



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:48 PM GMT

PDB ID : 2EXY
Title : Crystal structure of the E148Q Mutant of EcClC, Fab complexed in absence of bound ions
Authors : Lobet, S.; Dutzler, R.
Deposited on : 2005-11-09
Resolution : 3.10 Å(reported)

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

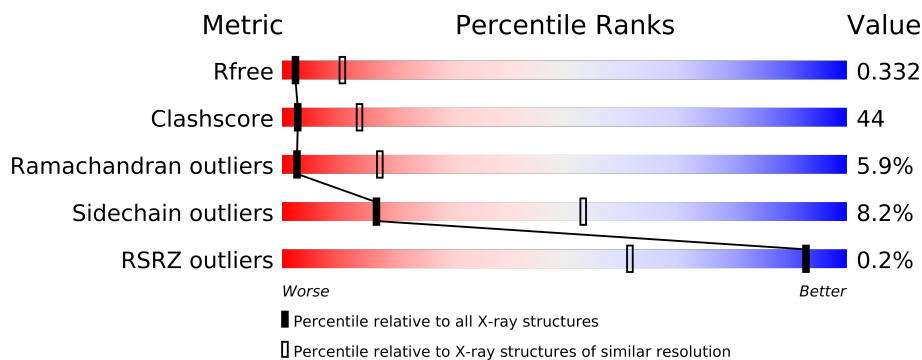
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1007 (3.18-3.02) |
| Clashscore | 79885 | 1078 (3.16-3.04) |
| Ramachandran outliers | 78287 | 1044 (3.16-3.04) |
| Sidechain outliers | 78261 | 1044 (3.16-3.04) |
| RSRZ outliers | 66119 | 1008 (3.18-3.02) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 473 | |
| 1 | B | 473 | |
| 2 | C | 222 | |
| 2 | E | 222 | |
| 3 | D | 211 | |
| 3 | F | 211 | |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13223 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H(+)/Cl(-) exchange transporter clcA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 444 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3333 | 2190 | 561 | 562 | 20 | | | |
| 1 | B | 441 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3304 | 2174 | 554 | 556 | 20 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| A | 148 | GLN | GLU | ENGINEERED | UNP P37019 |
| B | 148 | GLN | GLU | ENGINEERED | UNP P37019 |

- Molecule 2 is a protein called Fab Fragment (Heavy Chain).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | C | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1672 | 1077 | 274 | 315 | 6 | | | |
| 2 | E | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1672 | 1077 | 274 | 315 | 6 | | | |

- Molecule 3 is a protein called Fab Fragment (Light Chain).

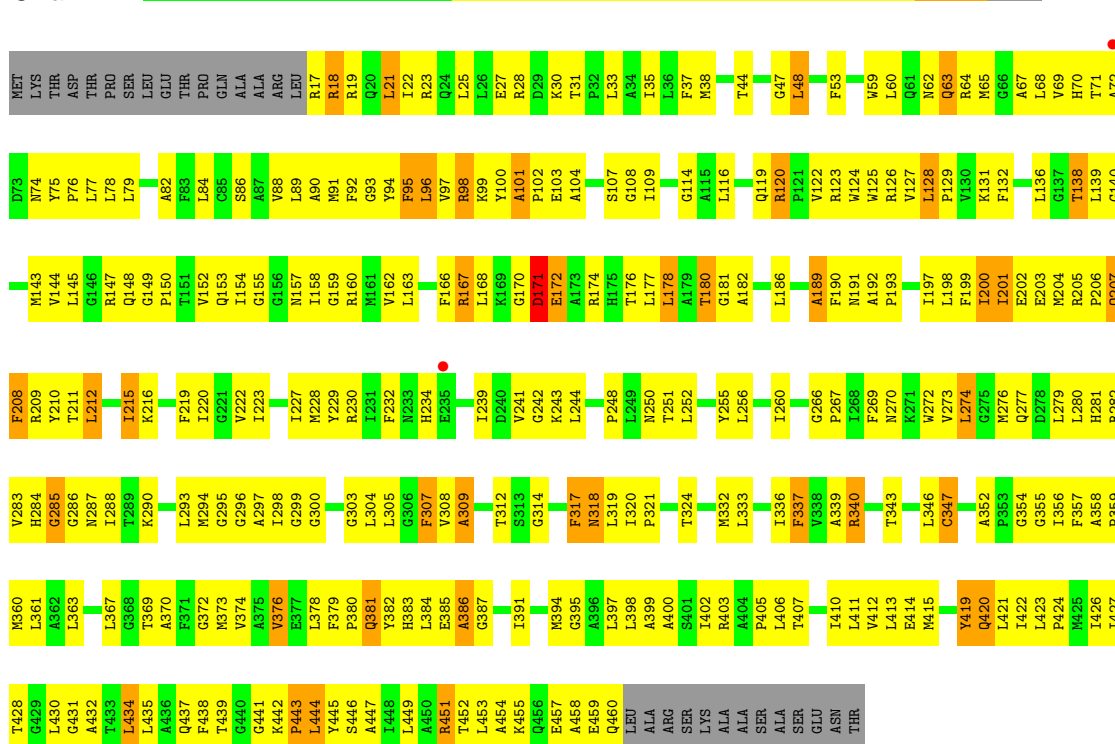
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | D | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1621 | 1008 | 271 | 334 | 8 | | | |
| 3 | F | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1621 | 1008 | 271 | 334 | 8 | | | |

3 Residue-property plots

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

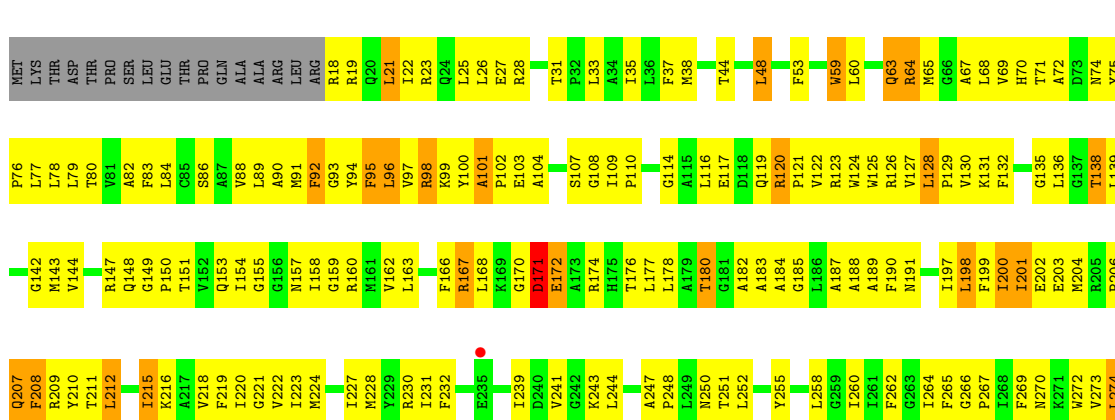
- Molecule 1: H(+)/Cl(-) exchange transporter clcA

