



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:30 am GMT

PDB ID : 1M1G
Title : Crystal Structure of Aquifex aeolicus N-utilization substance G (NusG), Space Group P2(1)
Authors : Steiner, T.; Kaiser, J.T.; Marinkovic, S.; Huber, R.; Wahl, M.C.
Deposited on : 2002-06-19
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

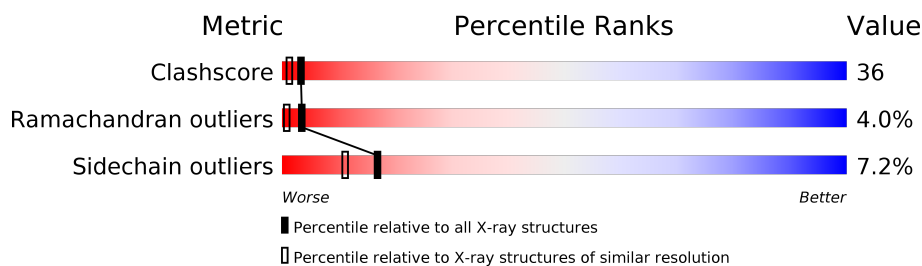
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 112137 | 7775 (2.00-2.00) |
| Ramachandran outliers | 110173 | 7679 (2.00-2.00) |
| Sidechain outliers | 110143 | 7678 (2.00-2.00) |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 248 | |
| 1 | B | 248 | |
| 1 | C | 248 | |
| 1 | D | 248 | |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8718 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 Transcription antitermination protein nusG.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 240 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1899 | 1214 | 323 | 354 | 8 | | | |
| 1 | B | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1917 | 1224 | 326 | 359 | 8 | | | |
| 1 | C | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1933 | 1234 | 329 | 362 | 8 | | | |
| 1 | D | 239 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1891 | 1208 | 322 | 353 | 8 | | | |

- Molecule 2 is water.

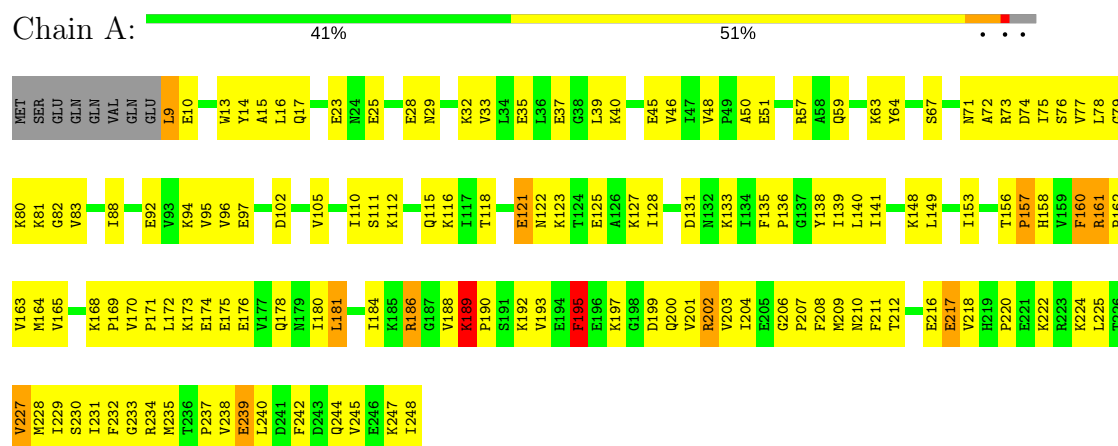
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 2 | A | 220 | Total | O | 0 | 0 |
| | | | 220 | 220 | | |
| 2 | B | 338 | Total | O | 0 | 0 |
| | | | 338 | 338 | | |
| 2 | C | 300 | Total | O | 0 | 0 |
| | | | 300 | 300 | | |
| 2 | D | 220 | Total | O | 0 | 0 |
| | | | 220 | 220 | | |

3 Residue-property plots [i](#)

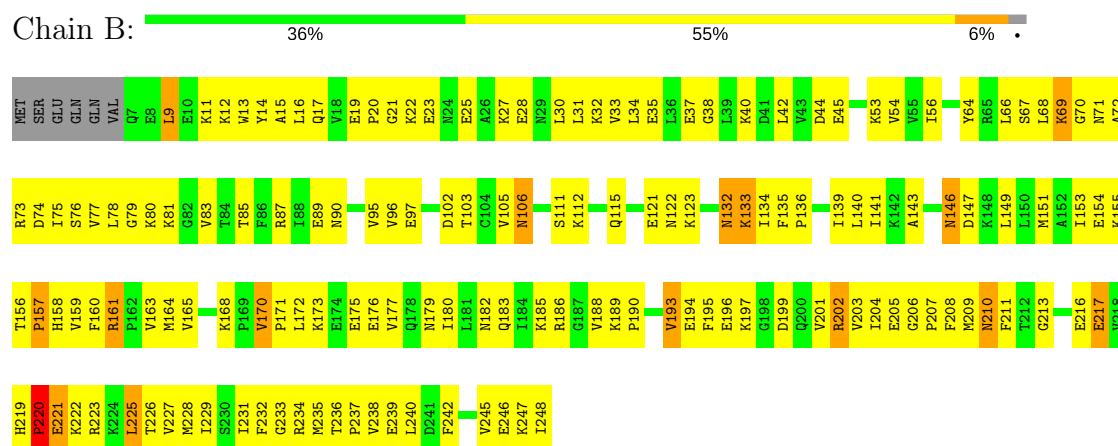
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

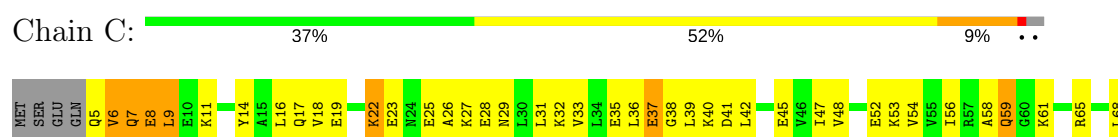
• Molecule 1: Transcription antitermination protein nusG

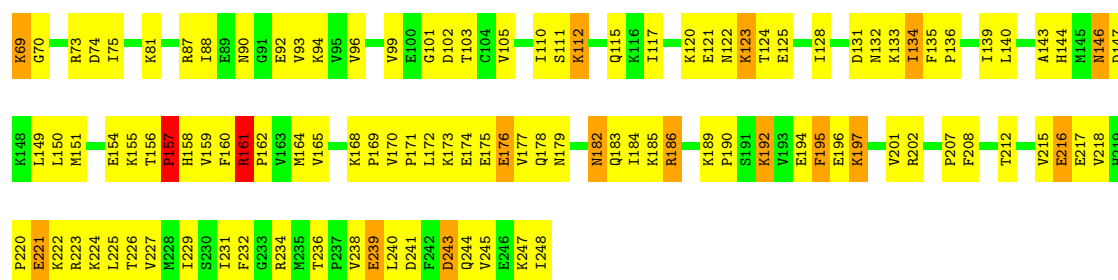


• Molecule 1: Transcription antitermination protein nusG



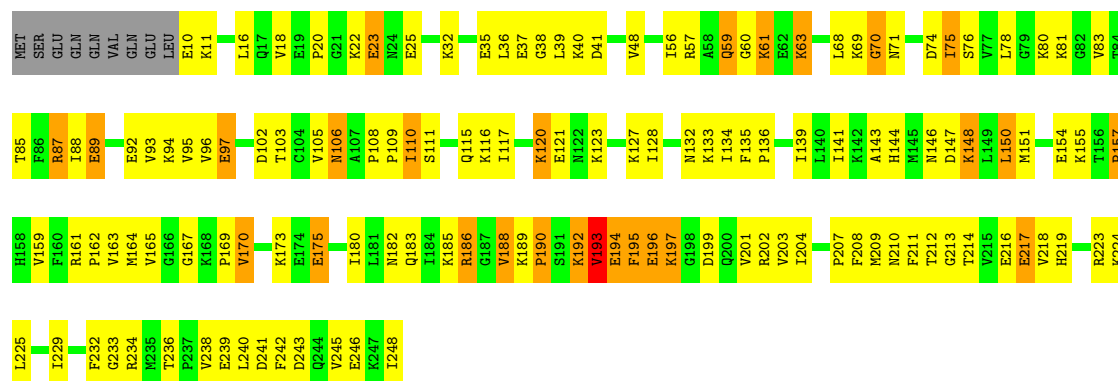
• Molecule 1: Transcription antitermination protein nusG





• Molecule 1: Transcription antitermination protein nusG

Chain D: 42% 44% 10%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 87.50Å 54.40Å 113.20Å 90.00° 89.30° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.00 | Depositor |
| % Data completeness (in resolution range) | 94.9 (30.00-2.00) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.08 | Depositor |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.251 , 0.274 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 8718 | wwPDB-VP |
| Average B, all atoms (Å ²) | 44.0 | wwPDB-VP |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 | 0.38 | 0/1928 | 0.64 | 0/2592 |
| 1 | B | 0.38 | 0/1946 | 0.65 | 1/2616 (0.0%) |
| 1 | C | 0.38 | 0/1962 | 0.64 | 0/2638 |
| 1 | D | 0.38 | 0/1920 | 0.67 | 0/2581 |
| All | All | 0.38 | 0/7756 | 0.65 | 1/10427 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1 | B | 225 | LEU | CA-CB-CG | 5.25 | 127.37 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1899 | 0 | 1994 | 105 | 322 |
| 1 | B | 1917 | 0 | 2008 | 157 | 388 |
| 1 | C | 1933 | 0 | 2025 | 159 | 134 |
| 1 | D | 1891 | 0 | 1983 | 140 | 102 |
| 2 | A | 220 | 0 | 0 | 28 | 50 |
| 2 | B | 338 | 0 | 0 | 50 | 69 |
| 2 | C | 300 | 0 | 0 | 48 | 42 |
| 2 | D | 220 | 0 | 0 | 45 | 9 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 8718 | 0 | 8010 | 561 | 598 |

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 36.

