



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 08:49 AM EDT

PDB ID : 2A0F
Title : Structure of D236A mutant E. coli Aspartate Transcarbamoylase in presence of Phosphonoacetamide at 2.90 Å resolution
Authors : Stieglitz, K.A.; Dusinger, K.J.; Cardia, J.P.; Tsuruta, H.; Kantrowitz, E.R.
Deposited on : 2005-06-16
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

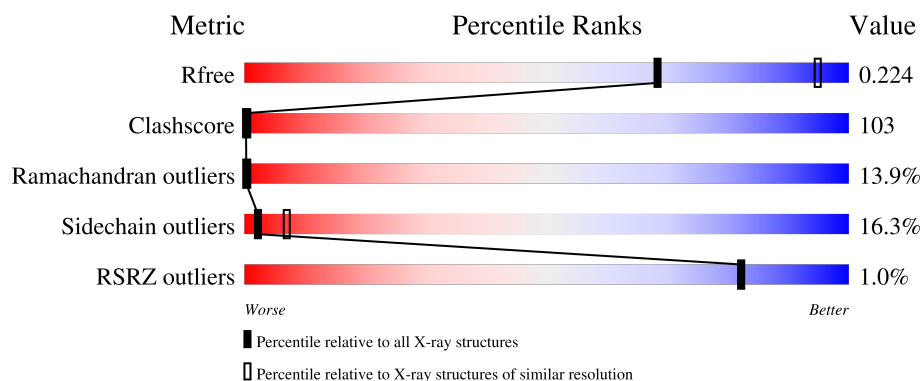
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

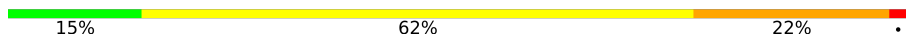

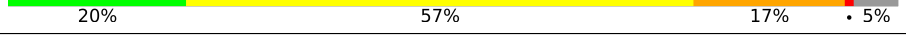

The reported resolution of this entry is 2.90 Å.

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} | 130704 | 1957 (2.90-2.90) |
| Clashscore | 141614 | 2172 (2.90-2.90) |
| Ramachandran outliers | 138981 | 2115 (2.90-2.90) |
| Sidechain outliers | 138945 | 2117 (2.90-2.90) |
| RSRZ outliers | 127900 | 1906 (2.90-2.90) |

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 310 |  15% 62% 22% • |
| 1 | C | 310 |  15% 61% 22% • |
| 2 | B | 153 |  20% 57% 17% • 5% |
| 2 | D | 153 |  12% 62% 19% • 5% |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7489 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 Aspartate carbamoyltransferase catalytic chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2412 | 1526 | 423 | 454 | 9 | | | |
| 1 | C | 310 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2412 | 1526 | 423 | 454 | 9 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 236 | ALA | ASP | engineered mutation | UNP P0A786 |
| C | 236 | ALA | ASP | engineered mutation | UNP P0A786 |

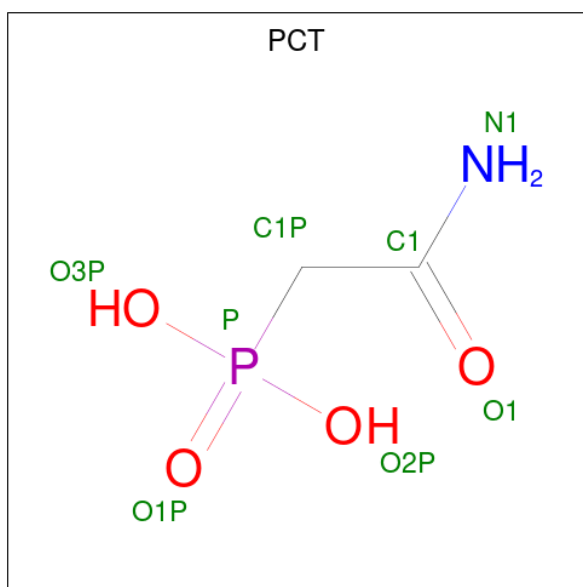
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1138 | 714 | 201 | 218 | 5 | | | |
| 2 | D | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1138 | 714 | 201 | 218 | 5 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| B | 1 | MET | - | initiating methionine | UNP P0A7F3 |
| D | 1 | MET | - | initiating methionine | UNP P0A7F3 |

- Molecule 3 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula: C₂H₆NO₄P).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 8 | 2 | 1 | 4 | 1 | | |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4 | B | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | D | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

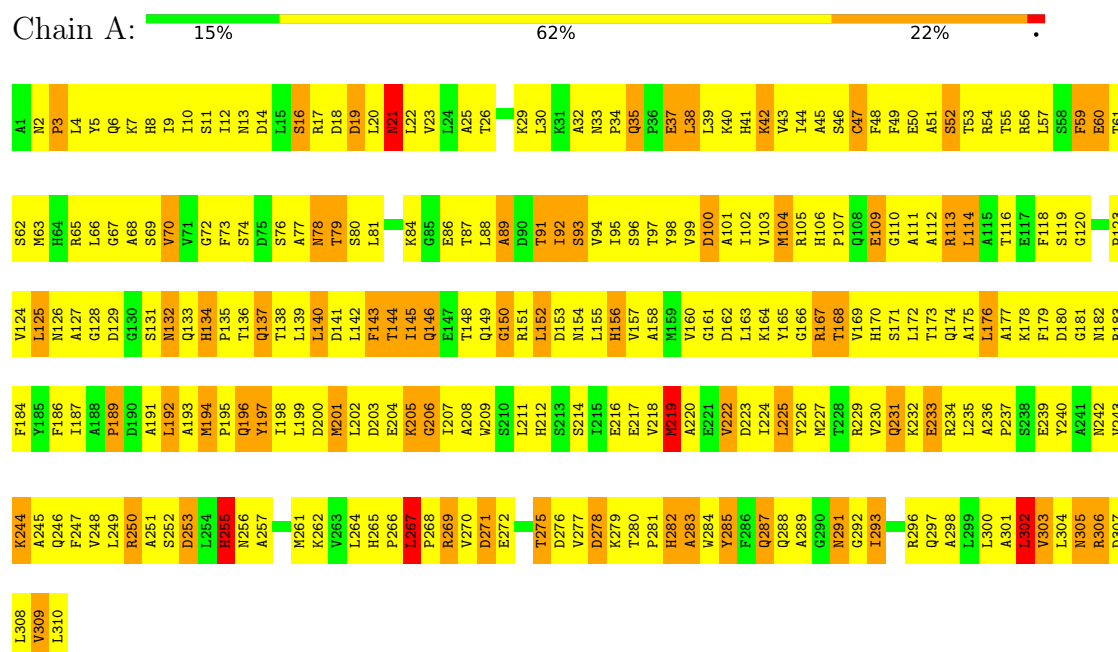
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5 | A | 130 | Total | O | 0 | 0 |
| | | | 130 | 130 | | |
| 5 | B | 82 | Total | O | 0 | 0 |
| | | | 82 | 82 | | |
| 5 | C | 110 | Total | O | 0 | 0 |
| | | | 110 | 110 | | |
| 5 | D | 57 | Total | O | 0 | 0 |
| | | | 57 | 57 | | |

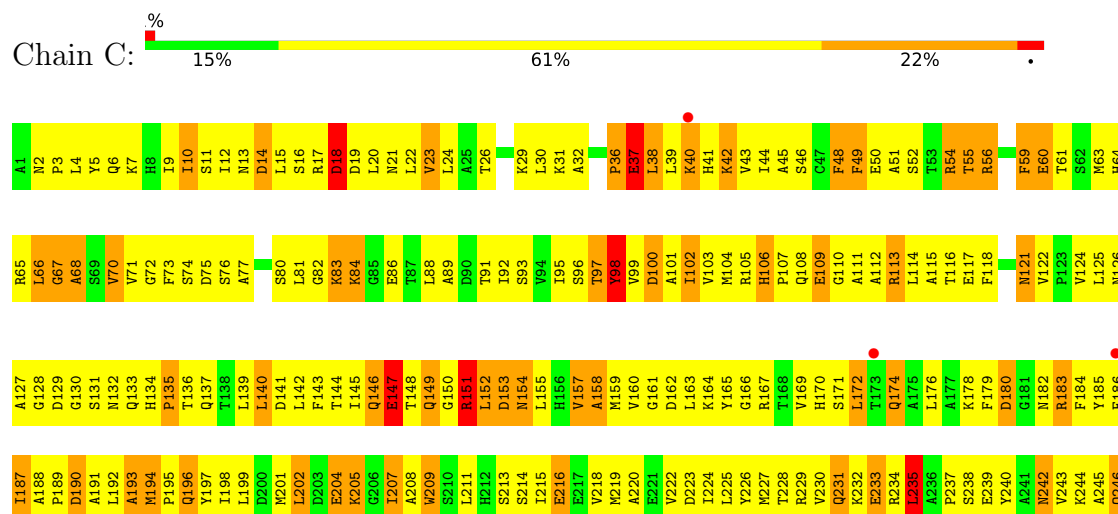
3 Residue-property plots

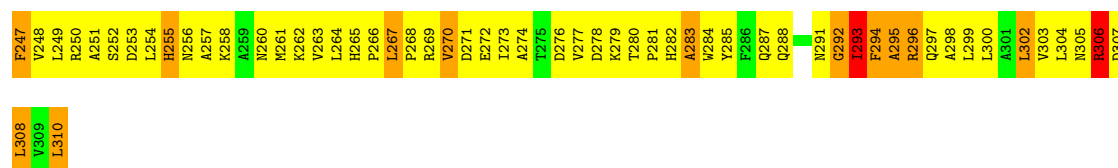
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Aspartate carbamoyltransferase catalytic chain

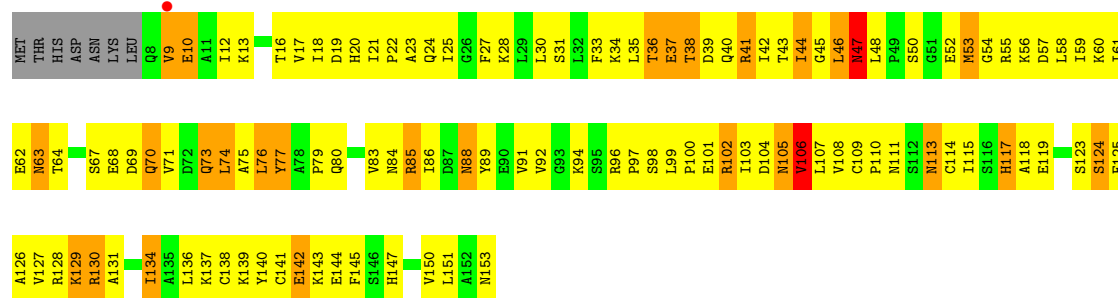


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

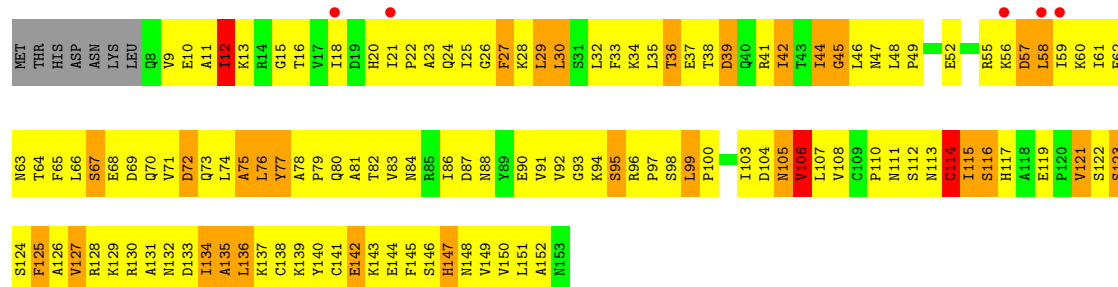
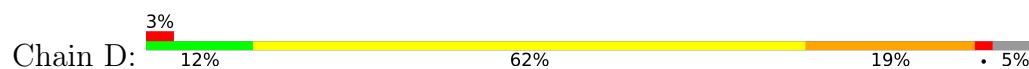




• Molecule 2: Aspartate carbamoyltransferase regulatory chain



• Molecule 2: Aspartate carbamoyltransferase regulatory chain



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 3 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 120.45Å 120.45Å 155.24Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 30.00 – 2.90 36.73 – 2.79 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (30.00-2.90) 80.8 (36.73-2.79) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.71 (at 2.81Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.217 , 0.279 0.209 , 0.224 | Depositor DCC |
| R_{free} test set | 2697 reflections (10.14%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 70.3 | Xtriage |
| Anisotropy | 0.131 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.22 , 122.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$ | Xtriage |
| Estimated twinning fraction | 0.427 for -h,-k,l | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 7489 | wwPDB-VP |
| Average B, all atoms (Å ²) | 76.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCT, ZN

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 | 0.62 | 1/2458 (0.0%) | 0.83 | 1/3335 (0.0%) |
| 1 | C | 0.53 | 3/2458 (0.1%) | 0.71 | 0/3335 |
| 2 | B | 0.52 | 0/1155 | 0.75 | 1/1561 (0.1%) |
| 2 | D | 0.44 | 0/1155 | 0.68 | 0/1561 |
| All | All | 0.55 | 4/7226 (0.1%) | 0.75 | 2/9792 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | C | 60 | GLU | CD-OE2 | 7.41 | 1.33 | 1.25 |
| 1 | A | 60 | GLU | CD-OE2 | 6.51 | 1.32 | 1.25 |
| 1 | C | 147 | GLU | CG-CD | 5.70 | 1.60 | 1.51 |
| 1 | C | 147 | GLU | CD-OE1 | 5.10 | 1.31 | 1.25 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 140 | LEU | CA-CB-CG | 6.34 | 129.88 | 115.30 |
| 2 | B | 74 | LEU | CA-CB-CG | -5.01 | 103.78 | 115.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 98 | TYR | Sidechain |

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 | 2412 | 0 | 2423 | 452 | 0 |
| 1 | C | 2412 | 0 | 2423 | 578 | 0 |
| 2 | B | 1138 | 0 | 1152 | 209 | 0 |
| 2 | D | 1138 | 0 | 1154 | 295 | 0 |
| 3 | A | 8 | 0 | 4 | 3 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 130 | 0 | 0 | 22 | 0 |
| 5 | B | 82 | 0 | 0 | 18 | 0 |
| 5 | C | 110 | 0 | 0 | 32 | 0 |
| 5 | D | 57 | 0 | 0 | 3 | 0 |
| All | All | 7489 | 0 | 7156 | 1476 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 103.