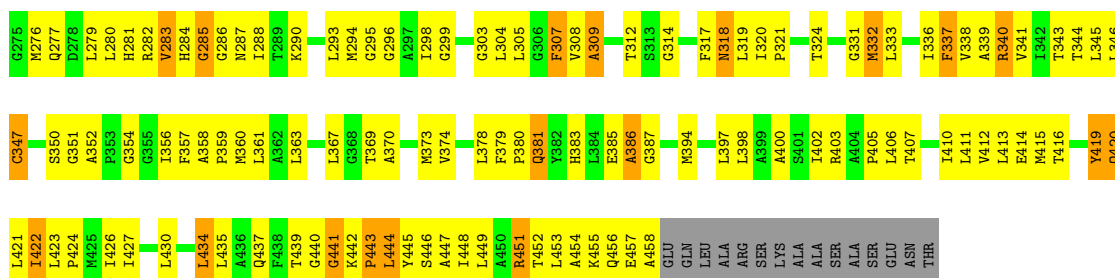
Chain A:



- Molecule 1: H(+)/Cl(-) exchange transporter clcA

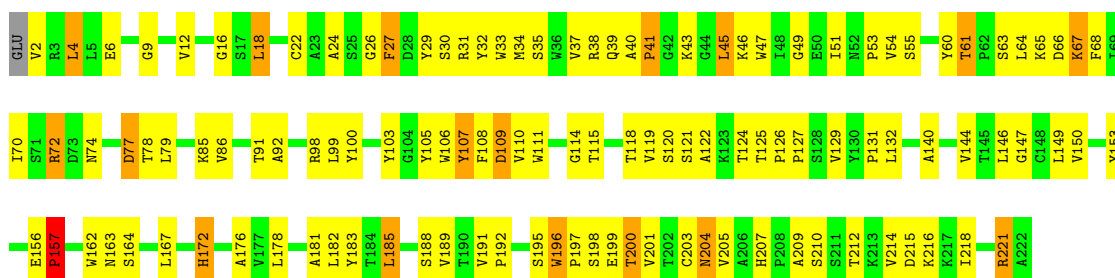
Chain B:





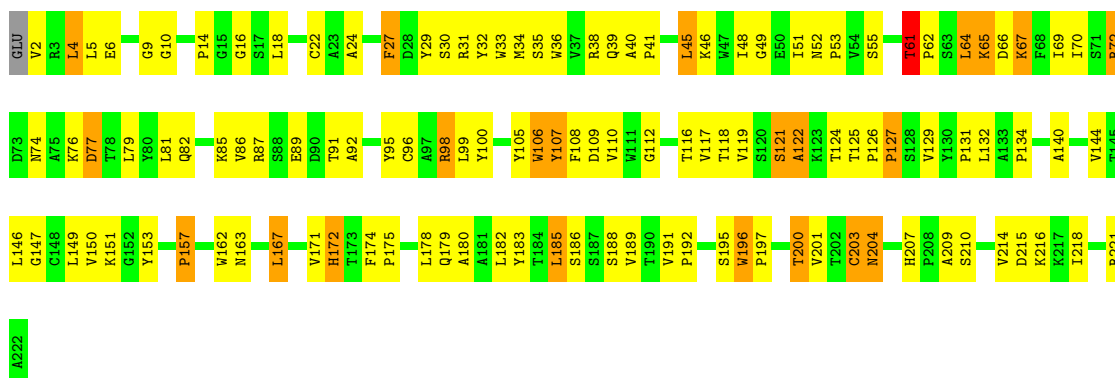
• Molecule 2: Fab Fragment (Heavy Chain)

Chain C:



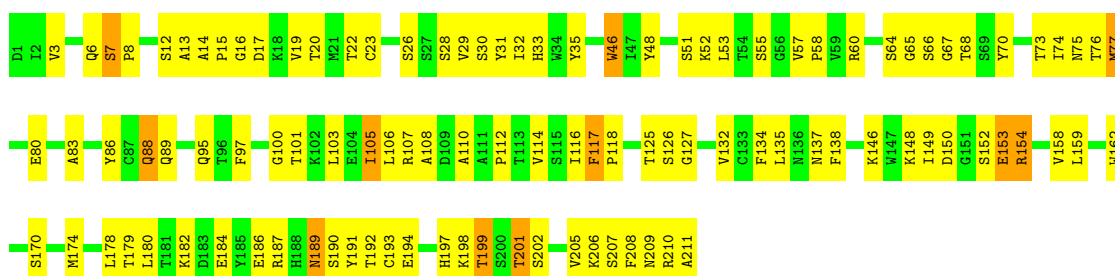
• Molecule 2: Fab Fragment (Heavy Chain)

Chain E:



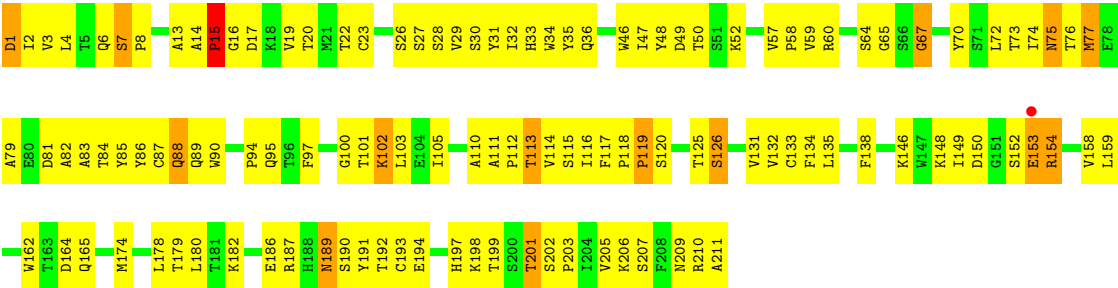
• Molecule 3: Fab Fragment (Light Chain)

Chain D:



• Molecule 3: Fab Fragment (Light Chain)