All (561) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:207:PRO:CG | 2:D:365:HOH:O | 1.84 | 1.24 |
| 1:B:235:MET:HB3 | 2:B:267:HOH:O | 1.09 | 1.23 |
| 1:D:212:THR:C | 2:D:320:HOH:O | 1.75 | 1.22 |
| 1:D:213:GLY:N | 2:D:320:HOH:O | 1.74 | 1.18 |
| 1:D:217:GLU:HB2 | 2:D:423:HOH:O | 1.44 | 1.15 |
| 1:B:168:LYS:O | 2:B:362:HOH:O | 1.68 | 1.10 |
| 1:C:103:THR:HG23 | 2:C:445:HOH:O | 1.53 | 1.07 |
| 1:D:207:PRO:HG2 | 2:D:365:HOH:O | 1.44 | 1.06 |
| 1:B:201:VAL:HG13 | 2:B:260:HOH:O | 1.53 | 1.05 |
| 1:D:190:PRO:HA | 2:D:395:HOH:O | 1.57 | 1.04 |
| 1:B:228:MET:HE2 | 2:B:267:HOH:O | 1.60 | 1.00 |
| 1:D:151:MET:O | 1:D:155:LYS:HD3 | 1.62 | 1.00 |
| 1:B:228:MET:CE | 2:B:267:HOH:O | 2.09 | 0.99 |
| 1:D:243:ASP:OD2 | 2:D:373:HOH:O | 1.84 | 0.94 |
| 1:C:215:VAL:HB | 2:C:522:HOH:O | 1.67 | 0.93 |
| 1:C:247:LYS:O | 1:C:248:ILE:HG12 | 1.68 | 0.93 |
| 1:C:112:LYS:HD2 | 1:C:112:LYS:H | 1.32 | 0.93 |
| 1:B:67:SER:OG | 2:B:395:HOH:O | 1.87 | 0.92 |
| 1:B:140:LEU:HD11 | 1:B:180:ILE:HD11 | 1.51 | 0.92 |
| 1:D:213:GLY:CA | 2:D:320:HOH:O | 2.09 | 0.92 |
| 1:A:195:PHE:O | 1:A:218:VAL:HG21 | 1.70 | 0.92 |
| 1:D:189:LYS:HB3 | 2:D:395:HOH:O | 1.69 | 0.91 |
| 1:B:205:GLU:OE1 | 2:B:297:HOH:O | 1.87 | 0.91 |
| 1:C:111:SER:H | 1:C:115:GLN:HE22 | 1.12 | 0.89 |
| 1:B:219:HIS:O | 2:B:426:HOH:O | 1.90 | 0.89 |
| 1:D:214:THR:HG21 | 2:D:277:HOH:O | 1.74 | 0.87 |
| 1:B:42:LEU:HB2 | 2:B:295:HOH:O | 1.74 | 0.86 |
| 1:A:206:GLY:C | 2:A:267:HOH:O | 2.15 | 0.85 |
| 1:A:204:ILE:HG12 | 2:A:439:HOH:O | 1.76 | 0.85 |
| 1:B:197:LYS:CE | 2:B:330:HOH:O | 2.24 | 0.84 |
| 1:B:67:SER:CB | 2:B:395:HOH:O | 2.25 | 0.84 |
| 1:B:69:LYS:HD3 | 1:B:70:GLY:N | 1.92 | 0.84 |
| 1:C:111:SER:H | 1:C:115:GLN:NE2 | 1.74 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:202:ARG:HG3 | 2:C:314:HOH:O | 1.77 | 0.83 |
| 1:B:197:LYS:HE3 | 2:B:330:HOH:O | 1.78 | 0.82 |
| 1:D:189:LYS:HB3 | 1:D:190:PRO:HA | 1.61 | 0.82 |
| 1:D:92:GLU:HG2 | 2:D:448:HOH:O | 1.79 | 0.81 |
| 1:A:201:VAL:HG12 | 1:A:247:LYS:HA | 1.61 | 0.81 |
| 1:C:212:THR:HG23 | 2:C:314:HOH:O | 1.80 | 0.80 |
| 1:B:197:LYS:NZ | 1:B:216:GLU:HG3 | 1.97 | 0.80 |
| 1:D:213:GLY:HA2 | 2:D:320:HOH:O | 1.75 | 0.80 |
| 1:B:202:ARG:HH22 | 1:B:204:ILE:HG22 | 1.47 | 0.80 |
| 1:C:134:ILE:HG12 | 2:C:381:HOH:O | 1.82 | 0.79 |
| 1:D:11:LYS:HD3 | 1:D:143:ALA:HA | 1.63 | 0.79 |
| 1:C:239:GLU:HG3 | 2:C:299:HOH:O | 1.82 | 0.79 |
| 1:A:186:ARG:HD3 | 1:A:186:ARG:N | 1.97 | 0.78 |
| 1:B:16:LEU:HB2 | 1:B:139:ILE:CG2 | 2.14 | 0.78 |
| 1:C:105:VAL:HB | 2:C:265:HOH:O | 1.84 | 0.78 |
| 1:C:146:ASN:ND2 | 1:C:149:LEU:H | 1.80 | 0.77 |
| 1:C:192:LYS:HD3 | 1:C:192:LYS:H | 1.49 | 0.77 |
| 1:B:112:LYS:O | 1:B:115:GLN:HB2 | 1.85 | 0.76 |
| 1:D:163:VAL:O | 1:D:170:VAL:HG23 | 1.86 | 0.76 |
| 1:D:111:SER:HA | 2:D:436:HOH:O | 1.86 | 0.76 |
| 1:C:146:ASN:HD21 | 1:C:149:LEU:H | 1.34 | 0.75 |
| 1:C:32:LYS:O | 1:C:36:LEU:HD23 | 1.87 | 0.75 |
| 1:A:186:ARG:HD3 | 1:A:186:ARG:H | 1.51 | 0.75 |
| 1:C:112:LYS:NZ | 2:C:451:HOH:O | 2.20 | 0.75 |
| 1:A:188:VAL:O | 1:A:189:LYS:HB2 | 1.87 | 0.74 |
| 1:B:32:LYS:HD3 | 2:B:273:HOH:O | 1.87 | 0.74 |
| 1:B:189:LYS:HZ2 | 1:B:189:LYS:HB2 | 1.52 | 0.74 |
| 1:B:228:MET:SD | 2:B:267:HOH:O | 2.40 | 0.74 |
| 1:B:199:ASP:O | 2:B:260:HOH:O | 2.06 | 0.73 |
| 1:A:201:VAL:HB | 1:A:245:VAL:HG22 | 1.71 | 0.73 |
| 1:D:207:PRO:CD | 2:D:365:HOH:O | 2.25 | 0.73 |
| 1:D:147:ASP:O | 1:D:151:MET:HG3 | 1.87 | 0.73 |
| 1:B:11:LYS:HD3 | 1:B:143:ALA:HA | 1.71 | 0.73 |
| 1:B:67:SER:HB2 | 2:B:395:HOH:O | 1.85 | 0.73 |
| 1:C:48:VAL:HG22 | 2:C:546:HOH:O | 1.89 | 0.72 |
| 1:A:202:ARG:HG3 | 2:A:445:HOH:O | 1.88 | 0.72 |
| 1:D:74:ASP:OD1 | 1:D:87:ARG:HD3 | 1.90 | 0.72 |
| 1:C:59:GLN:HG2 | 1:C:123:LYS:HB3 | 1.71 | 0.72 |
| 1:A:112:LYS:O | 1:A:115:GLN:HG2 | 1.89 | 0.72 |
| 1:A:71:ASN:HB2 | 2:A:295:HOH:O | 1.90 | 0.71 |
| 1:B:111:SER:H | 1:B:115:GLN:HE22 | 1.38 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:78:LEU:HD23 | 1:B:83:VAL:HG12 | 1.71 | 0.71 |
| 1:B:227:VAL:HG21 | 1:B:240:LEU:HD12 | 1.72 | 0.71 |
| 1:A:227:VAL:HG13 | 1:A:238:VAL:HG13 | 1.72 | 0.71 |
| 1:B:165:VAL:HB | 2:B:406:HOH:O | 1.89 | 0.71 |
| 1:C:19:GLU:HG2 | 1:C:22:LYS:HD2 | 1.69 | 0.71 |
| 1:A:81:LYS:HB2 | 2:A:296:HOH:O | 1.90 | 0.71 |
| 1:B:74:ASP:CG | 2:B:257:HOH:O | 2.28 | 0.71 |
| 1:D:190:PRO:CA | 2:D:395:HOH:O | 2.27 | 0.71 |
| 1:D:141:ILE:HB | 2:D:450:HOH:O | 1.91 | 0.70 |
| 1:B:163:VAL:O | 1:B:170:VAL:HG23 | 1.90 | 0.70 |
| 1:B:189:LYS:HZ2 | 1:B:189:LYS:CB | 2.04 | 0.70 |
| 1:B:196:GLU:HG2 | 1:B:199:ASP:OD2 | 1.91 | 0.70 |
| 1:A:16:LEU:HD11 | 1:A:141:ILE:HD13 | 1.73 | 0.70 |
| 1:D:195:PHE:O | 1:D:218:VAL:HG21 | 1.92 | 0.70 |
| 1:D:175:GLU:H | 1:D:175:GLU:CD | 1.92 | 0.70 |
| 1:C:172:LEU:HG | 2:C:509:HOH:O | 1.90 | 0.69 |
| 1:D:68:LEU:HD11 | 2:D:436:HOH:O | 1.92 | 0.69 |
| 1:B:69:LYS:HD3 | 1:B:70:GLY:H | 1.57 | 0.69 |
| 1:B:35:GLU:N | 1:B:40:LYS:HE2 | 2.07 | 0.69 |
| 1:D:162:PRO:HD2 | 1:D:164:MET:HE1 | 1.74 | 0.69 |
| 1:D:134:ILE:HG12 | 2:D:301:HOH:O | 1.93 | 0.68 |
| 1:A:222:LYS:O | 1:A:224:LYS:HG2 | 1.94 | 0.68 |
| 1:A:127:LYS:HB2 | 2:A:265:HOH:O | 1.93 | 0.68 |
| 1:C:222:LYS:O | 1:C:224:LYS:HG2 | 1.95 | 0.67 |
| 1:A:180:ILE:O | 1:A:184:ILE:HG12 | 1.94 | 0.67 |
| 1:B:170:VAL:HG13 | 2:B:406:HOH:O | 1.94 | 0.67 |
| 1:C:173:LYS:HB3 | 2:C:489:HOH:O | 1.94 | 0.67 |
| 1:D:162:PRO:HD2 | 1:D:164:MET:CE | 2.25 | 0.67 |
| 1:B:197:LYS:HE2 | 2:B:330:HOH:O | 1.93 | 0.67 |
| 1:D:208:PHE:CE1 | 1:D:238:VAL:HG21 | 2.30 | 0.66 |
| 1:C:201:VAL:HB | 1:C:245:VAL:HG22 | 1.77 | 0.66 |
| 1:B:149:LEU:HD22 | 2:B:295:HOH:O | 1.95 | 0.66 |
| 1:B:197:LYS:HZ3 | 1:B:216:GLU:HG3 | 1.59 | 0.66 |
| 1:D:56:ILE:HD13 | 1:D:75:ILE:HD12 | 1.78 | 0.66 |
| 1:C:112:LYS:H | 1:C:112:LYS:CD | 2.05 | 0.66 |
| 1:D:207:PRO:HD2 | 2:D:365:HOH:O | 1.91 | 0.66 |
| 1:D:241:ASP:O | 1:D:245:VAL:HG12 | 1.96 | 0.66 |
| 1:B:23:GLU:HG3 | 1:B:132:ASN:OD1 | 1.96 | 0.65 |
| 1:D:148:LYS:O | 1:D:148:LYS:HE3 | 1.96 | 0.65 |
| 1:C:248:ILE:O | 1:C:248:ILE:HG13 | 1.96 | 0.65 |
| 1:B:74:ASP:OD2 | 2:B:257:HOH:O | 2.13 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:244:GLN:HG3 | 2:C:530:HOH:O | 1.95 | 0.65 |
| 1:B:186:ARG:NH1 | 2:B:338:HOH:O | 2.29 | 0.65 |
| 1:B:27:LYS:HE2 | 1:B:31:LEU:HD11 | 1.78 | 0.65 |
| 1:B:34:LEU:N | 2:B:477:HOH:O | 2.30 | 0.64 |
| 1:B:54:VAL:HG23 | 2:B:547:HOH:O | 1.97 | 0.64 |
| 1:C:134:ILE:O | 1:C:136:PRO:HD3 | 1.97 | 0.64 |
| 1:A:227:VAL:HB | 2:A:451:HOH:O | 1.97 | 0.64 |
| 1:B:223:ARG:HG3 | 2:B:523:HOH:O | 1.97 | 0.64 |
| 1:D:59:GLN:NE2 | 1:D:80:LYS:HB2 | 2.12 | 0.64 |
| 1:B:235:MET:CB | 2:B:267:HOH:O | 1.89 | 0.63 |
| 1:B:80:LYS:HE3 | 1:B:123:LYS:HG3 | 1.79 | 0.63 |
| 1:C:5:GLN:HG2 | 1:C:6:VAL:HG23 | 1.80 | 0.63 |
| 1:D:154:GLU:HB2 | 2:D:355:HOH:O | 1.98 | 0.63 |
| 1:B:53:LYS:HE2 | 2:B:325:HOH:O | 1.99 | 0.63 |
| 1:D:132:ASN:O | 1:D:136:PRO:HG3 | 1.99 | 0.63 |
| 1:C:194:GLU:O | 1:C:195:PHE:HB2 | 1.98 | 0.62 |
| 1:B:111:SER:H | 1:B:115:GLN:NE2 | 1.96 | 0.62 |
| 1:B:31:LEU:C | 2:B:477:HOH:O | 2.37 | 0.62 |
| 1:B:16:LEU:HB2 | 1:B:139:ILE:HG22 | 1.82 | 0.62 |
| 1:D:61:LYS:HD3 | 1:D:63:LYS:HE3 | 1.81 | 0.62 |
| 1:B:201:VAL:HB | 1:B:245:VAL:HG13 | 1.81 | 0.62 |
| 1:C:218:VAL:O | 1:C:220:PRO:HD3 | 1.99 | 0.62 |
| 1:D:204:ILE:HG12 | 2:D:432:HOH:O | 1.99 | 0.62 |
| 1:A:9:LEU:N | 1:A:9:LEU:HD23 | 2.15 | 0.62 |
| 1:A:164:MET:HB2 | 1:A:168:LYS:O | 2.00 | 0.62 |
| 1:A:48:VAL:HG13 | 2:A:446:HOH:O | 2.00 | 0.61 |
| 1:D:59:GLN:HE21 | 1:D:80:LYS:HB2 | 1.64 | 0.61 |
| 1:B:68:LEU:N | 2:B:547:HOH:O | 2.33 | 0.61 |
| 1:D:182:ASN:O | 1:D:186:ARG:HB2 | 2.00 | 0.61 |
| 1:B:64:TYR:CE1 | 1:B:75:ILE:HD11 | 2.35 | 0.61 |
| 1:B:201:VAL:HB | 1:B:245:VAL:CG1 | 2.30 | 0.61 |
| 1:B:219:HIS:O | 1:B:221:GLU:N | 2.34 | 0.61 |
| 1:C:151:MET:O | 1:C:155:LYS:HG2 | 2.00 | 0.61 |
| 1:C:6:VAL:O | 1:C:8:GLU:N | 2.34 | 0.61 |
| 1:D:141:ILE:O | 1:D:141:ILE:HG13 | 2.00 | 0.61 |
| 1:D:194:GLU:CD | 2:D:364:HOH:O | 2.40 | 0.61 |
| 1:D:167:GLY:HA2 | 2:D:273:HOH:O | 2.00 | 0.61 |
| 1:C:146:ASN:HD22 | 1:C:146:ASN:C | 2.03 | 0.60 |
| 1:C:150:LEU:O | 1:C:154:GLU:HG3 | 2.01 | 0.60 |
| 1:A:164:MET:HG2 | 2:A:258:HOH:O | 2.01 | 0.60 |
| 1:C:182:ASN:ND2 | 1:C:186:ARG:HB2 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:203:VAL:HB | 1:D:208:PHE:O | 2.00 | 0.60 |
| 1:D:110:ILE:HG12 | 1:D:128:ILE:HD11 | 1.82 | 0.60 |
| 1:D:194:GLU:O | 1:D:195:PHE:HB2 | 2.01 | 0.60 |
| 1:A:204:ILE:O | 1:A:204:ILE:HG13 | 2.00 | 0.60 |
| 1:D:212:THR:O | 2:D:320:HOH:O | 2.01 | 0.59 |
| 1:D:57:ARG:NH2 | 1:D:57:ARG:HB3 | 2.17 | 0.59 |
| 1:C:158:HIS:HB2 | 2:C:352:HOH:O | 2.03 | 0.59 |
| 1:B:183:GLN:O | 1:B:189:LYS:HD3 | 2.03 | 0.59 |
| 1:C:234:ARG:HG3 | 1:C:234:ARG:HH21 | 1.67 | 0.59 |
| 1:B:199:ASP:C | 2:B:260:HOH:O | 2.41 | 0.59 |
| 1:D:120:LYS:NZ | 1:D:120:LYS:HB3 | 2.18 | 0.59 |
| 1:D:165:VAL:HG23 | 1:D:170:VAL:HG21 | 1.84 | 0.59 |
| 1:A:164:MET:HB3 | 1:A:169:PRO:HA | 1.84 | 0.59 |
| 1:A:206:GLY:O | 2:A:267:HOH:O | 2.16 | 0.59 |
| 1:D:190:PRO:CB | 2:D:395:HOH:O | 2.48 | 0.59 |
| 1:D:216:GLU:O | 1:D:217:GLU:HB3 | 2.03 | 0.59 |
| 1:A:174:GLU:O | 1:A:178:GLN:HG3 | 2.03 | 0.58 |
| 1:B:68:LEU:HB2 | 2:B:547:HOH:O | 2.03 | 0.58 |
| 1:C:69:LYS:HE2 | 1:C:70:GLY:H | 1.67 | 0.58 |
| 1:A:161:ARG:HG3 | 1:A:162:PRO:O | 2.02 | 0.58 |
| 1:B:146:ASN:ND2 | 1:B:149:LEU:H | 2.01 | 0.58 |
| 1:D:196:GLU:HG2 | 2:D:462:HOH:O | 2.01 | 0.58 |
| 1:A:48:VAL:HG22 | 2:A:446:HOH:O | 2.02 | 0.58 |
| 1:A:245:VAL:HG13 | 1:A:245:VAL:O | 2.03 | 0.58 |
| 1:B:165:VAL:HG23 | 1:B:170:VAL:CG2 | 2.33 | 0.58 |
| 1:C:222:LYS:HA | 2:C:541:HOH:O | 2.03 | 0.58 |
| 1:D:18:VAL:HG12 | 1:D:159:VAL:HG22 | 1.84 | 0.58 |
| 1:A:207:PRO:N | 2:A:267:HOH:O | 2.34 | 0.58 |
| 1:A:218:VAL:HG13 | 1:A:225:LEU:CD1 | 2.34 | 0.58 |
| 1:D:209:MET:HG2 | 1:D:210:ASN:OD1 | 2.04 | 0.58 |
| 1:B:112:LYS:H | 1:B:115:GLN:NE2 | 2.02 | 0.58 |
| 1:B:112:LYS:H | 1:B:115:GLN:HE21 | 1.52 | 0.57 |
| 1:D:22:LYS:HB3 | 1:D:25:GLU:HB2 | 1.86 | 0.57 |
| 1:D:196:GLU:HB2 | 2:D:439:HOH:O | 2.04 | 0.57 |
| 1:B:197:LYS:HZ1 | 1:B:216:GLU:HG3 | 1.67 | 0.57 |
| 1:C:161:ARG:HD2 | 1:C:164:MET:CE | 2.34 | 0.57 |
| 1:C:184:ILE:HG21 | 2:C:504:HOH:O | 2.04 | 0.57 |
| 1:C:131:ASP:OD1 | 1:C:133:LYS:HE2 | 2.05 | 0.57 |
| 1:D:185:LYS:HG2 | 2:D:255:HOH:O | 2.05 | 0.57 |
| 1:B:16:LEU:HB2 | 1:B:139:ILE:HG23 | 1.85 | 0.57 |
| 1:A:222:LYS:NZ | 1:A:222:LYS:HB3 | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:69:LYS:HD3 | 1:D:70:GLY:N | 2.20 | 0.57 |
| 1:C:221:GLU:OE1 | 1:C:221:GLU:HA | 2.04 | 0.57 |
| 1:D:10:GLU:HA | 2:D:409:HOH:O | 2.04 | 0.57 |
| 1:A:203:VAL:HB | 1:A:208:PHE:O | 2.05 | 0.56 |
| 1:A:216:GLU:O | 1:A:217:GLU:HB3 | 2.05 | 0.56 |
| 1:D:162:PRO:HB2 | 1:D:164:MET:HE2 | 1.86 | 0.56 |
| 1:A:110:ILE:CD1 | 1:A:116:LYS:HA | 2.35 | 0.56 |
| 1:D:201:VAL:HB | 1:D:245:VAL:HG23 | 1.87 | 0.56 |
| 1:D:85:THR:HB | 1:D:97:GLU:HG3 | 1.86 | 0.56 |
| 1:C:185:LYS:HZ2 | 1:C:186:ARG:NE | 2.03 | 0.56 |
| 1:C:160:PHE:HB2 | 2:C:310:HOH:O | 2.03 | 0.56 |
| 1:D:80:LYS:HZ2 | 1:D:81:LYS:HE3 | 1.70 | 0.56 |
| 1:C:144:HIS:HD2 | 2:C:520:HOH:O | 1.87 | 0.56 |
| 1:A:95:VAL:HG12 | 1:A:105:VAL:HG12 | 1.86 | 0.56 |
| 1:B:182:ASN:O | 1:B:186:ARG:HD3 | 2.06 | 0.56 |
| 1:C:88:ILE:HA | 1:C:92:GLU:O | 2.06 | 0.56 |
| 1:D:204:ILE:HG23 | 2:D:432:HOH:O | 2.05 | 0.56 |
| 1:A:180:ILE:HG13 | 1:A:181:LEU:N | 2.19 | 0.56 |
| 1:C:16:LEU:HD23 | 1:C:162:PRO:HB3 | 1.88 | 0.56 |
| 1:C:216:GLU:O | 1:C:226:THR:HB | 2.05 | 0.56 |
| 1:D:110:ILE:HB | 1:D:115:GLN:HB3 | 1.86 | 0.56 |
| 1:D:197:LYS:HD2 | 1:D:216:GLU:HA | 1.88 | 0.56 |
| 1:B:219:HIS:NE2 | 1:B:226:THR:OG1 | 2.39 | 0.55 |
| 1:A:231:ILE:O | 1:A:232:PHE:HB2 | 2.06 | 0.55 |
| 1:C:69:LYS:HA | 1:C:69:LYS:HE2 | 1.88 | 0.55 |
| 1:D:80:LYS:NZ | 1:D:81:LYS:HE3 | 2.22 | 0.55 |
| 1:A:188:VAL:O | 1:A:190:PRO:HA | 2.05 | 0.55 |
| 1:B:53:LYS:HA | 2:B:547:HOH:O | 2.06 | 0.55 |
| 1:D:193:VAL:HB | 1:D:196:GLU:HB3 | 1.89 | 0.55 |
| 1:B:165:VAL:HG23 | 1:B:170:VAL:HG22 | 1.88 | 0.55 |
| 1:C:23:GLU:HB3 | 2:C:546:HOH:O | 2.05 | 0.55 |
| 1:A:110:ILE:HD13 | 1:A:116:LYS:HA | 1.89 | 0.55 |
| 1:C:19:GLU:HB3 | 1:C:22:LYS:HG3 | 1.88 | 0.55 |
| 1:B:235:MET:CA | 2:B:267:HOH:O | 2.37 | 0.55 |
| 1:B:163:VAL:HG12 | 1:B:170:VAL:CG2 | 2.36 | 0.55 |
| 1:C:161:ARG:HD2 | 1:C:164:MET:HE3 | 1.89 | 0.55 |
| 1:C:17:GLN:HB2 | 1:C:161:ARG:HH11 | 1.72 | 0.55 |
| 1:C:22:LYS:HE2 | 2:C:345:HOH:O | 2.06 | 0.55 |
| 1:C:26:ALA:N | 2:C:352:HOH:O | 2.39 | 0.55 |
| 1:C:74:ASP:C | 1:C:75:ILE:HD12 | 2.26 | 0.55 |
| 1:C:201:VAL:HB | 1:C:245:VAL:CG2 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:239:GLU:HG2 | 2:B:580:HOH:O | 2.08 | 0.54 |
| 1:C:160:PHE:C | 1:C:161:ARG:HG3 | 2.27 | 0.54 |
| 1:B:134:ILE:C | 1:B:136:PRO:HD3 | 2.28 | 0.54 |
| 1:D:120:LYS:HD2 | 1:D:120:LYS:H | 1.73 | 0.54 |
| 1:D:87:ARG:HG2 | 1:D:89:GLU:HG3 | 1.88 | 0.54 |
| 1:B:196:GLU:HG2 | 1:B:199:ASP:CG | 2.27 | 0.54 |
| 1:C:194:GLU:O | 1:C:195:PHE:CB | 2.54 | 0.54 |
| 1:C:220:PRO:HG3 | 2:C:374:HOH:O | 2.06 | 0.54 |
| 1:D:224:LYS:HD2 | 1:D:241:ASP:OD2 | 2.07 | 0.54 |
| 1:D:69:LYS:C | 1:D:69:LYS:HD3 | 2.27 | 0.54 |
| 1:C:112:LYS:HD2 | 1:C:112:LYS:N | 2.12 | 0.54 |
| 1:C:185:LYS:O | 1:C:186:ARG:HB2 | 2.07 | 0.54 |
| 1:B:216:GLU:O | 1:B:217:GLU:HB3 | 2.08 | 0.54 |
| 1:D:110:ILE:HG12 | 1:D:128:ILE:CD1 | 2.37 | 0.54 |
| 1:C:229:ILE:HD12 | 1:C:238:VAL:HG11 | 1.89 | 0.54 |
| 1:D:183:GLN:HB2 | 2:D:256:HOH:O | 2.08 | 0.53 |
| 1:C:160:PHE:O | 1:C:161:ARG:HG3 | 2.08 | 0.53 |
| 1:A:202:ARG:CG | 2:A:445:HOH:O | 2.49 | 0.53 |
| 1:C:182:ASN:ND2 | 1:C:186:ARG:CB | 2.72 | 0.53 |
| 1:B:15:ALA:HB2 | 1:B:172:LEU:HD11 | 1.90 | 0.53 |
| 1:C:11:LYS:HD3 | 1:C:143:ALA:HA | 1.89 | 0.53 |
| 1:C:6:VAL:O | 1:C:8:GLU:HG2 | 2.09 | 0.53 |
| 1:D:193:VAL:HG11 | 2:D:439:HOH:O | 2.08 | 0.53 |
| 1:C:161:ARG:HG2 | 2:C:447:HOH:O | 2.09 | 0.52 |
| 1:B:9:LEU:HA | 2:B:363:HOH:O | 2.10 | 0.52 |
| 1:C:182:ASN:HD22 | 1:C:186:ARG:HB2 | 1.74 | 0.52 |
| 1:C:81:LYS:HD2 | 2:C:484:HOH:O | 2.09 | 0.52 |
| 1:D:151:MET:HE2 | 2:D:253:HOH:O | 2.09 | 0.52 |
| 1:A:71:ASN:O | 1:A:73:ARG:HG2 | 2.09 | 0.52 |
| 1:A:110:ILE:HD12 | 1:A:128:ILE:HG12 | 1.91 | 0.52 |
| 1:C:73:ARG:HD3 | 2:C:482:HOH:O | 2.09 | 0.52 |
| 1:A:23:GLU:HB3 | 2:A:446:HOH:O | 2.09 | 0.52 |
| 1:B:30:LEU:O | 1:B:33:VAL:HG12 | 2.10 | 0.52 |
| 1:C:176:GLU:HA | 1:C:176:GLU:OE1 | 2.08 | 0.52 |
| 1:A:75:ILE:HG23 | 1:A:75:ILE:O | 2.10 | 0.52 |
| 1:B:23:GLU:H | 1:B:23:GLU:CD | 2.13 | 0.52 |
| 1:B:54:VAL:HG12 | 1:B:56:ILE:CD1 | 2.39 | 0.52 |
| 1:B:78:LEU:CD2 | 1:B:83:VAL:HG12 | 2.37 | 0.52 |
| 1:B:195:PHE:O | 1:B:196:GLU:HB3 | 2.10 | 0.51 |
| 1:C:185:LYS:NZ | 1:C:186:ARG:NE | 2.58 | 0.51 |
| 1:D:248:ILE:HG22 | 1:D:248:ILE:OXT | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:GLU:HG2 | 1:A:111:SER:HB3 | 1.91 | 0.51 |