All (1476) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:111:ASN:HD22 | 2:D:114:CYS:HB2 | 1.07 | 1.16 |
| 1:A:158:ALA:HB2 | 1:A:222:VAL:HG11 | 1.26 | 1.11 |
| 2:D:82:THR:HA | 2:D:96:ARG:HH12 | 1.11 | 1.08 |
| 2:B:44:ILE:HG23 | 2:D:44:ILE:HB | 1.37 | 1.06 |
| 2:D:20:HIS:HB3 | 2:D:80:GLN:HG2 | 1.37 | 1.05 |
| 1:C:270:VAL:HG13 | 1:C:271:ASP:H | 1.20 | 1.04 |
| 2:B:75:ALA:HB1 | 2:B:99:LEU:HD12 | 1.36 | 1.03 |
| 1:C:249:LEU:HG | 1:C:254:LEU:HD11 | 1.40 | 1.02 |
| 1:C:26:THR:O | 1:C:30:LEU:HG | 1.58 | 1.02 |
| 1:A:229:ARG:HH21 | 1:A:270:VAL:HG21 | 1.22 | 1.02 |
| 1:C:20:LEU:H | 1:C:20:LEU:HD12 | 1.23 | 1.02 |
| 1:A:164:LYS:HA | 1:A:195:PRO:HD3 | 1.42 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:76:LEU:H | 2:B:76:LEU:HD23 | 1.23 | 1.01 |
| 2:D:74:LEU:HG | 2:D:97:PRO:HB3 | 1.40 | 1.00 |
| 1:C:12:ILE:HD11 | 1:C:135:PRO:HA | 1.43 | 1.00 |
| 1:A:189:PRO:HG2 | 1:A:192:LEU:HD12 | 1.42 | 0.99 |
| 1:C:219:MET:HB3 | 1:C:256:ASN:HD21 | 1.26 | 0.99 |
| 2:D:103:ILE:HB | 2:D:125:PHE:H | 1.26 | 0.99 |
| 2:D:146:SER:HB2 | 2:D:148:ASN:HD22 | 1.28 | 0.98 |
| 1:A:216:GLU:O | 1:A:219:MET:HB2 | 1.61 | 0.98 |
| 1:C:9:ILE:HB | 1:C:125:LEU:HA | 1.43 | 0.97 |
| 1:C:139:LEU:HA | 1:C:142:LEU:HD12 | 1.42 | 0.97 |
| 1:C:60:GLU:HA | 1:C:63:MET:SD | 2.05 | 0.97 |
| 1:C:264:LEU:HD12 | 1:C:288:GLN:HB2 | 1.46 | 0.97 |
| 2:D:111:ASN:ND2 | 2:D:114:CYS:HB2 | 1.79 | 0.97 |
| 2:B:43:THR:HA | 2:D:45:GLY:HA2 | 1.44 | 0.97 |
| 1:A:145:ILE:HG23 | 1:A:224:ILE:HD12 | 1.44 | 0.97 |
| 1:A:3:PRO:HD2 | 1:A:22:LEU:HD21 | 1.44 | 0.96 |
| 2:D:46:LEU:HD23 | 2:D:46:LEU:H | 1.29 | 0.96 |
| 1:A:8:HIS:CD2 | 1:A:123:PRO:HA | 2.01 | 0.96 |
| 1:A:219:MET:HB3 | 1:A:256:ASN:HD21 | 1.30 | 0.96 |
| 1:C:199:LEU:HA | 1:C:202:LEU:HD21 | 1.48 | 0.95 |
| 1:C:121:ASN:H | 1:C:121:ASN:HD22 | 1.15 | 0.94 |
| 1:A:267:LEU:HD23 | 1:A:268:PRO:HA | 1.47 | 0.93 |
| 1:C:237:PRO:HA | 1:C:240:TYR:CE2 | 2.03 | 0.93 |
| 1:A:52:SER:OG | 1:A:55:THR:HG22 | 1.69 | 0.92 |
| 2:D:137:LYS:HA | 2:D:144:GLU:HA | 1.50 | 0.92 |
| 1:C:55:THR:O | 1:C:59:PHE:HB2 | 1.70 | 0.91 |
| 2:D:82:THR:HA | 2:D:96:ARG:NH1 | 1.85 | 0.91 |
| 1:A:109:GLU:HB3 | 2:B:141:CYS:HB3 | 1.52 | 0.91 |
| 1:C:219:MET:HB3 | 1:C:256:ASN:ND2 | 1.84 | 0.91 |
| 1:C:92:ILE:HG21 | 1:C:115:ALA:O | 1.71 | 0.91 |
| 1:C:92:ILE:HG13 | 1:C:115:ALA:HA | 1.51 | 0.90 |
| 1:C:237:PRO:HA | 1:C:240:TYR:CZ | 2.07 | 0.90 |
| 1:C:169:VAL:HA | 1:C:172:LEU:HD13 | 1.53 | 0.90 |
| 2:B:102:ARG:HB3 | 2:B:126:ALA:HA | 1.53 | 0.90 |
| 1:C:19:ASP:O | 1:C:22:LEU:HB3 | 1.72 | 0.90 |
| 2:D:76:LEU:HB3 | 2:D:134:ILE:HG21 | 1.51 | 0.90 |
| 1:A:91:THR:O | 1:A:95:ILE:HG12 | 1.70 | 0.89 |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:N | 1.87 | 0.89 |
| 1:C:169:VAL:HB | 1:C:172:LEU:HD22 | 1.53 | 0.88 |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:HB | 1.52 | 0.88 |
| 1:C:118:PHE:HB2 | 5:C:329:HOH:O | 1.73 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:59:PHE:O | 1:C:63:MET:HG3 | 1.74 | 0.88 |
| 1:C:152:LEU:H | 1:C:152:LEU:HD12 | 1.37 | 0.88 |
| 2:B:41:ARG:HG3 | 2:D:48:LEU:HD22 | 1.56 | 0.87 |
| 1:C:109:GLU:HB2 | 2:D:141:CYS:SG | 2.13 | 0.87 |
| 2:D:111:ASN:ND2 | 2:D:114:CYS:H | 1.72 | 0.87 |
| 1:C:151:ARG:HH11 | 1:C:155:LEU:HD11 | 1.39 | 0.87 |
| 1:A:219:MET:HB3 | 1:A:256:ASN:ND2 | 1.89 | 0.87 |
| 2:B:27:PHE:N | 2:B:46:LEU:HD21 | 1.90 | 0.87 |
| 1:A:48:PHE:HE2 | 1:A:55:THR:HG23 | 1.38 | 0.86 |
| 1:C:228:THR:HA | 1:C:266:PRO:HG2 | 1.57 | 0.86 |
| 2:D:78:ALA:HB3 | 2:D:81:ALA:HB2 | 1.58 | 0.86 |
| 1:C:285:TYR:HA | 1:C:288:GLN:OE1 | 1.76 | 0.86 |
| 1:C:121:ASN:HD22 | 1:C:121:ASN:N | 1.69 | 0.86 |
| 1:A:94:VAL:HG23 | 1:A:95:ILE:HD13 | 1.57 | 0.85 |
| 1:C:157:VAL:HG12 | 1:C:158:ALA:H | 1.41 | 0.85 |
| 1:A:200:ASP:O | 1:A:203:ASP:HB2 | 1.75 | 0.85 |
| 2:B:21:ILE:HB | 2:B:57:ASP:HB2 | 1.58 | 0.85 |
| 2:B:41:ARG:HA | 2:D:47:ASN:HB2 | 1.57 | 0.85 |
| 2:D:56:LYS:HD2 | 2:D:57:ASP:N | 1.92 | 0.84 |
| 2:D:42:ILE:HA | 2:D:60:LYS:O | 1.76 | 0.84 |
| 1:C:207:ILE:HG13 | 1:C:208:ALA:H | 1.38 | 0.84 |
| 1:C:248:VAL:HG12 | 1:C:249:LEU:H | 1.43 | 0.84 |
| 1:C:109:GLU:HB3 | 5:C:419:HOH:O | 1.77 | 0.84 |
| 1:A:183:ARG:HH21 | 1:A:183:ARG:HG3 | 1.43 | 0.83 |
| 1:C:104:MET:SD | 1:C:112:ALA:HA | 2.17 | 0.83 |
| 1:A:51:ALA:O | 1:A:52:SER:HB2 | 1.76 | 0.83 |
| 1:A:54:ARG:HB2 | 3:A:1311:PCT:O3P | 1.79 | 0.83 |
| 1:C:13:ASN:N | 1:C:174:GLN:HE22 | 1.75 | 0.83 |
| 2:D:82:THR:CA | 2:D:96:ARG:HH12 | 1.92 | 0.83 |
| 1:A:92:ILE:HG22 | 1:A:93:SER:N | 1.94 | 0.83 |
| 1:C:264:LEU:HB3 | 1:C:288:GLN:CD | 1.99 | 0.82 |
| 2:D:29:LEU:C | 2:D:30:LEU:HD13 | 2.00 | 0.82 |
| 2:D:138:CYS:SG | 2:D:141:CYS:HB2 | 2.19 | 0.82 |
| 2:B:70:GLN:H | 2:B:70:GLN:NE2 | 1.77 | 0.82 |
| 1:C:183:ARG:HE | 1:C:208:ALA:HB1 | 1.44 | 0.82 |
| 1:A:8:HIS:ND1 | 1:A:116:THR:HG22 | 1.95 | 0.81 |
| 1:C:64:HIS:CD2 | 1:C:70:VAL:HG23 | 2.14 | 0.81 |
| 1:C:109:GLU:OE1 | 1:C:132:ASN:HB2 | 1.81 | 0.81 |
| 1:A:10:ILE:HG13 | 1:A:11:SER:N | 1.95 | 0.81 |
| 1:A:138:THR:HG23 | 1:A:172:LEU:HA | 1.63 | 0.81 |
| 2:B:137:LYS:HA | 2:B:144:GLU:HA | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:164:LYS:HB2 | 1:C:192:LEU:HA | 1.62 | 0.81 |
| 1:C:264:LEU:HD11 | 1:C:284:TRP:HB3 | 1.63 | 0.81 |
| 2:D:104:ASP:O | 2:D:106:VAL:HG23 | 1.82 | 0.80 |
| 1:A:116:THR:HA | 1:A:119:SER:OG | 1.82 | 0.80 |
| 2:B:70:GLN:H | 2:B:70:GLN:HE21 | 1.29 | 0.80 |
| 1:A:243:VAL:HG13 | 1:A:244:LYS:H | 1.47 | 0.80 |
| 1:C:91:THR:O | 1:C:95:ILE:HG13 | 1.82 | 0.79 |
| 2:D:20:HIS:HB3 | 2:D:80:GLN:CG | 2.12 | 0.79 |
| 1:C:142:LEU:HD23 | 1:C:145:ILE:CD1 | 2.12 | 0.79 |
| 2:B:141:CYS:O | 2:B:143:LYS:HG2 | 1.82 | 0.79 |
| 1:C:96:SER:O | 1:C:122:VAL:HG11 | 1.83 | 0.79 |
| 2:D:146:SER:HB2 | 2:D:148:ASN:ND2 | 1.97 | 0.79 |
| 1:C:218:VAL:O | 1:C:222:VAL:HG13 | 1.82 | 0.79 |
| 1:C:48:PHE:HZ | 1:C:52:SER:H | 1.30 | 0.79 |
| 1:A:3:PRO:CD | 1:A:22:LEU:HD21 | 2.13 | 0.79 |
| 2:B:39:ASP:HA | 2:D:55:ARG:HH22 | 1.47 | 0.79 |
| 1:C:124:VAL:HG12 | 1:C:125:LEU:N | 1.97 | 0.78 |
| 1:C:225:LEU:HB2 | 1:C:261:MET:SD | 2.24 | 0.78 |
| 1:A:229:ARG:NH2 | 1:A:270:VAL:HG21 | 1.98 | 0.78 |
| 2:D:126:ALA:O | 2:D:127:VAL:HG13 | 1.83 | 0.78 |
| 1:A:80:SER:O | 1:A:84:LYS:HB2 | 1.82 | 0.78 |
| 1:A:109:GLU:OE1 | 2:B:113:ASN:ND2 | 2.17 | 0.78 |
| 1:C:108:GLN:NE2 | 2:D:115:ILE:HD12 | 1.99 | 0.78 |
| 1:A:20:LEU:HD12 | 1:A:179:PHE:HZ | 1.46 | 0.78 |
| 1:C:132:ASN:OD1 | 2:D:143:LYS:NZ | 2.16 | 0.78 |
| 2:B:141:CYS:O | 2:B:143:LYS:N | 2.17 | 0.77 |
| 1:C:105:ARG:HH11 | 1:C:167:ARG:HH12 | 1.29 | 0.77 |
| 2:D:15:GLY:HA2 | 2:D:64:THR:O | 1.85 | 0.77 |
| 2:B:69:ASP:O | 2:B:73:GLN:HG3 | 1.83 | 0.77 |
| 1:C:183:ARG:HA | 1:C:208:ALA:HB3 | 1.66 | 0.77 |
| 2:B:30:LEU:HG | 2:D:27:PHE:CZ | 2.19 | 0.77 |
| 2:D:96:ARG:HG3 | 2:D:97:PRO:HD2 | 1.65 | 0.77 |
| 1:A:105:ARG:HB2 | 1:A:127:ALA:HB3 | 1.64 | 0.77 |
| 1:A:287:GLN:HE21 | 1:A:287:GLN:N | 1.82 | 0.77 |
| 1:A:302:LEU:HD23 | 1:A:302:LEU:H | 1.50 | 0.77 |
| 1:A:81:LEU:HG | 1:A:86:GLU:O | 1.85 | 0.77 |
| 1:C:171:SER:O | 1:C:174:GLN:HG3 | 1.85 | 0.77 |
| 2:B:44:ILE:HD11 | 2:B:46:LEU:HD23 | 1.65 | 0.77 |
| 1:C:264:LEU:CD1 | 1:C:284:TRP:HB3 | 2.14 | 0.77 |
| 1:C:160:VAL:HG12 | 1:C:161:GLY:H | 1.50 | 0.77 |
| 2:D:41:ARG:HB3 | 2:D:62:GLU:HB2 | 1.67 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:36:THR:HB | 2:D:27:PHE:CD2 | 2.20 | 0.77 |
| 1:C:264:LEU:HD12 | 1:C:288:GLN:CB | 2.15 | 0.77 |
| 1:A:38:LEU:HD23 | 1:A:38:LEU:O | 1.84 | 0.76 |
| 1:C:43:VAL:HG12 | 1:C:99:VAL:HG12 | 1.67 | 0.76 |
| 1:A:61:THR:HG22 | 1:A:65:ARG:HD2 | 1.67 | 0.76 |
| 2:B:30:LEU:HG | 2:D:27:PHE:HZ | 1.47 | 0.76 |
| 1:C:56:ARG:HG2 | 1:C:56:ARG:NH2 | 1.99 | 0.76 |
| 1:C:44:ILE:HG13 | 1:C:101:ALA:HB3 | 1.68 | 0.76 |
| 1:C:56:ARG:HG2 | 1:C:56:ARG:HH21 | 1.50 | 0.76 |
| 1:C:146:GLN:HA | 1:C:150:GLY:HA2 | 1.68 | 0.76 |
| 1:C:45:ALA:HB2 | 1:C:99:VAL:HG11 | 1.66 | 0.76 |
| 1:A:156:HIS:ND1 | 1:A:156:HIS:N | 2.31 | 0.75 |
| 1:A:26:THR:HA | 1:A:29:LYS:HE3 | 1.68 | 0.75 |
| 1:A:109:GLU:HG3 | 1:A:132:ASN:HB2 | 1.67 | 0.75 |
| 1:C:142:LEU:HD23 | 1:C:145:ILE:HD11 | 1.68 | 0.75 |
| 2:D:24:GLN:NE2 | 2:D:47:ASN:HD21 | 1.85 | 0.75 |
| 1:C:159:MET:CE | 1:C:172:LEU:HD23 | 2.16 | 0.75 |
| 1:A:43:VAL:HA | 1:A:69:SER:O | 1.85 | 0.75 |
| 2:B:34:LYS:HB3 | 2:B:37:GLU:HB2 | 1.69 | 0.75 |
| 5:B:204:HOH:O | 2:D:39:ASP:HA | 1.85 | 0.75 |
| 2:D:62:GLU:HG2 | 2:D:63:ASN:ND2 | 2.02 | 0.75 |
| 2:D:119:GLU:O | 2:D:121:VAL:HG13 | 1.86 | 0.75 |
| 1:A:166:GLY:HA2 | 1:A:231:GLN:NE2 | 2.01 | 0.75 |
| 2:B:76:LEU:H | 2:B:76:LEU:CD2 | 2.00 | 0.75 |
| 1:A:2:ASN:CG | 1:A:5:TYR:HB2 | 2.08 | 0.74 |
| 1:A:81:LEU:O | 1:A:81:LEU:HD23 | 1.86 | 0.74 |
| 1:C:20:LEU:C | 1:C:24:LEU:HG | 2.07 | 0.74 |
| 1:C:132:ASN:HA | 1:C:170:HIS:ND1 | 2.01 | 0.74 |
| 1:C:214:SER:HB2 | 1:C:216:GLU:HG3 | 1.69 | 0.74 |
| 1:A:267:LEU:CD2 | 1:A:268:PRO:HA | 2.16 | 0.74 |
| 2:B:45:GLY:HA3 | 2:B:48:LEU:HD11 | 1.68 | 0.74 |
| 2:B:75:ALA:CB | 2:B:99:LEU:HD12 | 2.16 | 0.74 |
| 1:C:149:GLN:HB2 | 5:C:326:HOH:O | 1.87 | 0.74 |
| 1:C:270:VAL:HG13 | 1:C:271:ASP:N | 2.01 | 0.74 |
| 1:A:48:PHE:CE2 | 1:A:55:THR:HG23 | 2.22 | 0.74 |
| 1:C:245:ALA:HB2 | 1:C:272:GLU:OE1 | 1.87 | 0.74 |
| 2:D:41:ARG:HB3 | 2:D:62:GLU:CB | 2.17 | 0.74 |
| 1:C:152:LEU:HD12 | 1:C:152:LEU:N | 2.03 | 0.74 |
| 2:B:42:ILE:HB | 2:D:46:LEU:HD21 | 1.70 | 0.74 |
| 1:C:228:THR:HA | 1:C:266:PRO:CG | 2.18 | 0.74 |
| 1:A:231:GLN:HB3 | 1:A:234:ARG:HB2 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:174:GLN:O | 1:C:178:LYS:HE2 | 1.87 | 0.73 |
| 1:A:2:ASN:ND2 | 1:A:5:TYR:HB2 | 2.03 | 0.73 |
| 1:A:59:PHE:HE2 | 1:A:300:LEU:HD21 | 1.54 | 0.73 |
| 1:A:269:ARG:HH12 | 1:A:275:THR:HA | 1.53 | 0.73 |
| 1:C:146:GLN:HA | 1:C:150:GLY:CA | 2.18 | 0.73 |
| 1:C:187:ILE:HD13 | 1:C:215:ILE:CD1 | 2.19 | 0.73 |
| 1:C:296:ARG:C | 1:C:300:LEU:HG | 2.09 | 0.73 |
| 2:D:148:ASN:O | 2:D:152:ALA:HB2 | 1.87 | 0.73 |
| 2:B:30:LEU:HD22 | 2:B:44:ILE:CD1 | 2.18 | 0.73 |
| 2:D:138:CYS:HB3 | 2:D:143:LYS:H | 1.53 | 0.73 |
| 1:C:249:LEU:HG | 1:C:254:LEU:CD1 | 2.17 | 0.73 |
| 1:A:4:LEU:HD12 | 1:A:302:LEU:HD12 | 1.70 | 0.72 |
| 1:A:141:ASP:O | 1:A:145:ILE:HG12 | 1.88 | 0.72 |
| 1:A:155:LEU:HD22 | 1:A:223:ASP:CG | 2.10 | 0.72 |
| 2:B:44:ILE:HG23 | 2:D:44:ILE:CB | 2.16 | 0.72 |
| 1:C:308:LEU:HD13 | 1:C:308:LEU:O | 1.89 | 0.72 |
| 1:A:237:PRO:HA | 1:A:240:TYR:CD1 | 2.24 | 0.72 |
| 1:C:287:GLN:H | 1:C:287:GLN:NE2 | 1.86 | 0.72 |
| 1:A:8:HIS:NE2 | 1:A:123:PRO:HA | 2.03 | 0.72 |
| 1:C:44:ILE:CG1 | 1:C:101:ALA:HB3 | 2.20 | 0.72 |
| 1:C:151:ARG:HH11 | 1:C:155:LEU:CD1 | 2.03 | 0.72 |
| 1:C:158:ALA:HA | 1:C:185:TYR:O | 1.89 | 0.72 |
| 1:C:227:MET:O | 1:C:266:PRO:HD3 | 1.89 | 0.72 |
| 1:C:245:ALA:HB1 | 5:C:338:HOH:O | 1.90 | 0.72 |
| 1:C:310:LEU:N | 1:C:310:LEU:HD12 | 2.05 | 0.72 |
| 1:C:169:VAL:CA | 1:C:172:LEU:HD13 | 2.20 | 0.71 |
| 1:C:296:ARG:O | 1:C:300:LEU:HG | 1.90 | 0.71 |
| 2:D:135:ALA:HB1 | 2:D:145:PHE:O | 1.89 | 0.71 |
| 1:C:226:TYR:CZ | 1:C:266:PRO:HG3 | 2.24 | 0.71 |
| 1:C:66:LEU:HD11 | 1:C:297:GLN:HA | 1.73 | 0.71 |
| 2:D:74:LEU:CG | 2:D:97:PRO:HB3 | 2.18 | 0.71 |
| 1:A:26:THR:HA | 1:A:29:LYS:CE | 2.21 | 0.71 |
| 1:C:163:LEU:HG | 1:C:188:ALA:HB2 | 1.71 | 0.71 |
| 2:B:85:ARG:NH2 | 2:B:85:ARG:HB2 | 2.05 | 0.71 |
| 2:D:29:LEU:O | 2:D:30:LEU:HD13 | 1.90 | 0.71 |
| 1:A:165:TYR:HE2 | 1:A:235:LEU:HD23 | 1.55 | 0.71 |
| 1:C:285:TYR:HA | 1:C:288:GLN:HB3 | 1.69 | 0.71 |
| 1:C:105:ARG:NH1 | 1:C:167:ARG:HH12 | 1.89 | 0.71 |
| 1:A:216:GLU:OE2 | 1:A:253:ASP:HA | 1.89 | 0.71 |
| 1:A:280:THR:HB | 1:A:281:PRO:CD | 2.21 | 0.71 |
| 1:A:288:GLN:O | 1:A:288:GLN:HG2 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:99:LEU:CD1 | 2:D:129:LYS:HE3 | 2.21 | 0.71 |
| 1:C:218:VAL:O | 1:C:218:VAL:HG12 | 1.91 | 0.70 |
| 1:C:164:LYS:HD3 | 1:C:191:ALA:O | 1.91 | 0.70 |
| 1:C:20:LEU:O | 1:C:24:LEU:HG | 1.91 | 0.70 |
| 1:C:134:HIS:CE1 | 1:C:137:GLN:HB2 | 2.27 | 0.70 |
| 1:C:139:LEU:CA | 1:C:142:LEU:HD12 | 2.21 | 0.70 |
| 1:C:160:VAL:HG12 | 1:C:161:GLY:N | 2.05 | 0.70 |
| 2:D:128:ARG:O | 2:D:130:ARG:HG3 | 1.91 | 0.70 |
| 1:A:229:ARG:HH21 | 1:A:270:VAL:CG2 | 2.01 | 0.70 |
| 1:A:128:GLY:HA2 | 1:A:133:GLN:O | 1.91 | 0.70 |
| 1:A:164:LYS:HA | 1:A:195:PRO:CD | 2.20 | 0.70 |
| 1:A:187:ILE:N | 1:A:187:ILE:HD12 | 2.07 | 0.70 |
| 1:A:230:VAL:O | 1:A:232:LYS:N | 2.24 | 0.70 |
| 1:C:142:LEU:HA | 1:C:145:ILE:CD1 | 2.22 | 0.70 |
| 1:A:267:LEU:HD23 | 1:A:269:ARG:H | 1.55 | 0.69 |
| 1:A:287:GLN:NE2 | 1:A:287:GLN:H | 1.90 | 0.69 |
| 1:C:111:ALA:O | 1:C:114:LEU:HB3 | 1.91 | 0.69 |
| 1:C:195:PRO:O | 1:C:199:LEU:HG | 1.91 | 0.69 |
| 1:C:30:LEU:HD12 | 1:C:298:ALA:HA | 1.74 | 0.69 |
| 1:C:222:VAL:HG21 | 1:C:225:LEU:HD13 | 1.75 | 0.69 |
| 2:D:138:CYS:O | 2:D:142:GLU:HA | 1.93 | 0.69 |
| 1:A:160:VAL:HG23 | 1:A:227:MET:SD | 2.32 | 0.69 |
| 2:B:46:LEU:O | 2:D:42:ILE:HG13 | 1.93 | 0.69 |
| 2:B:70:GLN:HA | 2:B:73:GLN:OE1 | 1.93 | 0.69 |
| 2:B:75:ALA:HB2 | 2:B:97:PRO:O | 1.92 | 0.69 |
| 1:C:133:GLN:O | 1:C:167:ARG:HB2 | 1.92 | 0.69 |
| 1:C:124:VAL:CG1 | 1:C:125:LEU:N | 2.55 | 0.69 |
| 1:A:2:ASN:HD22 | 1:A:306:ARG:CA | 2.06 | 0.69 |
| 1:C:50:GLU:OE2 | 1:C:107:PRO:HA | 1.93 | 0.69 |
| 1:A:9:ILE:HD13 | 1:A:125:LEU:HG | 1.74 | 0.69 |
| 1:C:11:SER:HA | 1:C:133:GLN:OE1 | 1.92 | 0.69 |
| 1:A:184:PHE:O | 1:A:209:TRP:HA | 1.93 | 0.69 |
| 2:B:70:GLN:HE21 | 2:B:70:GLN:N | 1.90 | 0.69 |
| 2:D:12:ILE:HD13 | 2:D:12:ILE:H | 1.58 | 0.69 |
| 2:D:105:ASN:HA | 2:D:123:SER:O | 1.92 | 0.69 |
| 1:C:169:VAL:HA | 1:C:172:LEU:CD1 | 2.23 | 0.68 |
| 1:C:228:THR:HA | 1:C:266:PRO:CD | 2.23 | 0.68 |
| 1:C:248:VAL:HG12 | 1:C:249:LEU:N | 2.07 | 0.68 |
| 1:A:153:ASP:OD1 | 1:A:179:PHE:HB3 | 1.92 | 0.68 |
| 1:C:112:ALA:C | 1:C:114:LEU:H | 1.97 | 0.68 |
| 1:C:132:ASN:N | 5:C:419:HOH:O | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:PHE:HB2 | 1:A:107:PRO:HD2 | 1.76 | 0.68 |
| 1:C:124:VAL:CG1 | 1:C:125:LEU:H | 2.06 | 0.68 |
| 1:A:2:ASN:ND2 | 1:A:306:ARG:HA | 2.09 | 0.68 |
| 1:A:8:HIS:CE1 | 1:A:116:THR:HG22 | 2.29 | 0.68 |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:HD13 | 1.76 | 0.68 |
| 1:A:202:LEU:HB3 | 1:A:207:ILE:HB | 1.75 | 0.68 |
| 1:A:255:HIS:CD2 | 1:A:255:HIS:H | 2.11 | 0.68 |
| 1:A:287:GLN:HE21 | 1:A:287:GLN:H | 1.42 | 0.68 |
| 1:C:9:ILE:HG21 | 1:C:125:LEU:HG | 1.76 | 0.68 |
| 1:A:47:CYS:HB3 | 1:A:73:PHE:CZ | 2.29 | 0.67 |
| 2:B:36:THR:HB | 2:D:27:PHE:CE2 | 2.28 | 0.67 |
| 2:B:41:ARG:HD3 | 2:D:48:LEU:HD13 | 1.76 | 0.67 |
| 1:C:43:VAL:C | 1:C:44:ILE:HD12 | 2.15 | 0.67 |
| 1:C:159:MET:O | 1:C:163:LEU:HD11 | 1.93 | 0.67 |
| 1:C:295:ALA:O | 1:C:297:GLN:N | 2.27 | 0.67 |
| 1:A:92:ILE:CG2 | 1:A:93:SER:N | 2.58 | 0.67 |
| 1:C:250:ARG:HB2 | 1:C:252:SER:OG | 1.94 | 0.67 |
| 1:A:45:ALA:HB1 | 1:A:47:CYS:SG | 2.35 | 0.67 |
| 1:C:42:LYS:HA | 1:C:100:ASP:OD1 | 1.94 | 0.67 |
| 1:C:262:LYS:HG3 | 1:C:282:HIS:HA | 1.77 | 0.67 |
| 1:C:269:ARG:HD3 | 1:C:273:ILE:H | 1.57 | 0.67 |
| 2:B:129:LYS:C | 2:B:129:LYS:HE3 | 2.15 | 0.67 |
| 2:D:66:LEU:HD22 | 2:D:83:VAL:HG21 | 1.77 | 0.67 |
| 1:C:17:ARG:HG3 | 1:C:18:ASP:H | 1.58 | 0.67 |
| 1:C:266:PRO:O | 1:C:267:LEU:HB2 | 1.94 | 0.67 |
| 2:B:84:ASN:O | 2:B:86:ILE:HG13 | 1.94 | 0.67 |
| 1:C:102:ILE:HD13 | 1:C:102:ILE:N | 2.09 | 0.67 |
| 1:A:201:MET:HG2 | 1:A:205:LYS:HD2 | 1.77 | 0.67 |
| 2:B:50:SER:HA | 2:B:56:LYS:HE2 | 1.75 | 0.67 |
| 1:C:160:VAL:HG12 | 5:C:338:HOH:O | 1.95 | 0.67 |
| 1:C:202:LEU:HA | 1:C:205:LYS:NZ | 2.10 | 0.67 |
| 1:C:223:ASP:C | 1:C:261:MET:HG2 | 2.16 | 0.67 |
| 1:A:29:LYS:HB2 | 1:A:29:LYS:HZ2 | 1.60 | 0.67 |
| 2:B:138:CYS:SG | 5:B:221:HOH:O | 2.53 | 0.67 |
| 1:A:110:GLY:HA2 | 1:A:129:ASP:OD1 | 1.96 | 0.66 |
| 2:B:69:ASP:HB3 | 2:B:70:GLN:HE21 | 1.59 | 0.66 |
| 1:C:20:LEU:H | 1:C:20:LEU:CD1 | 2.02 | 0.66 |
| 1:C:29:LYS:HD3 | 1:C:310:LEU:HB2 | 1.77 | 0.66 |
| 1:C:114:LEU:HD13 | 1:C:114:LEU:C | 2.15 | 0.66 |
| 2:B:62:GLU:C | 2:B:64:THR:H | 1.98 | 0.66 |
| 1:C:112:ALA:O | 1:C:114:LEU:N | 2.28 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:30:LEU:HD22 | 2:B:44:ILE:HD13 | 1.78 | 0.66 |
| 1:C:162:ASP:HB3 | 1:C:230:VAL:HA | 1.76 | 0.66 |
| 1:C:231:GLN:H | 1:C:231:GLN:NE2 | 1.93 | 0.66 |
| 2:D:34:LYS:HB3 | 2:D:37:GLU:OE1 | 1.95 | 0.66 |
| 1:C:222:VAL:HG23 | 1:C:261:MET:HG3 | 1.77 | 0.66 |
| 2:D:107:LEU:HD21 | 2:D:136:LEU:HD22 | 1.77 | 0.66 |
| 1:A:2:ASN:N | 1:A:306:ARG:O | 2.26 | 0.66 |
| 1:C:89:ALA:HB1 | 1:C:118:PHE:CG | 2.30 | 0.66 |
| 1:A:229:ARG:HH22 | 1:A:232:LYS:HE3 | 1.59 | 0.66 |
| 2:D:132:ASN:ND2 | 2:D:133:ASP:H | 1.93 | 0.66 |
| 1:A:5:TYR:C | 1:A:7:LYS:H | 1.98 | 0.66 |
| 1:A:138:THR:O | 1:A:142:LEU:HG | 1.96 | 0.66 |
| 1:C:151:ARG:NH1 | 1:C:155:LEU:HD21 | 2.11 | 0.66 |
| 1:A:99:VAL:HG23 | 1:A:101:ALA:H | 1.61 | 0.66 |
| 1:A:158:ALA:HB2 | 1:A:222:VAL:CG1 | 2.17 | 0.66 |
| 2:B:17:VAL:HG13 | 2:B:59:ILE:O | 1.95 | 0.66 |
| 1:C:59:PHE:CD1 | 1:C:296:ARG:HD3 | 2.30 | 0.65 |
| 1:C:88:LEU:O | 1:C:92:ILE:HG12 | 1.95 | 0.65 |
| 1:C:132:ASN:HA | 1:C:170:HIS:CE1 | 2.30 | 0.65 |
| 2:D:107:LEU:HD11 | 2:D:151:LEU:HD21 | 1.78 | 0.65 |
| 1:C:38:LEU:HD12 | 1:C:39:LEU:CD1 | 2.26 | 0.65 |
| 1:A:111:ALA:O | 1:A:114:LEU:HB2 | 1.97 | 0.65 |
| 1:A:308:LEU:HD23 | 1:A:309:VAL:O | 1.96 | 0.65 |
| 1:A:138:THR:OG1 | 1:A:171:SER:HB3 | 1.96 | 0.65 |
| 1:A:284:TRP:CD1 | 1:A:287:GLN:HB2 | 2.31 | 0.65 |
| 1:C:237:PRO:HG3 | 1:C:240:TYR:OH | 1.96 | 0.65 |
| 2:D:127:VAL:HG21 | 2:D:129:LYS:HZ2 | 1.61 | 0.65 |
| 1:A:183:ARG:NH2 | 1:A:208:ALA:O | 2.29 | 0.65 |
| 1:A:293:ILE:O | 1:A:297:GLN:HB2 | 1.97 | 0.65 |
| 2:B:30:LEU:HD12 | 2:B:35:LEU:HB2 | 1.78 | 0.65 |
| 1:C:100:ASP:O | 1:C:122:VAL:HG13 | 1.96 | 0.65 |
| 2:D:103:ILE:HB | 2:D:125:PHE:N | 2.07 | 0.65 |
| 2:D:125:PHE:CE2 | 2:D:138:CYS:HA | 2.32 | 0.65 |
| 2:B:13:LYS:HG3 | 2:B:89:TYR:CE1 | 2.32 | 0.64 |
| 1:A:26:THR:HA | 1:A:29:LYS:NZ | 2.12 | 0.64 |
| 1:A:129:ASP:O | 1:A:132:ASN:HB3 | 1.98 | 0.64 |
| 2:B:41:ARG:HA | 2:D:47:ASN:CB | 2.27 | 0.64 |
| 1:C:179:PHE:HD1 | 1:C:180:ASP:N | 1.95 | 0.64 |
| 1:C:205:LYS:H | 1:C:205:LYS:HD2 | 1.62 | 0.64 |
| 1:C:230:VAL:O | 1:C:232:LYS:N | 2.30 | 0.64 |
| 1:C:263:VAL:HB | 1:C:283:ALA:HA | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:59:PHE:CE1 | 1:C:296:ARG:NH2 | 2.65 | 0.64 |
| 2:D:76:LEU:HB3 | 2:D:134:ILE:CG2 | 2.25 | 0.64 |
| 2:D:13:LYS:HA | 2:D:88:ASN:HA | 1.78 | 0.64 |
| 1:A:169:VAL:O | 1:A:170:HIS:C | 2.36 | 0.64 |
| 1:C:162:ASP:OD2 | 1:C:165:TYR:HB2 | 1.98 | 0.64 |
| 1:A:25:ALA:O | 1:A:29:LYS:HG3 | 1.97 | 0.64 |
| 1:A:269:ARG:NH1 | 1:A:275:THR:HA | 2.12 | 0.64 |
| 1:C:227:MET:SD | 1:C:272:GLU:HB3 | 2.36 | 0.64 |
| 2:D:114:CYS:O | 2:D:116:SER:N | 2.30 | 0.64 |
| 2:D:86:ILE:HG23 | 2:D:90:GLU:C | 2.17 | 0.64 |
| 2:D:103:ILE:CB | 2:D:125:PHE:H | 2.04 | 0.64 |
| 1:A:229:ARG:HH12 | 1:A:232:LYS:HG2 | 1.63 | 0.64 |
| 1:A:40:LYS:O | 1:A:42:LYS:N | 2.31 | 0.64 |
| 1:A:292:GLY:O | 1:A:293:ILE:C | 2.35 | 0.64 |
| 1:C:48:PHE:HZ | 1:C:52:SER:N | 1.96 | 0.64 |
| 1:C:144:THR:HA | 1:C:147:GLU:HB2 | 1.80 | 0.63 |
| 1:C:157:VAL:O | 1:C:185:TYR:HB2 | 1.98 | 0.63 |
| 1:A:134:HIS:HB2 | 1:A:167:ARG:HB2 | 1.80 | 0.63 |
| 2:B:53:MET:SD | 2:B:54:GLY:N | 2.71 | 0.63 |
| 1:C:11:SER:CB | 1:C:133:GLN:HG3 | 2.27 | 0.63 |
| 1:C:274:ALA:O | 1:C:277:VAL:HG23 | 1.98 | 0.63 |
| 2:D:135:ALA:HA | 2:D:147:HIS:H | 1.63 | 0.63 |
| 2:B:68:GLU:HA | 2:B:71:VAL:CG2 | 2.27 | 0.63 |
| 1:C:171:SER:HA | 1:C:174:GLN:HG2 | 1.80 | 0.63 |
| 2:D:48:LEU:HB2 | 2:D:56:LYS:HZ2 | 1.61 | 0.63 |
| 1:C:183:ARG:NE | 1:C:208:ALA:HB1 | 2.13 | 0.63 |
| 1:A:23:VAL:HA | 1:A:302:LEU:HD11 | 1.81 | 0.63 |
| 1:A:113:ARG:HH22 | 2:B:139:LYS:HB2 | 1.62 | 0.63 |