Chain F:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 219.64Å 119.79Å 151.30Å 90.00° 128.09° 90.00° | Depositor |
| Resolution (Å) | 19.97 – 3.10 49.45 – 3.10 | Depositor EDS |
| % Data completeness (in resolution range) | 95.6 (19.97-3.10) 95.5 (49.45-3.10) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.80 (at 3.12Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.328 , 0.352 0.308 , 0.332 | Depositor DCC |
| R_{free} test set | 2591 reflections (4.84%) | DCC |
| Wilson B-factor (Å ²) | 82.6 | Xtriage |
| Anisotropy | 0.573 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 56.7 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$ | Xtriage |
| Outliers | 0 of 53580 reflections | Xtriage |
| F_o, F_c correlation | 0.88 | EDS |
| Total number of atoms | 13223 | wwPDB-VP |
| Average B, all atoms (Å ²) | 77.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.50 | 0/3405 | 0.68 | 0/4621 |
| 1 | B | 0.51 | 0/3376 | 0.69 | 0/4583 |
| 2 | C | 0.77 | 1/1721 (0.1%) | 0.88 | 1/2355 (0.0%) |
| 2 | E | 0.77 | 4/1721 (0.2%) | 0.86 | 0/2355 |
| 3 | D | 0.62 | 0/1660 | 0.77 | 1/2257 (0.0%) |
| 3 | F | 0.74 | 1/1660 (0.1%) | 0.83 | 0/2257 |
| All | All | 0.63 | 6/13543 (0.0%) | 0.77 | 2/18428 (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 | B | 0 | 1 |
| 2 | E | 0 | 1 |
| 3 | F | 0 | 1 |
| All | All | 0 | 3 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | C | 61 | THR | CB-CG2 | -7.07 | 1.29 | 1.52 |
| 2 | E | 121 | SER | C-N | -6.33 | 1.19 | 1.34 |
| 2 | E | 121 | SER | C-O | 5.50 | 1.33 | 1.23 |
| 2 | E | 121 | SER | CA-C | 5.16 | 1.66 | 1.52 |
| 3 | F | 201 | THR | CB-CG2 | -5.14 | 1.35 | 1.52 |
| 2 | E | 61 | THR | CB-CG2 | -5.04 | 1.35 | 1.52 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | C | 61 | THR | OG1-CB-CG2 | -9.16 | 88.94 | 110.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3 | D | 201 | THR | OG1-CB-CG2 | -5.44 | 97.48 | 110.00 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 419 | TYR | Sidechain |
| 2 | E | 95 | TYR | Sidechain |
| 3 | F | 31 | TYR | Sidechain |