| 1:A:139:ILE:HG22 | 2:A:446:HOH:O | 2.09 | 0.51 |
| 1:A:25:GLU:HB2 | 2:A:253:HOH:O | 2.10 | 0.51 |
| 1:A:64:TYR:CZ | 1:A:75:ILE:HD11 | 2.45 | 0.51 |
| 1:B:16:LEU:HD21 | 1:B:153:ILE:HD13 | 1.92 | 0.51 |
| 1:B:245:VAL:HG12 | 1:B:246:GLU:N | 2.25 | 0.51 |
| 1:A:29:ASN:HB3 | 1:A:156:THR:HG23 | 1.93 | 0.51 |
| 1:D:57:ARG:NH2 | 1:D:60:GLY:O | 2.43 | 0.51 |
| 1:A:164:MET:HA | 1:A:170:VAL:HG23 | 1.91 | 0.51 |
| 1:A:201:VAL:HB | 1:A:245:VAL:CG2 | 2.40 | 0.51 |
| 1:C:182:ASN:HD21 | 1:C:186:ARG:HG2 | 1.76 | 0.51 |
| 1:C:207:PRO:HG2 | 1:C:208:PHE:CD1 | 2.46 | 0.51 |
| 1:C:224:LYS:HD2 | 1:C:241:ASP:OD2 | 2.11 | 0.51 |
| 1:C:241:ASP:HB2 | 2:C:530:HOH:O | 2.11 | 0.50 |
| 1:A:37:GLU:HB3 | 1:A:39:LEU:HG | 1.94 | 0.50 |
| 1:C:101:GLY:C | 1:C:121:GLU:HG3 | 2.31 | 0.50 |
| 1:C:53:LYS:HG3 | 1:C:131:ASP:OD1 | 2.11 | 0.50 |
| 1:A:29:ASN:O | 1:A:33:VAL:HG23 | 2.10 | 0.50 |
| 1:B:28:GLU:OE1 | 1:B:28:GLU:HA | 2.12 | 0.50 |
| 1:D:87:ARG:HB2 | 1:D:96:VAL:CG2 | 2.41 | 0.50 |
| 1:A:176:GLU:O | 1:A:180:ILE:HG23 | 2.11 | 0.50 |
| 1:A:45:GLU:HB2 | 2:A:307:HOH:O | 2.10 | 0.50 |
| 1:B:147:ASP:O | 1:B:151:MET:HG3 | 2.12 | 0.50 |
| 1:A:9:LEU:O | 1:A:10:GLU:HB3 | 2.11 | 0.50 |
| 1:D:238:VAL:HG22 | 1:D:239:GLU:N | 2.26 | 0.50 |
| 1:D:48:VAL:HG22 | 1:D:139:ILE:HG22 | 1.92 | 0.50 |
| 1:C:172:LEU:N | 1:C:172:LEU:HD22 | 2.26 | 0.50 |
| 1:D:110:ILE:O | 1:D:128:ILE:HD11 | 2.11 | 0.50 |
| 1:B:245:VAL:CG1 | 1:B:246:GLU:N | 2.74 | 0.50 |
| 1:B:44:ASP:C | 1:B:45:GLU:HG2 | 2.32 | 0.50 |
| 1:C:61:LYS:HB2 | 2:C:413:HOH:O | 2.12 | 0.50 |
| 1:C:140:LEU:HD13 | 1:C:177:VAL:HG13 | 1.94 | 0.50 |
| 1:D:155:LYS:HE2 | 2:D:253:HOH:O | 2.12 | 0.50 |
| 1:A:64:TYR:CE1 | 1:A:75:ILE:HD11 | 2.46 | 0.49 |
| 1:D:165:VAL:HG23 | 1:D:170:VAL:CG2 | 2.41 | 0.49 |
| 1:A:239:GLU:O | 1:A:240:LEU:HD23 | 2.12 | 0.49 |
| 1:D:245:VAL:HA | 2:D:432:HOH:O | 2.12 | 0.49 |
| 1:C:190:PRO:HD2 | 2:C:544:HOH:O | 2.12 | 0.49 |
| 1:D:57:ARG:HB3 | 1:D:57:ARG:HH21 | 1.77 | 0.49 |
| 1:D:88:ILE:HA | 1:D:92:GLU:O | 2.12 | 0.49 |
| 1:B:85:THR:O | 1:B:96:VAL:HG22 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:135:PHE:N | 1:B:136:PRO:HD3 | 2.27 | 0.49 |
| 1:B:95:VAL:HG12 | 1:B:105:VAL:HG12 | 1.93 | 0.49 |
| 1:D:225:LEU:O | 1:D:239:GLU:HA | 2.12 | 0.49 |
| 1:B:97:GLU:HG3 | 2:B:291:HOH:O | 2.13 | 0.49 |
| 1:C:189:LYS:HB2 | 1:C:189:LYS:NZ | 2.28 | 0.49 |
| 1:D:218:VAL:HG12 | 1:D:219:HIS:N | 2.28 | 0.49 |
| 1:B:34:LEU:HB3 | 1:B:40:LYS:HD3 | 1.95 | 0.48 |
| 1:C:208:PHE:HD2 | 2:C:502:HOH:O | 1.97 | 0.48 |
| 1:D:150:LEU:O | 1:D:154:GLU:HG2 | 2.12 | 0.48 |
| 1:D:57:ARG:CB | 1:D:57:ARG:HH21 | 2.26 | 0.48 |
| 1:D:75:ILE:HD13 | 1:D:75:ILE:C | 2.34 | 0.48 |
| 1:B:201:VAL:CG1 | 2:B:260:HOH:O | 2.32 | 0.48 |
| 1:B:25:GLU:OE2 | 1:B:25:GLU:N | 2.43 | 0.48 |
| 1:C:164:MET:HA | 1:C:170:VAL:HG23 | 1.95 | 0.48 |
| 1:A:186:ARG:NH2 | 2:A:257:HOH:O | 2.45 | 0.48 |
| 1:C:215:VAL:HG13 | 1:C:225:LEU:HD22 | 1.95 | 0.48 |
| 1:D:173:LYS:HG2 | 2:D:431:HOH:O | 2.13 | 0.48 |
| 1:D:25:GLU:HG2 | 2:D:257:HOH:O | 2.13 | 0.48 |
| 1:B:103:THR:O | 1:B:106:ASN:HB2 | 2.14 | 0.48 |
| 1:B:160:PHE:HA | 2:B:251:HOH:O | 2.13 | 0.48 |
| 1:C:135:PHE:HD2 | 2:C:450:HOH:O | 1.96 | 0.48 |
| 1:D:94:LYS:HB3 | 1:D:109:PRO:HB3 | 1.95 | 0.48 |
| 1:A:225:LEU:O | 1:A:239:GLU:HA | 2.14 | 0.48 |
| 1:D:135:PHE:CZ | 1:D:183:GLN:HG2 | 2.49 | 0.48 |
| 1:A:248:ILE:HG22 | 1:A:248:ILE:OXT | 2.14 | 0.48 |
| 1:A:45:GLU:CB | 2:A:307:HOH:O | 2.61 | 0.48 |
| 1:D:116:LYS:HE2 | 1:D:127:LYS:HD2 | 1.95 | 0.48 |
| 1:B:222:LYS:NZ | 1:B:222:LYS:CB | 2.76 | 0.48 |
| 1:D:110:ILE:HD12 | 1:D:117:ILE:HG13 | 1.96 | 0.48 |
| 1:C:28:GLU:HG3 | 2:C:263:HOH:O | 2.13 | 0.48 |
| 1:A:218:VAL:O | 1:A:220:PRO:HD3 | 2.14 | 0.48 |
| 1:B:163:VAL:HG12 | 1:B:170:VAL:HG23 | 1.95 | 0.48 |
| 1:C:69:LYS:CE | 1:C:70:GLY:H | 2.25 | 0.48 |
| 1:C:69:LYS:HG3 | 2:C:397:HOH:O | 2.13 | 0.48 |
| 1:B:164:MET:CB | 2:B:362:HOH:O | 2.45 | 0.47 |
| 1:B:103:THR:HA | 2:C:506:HOH:O | 2.14 | 0.47 |
| 1:C:111:SER:HB2 | 1:C:112:LYS:HD2 | 1.97 | 0.47 |
| 1:C:156:THR:HG23 | 1:C:157:PRO:HD2 | 1.96 | 0.47 |
| 1:A:186:ARG:HG2 | 1:A:186:ARG:O | 2.14 | 0.47 |
| 1:A:94:LYS:HG2 | 2:A:443:HOH:O | 2.13 | 0.47 |
| 1:B:146:ASN:HD22 | 1:B:146:ASN:H | 1.60 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:171:PRO:HB2 | 2:C:513:HOH:O | 2.13 | 0.47 |
| 1:B:164:MET:HB3 | 2:B:362:HOH:O | 2.13 | 0.47 |
| 1:B:202:ARG:NH2 | 1:B:204:ILE:HG22 | 2.23 | 0.47 |
| 1:B:225:LEU:HD22 | 1:B:242:PHE:HD1 | 1.80 | 0.47 |
| 1:D:110:ILE:HD13 | 1:D:110:ILE:H | 1.79 | 0.47 |
| 1:D:16:LEU:CD2 | 1:D:162:PRO:HG3 | 2.44 | 0.47 |
| 1:D:173:LYS:HD2 | 1:D:175:GLU:HG2 | 1.97 | 0.47 |
| 1:A:202:ARG:CD | 2:A:445:HOH:O | 2.48 | 0.47 |
| 1:B:175:GLU:O | 1:B:179:ASN:ND2 | 2.48 | 0.47 |
| 1:D:234:ARG:HG2 | 1:D:236:THR:OG1 | 2.15 | 0.47 |
| 1:B:102:ASP:CG | 1:B:121:GLU:HB3 | 2.35 | 0.47 |
| 1:B:222:LYS:HB3 | 1:B:222:LYS:NZ | 2.28 | 0.47 |
| 1:B:28:GLU:O | 1:B:32:LYS:HG2 | 2.14 | 0.47 |
| 1:B:79:GLY:HA3 | 1:B:122:ASN:ND2 | 2.30 | 0.47 |
| 1:C:131:ASP:HB3 | 1:C:133:LYS:HG3 | 1.97 | 0.47 |
| 1:C:140:LEU:HD22 | 2:C:509:HOH:O | 2.13 | 0.47 |
| 1:D:192:LYS:NZ | 1:D:192:LYS:HB3 | 2.30 | 0.47 |
| 1:C:165:VAL:HG23 | 1:C:170:VAL:HG21 | 1.96 | 0.47 |
| 1:C:52:GLU:OE2 | 1:C:185:LYS:HG3 | 2.15 | 0.47 |
| 1:D:105:VAL:HG21 | 2:D:269:HOH:O | 2.15 | 0.46 |
| 1:B:193:VAL:HG13 | 1:B:193:VAL:O | 2.15 | 0.46 |
| 1:A:149:LEU:O | 1:A:153:ILE:HG12 | 2.15 | 0.46 |
| 1:A:199:ASP:CG | 1:A:247:LYS:NZ | 2.68 | 0.46 |
| 1:B:156:THR:HG23 | 1:B:157:PRO:HD2 | 1.98 | 0.46 |
| 1:A:160:PHE:HB3 | 2:A:356:HOH:O | 2.16 | 0.46 |
| 1:A:180:ILE:CG1 | 1:A:181:LEU:N | 2.78 | 0.46 |
| 1:A:46:VAL:HG22 | 1:A:141:ILE:HG22 | 1.98 | 0.46 |
| 1:B:80:LYS:CE | 1:B:123:LYS:HG3 | 2.44 | 0.46 |
| 1:C:236:THR:HG23 | 2:C:351:HOH:O | 2.15 | 0.46 |
| 1:B:202:ARG:HH22 | 1:B:204:ILE:CG2 | 2.24 | 0.46 |
| 1:C:140:LEU:HD13 | 1:C:177:VAL:CG1 | 2.46 | 0.46 |
| 1:C:17:GLN:HG2 | 2:C:272:HOH:O | 2.14 | 0.46 |
| 1:C:146:ASN:ND2 | 1:C:146:ASN:C | 2.69 | 0.46 |
| 1:C:234:ARG:NH2 | 1:C:234:ARG:HG3 | 2.31 | 0.46 |
| 1:B:176:GLU:O | 1:B:180:ILE:HG23 | 2.14 | 0.46 |
| 1:B:80:LYS:HD2 | 2:B:382:HOH:O | 2.16 | 0.46 |
| 1:C:192:LYS:HD3 | 1:C:192:LYS:N | 2.25 | 0.46 |
| 1:C:33:VAL:O | 1:C:37:GLU:HB2 | 2.15 | 0.46 |
| 1:D:188:VAL:HG21 | 2:D:338:HOH:O | 2.15 | 0.46 |
| 1:D:223:ARG:HA | 1:D:242:PHE:CE1 | 2.51 | 0.46 |
| 1:A:127:LYS:HB3 | 2:A:405:HOH:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:228:MET:CE | 1:A:237:PRO:HB3 | 2.46 | 0.46 |
| 1:B:54:VAL:N | 2:B:547:HOH:O | 2.49 | 0.46 |
| 1:A:39:LEU:HD21 | 1:A:148:LYS:CD | 2.46 | 0.46 |
| 1:B:175:GLU:CD | 1:B:175:GLU:H | 2.20 | 0.46 |
| 1:B:220:PRO:O | 1:B:221:GLU:C | 2.53 | 0.46 |
| 1:C:158:HIS:CD2 | 2:C:352:HOH:O | 2.69 | 0.46 |
| 1:C:75:ILE:HD12 | 1:C:75:ILE:N | 2.32 | 0.45 |
| 1:D:163:VAL:HG21 | 2:D:430:HOH:O | 2.16 | 0.45 |
| 1:A:164:MET:HB2 | 1:A:168:LYS:C | 2.37 | 0.45 |
| 1:A:57:ARG:HG3 | 1:A:125:GLU:HG2 | 1.97 | 0.45 |
| 1:A:116:LYS:HB2 | 2:A:405:HOH:O | 2.17 | 0.45 |
| 1:A:192:LYS:HG3 | 1:A:192:LYS:O | 2.16 | 0.45 |
| 1:C:47:ILE:HG13 | 2:C:308:HOH:O | 2.17 | 0.45 |
| 1:D:189:LYS:CB | 1:D:190:PRO:HA | 2.41 | 0.45 |
| 1:D:56:ILE:CD1 | 1:D:75:ILE:HD12 | 2.46 | 0.45 |
| 1:C:216:GLU:O | 1:C:226:THR:O | 2.34 | 0.45 |
| 1:D:173:LYS:CD | 1:D:175:GLU:HG2 | 2.46 | 0.45 |
| 1:A:197:LYS:HG3 | 1:A:217:GLU:H | 1.81 | 0.45 |
| 1:A:78:LEU:HD23 | 1:A:83:VAL:HG12 | 1.98 | 0.45 |
| 1:B:141:ILE:O | 1:B:141:ILE:HG13 | 2.16 | 0.45 |
| 1:C:247:LYS:O | 1:C:248:ILE:CG1 | 2.52 | 0.45 |
| 1:A:51:GLU:OE1 | 1:A:67:SER:HB2 | 2.16 | 0.45 |
| 1:B:163:VAL:HG12 | 1:B:170:VAL:HG21 | 1.99 | 0.45 |
| 1:D:127:LYS:HE3 | 2:D:291:HOH:O | 2.17 | 0.45 |
| 1:D:224:LYS:C | 1:D:225:LEU:HD22 | 2.36 | 0.45 |
| 1:D:246:GLU:O | 1:D:246:GLU:HG3 | 2.17 | 0.45 |
| 1:A:160:PHE:O | 1:A:161:ARG:HG2 | 2.17 | 0.45 |
| 1:D:20:PRO:HB3 | 2:D:416:HOH:O | 2.17 | 0.45 |
| 1:A:102:ASP:OD2 | 1:A:121:GLU:HB2 | 2.16 | 0.45 |
| 1:A:17:GLN:NE2 | 1:A:161:ARG:NH2 | 2.65 | 0.45 |
| 1:B:31:LEU:O | 2:B:477:HOH:O | 2.21 | 0.45 |
| 1:C:215:VAL:CG1 | 1:C:225:LEU:HD22 | 2.47 | 0.45 |
| 1:B:219:HIS:O | 1:B:220:PRO:C | 2.55 | 0.45 |
| 1:B:247:LYS:O | 1:B:248:ILE:O | 2.35 | 0.45 |
| 1:A:13:TRP:HE1 | 1:A:174:GLU:HG3 | 1.81 | 0.44 |
| 1:B:204:ILE:CG2 | 1:B:246:GLU:HB2 | 2.47 | 0.44 |
| 1:D:102:ASP:OD2 | 1:D:121:GLU:HB3 | 2.17 | 0.44 |
| 1:A:244:GLN:C | 2:A:439:HOH:O | 2.55 | 0.44 |
| 1:B:64:TYR:CZ | 1:B:75:ILE:HD11 | 2.52 | 0.44 |
| 1:C:162:PRO:O | 1:C:164:MET:HE2 | 2.17 | 0.44 |
| 1:B:213:GLY:HA3 | 1:B:229:ILE:HA | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:14:TYR:HA | 1:C:172:LEU:CD2 | 2.46 | 0.44 |
| 1:C:184:ILE:HD13 | 2:C:504:HOH:O | 2.16 | 0.44 |
| 1:B:87:ARG:HG2 | 1:B:89:GLU:HG3 | 1.99 | 0.44 |
| 1:B:185:LYS:HG2 | 2:B:552:HOH:O | 2.18 | 0.44 |
| 1:C:16:LEU:HA | 1:C:162:PRO:HA | 2.00 | 0.44 |
| 1:C:27:LYS:O | 1:C:31:LEU:HG | 2.18 | 0.44 |
| 1:B:209:MET:O | 1:B:210:ASN:HB2 | 2.17 | 0.44 |
| 1:C:215:VAL:HG22 | 1:C:227:VAL:HG12 | 2.00 | 0.44 |
| 1:D:133:LYS:HG3 | 1:D:190:PRO:HD2 | 1.99 | 0.44 |
| 1:D:135:PHE:CE1 | 1:D:180:ILE:HG23 | 2.52 | 0.44 |
| 1:A:133:LYS:HD2 | 2:A:268:HOH:O | 2.16 | 0.44 |
| 1:B:203:VAL:HA | 2:B:385:HOH:O | 2.17 | 0.44 |
| 1:B:64:TYR:HB3 | 1:B:66:LEU:CD1 | 2.47 | 0.44 |
| 1:C:196:GLU:HA | 1:C:218:VAL:HG21 | 1.98 | 0.44 |
| 1:C:25:GLU:HG3 | 2:C:524:HOH:O | 2.17 | 0.44 |
| 2:C:276:HOH:O | 1:D:155:LYS:HE3 | 2.17 | 0.44 |
| 1:B:16:LEU:HD22 | 1:B:153:ILE:HG21 | 1.99 | 0.44 |
| 1:B:219:HIS:NE2 | 1:B:239:GLU:OE1 | 2.51 | 0.44 |
| 1:B:219:HIS:CD2 | 1:B:239:GLU:OE1 | 2.71 | 0.44 |
| 1:D:192:LYS:O | 1:D:192:LYS:HG3 | 2.18 | 0.44 |
| 1:A:50:ALA:HB1 | 1:A:131:ASP:C | 2.38 | 0.44 |
| 1:B:189:LYS:HB2 | 1:B:189:LYS:NZ | 2.29 | 0.44 |
| 1:A:16:LEU:HD21 | 1:A:141:ILE:HD11 | 2.00 | 0.43 |
| 1:D:59:GLN:NE2 | 1:D:123:LYS:HG3 | 2.33 | 0.43 |
| 1:C:54:VAL:CG1 | 1:C:93:VAL:HG21 | 2.48 | 0.43 |
| 1:A:242:PHE:N | 1:A:242:PHE:CD1 | 2.87 | 0.43 |
| 1:A:195:PHE:HA | 1:A:195:PHE:HD2 | 1.70 | 0.43 |
| 1:B:216:GLU:O | 1:B:217:GLU:CB | 2.66 | 0.43 |
| 1:C:87:ARG:HB2 | 1:C:96:VAL:CG2 | 2.49 | 0.43 |
| 1:D:196:GLU:N | 1:D:199:ASP:OD2 | 2.51 | 0.43 |
| 1:D:218:VAL:HG13 | 1:D:225:LEU:CD1 | 2.48 | 0.43 |
| 1:A:28:GLU:O | 1:A:32:LYS:HG3 | 2.18 | 0.43 |
| 1:B:204:ILE:HG12 | 2:B:385:HOH:O | 2.17 | 0.43 |
| 1:C:182:ASN:HD21 | 1:C:186:ARG:CB | 2.30 | 0.43 |
| 1:D:192:LYS:O | 1:D:193:VAL:C | 2.56 | 0.43 |
| 1:B:13:TRP:CG | 1:B:177:VAL:HG21 | 2.53 | 0.43 |
| 1:B:54:VAL:HG22 | 1:B:68:LEU:HD13 | 2.00 | 0.43 |
| 1:C:19:GLU:HB3 | 1:C:158:HIS:HB3 | 2.01 | 0.43 |
| 1:B:228:MET:HE1 | 1:B:235:MET:C | 2.39 | 0.43 |
| 1:C:37:GLU:HB3 | 1:C:39:LEU:HG | 2.01 | 0.43 |
| 1:A:135:PHE:N | 1:A:136:PRO:HD3 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:216:GLU:O | 1:A:217:GLU:CB | 2.67 | 0.42 |
| 1:A:227:VAL:HG22 | 1:A:229:ILE:HG13 | 2.01 | 0.42 |
| 1:B:160:PHE:CG | 1:B:160:PHE:O | 2.72 | 0.42 |
| 1:A:13:TRP:HD1 | 2:A:280:HOH:O | 2.02 | 0.42 |
| 1:C:58:ALA:O | 1:C:59:GLN:HB2 | 2.20 | 0.42 |
| 1:D:211:PHE:HB3 | 1:D:229:ILE:HG23 | 2.01 | 0.42 |
| 1:B:194:GLU:HB3 | 1:B:242:PHE:CE2 | 2.54 | 0.42 |
| 1:C:134:ILE:C | 1:C:136:PRO:HD3 | 2.39 | 0.42 |
| 1:C:56:ILE:N | 1:C:56:ILE:HD12 | 2.34 | 0.42 |
| 1:B:228:MET:HE3 | 1:B:237:PRO:N | 2.34 | 0.42 |
| 1:B:74:ASP:OD1 | 1:B:87:ARG:HB2 | 2.18 | 0.42 |
| 1:C:29:ASN:HB3 | 1:C:157:PRO:HG2 | 2.01 | 0.42 |
| 1:B:38:GLY:HA2 | 2:B:256:HOH:O | 2.19 | 0.42 |
| 1:C:164:MET:HB3 | 1:C:169:PRO:HA | 2.02 | 0.42 |
| 1:D:241:ASP:C | 1:D:243:ASP:N | 2.72 | 0.42 |
| 1:B:12:LYS:HB2 | 1:B:14:TYR:CE1 | 2.55 | 0.42 |
| 1:C:164:MET:HB2 | 1:C:168:LYS:O | 2.20 | 0.42 |
| 1:C:243:ASP:N | 1:C:243:ASP:OD2 | 2.33 | 0.42 |
| 1:D:120:LYS:HZ3 | 1:D:120:LYS:HB3 | 1.85 | 0.42 |
| 1:B:160:PHE:O | 1:B:161:ARG:HG3 | 2.20 | 0.42 |
| 1:B:133:LYS:NZ | 1:B:189:LYS:HZ3 | 2.17 | 0.42 |
| 1:C:175:GLU:HA | 1:C:178:GLN:HG2 | 2.01 | 0.42 |
| 1:C:179:ASN:HB3 | 2:C:371:HOH:O | 2.18 | 0.42 |
| 1:C:231:ILE:O | 1:C:232:PHE:HB2 | 2.20 | 0.42 |
| 1:C:54:VAL:O | 1:C:65:ARG:HA | 2.19 | 0.42 |
| 1:D:141:ILE:HD12 | 2:D:450:HOH:O | 2.20 | 0.42 |
| 1:B:175:GLU:HG3 | 2:B:421:HOH:O | 2.20 | 0.42 |
| 1:C:99:VAL:O | 1:C:102:ASP:HB2 | 2.20 | 0.42 |
| 1:C:195:PHE:O | 1:C:218:VAL:HG11 | 2.20 | 0.42 |
| 1:C:40:LYS:HG2 | 2:C:278:HOH:O | 2.19 | 0.42 |
| 1:D:87:ARG:CG | 1:D:89:GLU:HG3 | 2.49 | 0.42 |
| 1:C:196:GLU:O | 1:C:197:LYS:C | 2.58 | 0.42 |
| 1:C:22:LYS:HB3 | 1:C:22:LYS:NZ | 2.35 | 0.42 |
| 1:D:164:MET:HE1 | 1:D:169:PRO:HG3 | 2.01 | 0.42 |
| 1:D:165:VAL:HB | 1:D:170:VAL:HG22 | 2.01 | 0.42 |
| 1:A:35:GLU:HG2 | 1:A:40:LYS:HE3 | 2.02 | 0.41 |
| 1:C:173:LYS:HE2 | 1:C:174:GLU:HB3 | 2.01 | 0.41 |
| 1:C:192:LYS:HD3 | 2:C:457:HOH:O | 2.19 | 0.41 |
| 1:C:18:VAL:HG12 | 1:C:159:VAL:HG22 | 2.02 | 0.41 |
| 1:C:202:ARG:NH2 | 2:C:314:HOH:O | 2.53 | 0.41 |
| 1:B:225:LEU:HD22 | 1:B:242:PHE:CD1 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:124:THR:O | 1:C:125:GLU:HB3 | 2.20 | 0.41 |
| 1:C:139:ILE:HG22 | 2:C:546:HOH:O | 2.19 | 0.41 |
| 1:D:23:GLU:HG2 | 2:D:286:HOH:O | 2.20 | 0.41 |
| 1:D:76:SER:HB3 | 1:D:83:VAL:CG1 | 2.50 | 0.41 |
| 1:D:95:VAL:HG23 | 1:D:117:ILE:HG21 | 2.03 | 0.41 |
| 1:B:34:LEU:CB | 1:B:40:LYS:HD3 | 2.49 | 0.41 |
| 1:D:87:ARG:HD2 | 2:D:466:HOH:O | 2.20 | 0.41 |
| 1:A:122:ASN:O | 1:A:123:LYS:HB2 | 2.20 | 0.41 |
| 1:A:25:GLU:HB3 | 1:A:158:HIS:CD2 | 2.56 | 0.41 |
| 1:B:193:VAL:O | 1:B:194:GLU:HB2 | 2.21 | 0.41 |
| 1:B:222:LYS:HB3 | 1:B:222:LYS:HZ3 | 1.86 | 0.41 |
| 1:D:59:GLN:HE22 | 1:D:123:LYS:HG3 | 1.85 | 0.41 |
| 1:A:230:SER:O | 1:A:231:ILE:HD13 | 2.21 | 0.41 |
| 1:B:53:LYS:CA | 2:B:547:HOH:O | 2.68 | 0.41 |
| 1:C:122:ASN:O | 1:C:123:LYS:HB2 | 2.20 | 0.41 |
| 1:C:156:THR:HG22 | 2:C:293:HOH:O | 2.21 | 0.41 |
| 1:C:28:GLU:O | 1:C:32:LYS:HD3 | 2.20 | 0.41 |
| 1:A:242:PHE:N | 1:A:242:PHE:HD1 | 2.18 | 0.41 |
| 1:C:221:GLU:C | 1:C:223:ARG:H | 2.19 | 0.41 |
| 1:C:239:GLU:O | 1:C:240:LEU:HD23 | 2.21 | 0.41 |
| 1:C:94:LYS:HA | 1:C:117:ILE:CD1 | 2.51 | 0.41 |
| 1:A:207:PRO:CA | 2:A:267:HOH:O | 2.67 | 0.41 |
| 1:A:72:ALA:HA | 1:A:88:ILE:O | 2.21 | 0.41 |
| 1:B:204:ILE:HG13 | 1:B:205:GLU:N | 2.36 | 0.41 |
| 1:D:196:GLU:HA | 1:D:218:VAL:HG23 | 2.03 | 0.41 |
| 1:D:61:LYS:CD | 1:D:63:LYS:HE3 | 2.49 | 0.41 |
| 1:C:110:ILE:HG13 | 1:C:128:ILE:HD11 | 2.02 | 0.40 |
| 1:C:16:LEU:CD2 | 1:C:162:PRO:HB3 | 2.51 | 0.40 |
| 1:C:164:MET:HB2 | 1:C:168:LYS:C | 2.41 | 0.40 |
| 1:C:221:GLU:C | 1:C:223:ARG:N | 2.72 | 0.40 |
| 1:D:87:ARG:O | 1:D:93:VAL:HA | 2.22 | 0.40 |
| 1:C:222:LYS:HG3 | 2:C:286:HOH:O | 2.22 | 0.40 |
| 1:D:203:VAL:HG22 | 1:D:240:LEU:HD11 | 2.03 | 0.40 |
| 1:A:222:LYS:HZ3 | 1:A:222:LYS:HB3 | 1.85 | 0.40 |
| 1:B:133:LYS:HE2 | 1:B:134:ILE:HD11 | 2.03 | 0.40 |
| 1:C:160:PHE:O | 1:C:161:ARG:O | 2.40 | 0.40 |