| 1:A:125:LEU:N | 1:A:125:LEU:CD1 | 2.60 | 0.63 |
| 2:B:38:THR:HG23 | 2:B:42:ILE:HD11 | 1.81 | 0.63 |
| 2:B:39:ASP:O | 2:D:47:ASN:HB3 | 1.98 | 0.63 |
| 2:B:86:ILE:HG12 | 2:B:91:VAL:HA | 1.80 | 0.63 |
| 1:C:5:TYR:HA | 1:C:303:VAL:HA | 1.81 | 0.63 |
| 1:A:223:ASP:O | 1:A:261:MET:HA | 1.99 | 0.62 |
| 2:D:46:LEU:H | 2:D:46:LEU:CD2 | 2.09 | 0.62 |
| 1:A:134:HIS:CE1 | 1:A:136:THR:OG1 | 2.52 | 0.62 |
| 1:A:176:LEU:HD12 | 1:A:184:PHE:CZ | 2.34 | 0.62 |
| 2:B:34:LYS:C | 2:B:36:THR:H | 2.01 | 0.62 |
| 2:B:39:ASP:CA | 2:D:55:ARG:HH22 | 2.12 | 0.62 |
| 2:D:56:LYS:HE2 | 2:D:58:LEU:HB3 | 1.81 | 0.62 |
| 2:B:71:VAL:HG23 | 5:B:190:HOH:O | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:48:LEU:HB2 | 2:D:56:LYS:NZ | 2.14 | 0.62 |
| 2:D:72:ASP:HA | 2:D:98:SER:O | 2.00 | 0.62 |
| 1:A:59:PHE:CE1 | 1:A:296:ARG:HG2 | 2.34 | 0.62 |
| 1:A:235:LEU:HB3 | 1:A:240:TYR:CE2 | 2.35 | 0.62 |
| 1:C:187:ILE:HD13 | 1:C:215:ILE:HD13 | 1.79 | 0.62 |
| 2:D:44:ILE:HG22 | 2:D:45:GLY:H | 1.63 | 0.62 |
| 2:D:110:PRO:HD3 | 2:D:150:VAL:HG13 | 1.81 | 0.62 |
| 2:D:128:ARG:NH1 | 2:D:130:ARG:HD2 | 2.15 | 0.62 |
| 1:A:111:ALA:HA | 2:B:115:ILE:HG21 | 1.81 | 0.62 |
| 1:A:201:MET:CG | 1:A:205:LYS:HD2 | 2.30 | 0.62 |
| 1:A:205:LYS:C | 1:A:207:ILE:H | 2.03 | 0.62 |
| 1:A:306:ARG:HG3 | 1:A:307:ASP:N | 2.14 | 0.62 |
| 2:B:104:ASP:O | 2:B:106:VAL:HG22 | 1.98 | 0.62 |
| 2:B:129:LYS:HZ1 | 2:B:131:ALA:N | 1.98 | 0.62 |
| 1:C:103:VAL:HA | 1:C:125:LEU:O | 1.99 | 0.62 |
| 1:C:306:ARG:HG3 | 1:C:307:ASP:H | 1.65 | 0.62 |
| 1:C:306:ARG:NH2 | 1:C:306:ARG:HB3 | 2.14 | 0.62 |
| 1:A:5:TYR:O | 1:A:7:LYS:N | 2.32 | 0.62 |
| 1:A:40:LYS:HA | 1:A:67:GLY:O | 2.00 | 0.62 |
| 1:A:161:GLY:O | 1:A:163:LEU:HG | 2.00 | 0.62 |
| 1:C:105:ARG:NH1 | 1:C:167:ARG:NH1 | 2.48 | 0.62 |
| 1:C:265:HIS:ND1 | 1:C:266:PRO:HD2 | 2.15 | 0.62 |
| 1:C:23:VAL:HG11 | 1:C:299:LEU:HD12 | 1.81 | 0.61 |
| 1:C:264:LEU:N | 1:C:264:LEU:HD22 | 2.14 | 0.61 |
| 1:A:186:PHE:O | 1:A:211:LEU:HD23 | 1.99 | 0.61 |
| 2:B:40:GLN:HB3 | 2:B:63:ASN:HD22 | 1.65 | 0.61 |
| 1:A:77:ALA:O | 1:A:79:THR:N | 2.28 | 0.61 |
| 2:B:20:HIS:NE2 | 2:B:52:GLU:CD | 2.54 | 0.61 |
| 1:C:65:ARG:NE | 5:C:351:HOH:O | 2.33 | 0.61 |
| 2:D:137:LYS:HE3 | 2:D:142:GLU:OE2 | 1.99 | 0.61 |
| 1:C:144:THR:HG21 | 1:C:288:GLN:HA | 1.83 | 0.61 |
| 1:C:306:ARG:CB | 1:C:306:ARG:HH21 | 2.14 | 0.61 |
| 2:D:73:GLN:O | 2:D:77:TYR:HB2 | 2.00 | 0.61 |
| 1:A:145:ILE:HG23 | 1:A:224:ILE:CD1 | 2.26 | 0.61 |
| 1:C:149:GLN:CB | 1:C:151:ARG:HH12 | 2.13 | 0.61 |
| 1:C:284:TRP:HD1 | 1:C:288:GLN:HB2 | 1.64 | 0.61 |
| 1:C:303:VAL:HG12 | 1:C:303:VAL:O | 2.01 | 0.61 |
| 2:D:81:ALA:O | 2:D:97:PRO:HD3 | 2.01 | 0.61 |
| 1:A:53:THR:O | 1:A:57:LEU:HD12 | 1.99 | 0.61 |
| 2:B:50:SER:OG | 2:B:53:MET:HB3 | 2.00 | 0.61 |
| 1:C:104:MET:HG3 | 1:C:126:ASN:HB2 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:99:LEU:HD22 | 2:D:99:LEU:O | 2.01 | 0.61 |
| 2:B:44:ILE:O | 2:D:44:ILE:HG12 | 2.01 | 0.61 |
| 1:C:9:ILE:HB | 1:C:125:LEU:CA | 2.27 | 0.61 |
| 2:D:138:CYS:HB3 | 2:D:143:LYS:N | 2.15 | 0.61 |
| 1:A:138:THR:CG2 | 1:A:172:LEU:HA | 2.31 | 0.60 |
| 1:A:183:ARG:HG3 | 1:A:183:ARG:NH2 | 2.10 | 0.60 |
| 1:A:284:TRP:HA | 1:A:287:GLN:NE2 | 2.16 | 0.60 |
| 1:C:176:LEU:C | 1:C:178:LYS:H | 2.05 | 0.60 |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:HG22 | 1.81 | 0.60 |
| 1:A:267:LEU:HD21 | 1:A:269:ARG:HG2 | 1.82 | 0.60 |
| 1:C:36:PRO:O | 1:C:38:LEU:N | 2.35 | 0.60 |
| 1:C:56:ARG:HH21 | 1:C:56:ARG:C | 2.04 | 0.60 |
| 1:C:269:ARG:NE | 1:C:273:ILE:HB | 2.15 | 0.60 |
| 1:A:245:ALA:HB2 | 1:A:271:ASP:OD2 | 2.00 | 0.60 |
| 1:C:125:LEU:O | 1:C:125:LEU:HD23 | 2.01 | 0.60 |
| 1:A:138:THR:HG23 | 1:A:172:LEU:CD1 | 2.31 | 0.60 |
| 1:A:291:ASN:HB2 | 5:A:1344:HOH:O | 2.00 | 0.60 |
| 2:B:105:ASN:C | 2:B:106:VAL:HG22 | 2.20 | 0.60 |
| 1:C:54:ARG:NH2 | 1:C:267:LEU:HD12 | 2.17 | 0.60 |
| 1:C:162:ASP:OD1 | 1:C:192:LEU:HD22 | 2.01 | 0.60 |
| 1:C:215:ILE:CG2 | 1:C:219:MET:HE2 | 2.31 | 0.60 |
| 1:A:39:LEU:HD13 | 1:A:304:LEU:HD12 | 1.83 | 0.60 |
| 1:A:49:PHE:CB | 1:A:107:PRO:HD2 | 2.31 | 0.60 |
| 2:B:27:PHE:HB2 | 2:D:36:THR:HG21 | 1.82 | 0.60 |
| 1:C:219:MET:HB3 | 1:C:256:ASN:CG | 2.20 | 0.60 |
| 1:C:17:ARG:HG3 | 1:C:18:ASP:N | 2.16 | 0.60 |
| 1:C:140:LEU:HD12 | 1:C:140:LEU:C | 2.21 | 0.60 |
| 2:D:28:LYS:HE2 | 2:D:32:LEU:HB2 | 1.82 | 0.60 |
| 1:A:4:LEU:O | 1:A:7:LYS:HB2 | 2.00 | 0.60 |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:CB | 2.31 | 0.60 |
| 1:C:38:LEU:HD12 | 1:C:39:LEU:HG | 1.83 | 0.60 |
| 1:C:162:ASP:CB | 1:C:230:VAL:HA | 2.31 | 0.60 |
| 2:D:149:VAL:HA | 2:D:152:ALA:HB3 | 1.83 | 0.60 |
| 1:C:189:PRO:HG3 | 1:C:246:GLN:OE1 | 2.02 | 0.60 |
| 1:C:199:LEU:O | 1:C:202:LEU:HG | 2.01 | 0.60 |
| 2:D:83:VAL:O | 2:D:94:LYS:HA | 2.01 | 0.60 |
| 1:A:267:LEU:HD23 | 1:A:269:ARG:N | 2.16 | 0.60 |
| 2:B:22:PRO:O | 2:B:25:ILE:HB | 2.02 | 0.60 |
| 2:B:42:ILE:HB | 2:D:46:LEU:CD2 | 2.31 | 0.60 |
| 2:B:105:ASN:OD1 | 2:B:105:ASN:O | 2.18 | 0.60 |
| 2:B:105:ASN:O | 2:B:106:VAL:HG13 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:183:ARG:NH2 | 1:C:184:PHE:O | 2.34 | 0.60 |
| 1:C:214:SER:HB2 | 1:C:216:GLU:OE2 | 2.02 | 0.60 |
| 1:C:270:VAL:CG1 | 1:C:271:ASP:H | 2.04 | 0.60 |
| 2:D:30:LEU:N | 2:D:30:LEU:HD22 | 2.16 | 0.60 |
| 1:A:119:SER:OG | 1:A:120:GLY:N | 2.35 | 0.59 |
| 2:B:21:ILE:CD1 | 2:B:59:ILE:HG12 | 2.32 | 0.59 |
| 1:C:13:ASN:N | 1:C:174:GLN:NE2 | 2.48 | 0.59 |
| 1:A:176:LEU:HD12 | 1:A:184:PHE:HZ | 1.68 | 0.59 |
| 1:C:195:PRO:HG2 | 1:C:198:ILE:HG12 | 1.82 | 0.59 |
| 2:D:138:CYS:SG | 2:D:141:CYS:N | 2.75 | 0.59 |
| 1:A:166:GLY:HA2 | 1:A:231:GLN:HE22 | 1.66 | 0.59 |
| 1:C:30:LEU:CD1 | 1:C:298:ALA:HA | 2.33 | 0.59 |
| 1:C:228:THR:CA | 1:C:266:PRO:HG2 | 2.30 | 0.59 |
| 1:A:172:LEU:O | 1:A:176:LEU:HG | 2.02 | 0.59 |
| 1:A:172:LEU:O | 1:A:175:ALA:HB3 | 2.03 | 0.59 |
| 2:B:21:ILE:HB | 2:B:57:ASP:CB | 2.30 | 0.59 |
| 1:C:214:SER:HB2 | 1:C:216:GLU:CG | 2.31 | 0.59 |
| 1:A:48:PHE:CE2 | 1:A:56:ARG:HB2 | 2.36 | 0.59 |
| 1:A:306:ARG:HG3 | 1:A:307:ASP:H | 1.66 | 0.59 |
| 1:C:45:ALA:HB1 | 1:C:72:GLY:H | 1.68 | 0.59 |
| 2:D:125:PHE:CD2 | 2:D:138:CYS:HA | 2.38 | 0.59 |
| 1:A:55:THR:HG21 | 1:A:105:ARG:HH11 | 1.68 | 0.59 |
| 1:C:56:ARG:HH21 | 1:C:56:ARG:CG | 2.16 | 0.59 |
| 1:A:44:ILE:CG2 | 1:A:103:VAL:HG23 | 2.33 | 0.59 |
| 1:A:229:ARG:HG3 | 1:A:270:VAL:HG23 | 1.85 | 0.59 |
| 2:B:16:THR:HG22 | 2:B:17:VAL:N | 2.18 | 0.59 |
| 1:C:89:ALA:HA | 5:C:329:HOH:O | 2.02 | 0.59 |
| 1:C:92:ILE:HA | 1:C:95:ILE:HB | 1.85 | 0.59 |
| 1:C:220:ALA:N | 1:C:256:ASN:ND2 | 2.50 | 0.59 |
| 2:D:99:LEU:HD13 | 2:D:129:LYS:HE3 | 1.85 | 0.59 |
| 1:A:23:VAL:HG22 | 1:A:302:LEU:CD1 | 2.33 | 0.59 |
| 1:C:141:ASP:O | 1:C:144:THR:N | 2.36 | 0.59 |
| 1:C:142:LEU:HA | 1:C:145:ILE:HG13 | 1.85 | 0.59 |
| 1:C:269:ARG:HD2 | 1:C:270:VAL:N | 2.18 | 0.59 |
| 1:A:140:LEU:HD13 | 1:A:288:GLN:O | 2.03 | 0.59 |
| 1:A:235:LEU:CB | 1:A:240:TYR:HE2 | 2.16 | 0.58 |
| 2:D:75:ALA:HA | 2:D:97:PRO:HB2 | 1.85 | 0.58 |
| 1:A:29:LYS:HB2 | 1:A:29:LYS:NZ | 2.18 | 0.58 |
| 1:A:49:PHE:HB2 | 1:A:106:HIS:HA | 1.84 | 0.58 |
| 2:B:30:LEU:HD22 | 2:B:44:ILE:HD12 | 1.84 | 0.58 |
| 1:C:131:SER:N | 5:C:419:HOH:O | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:136:THR:HB | 1:C:296:ARG:NH2 | 2.18 | 0.58 |
| 1:A:30:LEU:C | 1:A:32:ALA:N | 2.56 | 0.58 |
| 1:A:264:LEU:HD22 | 1:A:288:GLN:HG3 | 1.86 | 0.58 |
| 1:A:284:TRP:O | 1:A:288:GLN:N | 2.33 | 0.58 |
| 1:C:215:ILE:HG22 | 1:C:219:MET:HE2 | 1.84 | 0.58 |
| 2:D:84:ASN:ND2 | 2:D:91:VAL:HG11 | 2.17 | 0.58 |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:CB | 2.16 | 0.58 |
| 2:B:44:ILE:O | 2:D:44:ILE:N | 2.36 | 0.58 |
| 2:B:62:GLU:HG2 | 2:B:63:ASN:N | 2.18 | 0.58 |
| 1:A:164:LYS:CA | 1:A:195:PRO:HD3 | 2.26 | 0.58 |
| 2:D:115:ILE:C | 2:D:117:HIS:H | 2.07 | 0.58 |
| 1:C:144:THR:CG2 | 1:C:288:GLN:HA | 2.34 | 0.58 |
| 1:C:282:HIS:O | 1:C:284:TRP:N | 2.37 | 0.58 |
| 2:B:102:ARG:HA | 2:B:127:VAL:HG23 | 1.85 | 0.58 |
| 1:C:113:ARG:HA | 1:C:116:THR:OG1 | 2.04 | 0.58 |
| 2:D:66:LEU:HD13 | 2:D:83:VAL:HG21 | 1.84 | 0.58 |
| 2:D:111:ASN:ND2 | 2:D:114:CYS:N | 2.49 | 0.58 |
| 2:B:69:ASP:HB3 | 2:B:70:GLN:NE2 | 2.19 | 0.58 |
| 1:C:121:ASN:H | 1:C:121:ASN:ND2 | 1.94 | 0.58 |
| 1:C:179:PHE:CD1 | 1:C:180:ASP:N | 2.72 | 0.58 |
| 1:A:124:VAL:C | 1:A:125:LEU:HD12 | 2.24 | 0.58 |
| 2:D:12:ILE:HG23 | 2:D:41:ARG:NH2 | 2.19 | 0.58 |
| 2:B:18:ILE:HB | 2:B:21:ILE:HD11 | 1.85 | 0.57 |
| 1:A:2:ASN:HD22 | 1:A:306:ARG:C | 2.08 | 0.57 |
| 1:C:134:HIS:HB2 | 1:C:167:ARG:O | 2.04 | 0.57 |
| 1:C:152:LEU:HB2 | 1:C:179:PHE:CZ | 2.39 | 0.57 |
| 2:D:126:ALA:HB3 | 2:D:137:LYS:O | 2.04 | 0.57 |
| 1:A:296:ARG:O | 1:A:300:LEU:HG | 2.03 | 0.57 |
| 1:A:308:LEU:HD23 | 1:A:309:VAL:N | 2.19 | 0.57 |
| 1:C:184:PHE:HB2 | 1:C:209:TRP:HA | 1.87 | 0.57 |
| 2:B:50:SER:HB3 | 2:B:53:MET:C | 2.25 | 0.57 |
| 1:C:151:ARG:HH11 | 1:C:155:LEU:CG | 2.16 | 0.57 |
| 1:C:237:PRO:CA | 1:C:240:TYR:CZ | 2.85 | 0.57 |
| 1:A:177:ALA:HB2 | 1:A:202:LEU:HD23 | 1.86 | 0.57 |
| 1:C:4:LEU:HB3 | 1:C:22:LEU:CD2 | 2.35 | 0.57 |
| 1:C:23:VAL:HG12 | 1:C:302:LEU:HD12 | 1.85 | 0.57 |
| 1:C:112:ALA:C | 1:C:114:LEU:N | 2.57 | 0.57 |
| 1:C:188:ALA:O | 1:C:193:ALA:HB2 | 2.04 | 0.57 |
| 2:B:62:GLU:HG2 | 2:B:63:ASN:H | 1.69 | 0.57 |
| 1:C:66:LEU:HD11 | 1:C:297:GLN:CA | 2.34 | 0.57 |
| 1:C:207:ILE:HG13 | 1:C:208:ALA:N | 2.16 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:16:THR:HG22 | 2:D:65:PHE:HA | 1.86 | 0.57 |
| 2:D:143:LYS:HB2 | 2:D:145:PHE:CE1 | 2.39 | 0.57 |
| 1:A:26:THR:HG21 | 1:A:302:LEU:HD21 | 1.85 | 0.57 |
| 1:A:204:GLU:C | 1:A:206:GLY:H | 2.08 | 0.57 |
| 1:A:288:GLN:C | 5:A:1344:HOH:O | 2.43 | 0.57 |
| 1:C:89:ALA:HB1 | 1:C:118:PHE:CD2 | 2.40 | 0.57 |
| 1:C:115:ALA:HA | 5:C:329:HOH:O | 2.05 | 0.57 |
| 1:C:171:SER:HA | 1:C:174:GLN:CG | 2.35 | 0.57 |
| 1:C:237:PRO:O | 1:C:239:GLU:N | 2.38 | 0.57 |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:HG13 | 1.85 | 0.57 |
| 2:D:114:CYS:C | 2:D:116:SER:H | 2.08 | 0.57 |
| 1:A:189:PRO:HB3 | 1:A:242:ASN:ND2 | 2.18 | 0.57 |
| 1:C:44:ILE:CD1 | 1:C:101:ALA:HB3 | 2.34 | 0.57 |
| 1:A:163:LEU:HD13 | 1:A:194:MET:HB2 | 1.87 | 0.56 |
| 1:A:183:ARG:NE | 1:A:208:ALA:HB3 | 2.20 | 0.56 |
| 1:C:114:LEU:HD13 | 5:C:329:HOH:O | 2.05 | 0.56 |
| 1:C:254:LEU:O | 1:C:256:ASN:N | 2.35 | 0.56 |
| 2:D:128:ARG:HH12 | 2:D:130:ARG:CZ | 2.19 | 0.56 |
| 1:C:149:GLN:HB3 | 1:C:151:ARG:HH12 | 1.69 | 0.56 |
| 1:A:3:PRO:CG | 1:A:22:LEU:HD21 | 2.35 | 0.56 |
| 1:A:55:THR:HG21 | 1:A:105:ARG:HE | 1.70 | 0.56 |
| 1:A:138:THR:HG23 | 1:A:172:LEU:HD13 | 1.88 | 0.56 |
| 1:A:160:VAL:CG1 | 1:A:187:ILE:HB | 2.30 | 0.56 |
| 2:B:52:GLU:CD | 2:B:52:GLU:H | 2.09 | 0.56 |
| 2:B:128:ARG:O | 2:B:134:ILE:HG22 | 2.04 | 0.56 |
| 1:C:127:ALA:HA | 1:C:135:PRO:HD2 | 1.86 | 0.56 |
| 1:C:180:ASP:O | 1:C:182:ASN:OD1 | 2.24 | 0.56 |
| 1:A:285:TYR:HA | 1:A:288:GLN:OE1 | 2.06 | 0.56 |
| 1:C:3:PRO:O | 1:C:7:LYS:HD3 | 2.05 | 0.56 |
| 1:C:29:LYS:CD | 1:C:310:LEU:HB2 | 2.36 | 0.56 |
| 1:C:67:GLY:O | 1:C:68:ALA:HB2 | 2.05 | 0.56 |
| 1:C:237:PRO:C | 1:C:239:GLU:H | 2.09 | 0.56 |
| 2:D:125:PHE:CD1 | 2:D:136:LEU:HD13 | 2.40 | 0.56 |
| 1:A:248:VAL:HG13 | 1:A:271:ASP:O | 2.05 | 0.56 |
| 1:C:75:ASP:C | 1:C:77:ALA:H | 2.09 | 0.56 |
| 1:C:103:VAL:HG13 | 1:C:125:LEU:CD2 | 2.35 | 0.56 |
| 1:C:155:LEU:HD13 | 1:C:224:ILE:HD11 | 1.87 | 0.56 |
| 1:A:165:TYR:HB3 | 1:A:231:GLN:HG2 | 1.86 | 0.56 |
| 2:B:30:LEU:HD12 | 2:B:35:LEU:CB | 2.35 | 0.56 |
| 1:C:131:SER:O | 1:C:170:HIS:CE1 | 2.58 | 0.56 |
| 1:A:5:TYR:C | 1:A:7:LYS:N | 2.58 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:9:ILE:CG2 | 1:C:125:LEU:HG | 2.35 | 0.56 |
| 1:C:207:ILE:HG23 | 1:C:208:ALA:N | 2.20 | 0.56 |
| 2:B:12:ILE:HG12 | 2:B:13:LYS:N | 2.20 | 0.56 |
| 2:B:38:THR:CG2 | 2:B:42:ILE:HD11 | 2.34 | 0.56 |
| 1:C:60:GLU:CA | 1:C:63:MET:SD | 2.90 | 0.56 |
| 1:C:104:MET:HG3 | 1:C:126:ASN:CB | 2.35 | 0.56 |
| 1:C:171:SER:C | 1:C:174:GLN:HG3 | 2.25 | 0.56 |
| 2:D:96:ARG:NH2 | 2:D:97:PRO:HD2 | 2.21 | 0.56 |
| 2:D:137:LYS:HD2 | 2:D:142:GLU:O | 2.06 | 0.56 |
| 1:A:94:VAL:HG23 | 1:A:95:ILE:N | 2.19 | 0.56 |
| 1:C:44:ILE:HD11 | 1:C:101:ALA:HB3 | 1.88 | 0.56 |
| 1:C:104:MET:CE | 1:C:112:ALA:HA | 2.36 | 0.56 |
| 1:C:113:ARG:O | 1:C:117:GLU:HG3 | 2.06 | 0.56 |
| 2:D:24:GLN:NE2 | 2:D:47:ASN:ND2 | 2.54 | 0.56 |
| 1:A:2:ASN:HD22 | 1:A:306:ARG:HA | 1.67 | 0.56 |
| 1:A:78:ASN:HD22 | 1:A:78:ASN:N | 2.04 | 0.56 |
| 1:A:113:ARG:HG2 | 1:A:113:ARG:HH21 | 1.70 | 0.56 |
| 1:A:287:GLN:N | 1:A:287:GLN:NE2 | 2.50 | 0.55 |
| 1:C:135:PRO:HG2 | 1:C:136:THR:H | 1.70 | 0.55 |
| 1:C:273:ILE:HG21 | 1:C:285:TYR:OH | 2.06 | 0.55 |
| 2:D:138:CYS:HB3 | 2:D:142:GLU:N | 2.21 | 0.55 |
| 1:A:5:TYR:CE1 | 1:A:306:ARG:HB3 | 2.41 | 0.55 |
| 1:A:54:ARG:HH12 | 1:A:268:PRO:HB3 | 1.71 | 0.55 |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:HG | 1.70 | 0.55 |
| 1:A:196:GLN:C | 1:A:198:ILE:H | 2.09 | 0.55 |
| 1:C:253:ASP:OD1 | 1:C:254:LEU:HD12 | 2.05 | 0.55 |
| 1:A:20:LEU:HD12 | 1:A:179:PHE:CZ | 2.36 | 0.55 |
| 2:B:50:SER:HB3 | 2:B:53:MET:O | 2.06 | 0.55 |
| 1:C:228:THR:HA | 1:C:266:PRO:HD2 | 1.88 | 0.55 |
| 2:D:126:ALA:HB3 | 2:D:137:LYS:HB3 | 1.88 | 0.55 |
| 1:C:104:MET:CG | 1:C:126:ASN:HB2 | 2.35 | 0.55 |
| 1:C:178:LYS:HZ3 | 1:C:201:MET:CE | 2.20 | 0.55 |
| 2:D:15:GLY:HA3 | 2:D:61:ILE:O | 2.05 | 0.55 |
| 2:D:137:LYS:HD2 | 2:D:142:GLU:HG3 | 1.87 | 0.55 |
| 2:D:84:ASN:O | 2:D:86:ILE:HD12 | 2.06 | 0.55 |
| 1:A:166:GLY:O | 1:A:167:ARG:C | 2.45 | 0.55 |
| 1:C:46:SER:O | 1:C:72:GLY:HA3 | 2.07 | 0.55 |
| 1:C:219:MET:CB | 1:C:256:ASN:HD21 | 2.09 | 0.55 |
| 1:C:30:LEU:HD12 | 1:C:298:ALA:CA | 2.36 | 0.55 |
| 1:C:192:LEU:C | 1:C:194:MET:H | 2.11 | 0.55 |
| 1:C:226:TYR:OH | 1:C:266:PRO:HG3 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:67:SER:O | 2:D:71:VAL:HG23 | 2.07 | 0.55 |
| 1:A:59:PHE:O | 1:A:63:MET:HE2 | 2.06 | 0.55 |
| 2:B:41:ARG:HB2 | 2:D:47:ASN:O | 2.07 | 0.55 |
| 2:B:137:LYS:HA | 2:B:143:LYS:O | 2.07 | 0.55 |
| 1:C:9:ILE:HG22 | 1:C:135:PRO:HG3 | 1.89 | 0.55 |
| 1:C:11:SER:HB2 | 1:C:133:GLN:HG3 | 1.88 | 0.55 |
| 1:C:129:ASP:O | 5:C:419:HOH:O | 2.18 | 0.55 |
| 1:C:141:ASP:C | 1:C:143:PHE:N | 2.59 | 0.55 |
| 1:C:306:ARG:CG | 1:C:307:ASP:H | 2.19 | 0.55 |
| 2:D:59:ILE:N | 2:D:59:ILE:HD12 | 2.22 | 0.55 |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:CG2 | 2.37 | 0.55 |
| 2:D:105:ASN:O | 2:D:106:VAL:HG22 | 2.07 | 0.55 |
| 2:B:31:SER:HA | 2:D:27:PHE:HE1 | 1.72 | 0.55 |
| 1:C:280:THR:C | 1:C:282:HIS:H | 2.11 | 0.55 |
| 2:D:124:SER:HB2 | 2:D:139:LYS:HD3 | 1.89 | 0.55 |
| 2:D:127:VAL:CG2 | 2:D:129:LYS:HZ2 | 2.19 | 0.55 |
| 1:A:146:GLN:NE2 | 1:A:152:LEU:HG | 2.22 | 0.54 |
| 1:A:208:ALA:HA | 5:A:1437:HOH:O | 2.06 | 0.54 |
| 2:B:9:VAL:HG13 | 2:B:43:THR:HG21 | 1.88 | 0.54 |
| 1:A:235:LEU:HB3 | 1:A:240:TYR:HE2 | 1.72 | 0.54 |
| 1:C:142:LEU:HD23 | 1:C:145:ILE:HD12 | 1.88 | 0.54 |
| 1:C:148:THR:HB | 5:C:331:HOH:O | 2.08 | 0.54 |
| 1:C:151:ARG:HB3 | 1:C:151:ARG:NH2 | 2.22 | 0.54 |
| 1:C:152:LEU:H | 1:C:152:LEU:CD1 | 2.14 | 0.54 |
| 1:C:237:PRO:HA | 1:C:240:TYR:CD2 | 2.41 | 0.54 |
| 2:D:108:VAL:HG23 | 2:D:150:VAL:O | 2.07 | 0.54 |
| 1:A:10:ILE:HG13 | 1:A:11:SER:H | 1.72 | 0.54 |
| 1:A:92:ILE:HG22 | 1:A:93:SER:H | 1.67 | 0.54 |
| 1:A:155:LEU:HD22 | 1:A:223:ASP:OD2 | 2.06 | 0.54 |
| 1:A:168:THR:OG1 | 1:A:169:VAL:N | 2.40 | 0.54 |
| 2:B:85:ARG:HB2 | 2:B:85:ARG:HH21 | 1.71 | 0.54 |
| 1:C:26:THR:HA | 1:C:29:LYS:HG2 | 1.88 | 0.54 |
| 1:C:131:SER:HA | 1:C:167:ARG:HB3 | 1.88 | 0.54 |
| 1:C:160:VAL:CG1 | 1:C:161:GLY:H | 2.20 | 0.54 |
| 1:C:269:ARG:CD | 1:C:273:ILE:HB | 2.37 | 0.54 |
| 2:D:30:LEU:O | 2:D:34:LYS:HA | 2.07 | 0.54 |
| 2:D:122:SER:HB3 | 5:D:170:HOH:O | 2.07 | 0.54 |
| 1:A:8:HIS:ND1 | 1:A:116:THR:CG2 | 2.67 | 0.54 |
| 1:C:103:VAL:HG13 | 1:C:125:LEU:O | 2.05 | 0.54 |
| 1:C:20:LEU:HD12 | 1:C:20:LEU:N | 2.08 | 0.54 |
| 1:C:167:ARG:NH1 | 1:C:234:ARG:HH12 | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:13:LYS:CA | 2:D:88:ASN:HA | 2.37 | 0.54 |
| 2:D:74:LEU:HD11 | 2:D:81:ALA:HB1 | 1.90 | 0.54 |
| 1:A:59:PHE:HD2 | 1:A:63:MET:HE2 | 1.71 | 0.54 |
| 2:D:46:LEU:HD23 | 2:D:46:LEU:N | 2.11 | 0.54 |
| 2:D:127:VAL:HG12 | 2:D:136:LEU:HB3 | 1.88 | 0.54 |
| 1:A:47:CYS:HB3 | 1:A:73:PHE:CE2 | 2.42 | 0.54 |
| 2:B:62:GLU:O | 2:B:64:THR:N | 2.40 | 0.54 |
| 1:A:177:ALA:HB2 | 1:A:202:LEU:CD2 | 2.38 | 0.54 |
| 2:B:13:LYS:O | 2:B:88:ASN:N | 2.41 | 0.54 |
| 1:C:103:VAL:HG13 | 1:C:125:LEU:HD23 | 1.89 | 0.54 |
| 1:C:153:ASP:CG | 1:C:179:PHE:HE1 | 2.11 | 0.54 |
| 2:D:44:ILE:N | 2:D:44:ILE:HD13 | 2.23 | 0.54 |
| 2:D:99:LEU:HD11 | 2:D:129:LYS:HE3 | 1.89 | 0.54 |
| 2:D:125:PHE:CE1 | 2:D:136:LEU:HD13 | 2.43 | 0.54 |
| 1:A:129:ASP:CG | 1:A:132:ASN:HD22 | 2.11 | 0.54 |
| 1:A:139:LEU:O | 1:A:142:LEU:HB2 | 2.07 | 0.54 |
| 1:A:174:GLN:HG2 | 1:A:198:ILE:HG23 | 1.90 | 0.54 |
| 1:A:177:ALA:CB | 1:A:202:LEU:HD23 | 2.37 | 0.54 |
| 2:B:9:VAL:HG13 | 2:B:43:THR:CG2 | 2.38 | 0.54 |
| 2:B:27:PHE:HE1 | 2:D:34:LYS:HZ2 | 1.55 | 0.54 |
| 1:C:81:LEU:HA | 1:C:86:GLU:HB2 | 1.90 | 0.54 |
| 1:C:105:ARG:NH1 | 1:C:167:ARG:HH22 | 2.06 | 0.54 |
| 2:D:103:ILE:HG21 | 2:D:125:PHE:HB2 | 1.89 | 0.54 |
| 2:B:47:ASN:HB2 | 2:D:42:ILE:HD11 | 1.88 | 0.54 |
| 1:C:82:GLY:O | 1:C:83:LYS:C | 2.47 | 0.54 |
| 1:C:153:ASP:HA | 1:C:179:PHE:CE1 | 2.43 | 0.54 |
| 2:D:87:ASP:O | 2:D:88:ASN:HB3 | 2.07 | 0.54 |
| 2:D:111:ASN:ND2 | 2:D:114:CYS:CB | 2.63 | 0.54 |
| 1:A:109:GLU:O | 2:B:115:ILE:HG22 | 2.08 | 0.53 |
| 1:A:280:THR:HB | 1:A:281:PRO:HD2 | 1.89 | 0.53 |
| 1:C:96:SER:HB2 | 1:C:122:VAL:HB | 1.90 | 0.53 |
| 2:D:99:LEU:HD22 | 2:D:129:LYS:NZ | 2.22 | 0.53 |
| 2:B:129:LYS:NZ | 2:B:130:ARG:N | 2.57 | 0.53 |
| 1:C:265:HIS:N | 1:C:288:GLN:OE1 | 2.39 | 0.53 |
| 1:A:10:ILE:CG1 | 1:A:11:SER:N | 2.68 | 0.53 |
| 1:A:165:TYR:C | 1:A:231:GLN:HE21 | 2.11 | 0.53 |
| 1:A:225:LEU:HD12 | 1:A:226:TYR:N | 2.23 | 0.53 |
| 2:B:38:THR:HG21 | 2:B:61:ILE:HD11 | 1.91 | 0.53 |
| 1:C:306:ARG:HG3 | 1:C:307:ASP:N | 2.24 | 0.53 |
| 2:D:90:GLU:OE1 | 2:D:92:VAL:HG22 | 2.08 | 0.53 |
| 1:A:2:ASN:ND2 | 1:A:305:ASN:O | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:54:ARG:NH1 | 1:A:268:PRO:HB3 | 2.24 | 0.53 |
| 1:C:44:ILE:O | 1:C:70:VAL:HA | 2.08 | 0.53 |
| 1:C:49:PHE:HB2 | 1:C:105:ARG:O | 2.09 | 0.53 |
| 1:A:20:LEU:O | 1:A:22:LEU:N | 2.41 | 0.53 |
| 1:A:251:ALA:O | 1:A:253:ASP:N | 2.42 | 0.53 |
| 2:B:111:ASN:OD1 | 2:B:114:CYS:N | 2.41 | 0.53 |
| 1:C:45:ALA:CB | 1:C:99:VAL:HG11 | 2.38 | 0.53 |
| 1:C:92:ILE:HG22 | 1:C:118:PHE:O | 2.09 | 0.53 |
| 1:A:95:ILE:HD13 | 1:A:95:ILE:N | 2.23 | 0.53 |
| 1:A:284:TRP:HA | 1:A:287:GLN:CD | 2.28 | 0.53 |
| 1:C:162:ASP:OD2 | 1:C:231:GLN:HB2 | 2.09 | 0.53 |
| 1:A:113:ARG:HB3 | 2:B:140:TYR:HD1 | 1.74 | 0.53 |
| 1:C:4:LEU:HD21 | 1:C:299:LEU:CD1 | 2.39 | 0.53 |
| 1:C:64:HIS:NE2 | 1:C:70:VAL:HG23 | 2.24 | 0.53 |
| 1:C:145:ILE:HA | 5:C:320:HOH:O | 2.09 | 0.53 |
| 2:D:83:VAL:O | 2:D:83:VAL:HG13 | 2.09 | 0.53 |
| 1:C:262:LYS:O | 1:C:264:LEU:HD22 | 2.09 | 0.53 |
| 2:D:9:VAL:C | 2:D:11:ALA:H | 2.12 | 0.53 |
| 2:D:28:LYS:O | 2:D:30:LEU:N | 2.42 | 0.53 |
| 2:D:41:ARG:HB3 | 2:D:62:GLU:HB3 | 1.90 | 0.53 |
| 2:D:130:ARG:C | 2:D:132:ASN:H | 2.12 | 0.53 |
| 1:A:169:VAL:HG23 | 1:A:170:HIS:HD2 | 1.74 | 0.53 |
| 1:A:287:GLN:O | 5:A:1344:HOH:O | 2.19 | 0.53 |
| 1:C:106:HIS:ND1 | 1:C:108:GLN:OE1 | 2.37 | 0.53 |
| 2:B:129:LYS:HZ1 | 2:B:130:ARG:C | 2.12 | 0.53 |
| 2:B:141:CYS:N | 5:B:221:HOH:O | 2.15 | 0.53 |
| 1:C:250:ARG:O | 1:C:251:ALA:C | 2.47 | 0.53 |
| 2:D:41:ARG:H | 2:D:62:GLU:HB3 | 1.74 | 0.53 |
