.0 |
| 2 | B | 712 | PRO | 3.0 |
| 1 | A | 332 | LYS | 3.0 |
| 2 | B | 89 | GLU | 3.0 |
| 7 | I | 118 | ARG | 3.0 |
| 1 | A | 187 | LYS | 3.0 |
| 2 | B | 1099 | VAL | 3.0 |
| 2 | B | 103 | ASN | 3.0 |
| 2 | B | 871 | THR | 3.0 |
| 1 | A | 1401 | SER | 3.0 |
| 6 | H | 86 | ASP | 3.0 |
| 5 | F | 155 | LEU | 3.0 |
| 2 | B | 895 | ASP | 3.0 |
| 3 | C | 215 | GLU | 2.9 |
| 1 | A | 1400 | CYS | 2.9 |
| 1 | A | 1174 | PHE | 2.9 |
| 6 | H | 127 | GLY | 2.9 |
| 10 | L | 62 | LYS | 2.8 |
| 2 | B | 135 | ARG | 2.8 |
| 2 | B | 1183 | LYS | 2.8 |
| 1 | A | 247 | ARG | 2.7 |
| 2 | B | 1189 | ILE | 2.7 |
| 1 | A | 305 | ASP | 2.7 |
| 1 | A | 307 | ASP | 2.7 |
| 1 | A | 60 | SER | 2.7 |
| 2 | B | 465 | ASN | 2.7 |
| 7 | I | 120 | GLN | 2.7 |
| 6 | H | 62 | SER | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 336 | ILE | 2.7 |
| 1 | A | 72 | GLU | 2.7 |
| 2 | B | 106 | ASP | 2.6 |
| 2 | B | 875 | GLU | 2.6 |
| 2 | B | 426 | LYS | 2.6 |
| 1 | A | 129 | LYS | 2.6 |
| 2 | B | 1181 | GLU | 2.6 |
| 4 | E | 130 | ALA | 2.6 |
| 1 | A | 1094 | VAL | 2.6 |
| 6 | H | 110 | ASP | 2.6 |
| 1 | A | 36 | ARG | 2.6 |
| 6 | H | 108 | SER | 2.6 |
| 1 | A | 196 | GLU | 2.5 |
| 2 | B | 429 | PHE | 2.5 |
| 2 | B | 723 | VAL | 2.5 |
| 2 | B | 876 | LYS | 2.5 |
| 2 | B | 887 | HIS | 2.5 |
| 2 | B | 1222 | ARG | 2.5 |
| 1 | A | 1222 | ASN | 2.5 |
| 6 | H | 111 | LEU | 2.5 |
| 1 | A | 1256 | GLU | 2.4 |
| 6 | H | 138 | GLU | 2.4 |
| 1 | A | 1188 | GLN | 2.4 |
| 2 | B | 245 | GLU | 2.4 |
| 1 | A | 1449 | SER | 2.4 |
| 6 | H | 133 | ASN | 2.4 |
| 2 | B | 1176 | ASN | 2.4 |
| 6 | H | 13 | SER | 2.3 |
| 4 | E | 7 | ARG | 2.3 |
| 2 | B | 935 | ARG | 2.3 |
| 10 | L | 33 | GLU | 2.3 |
| 6 | H | 130 | ARG | 2.3 |
| 6 | H | 76 | THR | 2.3 |
| 6 | H | 89 | LEU | 2.3 |
| 2 | B | 263 | GLY | 2.3 |
| 1 | A | 1359 | ASP | 2.2 |
| 10 | L | 40 | LEU | 2.2 |
| 5 | F | 72 | LYS | 2.2 |
| 10 | L | 49 | LYS | 2.2 |
| 2 | B | 264 | SER | 2.2 |
| 9 | K | 54 | ARG | 2.2 |
| 4 | E | 51 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 39 | GLU | 2.2 |
| 4 | E | 114 | ASN | 2.2 |
| 2 | B | 1172 | ILE | 2.2 |
| 1 | A | 6 | TYR | 2.2 |
| 2 | B | 864 | LYS | 2.2 |
| 3 | C | 216 | GLY | 2.2 |
| 1 | A | 1203 | ASN | 2.2 |
| 6 | H | 126 | GLU | 2.2 |
| 10 | L | 41 | SER | 2.2 |
| 1 | A | 280 | GLU | 2.2 |
| 2 | B | 646 | LEU | 2.1 |
| 6 | H | 128 | ASN | 2.1 |
| 2 | B | 1186 | ASP | 2.1 |
| 2 | B | 959 | ASP | 2.1 |
| 6 | H | 32 | THR | 2.1 |
| 6 | H | 109 | LYS | 2.1 |
| 2 | B | 66 | ASP | 2.1 |
| 9 | K | 14 | GLU | 2.0 |
| 10 | L | 53 | HIS | 2.0 |
| 2 | B | 963 | PHE | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 11 | ILX | M | 1 | 10/11 | 0.84 | 0.33 | - | 72,74,79,80 | 0 |
| 11 | CSX | M | 6 | 7/8 | 0.74 | 0.24 | - | 80,82,84,86 | 0 |
| 11 | HYP | M | 8 | 8/9 | 0.91 | 0.20 | - | 70,72,72,73 | 0 |
| 11 | TRX | M | 2 | 15/16 | 0.88 | 0.23 | - | 75,77,79,80 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 12 | ZN | C | 3002 | 1/1 | 0.99 | 0.09 | -1.29 | 49,49,49,49 | 0 |
| 12 | ZN | B | 3007 | 1/1 | 0.99 | 0.07 | -1.32 | 64,64,64,64 | 0 |
| 12 | ZN | I | 3004 | 1/1 | 0.96 | 0.07 | -1.65 | 62,62,62,62 | 0 |
| 12 | ZN | J | 3001 | 1/1 | 0.99 | 0.12 | -1.68 | 46,46,46,46 | 0 |
| 12 | ZN | L | 3005 | 1/1 | 0.89 | 0.06 | -1.69 | 86,86,86,86 | 0 |
| 12 | ZN | A | 3008 | 1/1 | 0.97 | 0.12 | -1.73 | 81,81,81,81 | 0 |
| 12 | ZN | A | 3006 | 1/1 | 0.98 | 0.10 | -2.19 | 64,64,64,64 | 0 |
| 12 | ZN | I | 3003 | 1/1 | 0.99 | 0.08 | -2.42 | 45,45,45,45 | 0 |
| 13 | MN | A | 3009 | 1/1 | 0.72 | 0.34 | - | 149,149,149,149 | 0 |

6.5 Other polymers

There are no such residues in this entry.