All (598) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:165:VAL:CB | 1:B:238:VAL:CG1[2_757] | 0.11 | 2.09 |
| 1:D:195:PHE:CD2 | 2:A:260:HOH:O[2_646] | 0.20 | 2.00 |
| 1:B:207:PRO:C | 2:A:258:HOH:O[2_747] | 0.44 | 1.76 |
| 1:C:29:ASN:OD1 | 1:C:178:GLN:OE1[2_756] | 0.45 | 1.75 |
| 1:B:161:ARG:NH1 | 2:B:293:HOH:O[2_747] | 0.47 | 1.73 |
| 1:B:71:ASN:CG | 1:B:160:PHE:CA[2_757] | 0.47 | 1.73 |
| 1:B:71:ASN:CA | 1:B:160:PHE:CG[2_757] | 0.50 | 1.70 |
| 1:A:232:PHE:O | 2:B:255:HOH:O[2_757] | 0.50 | 1.70 |
| 1:A:170:VAL:CB | 1:B:231:ILE:CG1[2_757] | 0.52 | 1.68 |
| 1:A:172:LEU:CB | 1:B:232:PHE:C[2_757] | 0.53 | 1.67 |
| 1:B:234:ARG:CZ | 2:A:300:HOH:O[2_747] | 0.55 | 1.65 |
| 1:D:146:ASN:CB | 2:B:434:HOH:O[2_746] | 0.58 | 1.62 |
| 1:A:164:MET:O | 1:B:208:PHE:CD1[2_757] | 0.59 | 1.61 |
| 1:A:138:TYR:CZ | 1:B:210:ASN:CB[2_757] | 0.59 | 1.61 |
| 1:A:211:PHE:CD2 | 1:B:176:GLU:CB[2_757] | 0.62 | 1.58 |
| 1:A:232:PHE:CG | 1:B:15:ALA:CA[2_757] | 0.62 | 1.58 |
| 1:A:170:VAL:O | 1:B:231:ILE:CG2[2_757] | 0.63 | 1.57 |
| 1:A:231:ILE:CD1 | 1:B:176:GLU:OE2[2_757] | 0.64 | 1.56 |
| 1:A:232:PHE:CD2 | 1:B:15:ALA:CB[2_757] | 0.64 | 1.56 |
| 1:C:90:ASN:O | 1:C:151:MET:CE[2_746] | 0.66 | 1.54 |
| 1:A:234:ARG:CB | 1:B:163:VAL:CG1[2_757] | 0.66 | 1.54 |
| 1:A:172:LEU:CG | 1:B:232:PHE:N[2_757] | 0.70 | 1.50 |
| 1:D:242:PHE:O | 2:A:364:HOH:O[2_646] | 0.70 | 1.50 |
| 1:A:17:GLN:OE1 | 1:B:209:MET:CG[2_757] | 0.76 | 1.44 |
| 1:A:233:GLY:N | 1:B:170:VAL:O[2_757] | 0.77 | 1.43 |
| 1:A:211:PHE:CE2 | 1:B:176:GLU:CB[2_757] | 0.79 | 1.41 |
| 1:C:232:PHE:CE2 | 1:D:135:PHE:CD2[2_656] | 0.79 | 1.41 |
| 1:A:138:TYR:OH | 1:B:210:ASN:CA[2_757] | 0.79 | 1.41 |
| 1:A:212:THR:N | 2:B:413:HOH:O[2_757] | 0.79 | 1.41 |
| 1:A:164:MET:O | 1:B:208:PHE:CG[2_757] | 0.80 | 1.40 |
| 1:A:164:MET:CA | 1:B:208:PHE:CD2[2_757] | 0.80 | 1.40 |
| 1:A:172:LEU:CG | 1:B:232:PHE:CA[2_757] | 0.81 | 1.39 |
| 1:B:22:LYS:CD | 1:B:186:ARG:CD[2_747] | 0.82 | 1.38 |
| 2:B:296:HOH:O | 2:B:299:HOH:O[2_747] | 0.82 | 1.38 |
| 1:B:234:ARG:NE | 2:A:300:HOH:O[2_747] | 0.83 | 1.37 |
| 1:B:240:LEU:N | 2:B:264:HOH:O[2_757] | 0.86 | 1.34 |
| 1:A:233:GLY:C | 1:B:170:VAL:CB[2_757] | 0.87 | 1.33 |
| 1:A:232:PHE:C | 2:B:255:HOH:O[2_757] | 0.88 | 1.32 |
| 1:A:73:ARG:NH1 | 1:C:36:LEU:CD1[2_756] | 0.88 | 1.32 |
| 2:A:381:HOH:O | 2:C:334:HOH:O[2_756] | 0.88 | 1.32 |
| 1:A:138:TYR:CE1 | 1:B:210:ASN:ND2[2_757] | 0.89 | 1.31 |
| 1:A:172:LEU:CD2 | 1:B:232:PHE:N[2_757] | 0.89 | 1.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:185:LYS:CE | 2:C:307:HOH:O[2_746] | 0.89 | 1.31 |
| 1:B:72:ALA:CA | 1:B:160:PHE:CZ[2_757] | 0.90 | 1.30 |
| 1:B:237:PRO:CD | 1:D:103:THR:CB[2_756] | 0.92 | 1.28 |
| 1:B:217:GLU:OE1 | 2:D:310:HOH:O[2_756] | 0.92 | 1.28 |
| 1:A:211:PHE:CE1 | 1:B:176:GLU:C[2_757] | 0.93 | 1.27 |
| 1:A:14:TYR:C | 1:B:232:PHE:CE2[2_757] | 0.94 | 1.26 |
| 1:A:211:PHE:CE1 | 1:B:176:GLU:O[2_757] | 0.95 | 1.25 |
| 1:A:163:VAL:CG1 | 1:B:211:PHE:CD1[2_757] | 0.96 | 1.24 |
| 1:A:233:GLY:CA | 1:B:170:VAL:CA[2_757] | 0.97 | 1.23 |
| 1:D:233:GLY:CA | 2:C:395:HOH:O[2_646] | 0.97 | 1.23 |
| 1:A:163:VAL:CB | 1:B:211:PHE:CD1[2_757] | 0.98 | 1.22 |
| 1:B:74:ASP:O | 1:D:38:GLY:N[2_756] | 0.98 | 1.22 |
| 1:A:164:MET:C | 1:B:208:PHE:CD2[2_757] | 0.99 | 1.21 |
| 1:A:138:TYR:CE2 | 1:B:210:ASN:CB[2_757] | 1.00 | 1.20 |
| 1:B:208:PHE:N | 2:A:258:HOH:O[2_747] | 1.00 | 1.20 |
| 1:A:172:LEU:CB | 1:B:232:PHE:CA[2_757] | 1.00 | 1.20 |
| 1:B:238:VAL:CA | 1:D:106:ASN:OD1[2_756] | 1.01 | 1.19 |
| 1:A:232:PHE:CG | 1:B:15:ALA:N[2_757] | 1.01 | 1.19 |
| 1:B:71:ASN:CA | 1:B:160:PHE:CB[2_757] | 1.03 | 1.17 |
| 1:B:71:ASN:C | 1:B:160:PHE:CG[2_757] | 1.04 | 1.16 |
| 1:C:186:ARG:CG | 2:C:474:HOH:O[2_746] | 1.06 | 1.14 |
| 2:B:369:HOH:O | 2:C:315:HOH:O[1_556] | 1.06 | 1.14 |
| 1:B:75:ILE:C | 1:D:38:GLY:O[2_756] | 1.07 | 1.13 |
| 1:A:138:TYR:CD1 | 1:B:210:ASN:ND2[2_757] | 1.07 | 1.13 |
| 1:B:22:LYS:CE | 1:B:186:ARG:CZ[2_747] | 1.07 | 1.13 |
| 1:C:40:LYS:CA | 2:A:251:HOH:O[2_746] | 1.08 | 1.12 |
| 1:C:155:LYS:CB | 1:C:186:ARG:CZ[2_756] | 1.08 | 1.12 |
| 1:A:170:VAL:C | 1:B:231:ILE:CB[2_757] | 1.08 | 1.12 |
| 1:C:155:LYS:CG | 1:C:186:ARG:NH1[2_756] | 1.08 | 1.12 |
| 1:A:210:ASN:CA | 2:B:253:HOH:O[2_757] | 1.09 | 1.11 |
| 1:A:231:ILE:CD1 | 1:B:176:GLU:CD[2_757] | 1.09 | 1.11 |
| 1:B:72:ALA:N | 1:B:160:PHE:CE2[2_757] | 1.09 | 1.11 |
| 1:D:148:LYS:NZ | 2:B:340:HOH:O[2_746] | 1.09 | 1.11 |
| 1:D:40:LYS:CG | 2:B:271:HOH:O[2_746] | 1.10 | 1.10 |
| 1:B:75:ILE:CA | 1:D:38:GLY:O[2_756] | 1.11 | 1.09 |
| 1:A:170:VAL:CB | 1:B:231:ILE:CD1[2_757] | 1.12 | 1.08 |
| 1:A:163:VAL:CB | 1:B:211:PHE:CE1[2_757] | 1.13 | 1.07 |
| 1:C:232:PHE:CZ | 1:D:135:PHE:CG[2_656] | 1.13 | 1.07 |
| 1:A:75:ILE:CA | 1:C:38:GLY:O[2_756] | 1.14 | 1.06 |
| 1:A:75:ILE:C | 1:C:38:GLY:O[2_756] | 1.14 | 1.06 |
| 1:A:232:PHE:CD1 | 1:B:15:ALA:N[2_757] | 1.15 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:73:ARG:NH2 | 1:D:35:GLU:O[2_756] | 1.15 | 1.05 |
| 1:B:22:LYS:CE | 1:B:186:ARG:NH2[2_747] | 1.16 | 1.04 |
| 1:A:233:GLY:CA | 1:B:170:VAL:C[2_757] | 1.16 | 1.04 |
| 1:A:74:ASP:CG | 2:C:292:HOH:O[2_756] | 1.17 | 1.03 |
| 1:A:165:VAL:CG1 | 1:B:238:VAL:CA[2_757] | 1.17 | 1.03 |
| 1:A:17:GLN:CD | 1:B:209:MET:SD[2_757] | 1.18 | 1.02 |
| 1:A:211:PHE:CZ | 1:B:176:GLU:C[2_757] | 1.19 | 1.01 |
| 1:A:164:MET:C | 1:B:208:PHE:CG[2_757] | 1.19 | 1.01 |
| 1:A:138:TYR:CE1 | 1:B:210:ASN:CG[2_757] | 1.19 | 1.01 |
| 1:A:17:GLN:CD | 1:B:209:MET:CG[2_757] | 1.20 | 1.00 |
| 1:A:234:ARG:N | 1:B:170:VAL:CG2[2_757] | 1.20 | 1.00 |
| 1:A:15:ALA:N | 1:B:232:PHE:CE2[2_757] | 1.21 | 0.99 |
| 1:B:71:ASN:C | 1:B:160:PHE:CD1[2_757] | 1.21 | 0.99 |
| 1:A:170:VAL:CA | 1:B:231:ILE:CG1[2_757] | 1.21 | 0.99 |
| 1:A:138:TYR:CZ | 1:B:210:ASN:CG[2_757] | 1.22 | 0.98 |
| 1:A:165:VAL:CG1 | 1:D:106:ASN:OD1[1_566] | 1.22 | 0.98 |
| 1:A:172:LEU:CA | 1:B:232:PHE:C[2_757] | 1.22 | 0.98 |
| 1:B:161:ARG:CZ | 2:B:293:HOH:O[2_747] | 1.22 | 0.98 |
| 1:A:80:LYS:CG | 1:C:8:GLU:OE1[2_756] | 1.24 | 0.96 |
| 1:A:231:ILE:CA | 1:B:172:LEU:CD2[2_757] | 1.24 | 0.96 |
| 1:A:171:PRO:C | 1:B:231:ILE:O[2_757] | 1.24 | 0.96 |
| 1:B:74:ASP:O | 1:D:37:GLU:C[2_756] | 1.24 | 0.96 |
| 1:A:170:VAL:O | 1:B:231:ILE:CB[2_757] | 1.25 | 0.95 |
| 1:A:211:PHE:CD1 | 1:B:176:GLU:CA[2_757] | 1.25 | 0.95 |
| 1:A:74:ASP:O | 1:C:38:GLY:N[2_756] | 1.25 | 0.95 |
| 1:A:209:MET:O | 1:B:179:ASN:ND2[2_757] | 1.25 | 0.95 |
| 1:A:232:PHE:CD2 | 1:B:15:ALA:CA[2_757] | 1.26 | 0.94 |
| 1:C:40:LYS:N | 2:A:251:HOH:O[2_746] | 1.26 | 0.94 |
| 1:B:71:ASN:ND2 | 1:B:160:PHE:C[2_757] | 1.27 | 0.93 |
| 1:A:170:VAL:C | 1:B:231:ILE:CG2[2_757] | 1.27 | 0.93 |
| 1:A:233:GLY:C | 1:B:170:VAL:CG2[2_757] | 1.27 | 0.93 |
| 1:A:232:PHE:CD1 | 1:B:14:TYR:C[2_757] | 1.28 | 0.92 |
| 1:A:165:VAL:CG1 | 1:B:238:VAL:CB[2_757] | 1.28 | 0.92 |
| 2:A:302:HOH:O | 2:C:291:HOH:O[2_756] | 1.28 | 0.92 |
| 1:C:40:LYS:CG | 2:A:255:HOH:O[2_746] | 1.28 | 0.92 |
| 1:B:22:LYS:CE | 1:B:186:ARG:NE[2_747] | 1.29 | 0.91 |
| 1:B:71:ASN:C | 1:B:160:PHE:CD2[2_757] | 1.30 | 0.90 |
| 1:A:74:ASP:CB | 2:C:292:HOH:O[2_756] | 1.30 | 0.90 |
| 1:B:22:LYS:NZ | 1:B:186:ARG:NH2[2_747] | 1.30 | 0.90 |
| 1:C:40:LYS:C | 2:A:251:HOH:O[2_746] | 1.30 | 0.90 |
| 1:A:74:ASP:O | 1:C:38:GLY:CA[2_756] | 1.30 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:211:PHE:N | 2:B:546:HOH:O[2_757] | 1.31 | 0.89 |
| 1:D:242:PHE:C | 2:A:364:HOH:O[2_646] | 1.31 | 0.89 |
| 1:D:233:GLY:C | 2:C:395:HOH:O[2_646] | 1.31 | 0.89 |
| 1:B:219:HIS:CE1 | 1:D:108:PRO:CB[2_756] | 1.31 | 0.89 |
| 1:A:233:GLY:C | 1:B:170:VAL:CA[2_757] | 1.31 | 0.89 |
| 1:A:165:VAL:N | 1:B:208:PHE:CZ[2_757] | 1.32 | 0.88 |
| 1:A:172:LEU:CD2 | 1:B:231:ILE:C[2_757] | 1.32 | 0.88 |
| 1:B:71:ASN:N | 1:B:160:PHE:CB[2_757] | 1.32 | 0.88 |
| 1:A:164:MET:C | 1:B:208:PHE:CE2[2_757] | 1.32 | 0.88 |
| 1:B:71:ASN:CB | 1:B:160:PHE:CA[2_757] | 1.32 | 0.88 |
| 1:B:19:GLU:OE1 | 2:B:466:HOH:O[2_747] | 1.33 | 0.87 |
| 1:B:237:PRO:CD | 1:D:103:THR:CG2[2_756] | 1.33 | 0.87 |
| 1:A:64:TYR:OH | 1:C:40:LYS:CB[2_756] | 1.33 | 0.87 |
| 1:A:232:PHE:CD1 | 1:B:15:ALA:CA[2_757] | 1.33 | 0.87 |
| 1:D:41:ASP:N | 2:B:254:HOH:O[2_746] | 1.34 | 0.86 |
| 1:A:172:LEU:N | 1:B:231:ILE:O[2_757] | 1.34 | 0.86 |
| 1:B:71:ASN:OD1 | 1:B:159:VAL:O[2_757] | 1.34 | 0.86 |
| 1:A:211:PHE:C | 2:B:413:HOH:O[2_757] | 1.34 | 0.86 |
| 1:C:36:LEU:O | 2:C:262:HOH:O[2_756] | 1.34 | 0.86 |
| 2:B:268:HOH:O | 2:B:359:HOH:O[2_747] | 1.34 | 0.86 |
| 1:B:76:SER:OG | 1:D:39:LEU:CD2[2_756] | 1.34 | 0.86 |
| 1:B:72:ALA:N | 1:B:160:PHE:CZ[2_757] | 1.35 | 0.85 |
| 1:A:165:VAL:CG2 | 1:B:238:VAL:CG2[2_757] | 1.35 | 0.85 |
| 1:A:76:SER:OG | 1:C:39:LEU:CD2[2_756] | 1.36 | 0.84 |
| 1:B:73:ARG:CZ | 1:D:35:GLU:O[2_756] | 1.36 | 0.84 |
| 1:B:74:ASP:O | 1:D:38:GLY:CA[2_756] | 1.36 | 0.84 |
| 1:A:80:LYS:O | 1:C:9:LEU:CD2[2_756] | 1.36 | 0.84 |
| 1:B:71:ASN:CG | 1:B:160:PHE:N[2_757] | 1.36 | 0.84 |
| 1:A:211:PHE:CG | 1:B:176:GLU:CA[2_757] | 1.36 | 0.84 |
| 1:B:71:ASN:ND2 | 1:B:160:PHE:CA[2_757] | 1.37 | 0.83 |
| 1:A:165:VAL:N | 1:B:208:PHE:CE2[2_757] | 1.37 | 0.83 |
| 1:A:164:MET:CA | 1:B:208:PHE:CE2[2_757] | 1.37 | 0.83 |
| 1:B:165:VAL:CG1 | 2:C:545:HOH:O[1_556] | 1.38 | 0.82 |
| 1:D:40:LYS:C | 2:B:254:HOH:O[2_746] | 1.38 | 0.82 |
| 1:D:195:PHE:CE2 | 2:A:260:HOH:O[2_646] | 1.38 | 0.82 |
| 1:B:207:PRO:O | 2:A:258:HOH:O[2_747] | 1.38 | 0.82 |
| 1:B:71:ASN:ND2 | 1:B:160:PHE:N[2_757] | 1.38 | 0.82 |
| 1:A:233:GLY:O | 1:B:170:VAL:CG2[2_757] | 1.39 | 0.81 |
| 1:A:76:SER:N | 1:C:38:GLY:O[2_756] | 1.39 | 0.81 |
| 1:B:20:PRO:CG | 2:B:535:HOH:O[2_747] | 1.39 | 0.81 |
| 1:B:22:LYS:CD | 1:B:186:ARG:NE[2_747] | 1.39 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 2:A:254:HOH:O | 2:C:516:HOH:O[2_756] | 1.40 | 0.80 |
| 1:A:14:TYR:O | 1:B:232:PHE:CE2[2_757] | 1.40 | 0.80 |
| 1:C:232:PHE:CZ | 1:D:135:PHE:CD2[2_656] | 1.40 | 0.80 |
| 1:A:74:ASP:OD2 | 2:C:292:HOH:O[2_756] | 1.40 | 0.80 |
| 1:D:195:PHE:CG | 2:A:260:HOH:O[2_646] | 1.41 | 0.79 |
| 1:B:76:SER:N | 1:D:38:GLY:O[2_756] | 1.41 | 0.79 |
| 1:A:162:PRO:O | 1:B:207:PRO:O[2_757] | 1.41 | 0.79 |
| 1:C:9:LEU:O | 2:A:254:HOH:O[2_746] | 1.41 | 0.79 |
| 1:A:210:ASN:CG | 1:B:175:GLU:CG[2_757] | 1.41 | 0.79 |
| 1:B:71:ASN:OD1 | 1:B:159:VAL:C[2_757] | 1.41 | 0.79 |
| 1:B:72:ALA:C | 1:B:160:PHE:CZ[2_757] | 1.42 | 0.78 |
| 1:C:90:ASN:C | 1:C:151:MET:CE[2_746] | 1.42 | 0.78 |
| 1:A:77:VAL:CB | 1:C:41:ASP:OD2[2_756] | 1.42 | 0.78 |
| 1:A:234:ARG:CA | 1:B:170:VAL:CG2[2_757] | 1.42 | 0.78 |
| 1:A:172:LEU:C | 1:B:232:PHE:O[2_757] | 1.42 | 0.78 |
| 1:A:17:GLN:OE1 | 1:B:209:MET:SD[2_757] | 1.43 | 0.77 |
| 1:A:173:LYS:N | 1:B:233:GLY:CA[2_757] | 1.43 | 0.77 |
| 1:A:233:GLY:O | 1:B:170:VAL:CB[2_757] | 1.43 | 0.77 |
| 1:B:72:ALA:CA | 1:B:160:PHE:CE2[2_757] | 1.43 | 0.77 |
| 1:C:135:PHE:CD2 | 1:D:232:PHE:CZ[2_656] | 1.44 | 0.76 |
| 2:A:303:HOH:O | 2:C:306:HOH:O[2_756] | 1.44 | 0.76 |
| 1:A:165:VAL:CB | 1:B:238:VAL:CB[2_757] | 1.44 | 0.76 |
| 1:C:90:ASN:O | 1:C:151:MET:SD[2_746] | 1.44 | 0.76 |
| 1:B:21:GLY:O | 2:B:348:HOH:O[2_747] | 1.45 | 0.75 |
| 1:B:240:LEU:CG | 2:B:551:HOH:O[2_757] | 1.45 | 0.75 |
| 1:A:170:VAL:CG1 | 1:B:231:ILE:CG1[2_757] | 1.45 | 0.75 |
| 1:D:40:LYS:CB | 2:B:271:HOH:O[2_746] | 1.46 | 0.74 |
| 1:A:232:PHE:CD1 | 1:B:14:TYR:O[2_757] | 1.46 | 0.74 |
| 1:A:14:TYR:C | 1:B:232:PHE:CD2[2_757] | 1.47 | 0.73 |
| 1:A:209:MET:CB | 1:B:179:ASN:OD1[2_757] | 1.48 | 0.72 |
| 1:B:72:ALA:N | 1:B:160:PHE:CD2[2_757] | 1.48 | 0.72 |
| 1:D:202:ARG:CD | 2:C:503:HOH:O[2_646] | 1.48 | 0.72 |
| 1:B:71:ASN:OD1 | 1:B:160:PHE:N[2_757] | 1.48 | 0.72 |
| 1:A:211:PHE:CE1 | 1:B:176:GLU:CA[2_757] | 1.49 | 0.71 |
| 1:A:138:TYR:OH | 1:B:210:ASN:CB[2_757] | 1.49 | 0.71 |
| 1:B:78:LEU:CD1 | 1:D:11:LYS:CE[2_756] | 1.49 | 0.71 |
| 1:C:155:LYS:CB | 1:C:186:ARG:NH2[2_756] | 1.49 | 0.71 |