| 2:D:132:ASN:ND2 | 2:D:133:ASP:OD1 | 2.42 | 0.53 |
| 1:A:49:PHE:HA | 1:A:76:SER:HB2 | 1.90 | 0.52 |
| 1:A:309:VAL:HG22 | 5:A:1403:HOH:O | 2.08 | 0.52 |
| 1:C:178:LYS:NZ | 1:C:201:MET:CE | 2.73 | 0.52 |
| 2:D:137:LYS:CE | 2:D:142:GLU:HG3 | 2.39 | 0.52 |
| 1:C:184:PHE:HB3 | 1:C:186:PHE:CE1 | 2.44 | 0.52 |
| 1:A:2:ASN:ND2 | 1:A:5:TYR:CG | 2.77 | 0.52 |
| 1:A:146:GLN:HG2 | 1:A:152:LEU:HB3 | 1.90 | 0.52 |
| 1:A:229:ARG:CG | 1:A:270:VAL:HG23 | 2.39 | 0.52 |
| 1:A:278:ASP:HA | 1:A:285:TYR:OH | 2.09 | 0.52 |
| 2:B:17:VAL:HG13 | 2:B:60:LYS:HG2 | 1.91 | 0.52 |
| 1:C:136:THR:CB | 1:C:296:ARG:NH2 | 2.72 | 0.52 |
| 1:C:231:GLN:H | 1:C:231:GLN:HE21 | 1.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:287:GLN:HG2 | 5:A:1326:HOH:O | 2.09 | 0.52 |
| 2:B:128:ARG:HD3 | 5:B:201:HOH:O | 2.09 | 0.52 |
| 1:C:219:MET:HB3 | 1:C:256:ASN:OD1 | 2.08 | 0.52 |
| 2:D:24:GLN:HE21 | 2:D:47:ASN:HD21 | 1.58 | 0.52 |
| 2:D:107:LEU:HD21 | 2:D:136:LEU:CD2 | 2.39 | 0.52 |
| 2:D:124:SER:O | 2:D:139:LYS:HB3 | 2.09 | 0.52 |
| 1:A:76:SER:HA | 5:A:1399:HOH:O | 2.09 | 0.52 |
| 1:A:126:ASN:ND2 | 1:A:128:GLY:H | 2.07 | 0.52 |
| 1:C:155:LEU:HD13 | 1:C:224:ILE:CD1 | 2.40 | 0.52 |
| 1:C:201:MET:HA | 5:C:337:HOH:O | 2.09 | 0.52 |
| 1:A:201:MET:O | 1:A:202:LEU:C | 2.48 | 0.52 |
| 1:A:205:LYS:O | 1:A:207:ILE:N | 2.43 | 0.52 |
| 1:A:269:ARG:HH22 | 1:A:278:ASP:CG | 2.11 | 0.52 |
| 1:C:54:ARG:NE | 1:C:267:LEU:HB3 | 2.25 | 0.52 |
| 1:C:66:LEU:HG | 1:C:297:GLN:HG2 | 1.92 | 0.52 |
| 1:C:193:ALA:HB1 | 1:C:211:LEU:HD22 | 1.92 | 0.52 |
| 1:A:2:ASN:ND2 | 1:A:5:TYR:CB | 2.72 | 0.52 |
| 1:A:169:VAL:HG23 | 1:A:170:HIS:N | 2.25 | 0.52 |
| 1:C:38:LEU:HD12 | 1:C:39:LEU:CG | 2.39 | 0.52 |
| 1:C:45:ALA:HB1 | 1:C:72:GLY:N | 2.25 | 0.52 |
| 2:D:33:PHE:HB3 | 2:D:35:LEU:HG | 1.92 | 0.52 |
| 1:A:30:LEU:C | 1:A:32:ALA:H | 2.13 | 0.52 |
| 1:A:128:GLY:HA3 | 1:A:167:ARG:CZ | 2.40 | 0.52 |
| 1:C:92:ILE:O | 1:C:93:SER:C | 2.47 | 0.52 |
| 1:C:157:VAL:HG12 | 1:C:158:ALA:N | 2.17 | 0.52 |
| 1:A:265:HIS:O | 1:A:288:GLN:OE1 | 2.27 | 0.52 |
| 2:B:41:ARG:CD | 2:D:48:LEU:HD13 | 2.40 | 0.52 |
| 1:C:192:LEU:O | 1:C:194:MET:N | 2.36 | 0.52 |
| 1:C:202:LEU:HA | 1:C:205:LYS:HZ2 | 1.74 | 0.52 |
| 1:A:157:VAL:HA | 1:A:224:ILE:O | 2.10 | 0.52 |
| 2:B:18:ILE:HD12 | 2:B:18:ILE:N | 2.24 | 0.52 |
| 1:C:26:THR:HA | 1:C:29:LYS:CG | 2.40 | 0.52 |
| 2:D:86:ILE:HD12 | 2:D:86:ILE:H | 1.75 | 0.52 |
| 2:D:108:VAL:HG23 | 2:D:108:VAL:O | 2.10 | 0.52 |
| 1:A:187:ILE:HG23 | 1:A:212:HIS:O | 2.10 | 0.51 |
| 1:C:48:PHE:CZ | 1:C:52:SER:N | 2.70 | 0.51 |
| 1:C:155:LEU:HA | 5:C:363:HOH:O | 2.10 | 0.51 |
| 1:C:273:ILE:HG21 | 1:C:285:TYR:CZ | 2.45 | 0.51 |
| 2:D:24:GLN:HE21 | 2:D:47:ASN:ND2 | 2.08 | 0.51 |
| 1:A:16:SER:O | 1:A:178:LYS:HD3 | 2.11 | 0.51 |
| 1:A:26:THR:HG21 | 1:A:302:LEU:CD2 | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:103:ILE:O | 2:B:103:ILE:HG13 | 2.10 | 0.51 |
| 1:C:164:LYS:CB | 1:C:192:LEU:HA | 2.38 | 0.51 |
| 1:A:50:GLU:HG2 | 1:A:105:ARG:HD3 | 1.92 | 0.51 |
| 1:C:141:ASP:C | 1:C:143:PHE:H | 2.13 | 0.51 |
| 1:C:142:LEU:HA | 1:C:145:ILE:CG1 | 2.40 | 0.51 |
| 1:C:155:LEU:HD22 | 1:C:224:ILE:CD1 | 2.40 | 0.51 |
| 1:C:274:ALA:HB3 | 1:C:277:VAL:HG23 | 1.92 | 0.51 |
| 2:D:135:ALA:CB | 2:D:146:SER:HA | 2.40 | 0.51 |
| 1:A:23:VAL:O | 1:A:26:THR:HB | 2.10 | 0.51 |
| 2:B:109:CYS:SG | 2:B:110:PRO:HD2 | 2.50 | 0.51 |
| 1:C:136:THR:OG1 | 1:C:296:ARG:NH2 | 2.43 | 0.51 |
| 1:A:26:THR:OG1 | 1:A:302:LEU:HD21 | 2.10 | 0.51 |
| 1:A:177:ALA:O | 1:A:207:ILE:HD11 | 2.11 | 0.51 |
| 2:B:20:HIS:HA | 2:B:56:LYS:HD2 | 1.91 | 0.51 |
| 1:C:13:ASN:OD1 | 1:C:178:LYS:CE | 2.59 | 0.51 |
| 2:D:28:LYS:C | 2:D:30:LEU:H | 2.13 | 0.51 |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:CG1 | 2.40 | 0.51 |
| 2:B:21:ILE:O | 2:B:57:ASP:HB2 | 2.11 | 0.51 |
| 1:C:2:ASN:HB2 | 1:C:3:PRO:HD2 | 1.93 | 0.51 |
| 1:C:124:VAL:HG12 | 1:C:125:LEU:H | 1.64 | 0.51 |
| 1:C:178:LYS:HZ3 | 1:C:201:MET:HE1 | 1.75 | 0.51 |
| 1:C:188:ALA:HB3 | 1:C:193:ALA:HA | 1.92 | 0.51 |
| 2:B:28:LYS:C | 2:B:30:LEU:H | 2.12 | 0.51 |
| 1:A:279:LYS:HB2 | 5:A:1418:HOH:O | 2.11 | 0.51 |
| 2:B:27:PHE:H | 2:B:46:LEU:HD21 | 1.74 | 0.51 |
| 2:B:84:ASN:O | 2:B:86:ILE:N | 2.44 | 0.51 |
| 2:B:114:CYS:O | 2:B:117:HIS:HE1 | 1.93 | 0.51 |
| 1:C:4:LEU:HD23 | 1:C:303:VAL:HG22 | 1.93 | 0.51 |
| 1:C:159:MET:HE3 | 1:C:172:LEU:HD23 | 1.91 | 0.51 |
| 1:C:261:MET:C | 1:C:262:LYS:HD2 | 2.31 | 0.51 |
| 2:D:16:THR:CG2 | 2:D:65:PHE:HA | 2.41 | 0.51 |
| 2:D:34:LYS:O | 2:D:37:GLU:OE1 | 2.29 | 0.51 |
| 1:A:155:LEU:O | 1:A:182:ASN:HA | 2.10 | 0.51 |
| 1:A:191:ALA:C | 1:A:193:ALA:H | 2.14 | 0.51 |
| 1:C:291:ASN:O | 1:C:292:GLY:C | 2.49 | 0.51 |
| 2:D:45:GLY:O | 2:D:48:LEU:HD23 | 2.10 | 0.51 |
| 2:D:133:ASP:HB2 | 2:D:147:HIS:HE1 | 1.74 | 0.51 |
| 1:A:131:SER:HB2 | 1:A:165:TYR:HA | 1.93 | 0.51 |
| 2:B:36:THR:O | 2:D:24:GLN:NE2 | 2.43 | 0.51 |
| 1:C:46:SER:N | 1:C:72:GLY:HA3 | 2.26 | 0.51 |
| 1:C:136:THR:CB | 1:C:296:ARG:HH22 | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:129:ASP:OD2 | 1:A:132:ASN:HB3 | 2.10 | 0.50 |
| 1:C:186:PHE:C | 1:C:187:ILE:HG13 | 2.31 | 0.50 |
| 1:C:31:LYS:HZ3 | 1:C:143:PHE:HE2 | 1.53 | 0.50 |
| 1:C:80:SER:HA | 1:C:84:LYS:HB2 | 1.93 | 0.50 |
| 1:A:225:LEU:HD12 | 1:A:225:LEU:C | 2.32 | 0.50 |
| 1:A:16:SER:HA | 5:A:1389:HOH:O | 2.11 | 0.50 |
| 1:A:174:GLN:CG | 1:A:198:ILE:HG23 | 2.41 | 0.50 |
| 2:B:42:ILE:O | 2:D:46:LEU:N | 2.45 | 0.50 |
| 1:C:129:ASP:O | 1:C:130:GLY:C | 2.49 | 0.50 |
| 1:C:220:ALA:HB2 | 1:C:256:ASN:HD22 | 1.77 | 0.50 |
| 1:A:157:VAL:HG12 | 1:A:224:ILE:HB | 1.92 | 0.50 |
| 1:A:191:ALA:O | 1:A:193:ALA:N | 2.42 | 0.50 |
| 2:B:58:LEU:HD22 | 2:B:60:LYS:HG3 | 1.92 | 0.50 |
| 1:C:189:PRO:O | 1:C:192:LEU:N | 2.45 | 0.50 |
| 1:C:190:ASP:OD1 | 1:C:191:ALA:N | 2.36 | 0.50 |
| 2:D:125:PHE:O | 2:D:139:LYS:HB2 | 2.11 | 0.50 |
| 1:C:2:ASN:OD1 | 1:C:5:TYR:HB2 | 2.10 | 0.50 |
| 1:C:81:LEU:C | 1:C:81:LEU:HD23 | 2.32 | 0.50 |
| 1:C:155:LEU:HD23 | 1:C:223:ASP:CG | 2.32 | 0.50 |
| 1:C:224:ILE:N | 1:C:261:MET:HG2 | 2.26 | 0.50 |
| 2:D:137:LYS:CD | 2:D:142:GLU:HG3 | 2.42 | 0.50 |
| 2:D:149:VAL:HA | 2:D:152:ALA:CB | 2.42 | 0.50 |
| 1:A:16:SER:OG | 1:A:19:ASP:HB2 | 2.11 | 0.50 |
| 1:A:160:VAL:CG1 | 1:A:187:ILE:HD13 | 2.42 | 0.50 |
| 1:A:189:PRO:HD2 | 1:A:192:LEU:HB2 | 1.92 | 0.50 |
| 2:B:9:VAL:O | 2:B:10:GLU:HB2 | 2.11 | 0.50 |
| 2:B:96:ARG:HD2 | 2:B:97:PRO:HD2 | 1.93 | 0.50 |
| 1:C:263:VAL:HG23 | 1:C:282:HIS:HB3 | 1.94 | 0.50 |
| 2:B:83:VAL:HG11 | 2:B:85:ARG:NH1 | 2.26 | 0.50 |
| 2:B:36:THR:HG23 | 2:B:37:GLU:H | 1.77 | 0.49 |
| 1:C:26:THR:HA | 1:C:29:LYS:CD | 2.42 | 0.49 |
| 1:C:26:THR:CA | 1:C:29:LYS:HG2 | 2.42 | 0.49 |
| 1:C:43:VAL:O | 1:C:44:ILE:HD12 | 2.12 | 0.49 |
| 1:C:237:PRO:HA | 1:C:240:TYR:CE1 | 2.47 | 0.49 |
| 1:C:248:VAL:CG1 | 1:C:249:LEU:H | 2.19 | 0.49 |
| 1:C:295:ALA:O | 1:C:296:ARG:C | 2.49 | 0.49 |
| 1:A:128:GLY:HA3 | 1:A:167:ARG:NH2 | 2.27 | 0.49 |
| 2:B:55:ARG:O | 2:B:56:LYS:HB3 | 2.13 | 0.49 |
| 2:B:61:ILE:HG23 | 2:B:61:ILE:O | 2.11 | 0.49 |
| 1:C:21:ASN:HA | 1:C:24:LEU:HD12 | 1.94 | 0.49 |
| 1:C:26:THR:OG1 | 1:C:302:LEU:HD11 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:46:SER:O | 1:C:73:PHE:N | 2.45 | 0.49 |
| 1:A:2:ASN:ND2 | 1:A:306:ARG:CA | 2.70 | 0.49 |
| 1:A:48:PHE:CD2 | 1:A:105:ARG:HD2 | 2.47 | 0.49 |
| 1:A:109:GLU:OE2 | 1:A:132:ASN:HB2 | 2.12 | 0.49 |
| 1:A:134:HIS:ND1 | 1:A:136:THR:OG1 | 2.42 | 0.49 |
| 1:A:267:LEU:CD2 | 1:A:269:ARG:HG2 | 2.41 | 0.49 |
| 1:C:5:TYR:O | 1:C:6:GLN:HB2 | 2.12 | 0.49 |
| 1:C:38:LEU:HB3 | 1:C:39:LEU:HD12 | 1.94 | 0.49 |
| 1:C:140:LEU:O | 1:C:291:ASN:OD1 | 2.29 | 0.49 |
| 1:C:183:ARG:HA | 1:C:208:ALA:CB | 2.40 | 0.49 |
| 1:A:160:VAL:HA | 1:A:187:ILE:O | 2.12 | 0.49 |
| 1:A:243:VAL:O | 1:A:244:LYS:O | 2.29 | 0.49 |
| 1:C:159:MET:HE2 | 1:C:172:LEU:HD23 | 1.91 | 0.49 |
| 2:D:16:THR:HG21 | 2:D:66:LEU:HD12 | 1.94 | 0.49 |
| 1:A:39:LEU:HD21 | 1:A:301:ALA:HA | 1.94 | 0.49 |
| 1:C:61:THR:CG2 | 5:C:351:HOH:O | 2.60 | 0.49 |
| 1:C:234:ARG:C | 1:C:235:LEU:HD23 | 2.33 | 0.49 |
| 2:D:25:ILE:HG23 | 5:D:191:HOH:O | 2.12 | 0.49 |
| 1:A:78:ASN:HD22 | 1:A:78:ASN:H | 1.61 | 0.49 |
| 1:A:105:ARG:HG2 | 5:A:1388:HOH:O | 2.13 | 0.49 |
| 1:C:260:ASN:O | 1:C:262:LYS:HD2 | 2.12 | 0.49 |
| 1:A:137:GLN:NE2 | 1:A:266:PRO:HB3 | 2.28 | 0.49 |
| 1:A:183:ARG:NH2 | 1:A:183:ARG:CG | 2.74 | 0.49 |
| 2:B:12:ILE:HG12 | 2:B:13:LYS:H | 1.78 | 0.49 |
| 2:B:42:ILE:O | 2:D:45:GLY:HA2 | 2.12 | 0.49 |
| 1:A:202:LEU:HA | 1:A:207:ILE:HB | 1.94 | 0.49 |
| 1:A:302:LEU:HD23 | 1:A:302:LEU:N | 2.21 | 0.49 |
| 2:B:70:GLN:HB3 | 5:B:164:HOH:O | 2.13 | 0.49 |
| 1:C:60:GLU:O | 1:C:63:MET:HB2 | 2.13 | 0.49 |
| 1:C:109:GLU:CB | 5:C:419:HOH:O | 2.49 | 0.49 |
| 1:C:110:GLY:HA2 | 2:D:140:TYR:O | 2.12 | 0.49 |
| 1:C:128:GLY:HA2 | 1:C:133:GLN:O | 2.13 | 0.49 |
| 1:C:249:LEU:HD11 | 1:C:254:LEU:HD21 | 1.94 | 0.49 |
| 1:A:34:PRO:O | 1:A:35:GLN:HG3 | 2.13 | 0.49 |
| 1:A:160:VAL:CG2 | 1:A:227:MET:SD | 3.00 | 0.49 |
| 1:A:255:HIS:CD2 | 1:A:255:HIS:N | 2.75 | 0.49 |
| 1:A:267:LEU:HD23 | 1:A:268:PRO:CA | 2.33 | 0.49 |
| 1:C:5:TYR:CE2 | 1:C:305:ASN:N | 2.81 | 0.49 |
| 1:C:134:HIS:CE1 | 1:C:137:GLN:CB | 2.95 | 0.49 |
| 1:C:155:LEU:HD22 | 1:C:224:ILE:HD11 | 1.94 | 0.49 |
| 1:C:292:GLY:HA2 | 1:C:296:ARG:HG3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:33:PHE:O | 2:D:34:LYS:C | 2.51 | 0.49 |
| 1:A:92:ILE:HG21 | 1:A:118:PHE:HB2 | 1.94 | 0.49 |
| 1:C:229:ARG:O | 1:C:231:GLN:NE2 | 2.46 | 0.49 |
| 1:A:134:HIS:CE1 | 1:A:136:THR:HG1 | 2.31 | 0.48 |
| 1:A:202:LEU:CB | 1:A:207:ILE:HB | 2.41 | 0.48 |
| 1:C:13:ASN:HB2 | 1:C:174:GLN:NE2 | 2.27 | 0.48 |
| 1:C:160:VAL:CG1 | 1:C:161:GLY:N | 2.75 | 0.48 |
| 1:C:276:ASP:HA | 1:C:279:LYS:NZ | 2.27 | 0.48 |
| 1:A:9:ILE:HD12 | 1:A:9:ILE:N | 2.28 | 0.48 |
| 1:C:37:GLU:HA | 1:C:40:LYS:HE3 | 1.93 | 0.48 |
| 1:C:141:ASP:OD1 | 1:C:288:GLN:HG2 | 2.13 | 0.48 |
| 1:C:167:ARG:HG3 | 1:C:167:ARG:HH21 | 1.78 | 0.48 |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:CD1 | 2.43 | 0.48 |
| 1:A:289:ALA:N | 5:A:1344:HOH:O | 2.46 | 0.48 |
| 2:B:86:ILE:HA | 2:B:91:VAL:HA | 1.95 | 0.48 |
| 1:C:9:ILE:CB | 1:C:125:LEU:HG | 2.43 | 0.48 |
| 1:C:4:LEU:HD13 | 1:C:23:VAL:HG13 | 1.96 | 0.48 |
| 1:C:107:PRO:HB2 | 5:C:316:HOH:O | 2.13 | 0.48 |
| 1:C:142:LEU:HA | 1:C:145:ILE:HD12 | 1.94 | 0.48 |
| 1:C:219:MET:HE1 | 1:C:254:LEU:HG | 1.95 | 0.48 |
| 1:C:228:THR:HG23 | 1:C:266:PRO:HG2 | 1.96 | 0.48 |
| 1:C:260:ASN:O | 1:C:262:LYS:CD | 2.61 | 0.48 |
| 1:A:48:PHE:CZ | 1:A:56:ARG:HA | 2.49 | 0.48 |
| 1:A:55:THR:HB | 3:A:1311:PCT:C1 | 2.43 | 0.48 |
| 1:A:162:ASP:OD1 | 1:A:192:LEU:HD22 | 2.13 | 0.48 |
| 1:A:164:LYS:HD3 | 5:A:1376:HOH:O | 2.12 | 0.48 |
| 1:C:146:GLN:N | 1:C:146:GLN:OE1 | 2.47 | 0.48 |
| 1:A:13:ASN:OD1 | 1:A:174:GLN:CD | 2.51 | 0.48 |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:CG | 2.26 | 0.48 |
| 2:B:50:SER:OG | 2:B:56:LYS:HD3 | 2.13 | 0.48 |
| 1:C:49:PHE:CD1 | 1:C:49:PHE:N | 2.82 | 0.48 |
| 1:C:105:ARG:NH1 | 1:C:167:ARG:NH2 | 2.60 | 0.48 |
| 1:C:137:GLN:HG3 | 1:C:137:GLN:O | 2.14 | 0.48 |
| 1:A:167:ARG:HD2 | 5:A:1319:HOH:O | 2.13 | 0.48 |
| 1:C:65:ARG:C | 1:C:67:GLY:H | 2.16 | 0.48 |
| 1:C:231:GLN:NE2 | 1:C:231:GLN:N | 2.60 | 0.48 |
| 1:C:310:LEU:N | 1:C:310:LEU:CD1 | 2.74 | 0.48 |
| 2:D:147:HIS:HB2 | 2:D:151:LEU:CD1 | 2.44 | 0.48 |
| 1:A:87:THR:O | 1:A:91:THR:OG1 | 2.31 | 0.48 |
| 2:B:74:LEU:HB2 | 2:B:97:PRO:HB3 | 1.96 | 0.48 |
| 2:B:75:ALA:CB | 2:B:97:PRO:O | 2.60 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:92:ILE:HG13 | 1:C:115:ALA:CA | 2.32 | 0.48 |
| 1:C:125:LEU:HD23 | 1:C:125:LEU:C | 2.33 | 0.48 |
| 1:C:151:ARG:NH1 | 1:C:155:LEU:HD11 | 2.19 | 0.48 |
| 1:C:306:ARG:NH2 | 1:C:306:ARG:CB | 2.73 | 0.48 |
| 1:C:163:LEU:CG | 1:C:188:ALA:HB2 | 2.41 | 0.48 |
| 1:C:202:LEU:HA | 1:C:205:LYS:HZ3 | 1.77 | 0.48 |
| 1:C:245:ALA:O | 1:C:247:PHE:N | 2.46 | 0.48 |
| 1:A:106:HIS:HB3 | 1:A:111:ALA:HB3 | 1.95 | 0.48 |
| 2:B:30:LEU:O | 2:B:33:PHE:O | 2.31 | 0.48 |
| 2:B:47:ASN:O | 2:B:48:LEU:HD23 | 2.14 | 0.48 |
| 1:C:219:MET:O | 1:C:257:ALA:HA | 2.14 | 0.48 |
| 2:D:72:ASP:OD2 | 2:D:72:ASP:N | 2.46 | 0.48 |
| 1:A:57:LEU:O | 1:A:60:GLU:N | 2.47 | 0.47 |
| 1:A:165:TYR:CE2 | 1:A:235:LEU:HD23 | 2.43 | 0.47 |
| 1:C:228:THR:CB | 1:C:266:PRO:HG2 | 2.43 | 0.47 |
| 2:D:28:LYS:HE2 | 2:D:32:LEU:HD22 | 1.96 | 0.47 |
| 2:D:62:GLU:O | 2:D:63:ASN:HB2 | 2.13 | 0.47 |
| 2:D:86:ILE:HD12 | 2:D:86:ILE:N | 2.29 | 0.47 |
| 1:A:44:ILE:HG21 | 1:A:103:VAL:CG2 | 2.44 | 0.47 |
| 1:A:237:PRO:HD3 | 5:A:1392:HOH:O | 2.14 | 0.47 |
| 1:C:5:TYR:HE2 | 1:C:305:ASN:N | 2.12 | 0.47 |
| 1:C:26:THR:HG23 | 1:C:310:LEU:HD22 | 1.95 | 0.47 |
| 1:C:54:ARG:HH11 | 1:C:268:PRO:HD3 | 1.78 | 0.47 |
| 1:C:287:GLN:N | 1:C:287:GLN:CD | 2.67 | 0.47 |
| 2:D:28:LYS:HB3 | 2:D:32:LEU:HB3 | 1.97 | 0.47 |
| 2:D:137:LYS:HB2 | 2:D:144:GLU:CG | 2.44 | 0.47 |
| 1:A:50:GLU:HB3 | 1:A:107:PRO:HD3 | 1.96 | 0.47 |
| 1:A:109:GLU:HB3 | 2:B:141:CYS:CB | 2.34 | 0.47 |
| 1:A:197:TYR:CZ | 1:A:198:ILE:HD11 | 2.50 | 0.47 |
| 2:B:129:LYS:HE3 | 2:B:129:LYS:O | 2.14 | 0.47 |
| 1:C:146:GLN:HA | 1:C:150:GLY:N | 2.30 | 0.47 |
| 2:D:23:ALA:HB2 | 2:D:55:ARG:HG3 | 1.95 | 0.47 |
| 2:D:56:LYS:HD2 | 2:D:57:ASP:CA | 2.44 | 0.47 |
| 2:D:96:ARG:CZ | 2:D:96:ARG:HA | 2.44 | 0.47 |
| 1:A:160:VAL:HG22 | 1:A:225:LEU:HD11 | 1.95 | 0.47 |
| 1:A:170:HIS:H | 1:A:170:HIS:CD2 | 2.30 | 0.47 |
| 1:C:100:ASP:O | 1:C:122:VAL:CG1 | 2.62 | 0.47 |
| 1:C:291:ASN:O | 1:C:293:ILE:N | 2.47 | 0.47 |
| 2:D:149:VAL:O | 2:D:150:VAL:C | 2.53 | 0.47 |
| 1:A:41:HIS:O | 1:A:42:LYS:C | 2.53 | 0.47 |
| 1:A:48:PHE:HE2 | 1:A:55:THR:CG2 | 2.19 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:233:GLU:H | 1:A:233:GLU:CD | 2.17 | 0.47 |
| 1:C:80:SER:OG | 1:C:84:LYS:HD2 | 2.14 | 0.47 |
| 1:C:208:ALA:O | 1:C:209:TRP:HB3 | 2.14 | 0.47 |
| 1:C:253:ASP:OD1 | 1:C:254:LEU:CD1 | 2.63 | 0.47 |
| 1:C:287:GLN:NE2 | 1:C:287:GLN:N | 2.60 | 0.47 |
| 2:D:115:ILE:HG12 | 2:D:115:ILE:O | 2.15 | 0.47 |
| 1:A:3:PRO:C | 1:A:5:TYR:H | 2.16 | 0.47 |
| 1:A:119:SER:HG | 1:A:120:GLY:H | 1.60 | 0.47 |
| 2:B:21:ILE:HD13 | 2:B:59:ILE:HG12 | 1.96 | 0.47 |
| 2:B:42:ILE:O | 2:D:46:LEU:HD23 | 2.15 | 0.47 |
| 2:B:77:TYR:O | 2:B:79:PRO:HD3 | 2.14 | 0.47 |
| 2:B:84:ASN:HB3 | 2:B:91:VAL:HG13 | 1.96 | 0.47 |
| 2:B:141:CYS:C | 2:B:143:LYS:H | 2.18 | 0.47 |
| 1:C:89:ALA:HB1 | 1:C:118:PHE:CD1 | 2.49 | 0.47 |
| 1:C:108:GLN:HE22 | 2:D:115:ILE:HD12 | 1.74 | 0.47 |
| 1:C:126:ASN:ND2 | 1:C:128:GLY:H | 2.12 | 0.47 |
| 1:C:204:GLU:OE2 | 1:C:204:GLU:N | 2.48 | 0.47 |
| 1:C:237:PRO:C | 1:C:239:GLU:N | 2.68 | 0.47 |
| 1:C:249:LEU:O | 1:C:249:LEU:HD23 | 2.15 | 0.47 |
| 1:C:303:VAL:O | 1:C:304:LEU:HD23 | 2.15 | 0.47 |
| 2:D:104:ASP:O | 2:D:106:VAL:N | 2.48 | 0.47 |
| 2:D:146:SER:CB | 2:D:148:ASN:HD22 | 2.13 | 0.47 |
| 1:A:93:SER:O | 1:A:96:SER:OG | 2.33 | 0.47 |
| 2:B:18:ILE:HD13 | 2:B:59:ILE:HB | 1.97 | 0.47 |
| 2:B:86:ILE:HG12 | 2:B:91:VAL:HG22 | 1.95 | 0.47 |
| 1:C:43:VAL:O | 1:C:99:VAL:HA | 2.15 | 0.47 |
| 1:C:148:THR:HB | 1:C:149:GLN:OE1 | 2.15 | 0.47 |
| 1:A:4:LEU:O | 1:A:303:VAL:HG13 | 2.15 | 0.47 |
| 1:A:9:ILE:HB | 1:A:125:LEU:HA | 1.96 | 0.47 |
| 2:B:108:VAL:HA | 5:B:178:HOH:O | 2.15 | 0.47 |
| 1:C:66:LEU:CD1 | 1:C:300:LEU:HB2 | 2.45 | 0.47 |
| 2:D:12:ILE:HD13 | 2:D:12:ILE:N | 2.29 | 0.47 |
| 1:A:8:HIS:CD2 | 1:A:124:VAL:H | 2.33 | 0.47 |
| 1:C:253:ASP:CG | 1:C:254:LEU:HD12 | 2.34 | 0.47 |
| 2:D:114:CYS:C | 2:D:116:SER:N | 2.69 | 0.47 |
| 1:A:284:TRP:CG | 1:A:287:GLN:HB2 | 2.50 | 0.46 |
| 2:B:62:GLU:C | 2:B:64:THR:N | 2.67 | 0.46 |
| 2:B:86:ILE:HG12 | 2:B:91:VAL:CA | 2.42 | 0.46 |
| 2:B:137:LYS:HB2 | 2:B:144:GLU:OE2 | 2.15 | 0.46 |
| 2:B:137:LYS:HB2 | 2:B:144:GLU:CD | 2.36 | 0.46 |
| 1:C:23:VAL:HG12 | 1:C:302:LEU:CD1 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:44:ILE:HG13 | 1:C:101:ALA:O | 2.16 | 0.46 |
| 1:C:88:LEU:HD13 | 1:C:106:HIS:NE2 | 2.30 | 0.46 |
| 1:C:196:GLN:O | 1:C:196:GLN:OE1 | 2.33 | 0.46 |
| 1:C:264:LEU:HB3 | 1:C:288:GLN:OE1 | 2.15 | 0.46 |
| 2:D:16:THR:HG23 | 2:D:61:ILE:HD12 | 1.97 | 0.46 |
| 2:D:74:LEU:O | 2:D:75:ALA:O | 2.33 | 0.46 |
| 1:A:264:LEU:HD22 | 1:A:288:GLN:CG | 2.45 | 0.46 |
| 2:B:21:ILE:O | 2:B:57:ASP:N | 2.49 | 0.46 |
| 2:B:39:ASP:CG | 2:D:55:ARG:HH12 | 2.18 | 0.46 |
| 2:B:55:ARG:NH1 | 5:B:204:HOH:O | 2.47 | 0.46 |
| 2:D:113:ASN:O | 2:D:115:ILE:N | 2.48 | 0.46 |
| 1:A:23:VAL:HG22 | 1:A:302:LEU:HD12 | 1.98 | 0.46 |
| 1:A:176:LEU:HB2 | 1:A:184:PHE:HZ | 1.79 | 0.46 |
| 1:C:26:THR:C | 1:C:29:LYS:HG2 | 2.36 | 0.46 |
| 1:C:105:ARG:HH11 | 1:C:167:ARG:NH1 | 2.05 | 0.46 |
| 1:A:169:VAL:O | 1:A:173:THR:N | 2.42 | 0.46 |
| 1:C:10:ILE:O | 1:C:135:PRO:HD3 | 2.15 | 0.46 |
| 1:C:38:LEU:HD12 | 1:C:39:LEU:HD12 | 1.95 | 0.46 |
| 1:C:105:ARG:NH2 | 1:C:134:HIS:NE2 | 2.63 | 0.46 |
| 1:C:145:ILE:HB | 1:C:146:GLN:OE1 | 2.15 | 0.46 |
| 2:D:81:ALA:O | 2:D:96:ARG:NH2 | 2.48 | 0.46 |
| 2:D:135:ALA:HB1 | 2:D:146:SER:HA | 1.98 | 0.46 |
| 1:A:38:LEU:HD23 | 1:A:38:LEU:C | 2.36 | 0.46 |
| 1:A:131:SER:HB2 | 1:A:165:TYR:CA | 2.46 | 0.46 |
| 1:A:222:VAL:HG23 | 1:A:222:VAL:O | 2.15 | 0.46 |
| 2:B:59:ILE:HG22 | 2:B:60:LYS:N | 2.30 | 0.46 |
| 2:B:113:ASN:O | 2:B:114:CYS:C | 2.53 | 0.46 |
| 1:C:59:PHE:CE1 | 1:C:296:ARG:HD3 | 2.50 | 0.46 |
| 1:C:199:LEU:HD13 | 1:C:209:TRP:CE3 | 2.51 | 0.46 |
| 1:C:220:ALA:HA | 1:C:256:ASN:O | 2.15 | 0.46 |
| 1:A:243:VAL:HG22 | 1:A:244:LYS:N | 2.29 | 0.46 |
| 2:B:79:PRO:HG2 | 2:B:80:GLN:H | 1.80 | 0.46 |
| 2:D:127:VAL:CG1 | 2:D:136:LEU:HB3 | 2.46 | 0.46 |
| 1:A:152:LEU:HD12 | 1:A:152:LEU:H | 1.79 | 0.46 |
| 2:B:31:SER:HA | 2:D:27:PHE:CE1 | 2.51 | 0.46 |
| 1:C:21:ASN:HA | 1:C:24:LEU:HB2 | 1.97 | 0.46 |
| 1:C:288:GLN:O | 1:C:291:ASN:OD1 | 2.33 | 0.46 |
| 2:D:99:LEU:HD22 | 2:D:99:LEU:C | 2.36 | 0.46 |
| 2:B:56:LYS:HE3 | 5:B:228:HOH:O | 2.15 | 0.46 |
| 1:C:139:LEU:HA | 1:C:142:LEU:CD1 | 2.29 | 0.46 |
| 1:A:154:ASN:N | 1:A:181:GLY:O | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:LEU:HG | 1:A:176:LEU:H | 1.57 | 0.46 |
| 1:A:202:LEU:CA | 1:A:207:ILE:HB | 2.45 | 0.46 |
| 1:A:236:ALA:HA | 5:A:1392:HOH:O | 2.16 | 0.46 |
| 1:A:246:GLN:HB3 | 1:A:247:PHE:CD1 | 2.50 | 0.46 |
| 1:A:277:VAL:HA | 1:A:280:THR:HG23 | 1.97 | 0.46 |
| 2:B:117:HIS:O | 2:B:119:GLU:N | 2.49 | 0.46 |
| 1:C:195:PRO:HB2 | 1:C:197:TYR:CD2 | 2.50 | 0.46 |
| 2:D:66:LEU:CD2 | 2:D:83:VAL:HG21 | 2.44 | 0.46 |
| 2:D:84:ASN:O | 2:D:86:ILE:CD1 | 2.63 | 0.46 |
| 1:A:3:PRO:CG | 1:A:22:LEU:CD2 | 2.94 | 0.46 |
| 1:A:92:ILE:O | 1:A:94:VAL:N | 2.49 | 0.46 |
| 2:B:83:VAL:HG11 | 2:B:85:ARG:HH12 | 1.80 | 0.46 |
| 1:C:121:ASN:N | 1:C:121:ASN:ND2 | 2.43 | 0.46 |
| 1:C:280:THR:CG2 | 1:C:281:PRO:HD2 | 2.46 | 0.46 |
| 2:D:111:ASN:O | 2:D:117:HIS:CE1 | 2.69 | 0.46 |
| 1:A:12:ILE:HD13 | 5:A:1429:HOH:O | 2.16 | 0.45 |
| 1:A:44:ILE:HG21 | 1:A:103:VAL:HG23 | 1.97 | 0.45 |
| 1:C:227:MET:HG3 | 1:C:265:HIS:ND1 | 2.30 | 0.45 |
| 1:C:280:THR:C | 1:C:282:HIS:N | 2.70 | 0.45 |
| 2:D:143:LYS:CB | 2:D:145:PHE:CE1 | 2.99 | 0.45 |
| 1:A:30:LEU:O | 1:A:32:ALA:N | 2.50 | 0.45 |
| 1:A:92:ILE:CG2 | 1:A:118:PHE:HB2 | 2.46 | 0.45 |
| 1:A:132:ASN:ND2 | 2:B:142:GLU:OE1 | 2.37 | 0.45 |
| 1:A:249:LEU:HG | 1:A:250:ARG:N | 2.31 | 0.45 |
| 1:C:92:ILE:O | 1:C:95:ILE:N | 2.48 | 0.45 |
| 1:C:293:ILE:HB | 1:C:294:PHE:H | 1.62 | 0.45 |
| 2:D:34:LYS:HD3 | 2:D:37:GLU:OE2 | 2.16 | 0.45 |
| 2:D:110:PRO:HG3 | 2:D:150:VAL:HG22 | 1.97 | 0.45 |
| 2:D:146:SER:O | 2:D:148:ASN:N | 2.49 | 0.45 |
| 1:A:106:HIS:HA | 5:A:1388:HOH:O | 2.15 | 0.45 |
| 1:A:278:ASP:OD2 | 1:A:278:ASP:N | 2.49 | 0.45 |