5.2 Close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3333 | 0 | 3486 | 388 | 0 |
| 1 | B | 3304 | 0 | 3459 | 372 | 0 |
| 2 | C | 1672 | 0 | 1654 | 119 | 0 |
| 2 | E | 1672 | 0 | 1654 | 127 | 0 |
| 3 | D | 1621 | 0 | 1546 | 94 | 0 |
| 3 | F | 1621 | 0 | 1546 | 130 | 0 |
| All | All | 13223 | 0 | 13345 | 1156 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (1156) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:D:16:GLY:HA2 | 3:D:76:THR:HG23 | 1.28 | 1.06 |
| 1:A:381:GLN:NE2 | 1:A:381:GLN:H | 1.54 | 1.06 |
| 1:B:381:GLN:H | 1:B:381:GLN:NE2 | 1.53 | 1.05 |
| 3:F:192:THR:HA | 3:F:207:SER:HB3 | 1.37 | 1.05 |
| 1:A:223:ILE:HD11 | 1:B:426:ILE:HG22 | 1.39 | 1.04 |
| 1:A:28:ARG:HD2 | 1:B:207:GLN:HG2 | 1.40 | 1.03 |
| 2:C:45:LEU:H | 2:C:45:LEU:HD12 | 1.24 | 1.03 |
| 1:B:381:GLN:N | 1:B:381:GLN:HE21 | 1.57 | 1.01 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:207:GLN:HG2 | 1:B:28:ARG:HD2 | 1.43 | 1.00 |
| 3:F:194:GLU:HG2 | 3:F:205:VAL:HG12 | 1.42 | 0.99 |
| 3:D:194:GLU:HG2 | 3:D:205:VAL:HG12 | 1.44 | 0.99 |
| 1:A:381:GLN:N | 1:A:381:GLN:HE21 | 1.60 | 0.98 |
| 1:A:98:ARG:HH11 | 1:A:98:ARG:HB3 | 1.29 | 0.98 |
| 2:E:45:LEU:HD12 | 2:E:45:LEU:H | 1.26 | 0.98 |
| 3:F:7:SER:HB3 | 3:F:8:PRO:HD3 | 1.46 | 0.97 |
| 1:B:287:ASN:ND2 | 1:B:290:LYS:H | 1.62 | 0.96 |
| 1:B:120:ARG:HH11 | 1:B:120:ARG:HB3 | 1.28 | 0.95 |
| 3:F:16:GLY:HA2 | 3:F:76:THR:HG23 | 1.45 | 0.94 |
| 1:A:252:LEU:HD22 | 1:A:427:ILE:HD12 | 1.49 | 0.94 |
| 3:D:192:THR:HA | 3:D:207:SER:HB3 | 1.49 | 0.94 |
| 3:D:7:SER:HB3 | 3:D:8:PRO:HD3 | 1.49 | 0.93 |
| 1:B:98:ARG:HH11 | 1:B:98:ARG:HB3 | 1.34 | 0.92 |
| 1:B:154:ILE:O | 1:B:158:ILE:HG12 | 1.69 | 0.92 |
| 1:A:426:ILE:HG22 | 1:B:223:ILE:HD11 | 1.52 | 0.91 |
| 1:A:287:ASN:ND2 | 1:A:290:LYS:H | 1.69 | 0.91 |
| 1:A:75:TYR:HB3 | 1:A:76:PRO:HD3 | 1.51 | 0.90 |
| 2:C:127:PRO:HB3 | 2:C:153:TYR:HB3 | 1.53 | 0.90 |
| 1:A:220:ILE:HG12 | 1:B:430:LEU:HD21 | 1.55 | 0.89 |
| 1:A:274:LEU:HA | 1:A:277:GLN:HE21 | 1.37 | 0.88 |
| 1:A:274:LEU:O | 1:A:277:GLN:HG2 | 1.73 | 0.88 |
| 1:A:124:TRP:HA | 1:A:157:ASN:HD22 | 1.38 | 0.88 |
| 1:A:154:ILE:O | 1:A:158:ILE:HG12 | 1.74 | 0.88 |
| 1:A:430:LEU:HD21 | 1:B:220:ILE:HG12 | 1.55 | 0.88 |
| 1:A:305:LEU:HA | 1:A:308:VAL:HG22 | 1.55 | 0.88 |
| 1:B:75:TYR:HB3 | 1:B:76:PRO:HD3 | 1.54 | 0.88 |
| 1:B:124:TRP:HA | 1:B:157:ASN:HD22 | 1.39 | 0.87 |
| 1:B:305:LEU:HA | 1:B:308:VAL:HG22 | 1.58 | 0.86 |
| 1:B:68:LEU:HD21 | 1:B:82:ALA:HB2 | 1.58 | 0.86 |
| 3:F:110:ALA:O | 3:F:138:PHE:HA | 1.76 | 0.86 |
| 1:B:274:LEU:O | 1:B:277:GLN:HG2 | 1.75 | 0.85 |
| 3:F:14:ALA:O | 3:F:17:ASP:HB2 | 1.76 | 0.85 |
| 1:B:109:ILE:HD12 | 1:B:445:TYR:HE2 | 1.40 | 0.85 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:H | 1.17 | 0.85 |
| 1:B:198:LEU:HG | 1:B:410:ILE:HD12 | 1.59 | 0.84 |
| 1:A:274:LEU:HA | 1:A:277:GLN:NE2 | 1.93 | 0.84 |
| 1:A:198:LEU:HG | 1:A:410:ILE:HD12 | 1.57 | 0.84 |
| 1:A:381:GLN:HE21 | 1:A:381:GLN:H | 0.84 | 0.83 |
| 3:F:82:ALA:HB2 | 3:F:105:ILE:HD11 | 1.61 | 0.83 |
| 1:A:274:LEU:HD12 | 1:A:277:GLN:HE22 | 1.42 | 0.83 |
| 2:E:107:TYR:HB3 | 3:F:33:HIS:CD2 | 2.13 | 0.83 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:241:VAL:HG11 | 1:A:324:THR:HG21 | 1.61 | 0.83 |
| 1:A:18:ARG:NH1 | 1:B:457:GLU:HB3 | 1.96 | 0.81 |
| 2:C:132:LEU:HB2 | 2:C:147:GLY:O | 1.78 | 0.81 |
| 3:D:95:GLN:N | 3:D:95:GLN:OE1 | 2.14 | 0.81 |
| 2:E:204:ASN:HB3 | 2:E:215:ASP:OD1 | 1.80 | 0.81 |
| 1:B:120:ARG:HD3 | 1:B:453:LEU:CD1 | 2.11 | 0.81 |
| 1:A:279:LEU:HA | 1:A:282:ARG:HH11 | 1.46 | 0.81 |
| 1:A:223:ILE:HD11 | 1:B:426:ILE:CG2 | 2.09 | 0.81 |
| 2:E:127:PRO:HB3 | 2:E:153:TYR:HB3 | 1.63 | 0.80 |