| 1:A:211:PHE:CE2 | 1:B:176:GLU:CG[2_757] | 1.49 | 0.71 |
| 1:A:233:GLY:CA | 1:B:170:VAL:N[2_757] | 1.50 | 0.70 |
| 1:B:19:GLU:CD | 2:B:466:HOH:O[2_747] | 1.50 | 0.70 |
| 1:A:172:LEU:CA | 1:B:233:GLY:N[2_757] | 1.50 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:232:PHE:CG | 1:B:15:ALA:CB[2_757] | 1.51 | 0.69 |
| 1:D:40:LYS:CA | 2:B:254:HOH:O[2_746] | 1.51 | 0.69 |
| 1:A:172:LEU:CD1 | 1:B:232:PHE:CA[2_757] | 1.51 | 0.69 |
| 1:C:40:LYS:CB | 2:A:255:HOH:O[2_746] | 1.51 | 0.69 |
| 1:A:78:LEU:CD2 | 1:C:144:HIS:CB[2_756] | 1.52 | 0.68 |
| 1:A:208:PHE:O | 2:B:349:HOH:O[2_757] | 1.52 | 0.68 |
| 1:C:147:ASP:OD1 | 2:A:413:HOH:O[2_746] | 1.52 | 0.68 |
| 1:C:224:LYS:NZ | 1:D:248:ILE:OXT[2_656] | 1.52 | 0.68 |
| 1:A:209:MET:N | 1:B:179:ASN:CG[2_757] | 1.53 | 0.67 |
| 1:B:237:PRO:CG | 1:D:103:THR:CB[2_756] | 1.53 | 0.67 |
| 1:A:234:ARG:N | 1:B:170:VAL:CB[2_757] | 1.54 | 0.66 |
| 1:A:77:VAL:CG1 | 1:C:41:ASP:CB[2_756] | 1.54 | 0.66 |
| 1:A:232:PHE:CB | 1:B:15:ALA:N[2_757] | 1.54 | 0.66 |
| 1:B:234:ARG:NH2 | 2:A:300:HOH:O[2_747] | 1.54 | 0.66 |
| 1:A:165:VAL:CG1 | 1:B:238:VAL:CG1[2_757] | 1.54 | 0.66 |
| 1:A:209:MET:CA | 1:B:179:ASN:OD1[2_757] | 1.55 | 0.65 |
| 1:B:71:ASN:OD1 | 1:B:160:PHE:CA[2_757] | 1.56 | 0.64 |
| 1:A:210:ASN:C | 1:B:175:GLU:CB[2_757] | 1.56 | 0.64 |
| 1:C:147:ASP:CB | 2:A:413:HOH:O[2_746] | 1.57 | 0.63 |
| 1:A:165:VAL:CA | 1:B:238:VAL:CG1[2_757] | 1.57 | 0.63 |
| 1:B:71:ASN:O | 1:B:160:PHE:CE1[2_757] | 1.57 | 0.63 |
| 1:A:233:GLY:CA | 1:B:170:VAL:O[2_757] | 1.57 | 0.63 |
| 1:A:138:TYR:CZ | 1:B:210:ASN:CA[2_757] | 1.57 | 0.63 |
| 1:B:75:ILE:CA | 1:D:38:GLY:C[2_756] | 1.58 | 0.62 |
| 1:A:74:ASP:C | 1:C:37:GLU:O[2_756] | 1.58 | 0.62 |
| 1:A:80:LYS:C | 1:C:9:LEU:CG[2_756] | 1.58 | 0.62 |
| 1:D:40:LYS:N | 2:B:254:HOH:O[2_746] | 1.58 | 0.62 |
| 1:B:77:VAL:CB | 1:D:41:ASP:OD1[2_756] | 1.58 | 0.62 |
| 1:B:71:ASN:C | 1:B:160:PHE:CE1[2_757] | 1.58 | 0.62 |
| 1:B:64:TYR:OH | 1:D:40:LYS:CB[2_756] | 1.59 | 0.61 |
| 1:A:74:ASP:O | 1:C:37:GLU:C[2_756] | 1.59 | 0.61 |
| 1:A:165:VAL:CG2 | 1:B:238:VAL:CG1[2_757] | 1.59 | 0.61 |
| 1:A:164:MET:C | 1:B:208:PHE:CD1[2_757] | 1.59 | 0.61 |
| 1:B:73:ARG:NE | 1:D:36:LEU:O[2_756] | 1.59 | 0.61 |
| 1:C:135:PHE:CD1 | 1:D:232:PHE:CE1[2_656] | 1.59 | 0.61 |
| 1:B:71:ASN:CG | 1:B:160:PHE:C[2_757] | 1.60 | 0.60 |
| 1:D:245:VAL:O | 2:A:436:HOH:O[2_646] | 1.60 | 0.60 |
| 1:A:172:LEU:CB | 1:B:232:PHE:O[2_757] | 1.60 | 0.60 |
| 1:A:209:MET:C | 1:B:179:ASN:ND2[2_757] | 1.60 | 0.60 |
| 1:C:29:ASN:OD1 | 1:C:178:GLN:CD[2_756] | 1.61 | 0.59 |
| 1:B:233:GLY:CA | 2:A:344:HOH:O[2_747] | 1.61 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:19:GLU:CG | 2:B:466:HOH:O[2_747] | 1.61 | 0.59 |
| 1:A:172:LEU:CB | 1:B:233:GLY:N[2_757] | 1.62 | 0.58 |
| 1:A:83:VAL:CG1 | 1:C:144:HIS:ND1[2_756] | 1.62 | 0.58 |
| 1:C:39:LEU:CD2 | 2:A:266:HOH:O[2_746] | 1.62 | 0.58 |
| 1:A:74:ASP:CB | 1:C:37:GLU:O[2_756] | 1.62 | 0.58 |
| 1:C:232:PHE:CE2 | 1:D:135:PHE:CE2[2_656] | 1.62 | 0.58 |
| 1:A:211:PHE:CD2 | 1:B:176:GLU:CA[2_757] | 1.62 | 0.58 |
| 1:A:165:VAL:CG2 | 1:B:238:VAL:CB[2_757] | 1.63 | 0.57 |
| 1:C:29:ASN:CG | 1:C:178:GLN:OE1[2_756] | 1.63 | 0.57 |
| 1:C:147:ASP:CG | 2:A:413:HOH:O[2_746] | 1.63 | 0.57 |
| 1:A:172:LEU:CA | 1:B:232:PHE:O[2_757] | 1.63 | 0.57 |
| 1:C:39:LEU:CG | 2:A:266:HOH:O[2_746] | 1.64 | 0.56 |
| 1:B:71:ASN:O | 1:B:160:PHE:CD1[2_757] | 1.64 | 0.56 |
| 1:A:17:GLN:NE2 | 1:B:209:MET:SD[2_757] | 1.64 | 0.56 |
| 1:B:71:ASN:CA | 1:B:160:PHE:CD1[2_757] | 1.64 | 0.56 |
| 1:B:71:ASN:CB | 1:B:160:PHE:CB[2_757] | 1.65 | 0.55 |
| 1:B:74:ASP:C | 1:D:37:GLU:O[2_756] | 1.65 | 0.55 |
| 1:B:74:ASP:O | 1:D:37:GLU:O[2_756] | 1.66 | 0.54 |
| 1:A:80:LYS:CD | 1:C:8:GLU:OE1[2_756] | 1.66 | 0.54 |
| 1:A:14:TYR:CA | 1:B:232:PHE:CD2[2_757] | 1.66 | 0.54 |
| 1:A:170:VAL:CG2 | 1:B:231:ILE:CD1[2_757] | 1.66 | 0.54 |
| 1:D:233:GLY:O | 2:C:395:HOH:O[2_646] | 1.67 | 0.53 |
| 1:A:171:PRO:O | 1:B:234:ARG:CB[2_757] | 1.67 | 0.53 |
| 1:A:231:ILE:CD1 | 1:B:176:GLU:OE1[2_757] | 1.68 | 0.52 |
| 1:A:233:GLY:N | 1:B:170:VAL:C[2_757] | 1.68 | 0.52 |
| 1:C:155:LYS:CG | 1:C:186:ARG:CZ[2_756] | 1.68 | 0.52 |
| 1:A:232:PHE:CE1 | 1:B:14:TYR:O[2_757] | 1.68 | 0.52 |
| 1:C:36:LEU:C | 2:C:262:HOH:O[2_756] | 1.68 | 0.52 |
| 1:C:41:ASP:N | 2:A:251:HOH:O[2_746] | 1.68 | 0.52 |
| 1:A:164:MET:C | 1:B:208:PHE:CZ[2_757] | 1.68 | 0.52 |
| 1:C:135:PHE:CG | 1:D:232:PHE:CE1[2_656] | 1.69 | 0.51 |
| 1:A:75:ILE:CA | 1:C:38:GLY:C[2_756] | 1.69 | 0.51 |
| 1:A:233:GLY:O | 1:B:170:VAL:CA[2_757] | 1.69 | 0.51 |
| 1:C:185:LYS:CD | 2:C:307:HOH:O[2_746] | 1.69 | 0.51 |
| 1:B:71:ASN:C | 1:B:160:PHE:CE2[2_757] | 1.69 | 0.51 |
| 1:D:32:LYS:CD | 2:B:317:HOH:O[1_554] | 1.69 | 0.51 |
| 1:B:71:ASN:N | 1:B:160:PHE:CG[2_757] | 1.69 | 0.51 |
| 1:A:96:VAL:CG1 | 2:C:505:HOH:O[2_756] | 1.70 | 0.50 |
| 2:A:282:HOH:O | 2:D:334:HOH:O[2_656] | 1.70 | 0.50 |
| 1:A:231:ILE:CG1 | 1:B:176:GLU:OE2[2_757] | 1.70 | 0.50 |
| 1:A:163:VAL:CG1 | 1:B:211:PHE:CG[2_757] | 1.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:158:HIS:NE2 | 1:B:186:ARG:NH1[2_747] | 1.70 | 0.50 |
| 1:A:164:MET:N | 1:B:208:PHE:CD2[2_757] | 1.72 | 0.48 |
| 1:A:209:MET:N | 1:B:179:ASN:OD1[2_757] | 1.72 | 0.48 |
| 1:A:234:ARG:NH1 | 1:B:17:GLN:OE1[2_757] | 1.72 | 0.48 |
| 1:C:90:ASN:CB | 2:C:287:HOH:O[2_746] | 1.72 | 0.48 |
| 1:C:135:PHE:CE1 | 1:D:232:PHE:CE1[2_656] | 1.72 | 0.48 |
| 1:A:234:ARG:CG | 1:B:163:VAL:CG1[2_757] | 1.73 | 0.47 |
| 1:C:155:LYS:CB | 1:C:186:ARG:NE[2_756] | 1.73 | 0.47 |
| 1:B:72:ALA:C | 1:B:160:PHE:CE1[2_757] | 1.73 | 0.47 |
| 1:D:146:ASN:CG | 2:B:434:HOH:O[2_746] | 1.73 | 0.47 |
| 1:A:14:TYR:O | 1:B:232:PHE:CZ[2_757] | 1.73 | 0.47 |
| 1:C:35:GLU:OE2 | 2:A:323:HOH:O[2_746] | 1.73 | 0.47 |
| 1:A:172:LEU:CG | 1:B:231:ILE:C[2_757] | 1.74 | 0.46 |
| 1:A:164:MET:O | 1:B:208:PHE:CE1[2_757] | 1.74 | 0.46 |
| 1:A:209:MET:O | 1:B:179:ASN:CG[2_757] | 1.74 | 0.46 |
| 1:A:97:GLU:OE1 | 2:C:318:HOH:O[2_756] | 1.74 | 0.46 |
| 1:A:80:LYS:C | 1:C:9:LEU:CD2[2_756] | 1.75 | 0.45 |
| 1:B:22:LYS:CE | 1:B:186:ARG:CD[2_747] | 1.75 | 0.45 |
| 1:A:15:ALA:CB | 1:B:211:PHE:CE2[2_757] | 1.75 | 0.45 |
| 1:C:186:ARG:CD | 2:C:474:HOH:O[2_746] | 1.75 | 0.45 |
| 1:A:211:PHE:CD2 | 1:B:176:GLU:CG[2_757] | 1.75 | 0.45 |
| 1:C:186:ARG:CB | 2:C:474:HOH:O[2_746] | 1.75 | 0.45 |
| 1:A:80:LYS:CE | 1:C:8:GLU:OE1[2_756] | 1.75 | 0.45 |
| 1:B:71:ASN:CA | 1:B:160:PHE:CD2[2_757] | 1.75 | 0.45 |
| 1:A:210:ASN:C | 2:B:253:HOH:O[2_757] | 1.75 | 0.45 |
| 1:D:39:LEU:CG | 2:B:259:HOH:O[2_746] | 1.76 | 0.44 |
| 1:A:171:PRO:O | 1:B:234:ARG:N[2_757] | 1.76 | 0.44 |
| 1:A:210:ASN:OD1 | 1:B:175:GLU:CG[2_757] | 1.76 | 0.44 |
| 1:A:233:GLY:C | 1:B:170:VAL:N[2_757] | 1.76 | 0.44 |
| 1:B:234:ARG:NH1 | 2:A:300:HOH:O[2_747] | 1.76 | 0.44 |
| 1:B:71:ASN:CB | 1:B:160:PHE:C[2_757] | 1.77 | 0.43 |
| 1:A:211:PHE:CG | 1:B:176:GLU:CB[2_757] | 1.77 | 0.43 |
| 1:B:78:LEU:CD2 | 1:D:144:HIS:CB[2_756] | 1.77 | 0.43 |
| 1:B:239:GLU:C | 2:B:264:HOH:O[2_757] | 1.77 | 0.43 |
| 1:A:211:PHE:CZ | 1:B:176:GLU:CA[2_757] | 1.78 | 0.42 |
| 1:B:209:MET:CE | 2:A:447:HOH:O[2_747] | 1.78 | 0.42 |
| 1:A:74:ASP:CA | 1:C:37:GLU:O[2_756] | 1.78 | 0.42 |
| 1:A:170:VAL:CA | 1:B:231:ILE:CB[2_757] | 1.78 | 0.42 |
| 1:B:74:ASP:CB | 1:D:37:GLU:O[2_756] | 1.79 | 0.41 |
| 1:A:138:TYR:OH | 1:B:210:ASN:N[2_757] | 1.79 | 0.41 |
| 1:A:208:PHE:O | 1:B:179:ASN:ND2[2_757] | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:64:TYR:CE2 | 1:D:40:LYS:CE[2_756] | 1.79 | 0.41 |
| 1:A:172:LEU:O | 1:B:232:PHE:O[2_757] | 1.79 | 0.41 |
| 1:A:208:PHE:C | 1:B:179:ASN:ND2[2_757] | 1.79 | 0.41 |
| 1:A:172:LEU:CD1 | 1:B:232:PHE:N[2_757] | 1.80 | 0.40 |
| 1:A:211:PHE:CZ | 1:B:176:GLU:O[2_757] | 1.80 | 0.40 |
| 1:A:17:GLN:NE2 | 1:B:209:MET:CB[2_757] | 1.80 | 0.40 |
| 1:A:171:PRO:O | 1:B:234:ARG:CA[2_757] | 1.80 | 0.40 |
| 1:A:164:MET:C | 1:B:208:PHE:CE1[2_757] | 1.80 | 0.40 |
| 1:B:71:ASN:CB | 1:B:160:PHE:CG[2_757] | 1.80 | 0.40 |
| 1:A:73:ARG:NH1 | 1:C:36:LEU:CG[2_756] | 1.80 | 0.40 |
| 1:B:71:ASN:C | 1:B:160:PHE:CZ[2_757] | 1.80 | 0.40 |
| 1:C:151:MET:CG | 2:C:470:HOH:O[2_756] | 1.81 | 0.39 |
| 1:A:80:LYS:O | 1:C:9:LEU:CG[2_756] | 1.81 | 0.39 |
| 1:C:90:ASN:OD1 | 2:C:287:HOH:O[2_746] | 1.81 | 0.39 |
| 1:A:77:VAL:CB | 1:C:41:ASP:CG[2_756] | 1.82 | 0.38 |
| 1:A:211:PHE:CE2 | 1:B:176:GLU:CA[2_757] | 1.83 | 0.37 |
| 2:A:302:HOH:O | 2:C:306:HOH:O[2_756] | 1.84 | 0.36 |
| 1:A:17:GLN:CD | 1:B:209:MET:CB[2_757] | 1.84 | 0.36 |
| 1:A:231:ILE:C | 1:B:172:LEU:CD2[2_757] | 1.84 | 0.36 |
| 1:C:178:GLN:NE2 | 2:C:547:HOH:O[2_746] | 1.85 | 0.35 |
| 1:C:135:PHE:CG | 1:D:232:PHE:CZ[2_656] | 1.85 | 0.35 |
| 1:A:172:LEU:CG | 1:B:232:PHE:CB[2_757] | 1.85 | 0.35 |
| 1:A:210:ASN:C | 2:B:546:HOH:O[2_757] | 1.85 | 0.35 |
| 1:A:80:LYS:CE | 1:C:8:GLU:OE2[2_756] | 1.85 | 0.35 |
| 1:A:211:PHE:CZ | 1:B:177:VAL:N[2_757] | 1.85 | 0.35 |
| 1:A:15:ALA:N | 1:B:232:PHE:CD2[2_757] | 1.85 | 0.35 |
| 1:C:69:LYS:NZ | 2:C:249:HOH:O[2_746] | 1.86 | 0.34 |
| 1:B:72:ALA:N | 1:B:160:PHE:CE1[2_757] | 1.86 | 0.34 |
| 1:C:135:PHE:CD2 | 1:D:232:PHE:CE1[2_656] | 1.86 | 0.34 |
| 1:C:39:LEU:C | 2:A:251:HOH:O[2_746] | 1.86 | 0.34 |
| 1:A:80:LYS:CE | 1:C:8:GLU:CD[2_756] | 1.87 | 0.33 |
| 1:C:40:LYS:CA | 2:A:255:HOH:O[2_746] | 1.87 | 0.33 |
| 1:B:207:PRO:CA | 2:A:258:HOH:O[2_747] | 1.87 | 0.33 |
| 1:A:164:MET:CB | 1:B:208:PHE:CE2[2_757] | 1.87 | 0.33 |
| 1:A:210:ASN:ND2 | 1:B:175:GLU:CG[2_757] | 1.87 | 0.33 |
| 1:A:211:PHE:CZ | 1:B:176:GLU:CB[2_757] | 1.88 | 0.32 |
| 1:A:74:ASP:O | 1:C:37:GLU:O[2_756] | 1.88 | 0.32 |
| 1:A:171:PRO:O | 1:B:231:ILE:O[2_757] | 1.88 | 0.32 |
| 1:B:155:LYS:CE | 1:D:32:LYS:NZ[1_556] | 1.88 | 0.32 |
| 1:A:233:GLY:CA | 1:B:170:VAL:CB[2_757] | 1.88 | 0.32 |
| 1:B:217:GLU:OE2 | 1:D:108:PRO:CG[2_756] | 1.88 | 0.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:232:PHE:CE2 | 1:D:135:PHE:CG[2_656] | 1.89 | 0.31 |
| 1:B:237:PRO:CD | 1:D:103:THR:OG1[2_756] | 1.89 | 0.31 |
| 1:A:165:VAL:N | 1:B:208:PHE:CE1[2_757] | 1.89 | 0.31 |
| 1:A:138:TYR:CE1 | 1:B:210:ASN:CB[2_757] | 1.89 | 0.31 |
| 1:C:90:ASN:CG | 2:C:287:HOH:O[2_746] | 1.89 | 0.31 |
| 1:A:164:MET:O | 1:B:208:PHE:CD2[2_757] | 1.90 | 0.30 |
| 1:A:207:PRO:CB | 1:B:183:GLN:CD[2_757] | 1.90 | 0.30 |
| 1:A:232:PHE:CG | 1:B:15:ALA:C[2_757] | 1.90 | 0.30 |
| 1:C:135:PHE:CZ | 1:D:232:PHE:CE1[2_656] | 1.90 | 0.30 |
| 1:B:77:VAL:CG1 | 1:D:41:ASP:CB[2_756] | 1.90 | 0.30 |
| 1:A:210:ASN:O | 1:B:175:GLU:CB[2_757] | 1.90 | 0.30 |
| 1:A:234:ARG:CZ | 2:B:327:HOH:O[2_757] | 1.90 | 0.30 |
| 1:A:15:ALA:CA | 1:B:232:PHE:CE2[2_757] | 1.90 | 0.30 |
| 1:A:211:PHE:CB | 2:B:349:HOH:O[2_757] | 1.90 | 0.30 |
| 1:A:232:PHE:CA | 2:B:255:HOH:O[2_757] | 1.91 | 0.29 |
| 1:C:155:LYS:CB | 1:C:186:ARG:NH1[2_756] | 1.91 | 0.29 |
| 1:A:207:PRO:CB | 1:B:183:GLN:NE2[2_757] | 1.91 | 0.29 |
| 1:A:171:PRO:C | 1:B:234:ARG:CB[2_757] | 1.91 | 0.29 |
| 1:B:71:ASN:O | 1:B:160:PHE:CZ[2_757] | 1.91 | 0.29 |
| 1:B:173:LYS:N | 2:B:268:HOH:O[2_757] | 1.91 | 0.29 |
| 1:B:234:ARG:CD | 2:A:300:HOH:O[2_747] | 1.91 | 0.29 |
| 1:A:231:ILE:N | 1:B:172:LEU:CD2[2_757] | 1.92 | 0.28 |
| 1:B:90:ASN:ND2 | 2:B:399:HOH:O[2_757] | 1.92 | 0.28 |
| 1:B:188:VAL:CG2 | 2:B:305:HOH:O[2_757] | 1.92 | 0.28 |
| 1:B:75:ILE:CA | 1:D:38:GLY:CA[2_756] | 1.92 | 0.28 |
| 1:A:163:VAL:CA | 1:B:211:PHE:CE1[2_757] | 1.92 | 0.28 |
| 1:A:170:VAL:CG1 | 1:B:231:ILE:N[2_757] | 1.92 | 0.28 |
| 1:B:71:ASN:CB | 1:B:160:PHE:CD1[2_757] | 1.93 | 0.27 |
| 1:A:209:MET:N | 1:B:179:ASN:ND2[2_757] | 1.93 | 0.27 |
| 1:C:147:ASP:OD1 | 2:C:462:HOH:O[2_756] | 1.93 | 0.27 |
| 1:C:135:PHE:CZ | 1:D:232:PHE:CD1[2_656] | 1.93 | 0.27 |
| 1:B:71:ASN:ND2 | 1:B:161:ARG:N[2_757] | 1.93 | 0.27 |
| 1:B:238:VAL:C | 1:D:106:ASN:OD1[2_756] | 1.93 | 0.27 |
| 1:D:202:ARG:NH2 | 2:C:503:HOH:O[2_646] | 1.93 | 0.27 |