| 1:C:145:ILE:HG23 | 5:C:320:HOH:O | 2.16 | 0.45 |
| 1:C:151:ARG:CG | 1:C:153:ASP:HB2 | 2.46 | 0.45 |
| 2:D:16:THR:CG2 | 2:D:61:ILE:HD12 | 2.46 | 0.45 |
| 2:D:72:ASP:HB3 | 2:D:100:PRO:HD2 | 1.97 | 0.45 |
| 2:D:99:LEU:HD22 | 2:D:100:PRO:O | 2.16 | 0.45 |
| 1:A:283:ALA:O | 1:A:287:GLN:OE1 | 2.34 | 0.45 |
| 2:B:103:ILE:HG22 | 5:B:187:HOH:O | 2.16 | 0.45 |
| 1:C:205:LYS:HD2 | 1:C:205:LYS:N | 2.28 | 0.45 |
| 1:A:3:PRO:HB2 | 1:A:22:LEU:CD2 | 2.46 | 0.45 |
| 1:A:86:GLU:OE1 | 1:A:91:THR:HG23 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:103:VAL:HG22 | 1:A:125:LEU:HD13 | 1.97 | 0.45 |
| 2:B:44:ILE:HG13 | 5:B:188:HOH:O | 2.15 | 0.45 |
| 1:C:48:PHE:O | 1:C:74:SER:O | 2.34 | 0.45 |
| 1:C:265:HIS:CE1 | 1:C:266:PRO:HD2 | 2.52 | 0.45 |
| 2:D:149:VAL:O | 2:D:152:ALA:N | 2.50 | 0.45 |
| 1:C:157:VAL:O | 1:C:158:ALA:HB2 | 2.16 | 0.45 |
| 1:C:163:LEU:HB2 | 1:C:192:LEU:O | 2.17 | 0.45 |
| 1:C:176:LEU:C | 1:C:178:LYS:N | 2.70 | 0.45 |
| 2:D:13:LYS:C | 2:D:88:ASN:HA | 2.36 | 0.45 |
| 2:D:64:THR:HG22 | 2:D:65:PHE:N | 2.32 | 0.45 |
| 2:D:76:LEU:HD12 | 2:D:77:TYR:N | 2.32 | 0.45 |
| 2:D:128:ARG:HG2 | 2:D:128:ARG:HH21 | 1.82 | 0.45 |
| 1:A:2:ASN:OD1 | 1:A:5:TYR:HB2 | 2.15 | 0.45 |
| 1:A:10:ILE:HD12 | 1:A:113:ARG:CD | 2.47 | 0.45 |
| 1:A:39:LEU:HD12 | 1:A:66:LEU:HD12 | 1.99 | 0.45 |
| 1:A:81:LEU:HA | 1:A:86:GLU:HB3 | 1.99 | 0.45 |
| 1:A:189:PRO:HA | 1:A:246:GLN:OE1 | 2.17 | 0.45 |
| 1:C:59:PHE:CG | 1:C:296:ARG:HD3 | 2.51 | 0.45 |
| 1:C:154:ASN:O | 1:C:155:LEU:HG | 2.16 | 0.45 |
| 2:D:126:ALA:N | 2:D:137:LYS:O | 2.50 | 0.45 |
| 1:A:44:ILE:O | 1:A:70:VAL:HG23 | 2.17 | 0.45 |
| 1:A:49:PHE:CZ | 1:A:73:PHE:HZ | 2.35 | 0.45 |
| 1:A:109:GLU:HB2 | 2:B:114:CYS:HA | 1.98 | 0.45 |
| 1:A:146:GLN:NE2 | 1:A:151:ARG:C | 2.71 | 0.45 |
| 1:A:227:MET:CE | 1:A:272:GLU:HB2 | 2.47 | 0.45 |
| 1:A:284:TRP:O | 1:A:285:TYR:C | 2.55 | 0.45 |
| 1:C:249:LEU:HD23 | 1:C:249:LEU:C | 2.38 | 0.45 |
| 2:D:76:LEU:CB | 2:D:134:ILE:HG21 | 2.37 | 0.45 |
| 2:D:128:ARG:CZ | 2:D:130:ARG:HD2 | 2.47 | 0.45 |
| 2:D:141:CYS:O | 2:D:143:LYS:N | 2.49 | 0.45 |
| 1:A:109:GLU:CG | 1:A:132:ASN:HB2 | 2.41 | 0.45 |
| 2:B:41:ARG:HG3 | 2:D:48:LEU:CD2 | 2.37 | 0.45 |
| 2:B:61:ILE:HG23 | 2:B:64:THR:HB | 1.99 | 0.45 |
| 1:C:264:LEU:HD12 | 1:C:288:GLN:CG | 2.47 | 0.45 |
| 2:D:138:CYS:SG | 2:D:141:CYS:CB | 3.00 | 0.45 |
| 1:C:132:ASN:CB | 5:C:419:HOH:O | 2.65 | 0.44 |
| 1:C:262:LYS:O | 1:C:264:LEU:CD2 | 2.65 | 0.44 |
| 1:A:308:LEU:HD23 | 1:A:309:VAL:C | 2.38 | 0.44 |
| 2:B:114:CYS:O | 2:B:117:HIS:CE1 | 2.70 | 0.44 |
| 2:B:123:SER:O | 2:B:124:SER:HB2 | 2.17 | 0.44 |
| 1:C:31:LYS:HG3 | 5:C:391:HOH:O | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:151:ARG:CZ | 1:C:151:ARG:O | 2.65 | 0.44 |
| 1:C:226:TYR:O | 1:C:226:TYR:CD1 | 2.70 | 0.44 |
| 1:C:263:VAL:O | 1:C:264:LEU:HD13 | 2.17 | 0.44 |
| 2:D:69:ASP:OD2 | 2:D:70:GLN:NE2 | 2.49 | 0.44 |
| 2:D:125:PHE:HD1 | 2:D:136:LEU:HB2 | 1.82 | 0.44 |
| 1:A:39:LEU:O | 1:A:68:ALA:N | 2.50 | 0.44 |
| 1:A:237:PRO:HA | 1:A:240:TYR:CE1 | 2.52 | 0.44 |
| 2:B:12:ILE:CG1 | 2:B:13:LYS:N | 2.80 | 0.44 |
| 1:C:5:TYR:H | 1:C:7:LYS:HG2 | 1.82 | 0.44 |
| 1:C:61:THR:O | 1:C:64:HIS:HB2 | 2.16 | 0.44 |
| 2:D:9:VAL:HG13 | 2:D:9:VAL:O | 2.18 | 0.44 |
| 2:D:75:ALA:CA | 2:D:97:PRO:HB2 | 2.47 | 0.44 |
| 2:D:105:ASN:C | 2:D:106:VAL:HG22 | 2.37 | 0.44 |
| 1:A:59:PHE:CD2 | 1:A:63:MET:HE2 | 2.51 | 0.44 |
| 1:A:166:GLY:O | 1:A:168:THR:N | 2.50 | 0.44 |
| 1:A:169:VAL:HG23 | 1:A:170:HIS:H | 1.82 | 0.44 |
| 1:C:39:LEU:C | 1:C:41:HIS:H | 2.20 | 0.44 |
| 1:C:80:SER:CA | 1:C:84:LYS:HB2 | 2.47 | 0.44 |
| 1:C:151:ARG:HB3 | 1:C:151:ARG:HH21 | 1.82 | 0.44 |
| 2:D:58:LEU:C | 2:D:59:ILE:HD12 | 2.37 | 0.44 |
| 1:A:3:PRO:HG2 | 1:A:22:LEU:CD2 | 2.47 | 0.44 |
| 1:A:113:ARG:HG2 | 1:A:113:ARG:NH2 | 2.31 | 0.44 |
| 2:B:84:ASN:HB3 | 2:B:91:VAL:CG1 | 2.47 | 0.44 |
| 1:C:152:LEU:HB2 | 1:C:179:PHE:CE2 | 2.53 | 0.44 |
| 1:C:295:ALA:O | 1:C:298:ALA:N | 2.42 | 0.44 |
| 2:D:24:GLN:NE2 | 2:D:47:ASN:OD1 | 2.50 | 0.44 |
| 2:D:24:GLN:HE21 | 2:D:47:ASN:CG | 2.21 | 0.44 |
| 2:D:66:LEU:HD13 | 2:D:83:VAL:CG2 | 2.47 | 0.44 |
| 2:D:66:LEU:HB3 | 2:D:67:SER:H | 1.64 | 0.44 |
| 2:D:72:ASP:HB3 | 2:D:100:PRO:CD | 2.47 | 0.44 |
| 2:D:133:ASP:OD2 | 2:D:148:ASN:ND2 | 2.50 | 0.44 |
| 1:A:172:LEU:HG | 1:A:176:LEU:HD11 | 1.99 | 0.44 |
| 1:A:243:VAL:HG13 | 1:A:244:LYS:N | 2.25 | 0.44 |
| 1:C:234:ARG:HD3 | 5:C:406:HOH:O | 2.18 | 0.44 |
| 2:D:24:GLN:HG2 | 2:D:47:ASN:OD1 | 2.17 | 0.44 |
| 1:A:88:LEU:N | 2:B:119:GLU:OE1 | 2.49 | 0.44 |
| 2:B:34:LYS:C | 2:B:36:THR:N | 2.68 | 0.44 |
| 1:C:44:ILE:HG22 | 1:C:70:VAL:HG13 | 2.00 | 0.44 |
| 1:C:131:SER:O | 1:C:170:HIS:HE1 | 2.01 | 0.44 |
| 1:C:159:MET:HG2 | 1:C:172:LEU:CD2 | 2.48 | 0.44 |
| 2:D:41:ARG:CB | 2:D:62:GLU:HB3 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:ILE:O | 1:A:149:GLN:HB2 | 2.18 | 0.44 |
| 2:B:140:TYR:HB2 | 5:B:221:HOH:O | 2.17 | 0.44 |
| 1:C:38:LEU:C | 1:C:38:LEU:HD13 | 2.38 | 0.44 |
| 1:A:129:ASP:O | 1:A:129:ASP:OD2 | 2.35 | 0.44 |
| 1:A:195:PRO:HB2 | 1:A:198:ILE:CD1 | 2.48 | 0.44 |
| 2:B:16:THR:CG2 | 2:B:17:VAL:N | 2.81 | 0.44 |
| 2:B:43:THR:CG2 | 2:D:44:ILE:O | 2.66 | 0.44 |
| 2:B:50:SER:HA | 2:B:56:LYS:CE | 2.46 | 0.44 |
| 1:C:161:GLY:HA2 | 5:C:338:HOH:O | 2.18 | 0.44 |
| 1:C:227:MET:HE1 | 1:C:273:ILE:HD13 | 2.00 | 0.44 |
| 1:C:237:PRO:CA | 1:C:240:TYR:CE2 | 2.90 | 0.44 |
| 2:D:84:ASN:HD22 | 2:D:91:VAL:HG21 | 1.82 | 0.44 |
| 1:A:13:ASN:OD1 | 1:A:174:GLN:OE1 | 2.36 | 0.43 |
| 1:A:46:SER:H | 1:A:72:GLY:HA3 | 1.83 | 0.43 |
| 1:A:89:ALA:O | 1:A:93:SER:N | 2.45 | 0.43 |
| 1:A:143:PHE:CD1 | 1:A:143:PHE:C | 2.91 | 0.43 |
| 1:A:198:ILE:HD12 | 1:A:198:ILE:N | 2.33 | 0.43 |
| 1:A:236:ALA:HB3 | 1:A:239:GLU:OE2 | 2.18 | 0.43 |
| 2:B:17:VAL:CG1 | 2:B:58:LEU:HD21 | 2.48 | 0.43 |
| 1:C:250:ARG:O | 1:C:253:ASP:N | 2.47 | 0.43 |
| 1:C:274:ALA:H | 1:C:277:VAL:HG21 | 1.83 | 0.43 |
| 1:A:87:THR:HB | 2:B:119:GLU:OE2 | 2.18 | 0.43 |
| 1:A:94:VAL:CG2 | 1:A:95:ILE:N | 2.82 | 0.43 |
| 1:A:148:THR:OG1 | 1:A:149:GLN:HG2 | 2.17 | 0.43 |
| 1:A:280:THR:HA | 5:A:1411:HOH:O | 2.18 | 0.43 |
| 1:C:4:LEU:HD23 | 1:C:4:LEU:O | 2.18 | 0.43 |
| 1:C:227:MET:O | 1:C:266:PRO:CD | 2.62 | 0.43 |
| 1:C:284:TRP:CD1 | 1:C:284:TRP:O | 2.71 | 0.43 |
| 2:D:124:SER:CB | 2:D:139:LYS:HD3 | 2.48 | 0.43 |
| 1:A:21:ASN:OD1 | 1:A:21:ASN:N | 2.49 | 0.43 |
| 1:A:173:THR:HG21 | 1:A:194:MET:CE | 2.48 | 0.43 |
| 2:B:39:ASP:CG | 2:D:55:ARG:NH1 | 2.71 | 0.43 |
| 2:B:100:PRO:O | 2:B:127:VAL:HB | 2.18 | 0.43 |
| 1:C:150:GLY:O | 1:C:151:ARG:C | 2.57 | 0.43 |
| 2:D:41:ARG:NH2 | 2:D:60:LYS:HD3 | 2.34 | 0.43 |
| 1:A:17:ARG:HG2 | 1:A:179:PHE:CE1 | 2.53 | 0.43 |
| 1:A:133:GLN:HG3 | 2:B:142:GLU:OE1 | 2.19 | 0.43 |
| 1:C:46:SER:C | 1:C:72:GLY:HA3 | 2.39 | 0.43 |
| 1:C:112:ALA:O | 1:C:116:THR:HG23 | 2.18 | 0.43 |
| 1:A:220:ALA:HB2 | 1:A:256:ASN:HD22 | 1.83 | 0.43 |
| 1:C:16:SER:O | 1:C:19:ASP:OD2 | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:97:THR:O | 1:C:98:TYR:C | 2.57 | 0.43 |
| 1:A:81:LEU:HD12 | 1:A:88:LEU:HA | 2.01 | 0.43 |
| 1:A:102:ILE:O | 1:A:124:VAL:HA | 2.19 | 0.43 |
| 1:A:181:GLY:O | 1:A:182:ASN:CG | 2.57 | 0.43 |
| 2:B:19:ASP:HA | 2:B:58:LEU:HG | 2.00 | 0.43 |
| 1:C:66:LEU:HD12 | 1:C:300:LEU:HB2 | 2.00 | 0.43 |
| 1:C:66:LEU:HD21 | 1:C:297:GLN:HB3 | 1.99 | 0.43 |
| 1:C:126:ASN:HD21 | 1:C:128:GLY:C | 2.21 | 0.43 |
| 1:C:157:VAL:HA | 1:C:224:ILE:O | 2.19 | 0.43 |
| 1:C:218:VAL:O | 1:C:218:VAL:CG1 | 2.62 | 0.43 |
| 1:C:267:LEU:HD13 | 1:C:268:PRO:HA | 2.01 | 0.43 |
| 1:C:306:ARG:HH21 | 1:C:306:ARG:HB2 | 1.82 | 0.43 |
| 1:A:284:TRP:CD1 | 1:A:284:TRP:O | 2.71 | 0.43 |
| 1:C:114:LEU:C | 1:C:114:LEU:CD1 | 2.83 | 0.43 |
| 1:C:151:ARG:HG2 | 1:C:153:ASP:H | 1.84 | 0.43 |
| 2:D:9:VAL:C | 2:D:11:ALA:N | 2.71 | 0.43 |
| 1:A:110:GLY:C | 1:A:112:ALA:N | 2.70 | 0.43 |
| 1:A:167:ARG:HG3 | 1:A:168:THR:H | 1.82 | 0.43 |
| 1:C:12:ILE:HG22 | 1:C:12:ILE:O | 2.18 | 0.43 |
| 1:C:59:PHE:HE1 | 1:C:296:ARG:NH2 | 2.16 | 0.43 |
| 2:D:126:ALA:O | 2:D:136:LEU:CB | 2.66 | 0.43 |
| 2:D:132:ASN:CG | 2:D:133:ASP:H | 2.21 | 0.43 |
| 1:A:205:LYS:O | 1:A:207:ILE:HG12 | 2.18 | 0.43 |
| 1:C:45:ALA:CB | 1:C:72:GLY:H | 2.31 | 0.43 |
| 1:C:137:GLN:HG3 | 5:C:325:HOH:O | 2.18 | 0.43 |
| 1:C:244:LYS:HE3 | 5:C:376:HOH:O | 2.19 | 0.43 |
| 2:D:105:ASN:C | 2:D:106:VAL:CG2 | 2.87 | 0.43 |
| 2:D:111:ASN:O | 2:D:113:ASN:N | 2.52 | 0.43 |
| 1:A:2:ASN:OD1 | 1:A:5:TYR:N | 2.52 | 0.43 |
| 2:B:150:VAL:HG12 | 2:B:150:VAL:O | 2.18 | 0.43 |
| 1:C:169:VAL:C | 1:C:172:LEU:HD13 | 2.39 | 0.43 |
| 1:C:250:ARG:C | 1:C:252:SER:N | 2.71 | 0.43 |
| 2:D:76:LEU:HA | 2:D:134:ILE:HG13 | 2.01 | 0.43 |
| 1:A:5:TYR:CG | 1:A:306:ARG:HA | 2.54 | 0.42 |
| 1:A:183:ARG:CZ | 1:A:208:ALA:HB3 | 2.49 | 0.42 |
| 1:A:187:ILE:N | 1:A:187:ILE:CD1 | 2.75 | 0.42 |
| 1:A:309:VAL:HG23 | 1:A:310:LEU:N | 2.34 | 0.42 |
| 2:B:25:ILE:O | 2:B:25:ILE:HG22 | 2.19 | 0.42 |
| 2:B:107:LEU:HB2 | 2:B:125:PHE:CE1 | 2.54 | 0.42 |
| 1:C:130:GLY:O | 1:C:167:ARG:HD3 | 2.20 | 0.42 |
| 1:C:235:LEU:HD23 | 1:C:235:LEU:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:9:VAL:O | 2:D:11:ALA:N | 2.52 | 0.42 |
| 2:D:28:LYS:O | 2:D:32:LEU:N | 2.52 | 0.42 |
| 2:D:56:LYS:CD | 2:D:57:ASP:N | 2.74 | 0.42 |
| 1:A:26:THR:CG2 | 1:A:302:LEU:HD21 | 2.50 | 0.42 |
| 1:A:119:SER:HG | 1:A:120:GLY:N | 2.17 | 0.42 |
| 1:A:204:GLU:C | 1:A:206:GLY:N | 2.72 | 0.42 |
| 1:A:205:LYS:C | 1:A:207:ILE:N | 2.70 | 0.42 |
| 2:B:115:ILE:HA | 5:B:173:HOH:O | 2.19 | 0.42 |
| 1:C:4:LEU:HB3 | 1:C:22:LEU:HD23 | 2.01 | 0.42 |
| 1:C:252:SER:O | 1:C:255:HIS:CE1 | 2.73 | 0.42 |
| 1:C:261:MET:SD | 1:C:262:LYS:N | 2.92 | 0.42 |
| 2:D:99:LEU:CD2 | 2:D:129:LYS:NZ | 2.82 | 0.42 |
| 1:A:73:PHE:CD2 | 1:A:79:THR:HG21 | 2.55 | 0.42 |
| 1:A:261:MET:SD | 1:A:262:LYS:N | 2.92 | 0.42 |
| 1:A:265:HIS:HA | 1:A:266:PRO:HD2 | 1.75 | 0.42 |
| 2:B:12:ILE:CG1 | 2:B:13:LYS:H | 2.31 | 0.42 |
| 2:B:24:GLN:NE2 | 2:D:38:THR:O | 2.52 | 0.42 |
| 2:D:103:ILE:HG13 | 2:D:126:ALA:N | 2.34 | 0.42 |
| 1:A:23:VAL:HG22 | 1:A:302:LEU:HD11 | 2.01 | 0.42 |
| 1:A:92:ILE:O | 1:A:93:SER:C | 2.58 | 0.42 |
| 1:A:104:MET:O | 1:A:127:ALA:N | 2.47 | 0.42 |
| 1:A:149:GLN:O | 1:A:150:GLY:C | 2.58 | 0.42 |
| 1:A:174:GLN:HA | 1:A:201:MET:HE1 | 2.02 | 0.42 |
| 1:C:139:LEU:O | 1:C:142:LEU:N | 2.52 | 0.42 |
| 1:C:262:LYS:HB2 | 5:C:377:HOH:O | 2.19 | 0.42 |
| 1:C:263:VAL:O | 1:C:284:TRP:N | 2.42 | 0.42 |
| 2:D:12:ILE:HG23 | 2:D:41:ARG:HH21 | 1.83 | 0.42 |
| 2:D:26:GLY:O | 2:D:30:LEU:CD2 | 2.68 | 0.42 |
| 2:D:79:PRO:HG2 | 2:D:80:GLN:H | 1.84 | 0.42 |
| 2:D:137:LYS:HB2 | 2:D:144:GLU:CD | 2.39 | 0.42 |
| 1:A:22:LEU:HD12 | 5:A:1421:HOH:O | 2.20 | 0.42 |
| 1:A:187:ILE:HA | 5:A:1327:HOH:O | 2.19 | 0.42 |
| 2:B:42:ILE:HG12 | 2:B:61:ILE:HG13 | 2.01 | 0.42 |
| 1:C:45:ALA:HB3 | 1:C:102:ILE:HG22 | 2.00 | 0.42 |
| 1:C:132:ASN:CA | 1:C:170:HIS:ND1 | 2.76 | 0.42 |
| 2:D:16:THR:CB | 2:D:65:PHE:HA | 2.50 | 0.42 |
| 2:D:37:GLU:HB3 | 5:D:173:HOH:O | 2.18 | 0.42 |
| 1:A:109:GLU:CB | 2:B:114:CYS:HA | 2.49 | 0.42 |
| 1:A:196:GLN:C | 1:A:198:ILE:N | 2.72 | 0.42 |
| 1:A:255:HIS:HB3 | 5:A:1396:HOH:O | 2.19 | 0.42 |
| 2:B:28:LYS:C | 2:B:30:LEU:N | 2.72 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:76:LEU:HD23 | 2:B:76:LEU:N | 2.09 | 0.42 |
| 2:B:140:TYR:N | 5:B:221:HOH:O | 2.52 | 0.42 |
| 1:C:104:MET:HG3 | 1:C:126:ASN:OD1 | 2.20 | 0.42 |
| 1:C:167:ARG:HH11 | 1:C:234:ARG:HH22 | 1.68 | 0.42 |
| 1:C:285:TYR:CA | 1:C:288:GLN:OE1 | 2.60 | 0.42 |
| 2:D:107:LEU:CD1 | 2:D:151:LEU:HD21 | 2.47 | 0.42 |
| 1:A:131:SER:N | 1:A:234:ARG:NE | 2.67 | 0.42 |
| 1:A:186:PHE:C | 1:A:187:ILE:HD12 | 2.40 | 0.42 |
| 2:B:75:ALA:HB2 | 2:B:98:SER:O | 2.20 | 0.42 |
| 2:D:126:ALA:O | 2:D:127:VAL:CG1 | 2.62 | 0.42 |
| 1:A:89:ALA:O | 1:A:93:SER:OG | 2.38 | 0.42 |
| 1:A:217:GLU:C | 1:A:219:MET:H | 2.22 | 0.42 |
| 1:A:264:LEU:CD2 | 1:A:288:GLN:HB2 | 2.50 | 0.42 |
| 1:C:165:TYR:CE2 | 1:C:192:LEU:HD21 | 2.55 | 0.42 |
| 2:D:96:ARG:NH2 | 2:D:97:PRO:CD | 2.81 | 0.42 |
| 1:A:55:THR:HG21 | 1:A:105:ARG:NH1 | 2.33 | 0.42 |
| 2:B:39:ASP:CA | 2:D:55:ARG:NH2 | 2.81 | 0.42 |
| 2:B:129:LYS:C | 2:B:129:LYS:CE | 2.86 | 0.42 |
| 1:C:45:ALA:N | 1:C:99:VAL:HG11 | 2.35 | 0.42 |
| 1:C:127:ALA:HB1 | 1:C:136:THR:HG1 | 1.85 | 0.42 |
| 1:C:280:THR:O | 1:C:282:HIS:N | 2.53 | 0.42 |
| 2:D:16:THR:HB | 2:D:65:PHE:HA | 2.02 | 0.42 |
| 2:D:18:ILE:HG22 | 2:D:21:ILE:HD11 | 2.02 | 0.42 |
| 1:A:55:THR:HB | 3:A:1311:PCT:O1 | 2.19 | 0.42 |
| 1:A:109:GLU:OE2 | 1:A:132:ASN:CB | 2.68 | 0.42 |
| 1:A:214:SER:HB3 | 1:A:217:GLU:HG3 | 2.02 | 0.42 |
| 2:B:44:ILE:CG2 | 2:D:44:ILE:HB | 2.27 | 0.42 |
| 2:B:94:LYS:HD2 | 2:B:94:LYS:HA | 1.81 | 0.42 |
| 2:B:134:ILE:O | 2:B:147:HIS:HB3 | 2.20 | 0.42 |
| 2:B:136:LEU:O | 2:B:145:PHE:N | 2.53 | 0.42 |
| 1:C:48:PHE:CE2 | 1:C:51:ALA:HA | 2.55 | 0.42 |
| 1:C:172:LEU:O | 1:C:174:GLN:N | 2.43 | 0.42 |
| 1:A:280:THR:CB | 1:A:281:PRO:CD | 2.87 | 0.41 |
| 1:C:13:ASN:HB2 | 1:C:174:GLN:CD | 2.41 | 0.41 |
| 1:C:59:PHE:O | 1:C:60:GLU:C | 2.58 | 0.41 |
| 2:D:111:ASN:C | 2:D:113:ASN:N | 2.73 | 0.41 |
| 1:A:10:ILE:CG1 | 1:A:11:SER:H | 2.32 | 0.41 |
| 1:A:136:THR:HB | 1:A:296:ARG:HH11 | 1.84 | 0.41 |
| 1:A:202:LEU:H | 1:A:202:LEU:HG | 1.54 | 0.41 |
| 2:B:76:LEU:HG | 2:B:77:TYR:CD2 | 2.55 | 0.41 |
| 1:C:61:THR:HG21 | 5:C:351:HOH:O | 2.17 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:178:LYS:HA | 5:C:367:HOH:O | 2.21 | 0.41 |
| 1:C:223:ASP:C | 1:C:224:ILE:HG13 | 2.41 | 0.41 |
| 1:C:292:GLY:O | 1:C:296:ARG:HB2 | 2.20 | 0.41 |
| 1:A:277:VAL:O | 1:A:283:ALA:HB2 | 2.19 | 0.41 |
| 2:B:104:ASP:HB2 | 5:B:172:HOH:O | 2.19 | 0.41 |
| 1:C:26:THR:HG22 | 1:C:30:LEU:HG | 2.01 | 0.41 |
| 1:C:260:ASN:O | 5:C:331:HOH:O | 2.21 | 0.41 |
| 2:D:28:LYS:C | 2:D:30:LEU:N | 2.73 | 0.41 |
| 2:D:86:ILE:CG2 | 2:D:90:GLU:N | 2.84 | 0.41 |
| 2:D:143:LYS:HB3 | 2:D:145:PHE:CZ | 2.55 | 0.41 |
| 1:A:189:PRO:CG | 1:A:192:LEU:HD12 | 2.30 | 0.41 |
| 2:B:60:LYS:HG3 | 5:B:186:HOH:O | 2.19 | 0.41 |
| 1:C:6:GLN:H | 1:C:303:VAL:HG13 | 1.86 | 0.41 |
| 1:C:59:PHE:CE2 | 1:C:300:LEU:HD21 | 2.55 | 0.41 |
| 2:D:56:LYS:HD2 | 2:D:57:ASP:H | 1.77 | 0.41 |
| 1:A:219:MET:HE2 | 1:A:257:ALA:HA | 2.02 | 0.41 |
| 1:A:229:ARG:HD2 | 1:A:270:VAL:HG23 | 2.02 | 0.41 |
| 1:C:4:LEU:HA | 1:C:7:LYS:HG3 | 2.01 | 0.41 |
| 1:C:274:ALA:O | 1:C:277:VAL:CG2 | 2.67 | 0.41 |
| 2:D:134:ILE:H | 2:D:147:HIS:CE1 | 2.39 | 0.41 |
| 1:A:4:LEU:HD23 | 1:A:7:LYS:HD2 | 2.02 | 0.41 |
| 1:A:26:THR:CB | 1:A:302:LEU:HD21 | 2.50 | 0.41 |
| 1:A:176:LEU:CD1 | 1:A:184:PHE:CZ | 3.03 | 0.41 |
| 1:A:197:TYR:CE1 | 1:A:198:ILE:HD11 | 2.56 | 0.41 |
| 2:B:38:THR:HG23 | 2:B:38:THR:O | 2.21 | 0.41 |
| 1:C:60:GLU:O | 1:C:70:VAL:HG21 | 2.20 | 0.41 |
| 1:C:65:ARG:CZ | 5:C:351:HOH:O | 2.69 | 0.41 |
| 1:C:183:ARG:HG2 | 1:C:208:ALA:CB | 2.51 | 0.41 |
| 1:C:187:ILE:HG21 | 1:C:215:ILE:HD11 | 2.02 | 0.41 |
| 1:C:204:GLU:HG2 | 1:C:205:LYS:HZ2 | 1.85 | 0.41 |
| 1:C:229:ARG:HH12 | 1:C:233:GLU:CG | 2.34 | 0.41 |
| 2:D:67:SER:O | 2:D:71:VAL:CG2 | 2.68 | 0.41 |
| 2:D:68:GLU:O | 2:D:72:ASP:OD2 | 2.38 | 0.41 |
| 2:D:93:GLY:C | 2:D:95:SER:H | 2.24 | 0.41 |
| 2:D:99:LEU:CD2 | 2:D:129:LYS:HZ2 | 2.33 | 0.41 |
| 2:D:125:PHE:HB3 | 2:D:126:ALA:H | 1.55 | 0.41 |
| 2:D:141:CYS:C | 2:D:143:LYS:N | 2.73 | 0.41 |
| 1:A:114:LEU:CD2 | 2:B:115:ILE:HG23 | 2.50 | 0.41 |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:N | 2.19 | 0.41 |
| 1:A:196:GLN:HA | 1:A:199:LEU:HB2 | 2.02 | 0.41 |
| 1:C:12:ILE:C | 1:C:174:GLN:HE22 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:50:GLU:HB3 | 1:C:51:ALA:H | 1.65 | 0.41 |
| 1:C:88:LEU:HD22 | 1:C:106:HIS:NE2 | 2.36 | 0.41 |
| 1:C:109:GLU:C | 1:C:111:ALA:H | 2.24 | 0.41 |
| 1:C:186:PHE:HE1 | 1:C:209:TRP:HB2 | 1.86 | 0.41 |
| 1:A:41:HIS:O | 1:A:42:LYS:O | 2.39 | 0.41 |
| 2:B:30:LEU:HA | 2:B:35:LEU:HD12 | 2.01 | 0.41 |
| 2:B:58:LEU:HD23 | 2:B:59:ILE:O | 2.21 | 0.41 |
| 1:C:110:GLY:N | 1:C:129:ASP:OD1 | 2.49 | 0.41 |
| 1:C:157:VAL:CG1 | 1:C:158:ALA:H | 2.12 | 0.41 |
| 2:D:30:LEU:HB3 | 2:D:36:THR:OG1 | 2.21 | 0.41 |
| 1:A:10:ILE:HD12 | 1:A:113:ARG:HD2 | 2.02 | 0.41 |
| 1:A:56:ARG:HG2 | 1:A:60:GLU:OE2 | 2.21 | 0.41 |
| 1:A:110:GLY:C | 1:A:112:ALA:H | 2.24 | 0.41 |
| 1:A:126:ASN:HD22 | 1:A:135:PRO:HD2 | 1.86 | 0.41 |
| 1:C:26:THR:HA | 1:C:29:LYS:HD2 | 2.02 | 0.41 |
| 1:C:44:ILE:HG13 | 1:C:101:ALA:CB | 2.42 | 0.41 |
| 1:C:54:ARG:NH1 | 1:C:268:PRO:HD3 | 2.35 | 0.41 |
| 1:C:92:ILE:HD13 | 1:C:95:ILE:HD12 | 2.02 | 0.41 |
| 1:C:116:THR:HG22 | 1:C:124:VAL:HG11 | 2.03 | 0.41 |
| 1:C:126:ASN:ND2 | 1:C:126:ASN:C | 2.74 | 0.41 |
| 1:C:163:LEU:CD1 | 1:C:188:ALA:HB2 | 2.51 | 0.41 |
| 1:C:186:PHE:O | 1:C:187:ILE:HG13 | 2.21 | 0.41 |
| 2:D:111:ASN:C | 2:D:113:ASN:H | 2.23 | 0.41 |
| 2:B:23:ALA:C | 2:B:25:ILE:H | 2.23 | 0.41 |
| 1:C:214:SER:HB2 | 1:C:216:GLU:CD | 2.40 | 0.41 |
| 2:D:41:ARG:CB | 2:D:62:GLU:CB | 2.93 | 0.41 |
| 2:D:105:ASN:HA | 2:D:123:SER:C | 2.42 | 0.41 |
| 1:A:100:ASP:HB2 | 5:A:1410:HOH:O | 2.21 | 0.40 |
| 1:A:146:GLN:NE2 | 1:A:152:LEU:N | 2.68 | 0.40 |
| 1:A:176:LEU:HB2 | 1:A:184:PHE:CZ | 2.55 | 0.40 |
| 1:A:195:PRO:O | 1:A:198:ILE:HD13 | 2.22 | 0.40 |
| 1:A:266:PRO:O | 1:A:267:LEU:O | 2.38 | 0.40 |
| 2:B:34:LYS:HD3 | 2:B:37:GLU:OE2 | 2.21 | 0.40 |
| 2:B:138:CYS:CB | 5:B:221:HOH:O | 2.69 | 0.40 |
| 1:C:9:ILE:HB | 1:C:125:LEU:HG | 2.02 | 0.40 |
| 1:C:12:ILE:CD1 | 1:C:135:PRO:HA | 2.32 | 0.40 |
| 1:C:48:PHE:HB3 | 1:C:74:SER:O | 2.20 | 0.40 |
| 1:C:92:ILE:CD1 | 1:C:115:ALA:HB1 | 2.52 | 0.40 |
| 1:C:261:MET:O | 1:C:282:HIS:ND1 | 2.54 | 0.40 |
| 2:D:22:PRO:HB2 | 2:D:25:ILE:HG13 | 2.03 | 0.40 |
| 2:D:75:ALA:N | 2:D:97:PRO:HB2 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:141:CYS:C | 2:D:143:LYS:H | 2.25 | 0.40 |
| 1:A:55:THR:HG21 | 1:A:105:ARG:NE | 2.35 | 0.40 |
| 1:A:250:ARG:NH2 | 1:A:276:ASP:OD2 | 2.54 | 0.40 |
| 1:A:262:LYS:HG2 | 1:A:282:HIS:HA | 2.03 | 0.40 |
| 1:A:298:ALA:O | 1:A:302:LEU:CD2 | 2.69 | 0.40 |
| 5:B:165:HOH:O | 2:D:49:PRO:HG2 | 2.21 | 0.40 |
| 1:C:39:LEU:HD12 | 1:C:39:LEU:N | 2.36 | 0.40 |
| 1:C:132:ASN:O | 1:C:170:HIS:ND1 | 2.54 | 0.40 |
| 1:C:197:TYR:CE1 | 2:D:143:LYS:HA | 2.56 | 0.40 |
| 1:C:219:MET:CB | 1:C:256:ASN:ND2 | 2.72 | 0.40 |
| 2:D:65:PHE:HB3 | 2:D:66:LEU:H | 1.67 | 0.40 |
| 2:D:86:ILE:HG13 | 2:D:91:VAL:HG22 | 2.02 | 0.40 |
| 1:A:33:ASN:HA | 1:A:34:PRO:HD3 | 1.74 | 0.40 |
| 1:C:135:PRO:HG2 | 1:C:136:THR:N | 2.35 | 0.40 |
| 1:C:189:PRO:HD2 | 1:C:192:LEU:HD12 | 2.02 | 0.40 |
| 1:C:250:ARG:O | 1:C:252:SER:N | 2.54 | 0.40 |
| 1:C:264:LEU:CA | 1:C:288:GLN:OE1 | 2.70 | 0.40 |
| 1:C:271:ASP:O | 1:C:272:GLU:C | 2.59 | 0.40 |
| 1:A:12:ILE:HD11 | 1:A:135:PRO:HA | 2.04 | 0.40 |
| 1:A:160:VAL:O | 1:A:227:MET:HA | 2.21 | 0.40 |
| 1:A:229:ARG:HA | 1:A:272:GLU:OE2 | 2.21 | 0.40 |
| 1:A:277:VAL:HG12 | 1:A:285:TYR:OH | 2.21 | 0.40 |
| 1:C:164:LYS:HG3 | 1:C:195:PRO:HD3 | 2.02 | 0.40 |
| 2:D:34:LYS:HD3 | 2:D:37:GLU:CD | 2.42 | 0.40 |
| 2:B:46:LEU:HD12 | 2:D:42:ILE:CD1 | 2.52 | 0.40 |
| 2:B:117:HIS:ND1 | 2:B:117:HIS:N | 2.69 | 0.40 |
| 1:C:31:LYS:NZ | 1:C:143:PHE:CE2 | 2.80 | 0.40 |
| 1:C:246:GLN:HA | 5:C:314:HOH:O | 2.20 | 0.40 |
| 2:D:30:LEU:HD13 | 2:D:30:LEU:N | 2.34 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 308/310 (99%) | 200 (65%) | 73 (24%) | 35 (11%) | 0 | 1 |
| 1 | C | 308/310 (99%) | 187 (61%) | 70 (23%) | 51 (17%) | 0 | 0 |
| 2 | B | 144/153 (94%) | 82 (57%) | 44 (31%) | 18 (12%) | 0 | 0 |
| 2 | D | 144/153 (94%) | 88 (61%) | 34 (24%) | 22 (15%) | 0 | 0 |
| All | All | 904/926 (98%) | 557 (62%) | 221 (24%) | 126 (14%) | 0 | 0 |