| 1:B:120:ARG:NH1 | 1:B:120:ARG:HB3 | 1.95 | 0.80 |
| 2:C:207:HIS:CE1 | 2:C:209:ALA:HB3 | 2.16 | 0.80 |
| 1:A:123:ARG:HA | 1:A:125:TRP:CH2 | 2.17 | 0.80 |
| 2:C:172:HIS:HB2 | 2:C:188:SER:HB3 | 1.61 | 0.80 |
| 3:D:150:ASP:HA | 3:D:190:SER:HB3 | 1.62 | 0.80 |
| 1:B:449:LEU:O | 1:B:453:LEU:HB2 | 1.82 | 0.79 |
| 1:A:109:ILE:HD12 | 1:A:445:TYR:HE2 | 1.46 | 0.79 |
| 3:D:30:SER:HA | 3:D:70:TYR:OH | 1.83 | 0.79 |
| 1:B:241:VAL:HG11 | 1:B:324:THR:HG21 | 1.65 | 0.79 |
| 1:B:200:ILE:HG22 | 1:B:201:ILE:N | 1.97 | 0.79 |
| 1:B:201:ILE:HG21 | 1:B:215:ILE:HD11 | 1.63 | 0.78 |
| 3:F:111:ALA:N | 3:F:199:THR:HG21 | 1.98 | 0.78 |
| 1:A:120:ARG:HB3 | 1:A:120:ARG:HH11 | 1.48 | 0.78 |
| 1:B:120:ARG:CB | 1:B:120:ARG:HH11 | 1.95 | 0.78 |
| 1:A:44:THR:O | 1:A:48:LEU:HD22 | 1.83 | 0.78 |
| 1:A:449:LEU:O | 1:A:453:LEU:HB2 | 1.83 | 0.78 |
| 1:B:451:ARG:CB | 1:B:451:ARG:HH11 | 1.96 | 0.78 |
| 1:A:274:LEU:HD12 | 1:A:277:GLN:NE2 | 1.97 | 0.78 |
| 2:E:72:ARG:NH1 | 2:E:74:ASN:OD1 | 2.16 | 0.78 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:H | 1.27 | 0.78 |
| 3:F:95:GLN:OE1 | 3:F:95:GLN:N | 2.16 | 0.78 |
| 1:A:200:ILE:HG22 | 1:A:201:ILE:N | 1.97 | 0.78 |
| 1:A:98:ARG:NH1 | 1:A:98:ARG:HB3 | 1.99 | 0.77 |
| 1:B:260:ILE:HG23 | 1:B:435:LEU:HG | 1.64 | 0.77 |
| 2:C:107:TYR:HB3 | 3:D:33:HIS:CD2 | 2.20 | 0.77 |
| 1:B:279:LEU:HA | 1:B:282:ARG:HH11 | 1.49 | 0.77 |
| 1:A:281:HIS:HA | 1:A:284:HIS:CE1 | 2.20 | 0.77 |
| 1:A:200:ILE:HD12 | 1:A:204:MET:HG3 | 1.64 | 0.77 |
| 3:F:192:THR:CA | 3:F:207:SER:HB3 | 2.13 | 0.76 |
| 1:B:44:THR:O | 1:B:48:LEU:HD22 | 1.85 | 0.76 |
| 1:B:421:LEU:O | 1:B:424:PRO:HD2 | 1.84 | 0.76 |
| 1:A:68:LEU:HD21 | 1:A:82:ALA:HB2 | 1.66 | 0.76 |
| 1:B:65:MET:C | 1:B:67:ALA:H | 1.89 | 0.76 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:201:ILE:HG21 | 1:A:215:ILE:HD11 | 1.66 | 0.76 |
| 3:D:189:ASN:HD21 | 3:D:211:ALA:H | 1.31 | 0.76 |
| 2:E:45:LEU:N | 2:E:45:LEU:HD12 | 2.00 | 0.76 |
| 1:B:150:PRO:O | 1:B:154:ILE:HG13 | 1.85 | 0.76 |
| 1:B:374:VAL:HG12 | 1:B:378:LEU:CD1 | 2.16 | 0.76 |
| 1:A:374:VAL:HG12 | 1:A:378:LEU:CD1 | 2.16 | 0.75 |
| 1:A:423:LEU:HB3 | 1:A:424:PRO:HD3 | 1.69 | 0.75 |
| 2:C:126:PRO:HB3 | 2:C:210:SER:OG | 1.86 | 0.75 |
| 1:B:281:HIS:HA | 1:B:284:HIS:CE1 | 2.21 | 0.75 |
| 1:A:119:GLN:HB3 | 1:A:453:LEU:HD11 | 1.67 | 0.75 |
| 2:E:221:ARG:HH22 | 3:F:120:SER:HA | 1.51 | 0.75 |
| 3:F:189:ASN:HD21 | 3:F:211:ALA:H | 1.35 | 0.75 |
| 1:A:65:MET:C | 1:A:67:ALA:H | 1.90 | 0.74 |
| 1:B:274:LEU:HA | 1:B:277:GLN:HE21 | 1.50 | 0.74 |
| 1:B:109:ILE:HD12 | 1:B:445:TYR:CE2 | 2.23 | 0.74 |
| 2:C:207:HIS:HE1 | 2:C:209:ALA:HB3 | 1.49 | 0.74 |
| 1:B:252:LEU:HD22 | 1:B:427:ILE:HD12 | 1.68 | 0.74 |
| 2:E:45:LEU:HD11 | 3:F:86:TYR:CD1 | 2.23 | 0.74 |
| 3:D:14:ALA:O | 3:D:17:ASP:HB2 | 1.87 | 0.74 |
| 1:A:150:PRO:O | 1:A:154:ILE:HG13 | 1.88 | 0.74 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:HG3 | 1.53 | 0.73 |
| 1:B:123:ARG:HH21 | 1:B:126:ARG:HH11 | 1.35 | 0.73 |
| 2:C:18:LEU:HD23 | 2:C:18:LEU:H | 1.53 | 0.73 |
| 3:F:150:ASP:HA | 3:F:190:SER:HB3 | 1.69 | 0.73 |
| 1:A:120:ARG:HD3 | 1:A:453:LEU:HD13 | 1.70 | 0.73 |
| 1:A:18:ARG:O | 1:A:18:ARG:HG2 | 1.86 | 0.73 |
| 3:F:148:LYS:HB2 | 3:F:192:THR:OG1 | 1.89 | 0.72 |
| 3:F:7:SER:HB3 | 3:F:8:PRO:CD | 2.18 | 0.72 |
| 1:A:120:ARG:HD3 | 1:A:453:LEU:CD1 | 2.19 | 0.72 |
| 2:C:189:VAL:O | 2:C:189:VAL:HG13 | 1.90 | 0.72 |
| 2:C:51:ILE:HD11 | 2:C:55:SER:HB3 | 1.70 | 0.72 |
| 1:B:380:PRO:HD2 | 1:B:381:GLN:HE22 | 1.53 | 0.72 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:N | 1.87 | 0.72 |
| 3:F:1:ASP:HB3 | 3:F:94:PRO:HD2 | 1.69 | 0.72 |
| 1:A:28:ARG:HD2 | 1:B:207:GLN:CG | 2.17 | 0.72 |