| 1:A:78:LEU:CD1 | 1:C:11:LYS:CE[2_756] | 1.93 | 0.27 |
| 1:A:164:MET:CE | 1:B:207:PRO:CB[2_757] | 1.94 | 0.26 |
| 1:A:78:LEU:CD1 | 1:C:11:LYS:CG[2_756] | 1.94 | 0.26 |
| 1:A:165:VAL:N | 1:B:208:PHE:CD2[2_757] | 1.94 | 0.26 |
| 1:C:37:GLU:OE1 | 2:C:397:HOH:O[2_756] | 1.94 | 0.26 |
| 1:C:135:PHE:CE1 | 1:D:232:PHE:CD1[2_656] | 1.95 | 0.25 |
| 1:C:151:MET:SD | 2:C:470:HOH:O[2_756] | 1.95 | 0.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:D:40:LYS:CA | 2:B:271:HOH:O[2_746] | 1.95 | 0.25 |
| 1:B:74:ASP:C | 1:D:38:GLY:CA[2_756] | 1.95 | 0.25 |
| 1:A:138:TYR:OH | 1:B:210:ASN:CG[2_757] | 1.95 | 0.25 |
| 1:C:40:LYS:NZ | 2:A:323:HOH:O[2_746] | 1.95 | 0.25 |
| 1:A:210:ASN:N | 2:B:253:HOH:O[2_757] | 1.95 | 0.25 |
| 1:A:170:VAL:CG2 | 1:B:231:ILE:CG1[2_757] | 1.96 | 0.24 |
| 1:A:232:PHE:CE2 | 1:B:15:ALA:CB[2_757] | 1.96 | 0.24 |
| 1:C:135:PHE:CE2 | 1:D:232:PHE:CE1[2_656] | 1.97 | 0.23 |
| 1:A:210:ASN:ND2 | 2:B:421:HOH:O[2_757] | 1.97 | 0.23 |
| 1:A:230:SER:OG | 1:B:171:PRO:O[2_757] | 1.97 | 0.23 |
| 1:C:35:GLU:OE1 | 2:A:323:HOH:O[2_746] | 1.97 | 0.23 |
| 1:A:165:VAL:CA | 1:B:208:PHE:CE1[2_757] | 1.97 | 0.23 |
| 1:A:170:VAL:CB | 1:B:231:ILE:CB[2_757] | 1.97 | 0.23 |
| 1:B:73:ARG:NH1 | 1:D:35:GLU:O[2_756] | 1.97 | 0.23 |
| 1:A:209:MET:O | 1:B:175:GLU:O[2_757] | 1.97 | 0.23 |
| 1:C:185:LYS:NZ | 2:C:307:HOH:O[2_746] | 1.97 | 0.23 |
| 1:B:21:GLY:C | 2:B:348:HOH:O[2_747] | 1.98 | 0.22 |
| 1:B:168:LYS:NZ | 2:C:317:HOH:O[1_556] | 1.98 | 0.22 |
| 1:B:81:LYS:C | 2:D:271:HOH:O[2_756] | 1.98 | 0.22 |
| 1:A:210:ASN:O | 1:B:175:GLU:CG[2_757] | 1.98 | 0.22 |
| 1:C:35:GLU:OE1 | 2:A:287:HOH:O[2_746] | 1.98 | 0.22 |
| 1:A:77:VAL:CB | 1:C:41:ASP:CB[2_756] | 1.98 | 0.22 |
| 1:A:232:PHE:C | 1:B:170:VAL:O[2_757] | 1.99 | 0.21 |
| 1:C:232:PHE:CZ | 1:D:135:PHE:CD1[2_656] | 1.99 | 0.21 |
| 1:C:40:LYS:N | 2:A:255:HOH:O[2_746] | 1.99 | 0.21 |
| 1:A:164:MET:CA | 1:B:208:PHE:CG[2_757] | 1.99 | 0.21 |
| 1:B:71:ASN:CG | 1:B:160:PHE:CB[2_757] | 1.99 | 0.21 |
| 1:A:234:ARG:NE | 2:B:327:HOH:O[2_757] | 1.99 | 0.21 |
| 1:D:233:GLY:O | 2:C:473:HOH:O[2_646] | 1.99 | 0.21 |
| 1:D:146:ASN:CA | 2:B:434:HOH:O[2_746] | 1.99 | 0.21 |
| 1:A:232:PHE:CB | 1:B:15:ALA:CA[2_757] | 1.99 | 0.21 |
| 1:B:237:PRO:N | 1:D:103:THR:CG2[2_756] | 1.99 | 0.21 |
| 1:C:232:PHE:CZ | 1:D:135:PHE:CB[2_656] | 1.99 | 0.21 |
| 1:A:138:TYR:CZ | 1:B:210:ASN:ND2[2_757] | 1.99 | 0.21 |
| 1:B:72:ALA:N | 1:B:160:PHE:CG[2_757] | 2.00 | 0.20 |
| 1:A:172:LEU:CD1 | 1:B:232:PHE:CG[2_757] | 2.00 | 0.20 |
| 1:A:97:GLU:CD | 2:C:318:HOH:O[2_756] | 2.00 | 0.20 |
| 1:A:172:LEU:C | 1:B:232:PHE:C[2_757] | 2.00 | 0.20 |
| 1:A:17:GLN:NE2 | 1:B:209:MET:CG[2_757] | 2.00 | 0.20 |
| 1:B:22:LYS:NZ | 1:B:182:ASN:O[2_747] | 2.00 | 0.20 |
| 1:A:209:MET:CA | 1:B:179:ASN:CG[2_757] | 2.00 | 0.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:232:PHE:N | 1:B:172:LEU:CG[2_757] | 2.00 | 0.20 |
| 1:C:35:GLU:CD | 2:A:323:HOH:O[2_746] | 2.00 | 0.20 |
| 1:A:140:LEU:CD2 | 1:B:232:PHE:CE1[2_757] | 2.00 | 0.20 |
| 1:A:161:ARG:NH2 | 1:B:206:GLY:O[2_757] | 2.01 | 0.19 |
| 1:B:71:ASN:O | 1:B:160:PHE:CG[2_757] | 2.01 | 0.19 |
| 1:B:83:VAL:CG1 | 1:D:144:HIS:ND1[2_756] | 2.01 | 0.19 |
| 2:B:453:HOH:O | 2:D:276:HOH:O[2_756] | 2.01 | 0.19 |
| 1:B:219:HIS:CE1 | 1:D:108:PRO:CG[2_756] | 2.01 | 0.19 |
| 1:A:81:LYS:N | 1:C:9:LEU:CD2[2_756] | 2.01 | 0.19 |
| 1:A:77:VAL:N | 1:C:42:LEU:CD1[2_756] | 2.01 | 0.19 |
| 1:A:17:GLN:NE2 | 1:B:209:MET:CE[2_757] | 2.02 | 0.18 |
| 1:A:232:PHE:N | 1:B:172:LEU:CD2[2_757] | 2.02 | 0.18 |
| 1:B:235:MET:CG | 2:B:469:HOH:O[2_757] | 2.02 | 0.18 |
| 1:A:165:VAL:CG1 | 1:B:238:VAL:N[2_757] | 2.02 | 0.18 |
| 1:A:172:LEU:CD2 | 1:B:231:ILE:CA[2_757] | 2.02 | 0.18 |
| 1:C:25:GLU:OE1 | 1:C:174:GLU:OE1[2_756] | 2.02 | 0.18 |
| 1:A:211:PHE:CD1 | 1:B:176:GLU:C[2_757] | 2.02 | 0.18 |
| 1:A:232:PHE:CE2 | 1:B:15:ALA:CA[2_757] | 2.02 | 0.18 |
| 1:D:39:LEU:CD2 | 2:B:259:HOH:O[2_746] | 2.03 | 0.17 |
| 1:A:170:VAL:C | 1:B:231:ILE:CG1[2_757] | 2.03 | 0.17 |
| 1:A:164:MET:O | 1:B:208:PHE:CB[2_757] | 2.03 | 0.17 |
| 1:A:81:LYS:CA | 1:C:9:LEU:CD2[2_756] | 2.03 | 0.17 |
| 1:B:74:ASP:CA | 1:D:37:GLU:O[2_756] | 2.03 | 0.17 |
| 1:A:77:VAL:CG1 | 1:C:41:ASP:CG[2_756] | 2.03 | 0.17 |
| 1:A:75:ILE:CA | 1:C:38:GLY:CA[2_756] | 2.04 | 0.16 |
| 1:A:172:LEU:CB | 1:B:232:PHE:N[2_757] | 2.04 | 0.16 |
| 1:A:232:PHE:CA | 1:B:15:ALA:N[2_757] | 2.04 | 0.16 |
| 1:A:172:LEU:CG | 1:B:232:PHE:C[2_757] | 2.04 | 0.16 |
| 1:A:211:PHE:N | 1:B:175:GLU:CB[2_757] | 2.04 | 0.16 |
| 1:B:238:VAL:CB | 1:D:106:ASN:OD1[2_756] | 2.04 | 0.16 |
| 1:A:171:PRO:CB | 1:B:234:ARG:CB[2_757] | 2.05 | 0.15 |
| 1:A:172:LEU:C | 1:B:233:GLY:CA[2_757] | 2.05 | 0.15 |
| 1:A:172:LEU:CD1 | 1:B:232:PHE:CB[2_757] | 2.05 | 0.15 |
| 1:C:155:LYS:CE | 1:C:185:LYS:NZ[2_756] | 2.05 | 0.15 |
| 1:D:202:ARG:NE | 2:C:503:HOH:O[2_646] | 2.05 | 0.15 |
| 1:A:161:ARG:CD | 1:B:207:PRO:CA[2_757] | 2.05 | 0.15 |
| 1:B:22:LYS:CD | 1:B:186:ARG:CG[2_747] | 2.05 | 0.15 |
| 1:A:170:VAL:O | 1:B:231:ILE:CA[2_757] | 2.05 | 0.15 |
| 1:B:208:PHE:CA | 2:A:258:HOH:O[2_747] | 2.05 | 0.15 |
| 1:C:135:PHE:CE2 | 1:D:232:PHE:CZ[2_656] | 2.05 | 0.15 |
| 1:A:212:THR:CA | 2:B:413:HOH:O[2_757] | 2.05 | 0.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:81:LYS:N | 1:C:9:LEU:CD1[2_756] | 2.05 | 0.15 |
| 1:A:74:ASP:C | 1:C:38:GLY:CA[2_756] | 2.06 | 0.14 |
| 1:D:36:LEU:O | 2:B:358:HOH:O[2_746] | 2.06 | 0.14 |
| 1:A:211:PHE:CA | 2:B:413:HOH:O[2_757] | 2.06 | 0.14 |
| 1:D:148:LYS:CD | 2:B:336:HOH:O[2_746] | 2.06 | 0.14 |
| 1:A:80:LYS:CG | 1:C:8:GLU:CD[2_756] | 2.07 | 0.13 |
| 1:C:7:GLN:CG | 2:A:303:HOH:O[2_746] | 2.07 | 0.13 |
| 1:A:97:GLU:OE2 | 2:C:318:HOH:O[2_756] | 2.07 | 0.13 |
| 1:A:208:PHE:C | 1:B:179:ASN:CG[2_757] | 2.07 | 0.13 |
| 1:B:73:ARG:N | 1:B:160:PHE:CZ[2_757] | 2.07 | 0.13 |
| 1:A:200:GLN:OE1 | 1:C:120:LYS:NZ[2_756] | 2.07 | 0.13 |
| 1:A:211:PHE:O | 2:B:546:HOH:O[2_757] | 2.07 | 0.13 |
| 1:B:151:MET:CE | 2:D:321:HOH:O[1_556] | 2.08 | 0.12 |
| 1:B:74:ASP:C | 1:D:37:GLU:C[2_756] | 2.08 | 0.12 |
| 2:A:384:HOH:O | 2:D:328:HOH:O[1_566] | 2.08 | 0.12 |
| 1:B:161:ARG:NE | 2:B:293:HOH:O[2_747] | 2.08 | 0.12 |
| 1:A:211:PHE:CG | 1:B:176:GLU:N[2_757] | 2.08 | 0.12 |
| 1:B:71:ASN:ND2 | 1:B:160:PHE:O[2_757] | 2.08 | 0.12 |
| 1:D:148:LYS:CE | 2:B:340:HOH:O[2_746] | 2.08 | 0.12 |
| 2:B:274:HOH:O | 2:B:299:HOH:O[2_747] | 2.08 | 0.12 |
| 1:C:8:GLU:O | 2:A:254:HOH:O[2_746] | 2.08 | 0.12 |
| 1:A:233:GLY:N | 2:B:255:HOH:O[2_757] | 2.09 | 0.11 |
| 1:A:78:LEU:CD1 | 1:C:11:LYS:CD[2_756] | 2.09 | 0.11 |
| 1:A:78:LEU:CD2 | 1:C:144:HIS:CG[2_756] | 2.09 | 0.11 |
| 1:B:208:PHE:CE1 | 2:A:285:HOH:O[2_747] | 2.09 | 0.11 |
| 1:A:165:VAL:CA | 1:B:208:PHE:CZ[2_757] | 2.09 | 0.11 |
| 1:A:234:ARG:CB | 1:B:163:VAL:CB[2_757] | 2.09 | 0.11 |
| 1:A:232:PHE:CZ | 1:B:140:LEU:CD2[2_757] | 2.09 | 0.11 |
| 1:A:209:MET:C | 1:B:179:ASN:CG[2_757] | 2.09 | 0.11 |
| 1:A:63:LYS:CG | 1:C:41:ASP:OD1[2_756] | 2.09 | 0.11 |
| 1:B:238:VAL:CA | 1:D:106:ASN:CG[2_756] | 2.10 | 0.10 |
| 1:A:200:GLN:NE2 | 2:C:379:HOH:O[2_756] | 2.10 | 0.10 |
| 1:A:59:GLN:NE2 | 1:C:8:GLU:N[2_756] | 2.10 | 0.10 |
| 1:A:235:MET:N | 1:B:165:VAL:CG2[2_757] | 2.10 | 0.10 |
| 1:A:232:PHE:CE1 | 1:B:15:ALA:CA[2_757] | 2.10 | 0.10 |
| 1:B:154:GLU:OE2 | 1:D:36:LEU:CD2[1_556] | 2.10 | 0.10 |
| 1:C:37:GLU:N | 2:C:262:HOH:O[2_756] | 2.10 | 0.10 |
| 1:A:211:PHE:CA | 2:B:546:HOH:O[2_757] | 2.10 | 0.10 |
| 1:A:209:MET:C | 1:B:179:ASN:OD1[2_757] | 2.10 | 0.10 |
| 1:A:233:GLY:O | 1:B:170:VAL:N[2_757] | 2.11 | 0.09 |
| 1:A:163:VAL:CB | 1:B:211:PHE:CG[2_757] | 2.11 | 0.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:144:HIS:CE1 | 2:A:316:HOH:O[2_746] | 2.11 | 0.09 |
| 1:A:170:VAL:CG1 | 1:B:231:ILE:CB[2_757] | 2.11 | 0.09 |
| 1:B:240:LEU:CB | 2:B:551:HOH:O[2_757] | 2.11 | 0.09 |
| 1:B:155:LYS:NZ | 2:D:363:HOH:O[1_556] | 2.12 | 0.08 |
| 1:D:40:LYS:N | 2:B:271:HOH:O[2_746] | 2.12 | 0.08 |
| 1:B:217:GLU:CD | 2:D:310:HOH:O[2_756] | 2.12 | 0.08 |
| 1:B:240:LEU:CA | 2:B:264:HOH:O[2_757] | 2.12 | 0.08 |
| 1:A:211:PHE:CZ | 1:B:176:GLU:CG[2_757] | 2.12 | 0.08 |
| 1:A:82:GLY:N | 1:C:9:LEU:CD1[2_756] | 2.12 | 0.08 |
| 1:A:171:PRO:N | 1:B:231:ILE:CB[2_757] | 2.12 | 0.08 |
| 1:A:234:ARG:CA | 1:B:163:VAL:CG1[2_757] | 2.13 | 0.07 |
| 1:D:39:LEU:C | 2:B:254:HOH:O[2_746] | 2.13 | 0.07 |
| 1:A:81:LYS:N | 1:C:9:LEU:CG[2_756] | 2.13 | 0.07 |
| 1:C:90:ASN:CG | 1:C:147:ASP:O[2_746] | 2.13 | 0.07 |
| 1:A:209:MET:CA | 1:B:179:ASN:ND2[2_757] | 2.13 | 0.07 |
| 1:A:170:VAL:CA | 1:B:231:ILE:CD1[2_757] | 2.13 | 0.07 |
| 1:B:236:THR:CA | 1:D:103:THR:CG2[2_756] | 2.13 | 0.07 |
| 1:D:37:GLU:CA | 2:B:358:HOH:O[2_746] | 2.13 | 0.07 |
| 1:A:172:LEU:CB | 1:B:232:PHE:CB[2_757] | 2.14 | 0.06 |
| 1:B:240:LEU:N | 2:B:551:HOH:O[2_757] | 2.14 | 0.06 |
| 1:A:207:PRO:CB | 1:B:183:GLN:OE1[2_757] | 2.14 | 0.06 |
| 1:B:72:ALA:N | 1:B:160:PHE:CD1[2_757] | 2.14 | 0.06 |
| 1:B:89:GLU:OE2 | 2:B:452:HOH:O[2_757] | 2.14 | 0.06 |
| 1:A:82:GLY:CA | 1:C:144:HIS:NE2[2_756] | 2.14 | 0.06 |
| 1:A:163:VAL:CG2 | 1:B:211:PHE:CD1[2_757] | 2.14 | 0.06 |
| 1:A:64:TYR:CE2 | 1:C:40:LYS:CE[2_756] | 2.14 | 0.06 |
| 1:B:71:ASN:CA | 1:B:160:PHE:CA[2_757] | 2.14 | 0.06 |
| 1:A:74:ASP:C | 1:C:37:GLU:C[2_756] | 2.14 | 0.06 |
| 1:A:233:GLY:O | 1:B:170:VAL:CG1[2_757] | 2.14 | 0.06 |
| 1:C:39:LEU:O | 2:A:251:HOH:O[2_746] | 2.15 | 0.05 |
| 1:A:171:PRO:CB | 1:B:234:ARG:CG[2_757] | 2.15 | 0.05 |
| 1:C:182:ASN:ND2 | 2:C:474:HOH:O[2_746] | 2.15 | 0.05 |
| 1:B:72:ALA:CA | 1:B:160:PHE:CE1[2_757] | 2.15 | 0.05 |
| 1:B:73:ARG:NE | 1:D:36:LEU:C[2_756] | 2.15 | 0.05 |
| 1:A:14:TYR:C | 1:B:232:PHE:CZ[2_757] | 2.15 | 0.05 |
| 1:A:79:GLY:O | 1:C:9:LEU:CB[2_756] | 2.16 | 0.04 |
| 1:B:22:LYS:CD | 1:B:186:ARG:CZ[2_747] | 2.16 | 0.04 |
| 1:A:164:MET:N | 1:B:208:PHE:CA[2_757] | 2.16 | 0.04 |
| 1:A:77:VAL:CA | 1:C:41:ASP:CB[2_756] | 2.16 | 0.04 |
| 1:B:235:MET:SD | 2:B:469:HOH:O[2_757] | 2.16 | 0.04 |
| 1:A:172:LEU:CA | 1:B:231:ILE:O[2_757] | 2.16 | 0.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:240:LEU:CD2 | 2:B:551:HOH:O[2_757] | 2.16 | 0.04 |
| 1:A:59:GLN:NE2 | 1:C:7:GLN:C[2_756] | 2.16 | 0.04 |
| 1:C:90:ASN:O | 1:C:151:MET:CG[2_746] | 2.17 | 0.03 |
| 1:A:171:PRO:CG | 1:B:234:ARG:CG[2_757] | 2.17 | 0.03 |
| 1:B:237:PRO:CG | 1:D:103:THR:OG1[2_756] | 2.17 | 0.03 |
| 1:B:238:VAL:N | 1:D:106:ASN:OD1[2_756] | 2.17 | 0.03 |
| 1:A:138:TYR:OH | 1:B:210:ASN:C[2_757] | 2.17 | 0.03 |
| 1:A:170:VAL:CA | 1:B:231:ILE:CG2[2_757] | 2.17 | 0.03 |
| 1:A:172:LEU:CA | 1:B:233:GLY:CA[2_757] | 2.17 | 0.03 |
| 1:C:232:PHE:CD2 | 1:D:135:PHE:CD2[2_656] | 2.18 | 0.02 |
| 1:A:210:ASN:CB | 1:B:175:GLU:CB[2_757] | 2.18 | 0.02 |
| 1:B:72:ALA:O | 1:B:160:PHE:CE1[2_757] | 2.18 | 0.02 |
| 1:C:90:ASN:ND2 | 1:C:147:ASP:O[2_746] | 2.18 | 0.02 |
| 1:A:172:LEU:CD2 | 1:B:232:PHE:CA[2_757] | 2.18 | 0.02 |
| 1:A:173:LYS:NZ | 2:D:387:HOH:O[2_666] | 2.18 | 0.02 |
| 1:A:138:TYR:CD1 | 1:B:210:ASN:CG[2_757] | 2.18 | 0.02 |
| 1:A:210:ASN:O | 2:B:253:HOH:O[2_757] | 2.18 | 0.02 |
| 1:B:77:VAL:CB | 1:D:41:ASP:CG[2_756] | 2.18 | 0.02 |
| 1:B:73:ARG:NH2 | 1:D:35:GLU:C[2_756] | 2.18 | 0.02 |
| 1:B:75:ILE:N | 1:D:38:GLY:CA[2_756] | 2.18 | 0.02 |
| 1:B:78:LEU:CD1 | 1:D:11:LYS:NZ[2_756] | 2.19 | 0.01 |
| 1:C:90:ASN:OD1 | 1:C:147:ASP:CB[2_746] | 2.19 | 0.01 |
| 1:B:21:GLY:CA | 2:B:348:HOH:O[2_747] | 2.19 | 0.01 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 1 | A | 238/248 (96%) | 214 (90%) | 18 (8%) | 6 (2%) | 6 | 2 |
| 1 | B | 240/248 (97%) | 206 (86%) | 27 (11%) | 7 (3%) | 5 | 1 |
| 1 | C | 242/248 (98%) | 208 (86%) | 22 (9%) | 12 (5%) | 2 | 0 |
| 1 | D | 237/248 (96%) | 205 (86%) | 19 (8%) | 13 (6%) | 2 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------------|
| All | All | 957/992 (96%) | 833 (87%) | 86 (9%) | 38 (4%) | 3 1 |