All (126) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | GLN |
| 1 | A | 21 | ASN |
| 1 | A | 192 | LEU |
| 1 | A | 231 | GLN |
| 1 | A | 244 | LYS |
| 1 | A | 302 | LEU |
| 2 | B | 10 | GLU |
| 2 | B | 85 | ARG |
| 2 | B | 106 | VAL |
| 2 | B | 142 | GLU |
| 1 | C | 32 | ALA |
| 1 | C | 37 | GLU |
| 1 | C | 68 | ALA |
| 1 | C | 97 | THR |
| 1 | C | 98 | TYR |
| 1 | C | 190 | ASP |
| 1 | C | 209 | TRP |
| 1 | C | 213 | SER |
| 1 | C | 231 | GLN |
| 1 | C | 235 | LEU |
| 1 | C | 258 | LYS |
| 1 | C | 283 | ALA |
| 1 | C | 293 | ILE |
| 1 | C | 295 | ALA |
| 1 | C | 296 | ARG |
| 2 | D | 75 | ALA |
| 2 | D | 105 | ASN |
| 2 | D | 106 | VAL |
| 2 | D | 115 | ILE |
| 2 | D | 127 | VAL |
| 1 | A | 37 | GLU |
| 1 | A | 38 | LEU |
| 1 | A | 42 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 89 | ALA |
| 1 | A | 93 | SER |
| 1 | A | 132 | ASN |
| 1 | A | 150 | GLY |
| 1 | A | 197 | TYR |
| 1 | A | 201 | MET |
| 1 | A | 252 | SER |
| 1 | A | 267 | LEU |
| 1 | A | 309 | VAL |
| 2 | B | 41 | ARG |
| 2 | B | 67 | SER |
| 2 | B | 77 | TYR |
| 2 | B | 101 | GLU |
| 2 | B | 105 | ASN |
| 2 | B | 118 | ALA |
| 1 | C | 14 | ASP |
| 1 | C | 42 | LYS |
| 1 | C | 113 | ARG |
| 1 | C | 153 | ASP |
| 1 | C | 154 | ASN |
| 1 | C | 166 | GLY |
| 1 | C | 193 | ALA |
| 1 | C | 238 | SER |
| 1 | C | 255 | HIS |
| 1 | C | 306 | ARG |
| 2 | D | 29 | LEU |
| 2 | D | 114 | CYS |
| 2 | D | 123 | SER |
| 2 | D | 135 | ALA |
| 2 | D | 142 | GLU |
| 1 | A | 16 | SER |
| 1 | A | 52 | SER |
| 1 | A | 78 | ASN |
| 1 | A | 205 | LYS |
| 1 | A | 283 | ALA |
| 2 | B | 9 | VAL |
| 2 | B | 47 | ASN |
| 2 | B | 63 | ASN |
| 2 | B | 88 | ASN |
| 1 | C | 18 | ASP |
| 1 | C | 40 | LYS |
| 1 | C | 54 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 55 | THR |
| 1 | C | 135 | PRO |
| 1 | C | 151 | ARG |
| 1 | C | 157 | VAL |
| 1 | C | 158 | ALA |
| 1 | C | 172 | LEU |
| 1 | C | 194 | MET |
| 1 | C | 292 | GLY |
| 2 | D | 10 | GLU |
| 2 | D | 112 | SER |
| 2 | D | 131 | ALA |
| 2 | D | 147 | HIS |
| 1 | A | 167 | ARG |
| 1 | A | 219 | MET |
| 1 | A | 255 | HIS |
| 2 | B | 124 | SER |
| 1 | C | 67 | GLY |
| 1 | C | 246 | GLN |
| 2 | D | 42 | ILE |
| 2 | D | 67 | SER |
| 2 | D | 116 | SER |
| 1 | A | 3 | PRO |
| 1 | A | 271 | ASP |
| 2 | B | 73 | GLN |
| 2 | B | 130 | ARG |
| 1 | C | 36 | PRO |
| 1 | C | 71 | VAL |
| 1 | C | 83 | LYS |
| 1 | C | 84 | LYS |
| 1 | C | 242 | ASN |
| 1 | C | 302 | LEU |
| 2 | D | 95 | SER |
| 1 | A | 144 | THR |
| 1 | A | 168 | THR |
| 1 | A | 218 | VAL |
| 1 | C | 66 | LEU |
| 1 | C | 76 | SER |
| 1 | C | 267 | LEU |
| 2 | D | 12 | ILE |
| 1 | A | 206 | GLY |
| 1 | A | 222 | VAL |
| 2 | D | 45 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 134 | ILE |
| 1 | A | 293 | ILE |
| 1 | C | 10 | ILE |
| 1 | A | 189 | PRO |
| 2 | B | 92 | VAL |
| 1 | C | 270 | VAL |
| 2 | D | 121 | VAL |
| 1 | C | 187 | ILE |
| 1 | C | 207 | 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 | 260/260 (100%) | 209 (80%) | 51 (20%) | 1 | 4 |
| 1 | C | 260/260 (100%) | 218 (84%) | 42 (16%) | 2 | 7 |
| 2 | B | 129/137 (94%) | 112 (87%) | 17 (13%) | 4 | 12 |
| 2 | D | 129/137 (94%) | 112 (87%) | 17 (13%) | 4 | 12 |
| All | All | 778/794 (98%) | 651 (84%) | 127 (16%) | 2 | 7 |