| 2:E:41:PRO:HD3 | 2:E:92:ALA:HA | 1.72 | 0.72 |
| 2:E:132:LEU:HD21 | 3:F:132:VAL:HG21 | 1.72 | 0.72 |
| 2:C:2:VAL:HA | 2:C:26:GLY:HA3 | 1.71 | 0.72 |
| 2:E:126:PRO:HB3 | 2:E:210:SER:OG | 1.90 | 0.71 |
| 3:F:30:SER:HA | 3:F:70:TYR:OH | 1.90 | 0.71 |
| 1:B:119:GLN:HB3 | 1:B:453:LEU:HD11 | 1.72 | 0.71 |
| 2:C:124:THR:HG22 | 2:C:125:THR:N | 2.06 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:120:ARG:HD3 | 1:B:453:LEU:HD13 | 1.70 | 0.71 |
| 1:A:260:ILE:HG23 | 1:A:435:LEU:HG | 1.73 | 0.71 |
| 1:B:166:PHE:HB2 | 1:B:168:LEU:HD11 | 1.73 | 0.71 |
| 1:B:287:ASN:ND2 | 1:B:290:LYS:N | 2.38 | 0.71 |
| 3:D:20:THR:HG23 | 3:D:73:THR:OG1 | 1.90 | 0.71 |
| 1:B:320:ILE:HG21 | 1:B:394:MET:CE | 2.21 | 0.71 |
| 1:A:18:ARG:NH2 | 1:B:456:GLN:NE2 | 2.38 | 0.71 |
| 1:B:168:LEU:H | 1:B:168:LEU:HD12 | 1.56 | 0.70 |
| 2:C:72:ARG:NH1 | 2:C:74:ASN:OD1 | 2.24 | 0.70 |
| 1:A:451:ARG:HH11 | 1:A:451:ARG:CB | 2.04 | 0.70 |
| 2:C:45:LEU:N | 2:C:45:LEU:HD12 | 2.03 | 0.70 |
| 1:B:206:PRO:HG2 | 1:B:211:THR:OG1 | 1.91 | 0.70 |
| 1:B:144:VAL:HG21 | 1:B:343:THR:HB | 1.73 | 0.70 |
| 2:C:12:VAL:HG23 | 2:C:119:VAL:HG22 | 1.72 | 0.70 |
| 1:A:108:GLY:HA2 | 1:A:153:GLN:NE2 | 2.06 | 0.70 |
| 1:A:216:LYS:HD3 | 1:B:434:LEU:CD2 | 2.22 | 0.70 |
| 3:F:2:ILE:HD11 | 3:F:27:SER:HB2 | 1.74 | 0.70 |
| 1:B:381:GLN:H | 1:B:381:GLN:HE21 | 0.80 | 0.69 |
| 1:B:182:ALA:HB1 | 1:B:204:MET:CE | 2.22 | 0.69 |
| 1:A:144:VAL:HG21 | 1:A:343:THR:HB | 1.73 | 0.69 |
| 1:B:274:LEU:HA | 1:B:277:GLN:NE2 | 2.07 | 0.69 |
| 1:A:123:ARG:HH21 | 1:A:126:ARG:HH11 | 1.36 | 0.69 |
| 1:A:22:ILE:HD13 | 1:B:454:ALA:HB2 | 1.73 | 0.69 |
| 2:E:39:GLN:O | 2:E:92:ALA:HB1 | 1.92 | 0.69 |
| 3:D:65:GLY:HA3 | 3:D:70:TYR:HA | 1.75 | 0.69 |
| 1:A:18:ARG:NH2 | 1:B:456:GLN:HE21 | 1.90 | 0.69 |
| 3:D:148:LYS:HB2 | 3:D:192:THR:OG1 | 1.92 | 0.69 |
| 1:A:109:ILE:HD12 | 1:A:445:TYR:CE2 | 2.28 | 0.69 |
| 2:E:91:THR:OG1 | 2:E:119:VAL:HG23 | 1.91 | 0.69 |
| 1:A:426:ILE:CG2 | 1:B:223:ILE:HD11 | 2.22 | 0.69 |
| 1:A:79:LEU:H | 1:A:79:LEU:CD2 | 2.06 | 0.69 |
| 1:B:197:ILE:HD13 | 1:B:219:PHE:CE1 | 2.28 | 0.69 |
| 1:A:207:GLN:CG | 1:B:28:ARG:HD2 | 2.21 | 0.69 |
| 3:F:7:SER:HB2 | 3:F:22:THR:HB | 1.75 | 0.69 |
| 1:B:200:ILE:HD12 | 1:B:204:MET:HG3 | 1.74 | 0.69 |
| 2:C:39:GLN:O | 2:C:92:ALA:HB1 | 1.93 | 0.69 |
| 1:B:358:ALA:O | 1:B:361:LEU:HB2 | 1.91 | 0.68 |
| 1:B:274:LEU:HD12 | 1:B:277:GLN:NE2 | 2.07 | 0.68 |
| 2:E:18:LEU:H | 2:E:18:LEU:HD23 | 1.57 | 0.68 |
| 3:F:88:GLN:HB2 | 3:F:97:PHE:CD1 | 2.27 | 0.68 |
| 2:C:129:VAL:HG21 | 2:C:214:VAL:CG2 | 2.23 | 0.68 |
| 3:F:111:ALA:HB2 | 3:F:199:THR:HB | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:98:ARG:NH1 | 1:B:98:ARG:HB3 | 2.05 | 0.68 |
| 1:A:163:LEU:HD21 | 1:A:174:ARG:HG3 | 1.74 | 0.68 |
| 1:B:282:ARG:O | 1:B:284:HIS:N | 2.26 | 0.68 |
| 1:A:79:LEU:H | 1:A:79:LEU:HD22 | 1.58 | 0.68 |
| 1:B:274:LEU:HD12 | 1:B:277:GLN:HE22 | 1.59 | 0.68 |
| 3:F:192:THR:HA | 3:F:207:SER:CB | 2.19 | 0.68 |
| 1:B:79:LEU:H | 1:B:79:LEU:HD22 | 1.57 | 0.68 |
| 1:B:284:HIS:HA | 1:B:290:LYS:HB3 | 1.75 | 0.68 |
| 3:D:7:SER:HB3 | 3:D:8:PRO:CD | 2.23 | 0.68 |
| 1:A:182:ALA:HB1 | 1:A:204:MET:CE | 2.24 | 0.68 |
| 1:A:17:ARG:C | 1:A:17:ARG:HD2 | 2.14 | 0.68 |
| 1:A:380:PRO:HD2 | 1:A:381:GLN:HE22 | 1.59 | 0.67 |
| 1:B:172:GLU:O | 1:B:176:THR:HB | 1.93 | 0.67 |
| 1:A:458:ALA:N | 1:A:460:GLN:HE22 | 1.91 | 0.67 |
| 2:C:204:ASN:HB3 | 2:C:215:ASP:OD1 | 1.93 | 0.67 |
| 1:B:79:LEU:H | 1:B:79:LEU:CD2 | 2.07 | 0.67 |
| 1:B:374:VAL:HG12 | 1:B:378:LEU:HD11 | 1.77 | 0.67 |
| 1:A:120:ARG:HB3 | 1:A:120:ARG:NH1 | 2.09 | 0.67 |
| 1:A:421:LEU:O | 1:A:424:PRO:HD2 | 1.95 | 0.67 |