All (38) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 189 | LYS |
| 1 | B | 193 | VAL |
| 1 | B | 220 | PRO |
| 1 | C | 8 | GLU |
| 1 | C | 157 | PRO |
| 1 | C | 161 | ARG |
| 1 | D | 186 | ARG |
| 1 | D | 190 | PRO |
| 1 | D | 197 | LYS |
| 1 | A | 193 | VAL |
| 1 | C | 6 | VAL |
| 1 | C | 59 | GLN |
| 1 | C | 195 | PHE |
| 1 | C | 197 | LYS |
| 1 | D | 70 | GLY |
| 1 | D | 71 | ASN |
| 1 | D | 89 | GLU |
| 1 | A | 157 | PRO |
| 1 | A | 195 | PHE |
| 1 | A | 217 | GLU |
| 1 | B | 217 | GLU |
| 1 | C | 7 | GLN |
| 1 | C | 9 | LEU |
| 1 | D | 59 | GLN |
| 1 | D | 161 | ARG |
| 1 | D | 193 | VAL |
| 1 | B | 190 | PRO |
| 1 | C | 217 | GLU |
| 1 | C | 221 | GLU |
| 1 | D | 194 | GLU |
| 1 | B | 161 | ARG |
| 1 | C | 134 | ILE |
| 1 | D | 217 | GLU |
| 1 | B | 221 | GLU |
| 1 | D | 157 | PRO |
| 1 | D | 195 | PHE |
| 1 | A | 161 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 157 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 214/222 (96%) | 201 (94%) | 13 (6%) | 22 | 16 |
| 1 | B | 216/222 (97%) | 205 (95%) | 11 (5%) | 28 | 22 |
| 1 | C | 218/222 (98%) | 199 (91%) | 19 (9%) | 12 | 7 |
| 1 | D | 213/222 (96%) | 194 (91%) | 19 (9%) | 11 | 7 |
| All | All | 861/888 (97%) | 799 (93%) | 62 (7%) | 17 | 11 |