All (127) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 14 | ASP |
| 1 | A | 18 | ASP |
| 1 | A | 19 | ASP |
| 1 | A | 21 | ASN |
| 1 | A | 35 | GLN |
| 1 | A | 37 | GLU |
| 1 | A | 47 | CYS |
| 1 | A | 59 | PHE |
| 1 | A | 62 | SER |
| 1 | A | 70 | VAL |
| 1 | A | 74 | SER |
| 1 | A | 79 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 91 | THR |
| 1 | A | 92 | ILE |
| 1 | A | 97 | THR |
| 1 | A | 100 | ASP |
| 1 | A | 104 | MET |
| 1 | A | 109 | GLU |
| 1 | A | 113 | ARG |
| 1 | A | 114 | LEU |
| 1 | A | 125 | LEU |
| 1 | A | 134 | HIS |
| 1 | A | 137 | GLN |
| 1 | A | 143 | PHE |
| 1 | A | 144 | THR |
| 1 | A | 145 | ILE |
| 1 | A | 146 | GLN |
| 1 | A | 152 | LEU |
| 1 | A | 156 | HIS |
| 1 | A | 176 | LEU |
| 1 | A | 180 | ASP |
| 1 | A | 194 | MET |
| 1 | A | 196 | GLN |
| 1 | A | 219 | MET |
| 1 | A | 225 | LEU |
| 1 | A | 233 | GLU |
| 1 | A | 250 | ARG |
| 1 | A | 253 | ASP |
| 1 | A | 255 | HIS |
| 1 | A | 267 | LEU |
| 1 | A | 269 | ARG |
| 1 | A | 275 | THR |
| 1 | A | 278 | ASP |
| 1 | A | 282 | HIS |
| 1 | A | 285 | TYR |
| 1 | A | 287 | GLN |
| 1 | A | 291 | ASN |
| 1 | A | 302 | LEU |
| 1 | A | 303 | VAL |
| 1 | A | 305 | ASN |
| 1 | A | 306 | ARG |
| 2 | B | 36 | THR |
| 2 | B | 37 | GLU |
| 2 | B | 38 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 44 | ILE |
| 2 | B | 46 | LEU |
| 2 | B | 47 | ASN |
| 2 | B | 53 | MET |
| 2 | B | 70 | GLN |
| 2 | B | 76 | LEU |
| 2 | B | 102 | ARG |
| 2 | B | 106 | VAL |
| 2 | B | 113 | ASN |
| 2 | B | 117 | HIS |
| 2 | B | 129 | LYS |
| 2 | B | 134 | ILE |
| 2 | B | 151 | LEU |
| 2 | B | 153 | ASN |
| 1 | C | 14 | ASP |
| 1 | C | 15 | LEU |
| 1 | C | 18 | ASP |
| 1 | C | 23 | VAL |
| 1 | C | 37 | GLU |
| 1 | C | 38 | LEU |
| 1 | C | 48 | PHE |
| 1 | C | 49 | PHE |
| 1 | C | 56 | ARG |
| 1 | C | 59 | PHE |
| 1 | C | 70 | VAL |
| 1 | C | 98 | TYR |
| 1 | C | 100 | ASP |
| 1 | C | 102 | ILE |
| 1 | C | 106 | HIS |
| 1 | C | 109 | GLU |
| 1 | C | 121 | ASN |
| 1 | C | 140 | LEU |
| 1 | C | 146 | GLN |
| 1 | C | 147 | GLU |
| 1 | C | 149 | GLN |
| 1 | C | 151 | ARG |
| 1 | C | 152 | LEU |
| 1 | C | 174 | GLN |
| 1 | C | 180 | ASP |
| 1 | C | 183 | ARG |
| 1 | C | 196 | GLN |
| 1 | C | 202 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 204 | GLU |
| 1 | C | 205 | LYS |
| 1 | C | 216 | GLU |
| 1 | C | 233 | GLU |
| 1 | C | 235 | LEU |
| 1 | C | 242 | ASN |
| 1 | C | 243 | VAL |
| 1 | C | 247 | PHE |
| 1 | C | 278 | ASP |
| 1 | C | 293 | ILE |
| 1 | C | 294 | PHE |
| 1 | C | 306 | ARG |
| 1 | C | 308 | LEU |
| 1 | C | 310 | LEU |
| 2 | D | 12 | ILE |
| 2 | D | 27 | PHE |
| 2 | D | 30 | LEU |
| 2 | D | 36 | THR |
| 2 | D | 39 | ASP |
| 2 | D | 44 | ILE |
| 2 | D | 52 | GLU |
| 2 | D | 57 | ASP |
| 2 | D | 58 | LEU |
| 2 | D | 72 | ASP |
| 2 | D | 76 | LEU |
| 2 | D | 77 | TYR |
| 2 | D | 99 | LEU |
| 2 | D | 106 | VAL |
| 2 | D | 114 | CYS |
| 2 | D | 125 | PHE |
| 2 | D | 136 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 33 | ASN |
| 1 | A | 35 | GLN |
| 1 | A | 78 | ASN |
| 1 | A | 126 | ASN |
| 1 | A | 146 | GLN |
| 1 | A | 149 | GLN |
| 1 | A | 231 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 242 | ASN |
| 1 | A | 287 | GLN |
| 1 | A | 291 | ASN |
| 2 | B | 63 | ASN |
| 2 | B | 70 | GLN |
| 2 | B | 105 | ASN |
| 2 | B | 132 | ASN |
| 1 | C | 33 | ASN |
| 1 | C | 64 | HIS |
| 1 | C | 121 | ASN |
| 1 | C | 231 | GLN |
| 1 | C | 256 | ASN |
| 1 | C | 287 | GLN |
| 2 | D | 24 | GLN |
| 2 | D | 63 | ASN |
| 2 | D | 111 | ASN |
| 2 | D | 132 | ASN |
| 2 | D | 148 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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 | $\# Z > 2$ |
| 3 | PCT | A | 1311 | - | 7,7,7 | 2.81 | 3 (42%) | 9,10,10 | 0.93 | 0 |