| 1:A:199:PHE:HA | 1:A:407:THR:OG1 | 1.95 | 0.67 |
| 3:F:7:SER:CB | 3:F:8:PRO:HD3 | 2.22 | 0.66 |
| 1:B:451:ARG:HB3 | 1:B:451:ARG:HH11 | 1.59 | 0.66 |
| 2:E:129:VAL:HG21 | 2:E:214:VAL:CG2 | 2.25 | 0.66 |
| 3:D:13:ALA:HB3 | 3:D:77:MET:CE | 2.25 | 0.66 |
| 1:A:458:ALA:H | 1:A:460:GLN:HE22 | 1.43 | 0.66 |
| 1:A:97:VAL:HG22 | 1:A:104:ALA:HB3 | 1.76 | 0.66 |
| 1:A:434:LEU:CD2 | 1:B:216:LYS:HD3 | 2.25 | 0.66 |
| 3:F:148:LYS:HA | 3:F:152:SER:O | 1.96 | 0.66 |
| 2:C:18:LEU:N | 2:C:18:LEU:HD23 | 2.08 | 0.66 |
| 2:C:41:PRO:HD3 | 2:C:92:ALA:HA | 1.78 | 0.66 |
| 1:A:403:ARG:NH2 | 1:A:437:GLN:HB2 | 2.10 | 0.66 |
| 3:D:148:LYS:HA | 3:D:152:SER:O | 1.95 | 0.66 |
| 2:E:192:PRO:O | 2:E:195:SER:HB3 | 1.95 | 0.66 |
| 1:A:172:GLU:O | 1:A:176:THR:HB | 1.95 | 0.66 |
| 2:E:189:VAL:HG13 | 2:E:189:VAL:O | 1.95 | 0.66 |
| 1:A:403:ARG:HH22 | 1:A:437:GLN:HB2 | 1.60 | 0.66 |
| 3:D:192:THR:CA | 3:D:207:SER:HB3 | 2.25 | 0.66 |
| 1:A:266:GLY:HA3 | 1:A:400:ALA:HB1 | 1.78 | 0.66 |
| 2:C:45:LEU:HD11 | 3:D:86:TYR:CD1 | 2.31 | 0.65 |
| 1:A:282:ARG:O | 1:A:284:HIS:N | 2.29 | 0.65 |
| 1:A:403:ARG:HH22 | 1:A:437:GLN:CB | 2.09 | 0.65 |
| 1:A:332:MET:O | 1:A:336:ILE:HG13 | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:374:VAL:HG12 | 1:A:378:LEU:HD11 | 1.79 | 0.65 |
| 2:C:129:VAL:HG21 | 2:C:214:VAL:HG21 | 1.78 | 0.65 |
| 1:A:122:VAL:HG11 | 1:A:160:ARG:CB | 2.26 | 0.65 |
| 1:A:166:PHE:HB2 | 1:A:168:LEU:HD11 | 1.77 | 0.65 |
| 2:E:6:GLU:HA | 2:E:22:CYS:HA | 1.78 | 0.65 |
| 2:E:172:HIS:HB2 | 2:E:188:SER:HB3 | 1.77 | 0.65 |
| 1:A:411:LEU:O | 1:A:414:GLU:HB2 | 1.97 | 0.65 |
| 2:E:207:HIS:ND1 | 2:E:210:SER:HB3 | 2.12 | 0.65 |
| 1:A:197:ILE:HD13 | 1:A:219:PHE:CE1 | 2.32 | 0.65 |
| 3:F:22:THR:HG22 | 3:F:23:CYS:N | 2.12 | 0.65 |
| 1:B:423:LEU:HB3 | 1:B:424:PRO:HD3 | 1.79 | 0.65 |
| 1:B:108:GLY:HA2 | 1:B:153:GLN:NE2 | 2.12 | 0.65 |
| 3:D:22:THR:HG22 | 3:D:23:CYS:N | 2.12 | 0.65 |
| 1:A:374:VAL:HG12 | 1:A:378:LEU:HD12 | 1.79 | 0.65 |
| 1:B:114:GLY:HA2 | 1:B:449:LEU:HD21 | 1.79 | 0.65 |
| 2:E:35:SER:HB2 | 2:E:49:GLY:O | 1.97 | 0.65 |
| 1:B:23:ARG:O | 1:B:27:GLU:HB2 | 1.97 | 0.65 |
| 1:A:250:ASN:OD1 | 1:A:251:THR:HG23 | 1.96 | 0.65 |
| 1:A:357:PHE:CE1 | 1:A:398:LEU:HD22 | 2.31 | 0.64 |
| 1:A:114:GLY:HA2 | 1:A:449:LEU:HD21 | 1.79 | 0.64 |
| 1:A:168:LEU:HD12 | 1:A:168:LEU:H | 1.61 | 0.64 |
| 3:F:134:PHE:O | 3:F:135:LEU:HD23 | 1.97 | 0.64 |
| 2:E:34:MET:HB3 | 2:E:79:LEU:HD22 | 1.78 | 0.64 |
| 3:D:182:LYS:HG2 | 3:D:186:GLU:OE1 | 1.97 | 0.64 |
| 1:A:37:PHE:HD2 | 1:A:38:MET:HE2 | 1.62 | 0.64 |
| 2:E:146:LEU:HD12 | 2:E:201:VAL:HG11 | 1.79 | 0.64 |
| 2:E:2:VAL:O | 2:E:2:VAL:HG23 | 1.96 | 0.64 |
| 1:A:318:ASN:HD22 | 1:A:318:ASN:N | 1.95 | 0.64 |
| 1:B:119:GLN:O | 1:B:120:ARG:HD2 | 1.98 | 0.64 |
| 1:B:410:ILE:O | 1:B:414:GLU:HG2 | 1.98 | 0.64 |
| 1:A:220:ILE:CG1 | 1:B:430:LEU:HD21 | 2.26 | 0.64 |
| 1:A:18:ARG:HH11 | 1:B:457:GLU:HB3 | 1.62 | 0.64 |
| 1:B:250:ASN:OD1 | 1:B:251:THR:HG23 | 1.97 | 0.64 |
| 1:B:270:ASN:ND2 | 1:B:444:LEU:HD23 | 2.12 | 0.64 |
| 1:A:120:ARG:HH11 | 1:A:120:ARG:CB | 2.11 | 0.64 |
| 1:A:147:ARG:HG3 | 1:A:147:ARG:HH11 | 1.63 | 0.63 |
| 3:D:205:VAL:O | 3:D:206:LYS:HG2 | 1.98 | 0.63 |
| 2:E:132:LEU:HB2 | 2:E:147:GLY:O | 1.99 | 0.63 |
| 2:E:24:ALA:HB1 | 2:E:27:PHE:HE1 | 1.63 | 0.63 |
| 3:F:65:GLY:HA3 | 3:F:70:TYR:HA | 1.80 | 0.63 |
| 1:A:443:PRO:HB2 | 1:A:446:SER:HB2 | 1.80 | 0.63 |
| 1:B:166:PHE:HB2 | 1:B:168:LEU:CD1 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:454:ALA:HB2 | 1:B:22:ILE:HD13 | 1.79 | 0.63 |
| 2:C:192:PRO:O | 2:C:195:SER:HB3 | 1.98 | 0.63 |
| 2:E:207:HIS:CE1 | 2:E:209:ALA:HB3 | 2.34 | 0.63 |
| 3:D:179:THR:O | 3:D:180:LEU:HD23 | 1.97 | 0.63 |