All (62) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | LEU |
| 1 | A | 118 | THR |
| 1 | A | 121 | GLU |
| 1 | A | 157 | PRO |
| 1 | A | 160 | PHE |
| 1 | A | 175 | GLU |
| 1 | A | 181 | LEU |
| 1 | A | 186 | ARG |
| 1 | A | 189 | LYS |
| 1 | A | 195 | PHE |
| 1 | A | 202 | ARG |
| 1 | A | 227 | VAL |
| 1 | A | 239 | GLU |
| 1 | B | 9 | LEU |
| 1 | B | 37 | GLU |
| 1 | B | 69 | LYS |
| 1 | B | 106 | ASN |
| 1 | B | 132 | ASN |
| 1 | B | 133 | LYS |
| 1 | B | 146 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 170 | VAL |
| 1 | B | 202 | ARG |
| 1 | B | 210 | ASN |
| 1 | B | 220 | PRO |
| 1 | C | 22 | LYS |
| 1 | C | 37 | GLU |
| 1 | C | 45 | GLU |
| 1 | C | 68 | LEU |
| 1 | C | 69 | LYS |
| 1 | C | 112 | LYS |
| 1 | C | 123 | LYS |
| 1 | C | 132 | ASN |
| 1 | C | 146 | ASN |
| 1 | C | 157 | PRO |
| 1 | C | 161 | ARG |
| 1 | C | 176 | GLU |
| 1 | C | 182 | ASN |
| 1 | C | 183 | GLN |
| 1 | C | 186 | ARG |
| 1 | C | 192 | LYS |
| 1 | C | 216 | GLU |
| 1 | C | 239 | GLU |
| 1 | C | 243 | ASP |
| 1 | D | 23 | GLU |
| 1 | D | 61 | LYS |
| 1 | D | 63 | LYS |
| 1 | D | 75 | ILE |
| 1 | D | 78 | LEU |
| 1 | D | 87 | ARG |
| 1 | D | 97 | GLU |
| 1 | D | 106 | ASN |
| 1 | D | 110 | ILE |
| 1 | D | 120 | LYS |
| 1 | D | 148 | LYS |
| 1 | D | 150 | LEU |
| 1 | D | 157 | PRO |
| 1 | D | 170 | VAL |
| 1 | D | 175 | GLU |
| 1 | D | 188 | VAL |
| 1 | D | 192 | LYS |
| 1 | D | 193 | VAL |
| 1 | D | 196 | GLU |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 17 | GLN |
| 1 | A | 29 | ASN |
| 1 | A | 90 | ASN |
| 1 | A | 106 | ASN |
| 1 | A | 158 | HIS |
| 1 | A | 179 | ASN |
| 1 | B | 17 | GLN |
| 1 | B | 106 | ASN |
| 1 | B | 115 | GLN |
| 1 | B | 146 | ASN |
| 1 | B | 178 | GLN |
| 1 | B | 179 | ASN |
| 1 | B | 182 | ASN |
| 1 | C | 29 | ASN |
| 1 | C | 90 | ASN |
| 1 | C | 106 | ASN |
| 1 | C | 115 | GLN |
| 1 | C | 146 | ASN |
| 1 | C | 178 | GLN |
| 1 | C | 182 | ASN |
| 1 | C | 219 | HIS |
| 1 | D | 59 | GLN |
| 1 | D | 71 | ASN |
| 1 | D | 106 | ASN |
| 1 | D | 178 | GLN |
| 1 | D | 179 | ASN |
| 1 | D | 200 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.