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 |
|-----|------|-------|------|------|---------|----------|-------|
| 3 | PCT | A | 1311 | - | - | 1/4/5/5 | - |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3 | A | 1311 | PCT | P-O1P | 5.41 | 1.61 | 1.50 |
| 3 | A | 1311 | PCT | P-O2P | -3.47 | 1.47 | 1.54 |
| 3 | A | 1311 | PCT | P-O3P | 2.97 | 1.61 | 1.54 |

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 3 | A | 1311 | PCT | O1-C1-C1P-P |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3 | A | 1311 | PCT | 3 | 0 |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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 | 310/310 (100%) | -0.63 | 0 100 100 | 13, 49, 72, 89 | 0 |
| 1 | C | 310/310 (100%) | -0.50 | 3 (0%) 82 82 | 60, 90, 112, 137 | 0 |
| 2 | B | 146/153 (95%) | -0.48 | 1 (0%) 87 87 | 41, 78, 98, 102 | 0 |
| 2 | D | 146/153 (95%) | -0.24 | 5 (3%) 45 40 | 84, 104, 121, 127 | 0 |
| All | All | 912/926 (98%) | -0.50 | 9 (0%) 82 82 | 13, 82, 115, 137 | 0 |

All (9) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | D | 18 | ILE | 5.2 |
| 2 | D | 58 | LEU | 5.0 |
| 2 | D | 59 | ILE | 4.1 |
| 1 | C | 173 | THR | 3.9 |
| 2 | B | 9 | VAL | 2.8 |
| 2 | D | 56 | LYS | 2.7 |
| 1 | C | 186 | PHE | 2.5 |
| 2 | D | 21 | ILE | 2.3 |
| 1 | C | 40 | LYS | 2.1 |

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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. 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 | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3 | PCT | A | 1311 | 8/8 | 0.96 | 0.15 | 32,36,38,39 | 0 |
| 4 | ZN | D | 154 | 1/1 | 0.98 | 0.07 | 47,47,47,47 | 0 |
| 4 | ZN | B | 154 | 1/1 | 0.99 | 0.16 | 45,45,45,45 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.