| 3:D:114:VAL:O | 3:D:206:LYS:HD2 | 1.98 | 0.63 |
| 2:C:51:ILE:CD1 | 2:C:72:ARG:HD2 | 2.29 | 0.63 |
| 1:B:163:LEU:HD21 | 1:B:174:ARG:HG3 | 1.81 | 0.63 |
| 1:A:138:THR:HG22 | 1:A:143:MET:SD | 2.38 | 0.63 |
| 2:E:45:LEU:CD1 | 2:E:45:LEU:H | 2.09 | 0.62 |
| 1:A:320:ILE:HG21 | 1:A:394:MET:CE | 2.29 | 0.62 |
| 1:A:269:PHE:O | 1:A:273:VAL:HG12 | 1.99 | 0.62 |
| 1:B:266:GLY:HA3 | 1:B:400:ALA:HB1 | 1.81 | 0.62 |
| 3:F:20:THR:HG23 | 3:F:73:THR:OG1 | 1.99 | 0.62 |
| 3:F:190:SER:HA | 3:F:209:ASN:OD1 | 1.99 | 0.62 |
| 1:A:287:ASN:ND2 | 1:A:290:LYS:HG3 | 2.14 | 0.62 |
| 1:B:374:VAL:HG12 | 1:B:378:LEU:HD12 | 1.81 | 0.62 |
| 1:A:86:SER:OG | 1:A:303:GLY:HA3 | 1.99 | 0.62 |
| 3:D:7:SER:CB | 3:D:8:PRO:HD3 | 2.25 | 0.62 |
| 1:A:410:ILE:O | 1:A:414:GLU:HG2 | 1.99 | 0.62 |
| 3:F:111:ALA:HB2 | 3:F:199:THR:CB | 2.30 | 0.62 |
| 1:A:71:THR:HB | 1:A:77:LEU:HD23 | 1.81 | 0.62 |
| 1:B:279:LEU:O | 1:B:279:LEU:HD23 | 1.98 | 0.61 |
| 3:F:13:ALA:HB3 | 3:F:77:MET:CE | 2.29 | 0.61 |
| 1:B:199:PHE:HA | 1:B:407:THR:OG1 | 2.00 | 0.61 |
| 1:A:437:GLN:NE2 | 1:B:31:THR:H | 1.99 | 0.61 |
| 3:F:7:SER:CB | 3:F:22:THR:HB | 2.30 | 0.61 |
| 1:A:31:THR:H | 1:B:437:GLN:NE2 | 1.97 | 0.61 |
| 1:A:75:TYR:HB3 | 1:A:76:PRO:CD | 2.29 | 0.61 |
| 1:A:358:ALA:O | 1:A:361:LEU:HB2 | 1.99 | 0.61 |
| 1:A:357:PHE:CE1 | 1:A:398:LEU:HD13 | 2.35 | 0.61 |
| 1:B:243:LYS:HE2 | 1:B:420:GLN:OE1 | 2.00 | 0.61 |
| 1:A:23:ARG:O | 1:A:27:GLU:HB2 | 2.00 | 0.61 |
| 1:A:287:ASN:ND2 | 1:A:290:LYS:N | 2.47 | 0.61 |
| 1:A:216:LYS:HD3 | 1:B:434:LEU:HD22 | 1.82 | 0.61 |
| 2:E:18:LEU:N | 2:E:18:LEU:HD23 | 2.15 | 0.61 |
| 1:A:99:LYS:HB2 | 1:A:288:ILE:HD11 | 1.83 | 0.61 |
| 2:C:30:SER:C | 2:C:32:TYR:H | 2.04 | 0.61 |
| 2:C:129:VAL:CG2 | 2:C:214:VAL:HG21 | 2.30 | 0.61 |
| 1:B:147:ARG:HH11 | 1:B:147:ARG:HG3 | 1.65 | 0.61 |
| 1:B:443:PRO:HB2 | 1:B:446:SER:HB2 | 1.83 | 0.61 |
| 1:B:72:ALA:HA | 1:B:78:LEU:HD21 | 1.81 | 0.61 |
| 1:A:148:GLN:HE22 | 1:A:189:ALA:HB1 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:320:ILE:HG21 | 1:B:394:MET:HE3 | 1.82 | 0.61 |
| 1:A:166:PHE:HB2 | 1:A:168:LEU:CD1 | 2.30 | 0.61 |
| 1:A:72:ALA:HA | 1:A:78:LEU:HD21 | 1.83 | 0.61 |
| 1:A:413:LEU:HD11 | 1:A:419:TYR:HD1 | 1.65 | 0.60 |
| 1:A:298:ILE:CG2 | 1:A:346:LEU:HG | 2.31 | 0.60 |
| 1:B:176:THR:O | 1:B:180:THR:HG23 | 2.01 | 0.60 |
| 1:B:403:ARG:NH2 | 1:B:437:GLN:HB2 | 2.15 | 0.60 |
| 3:F:182:LYS:HG2 | 3:F:186:GLU:OE1 | 2.00 | 0.60 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:HG3 | 1.66 | 0.60 |
| 3:F:194:GLU:CG | 3:F:205:VAL:HG12 | 2.24 | 0.60 |
| 3:F:114:VAL:HG22 | 3:F:135:LEU:HD22 | 1.83 | 0.60 |
| 3:F:77:MET:SD | 3:F:103:LEU:HD21 | 2.41 | 0.60 |
| 2:C:185:LEU:HD12 | 2:C:185:LEU:O | 2.00 | 0.60 |
| 1:A:284:HIS:HA | 1:A:290:LYS:HB3 | 1.84 | 0.60 |
| 1:B:182:ALA:HB1 | 1:B:204:MET:HE3 | 1.84 | 0.60 |
| 2:C:6:GLU:HA | 2:C:22:CYS:HA | 1.82 | 0.60 |
| 1:A:190:PHE:CE2 | 1:A:411:LEU:HD21 | 2.37 | 0.60 |
| 3:F:95:GLN:H | 3:F:95:GLN:CD | 2.05 | 0.60 |
| 1:A:148:GLN:NE2 | 1:A:189:ALA:HB1 | 2.16 | 0.60 |
| 1:A:243:LYS:HE2 | 1:A:420:GLN:OE1 | 2.01 | 0.60 |
| 3:F:179:THR:O | 3:F:180:LEU:HD23 | 2.01 | 0.60 |
| 1:A:255:TYR:CD2 | 1:A:424:PRO:HB3 | 2.36 | 0.59 |
| 2:E:207:HIS:HE1 | 2:E:209:ALA:HB3 | 1.67 | 0.59 |
| 1:A:53:PHE:HE2 | 1:A:147:ARG:HB2 | 1.66 | 0.59 |
| 1:B:357:PHE:CE1 | 1:B:398:LEU:HD13 | 2.36 | 0.59 |
| 3:F:34:TRP:CZ3 | 3:F:87:CYS:HB3 | 2.37 | 0.59 |
| 2:E:129:VAL:CG2 | 2:E:214:VAL:HG21 | 2.32 | 0.59 |
| 3:F:114:VAL:HG12 | 3:F:115:SER:N | 2.17 | 0.59 |
| 3:F:116:ILE:HD13 | 3:F:193:CYS:HB2 | 1.84 | 0.59 |
| 2:C:51:ILE:HD13 | 2:C:72:ARG:HD2 | 1.84 | 0.59 |
| 1:B:318:ASN:HD22 | 1:B:319:LEU:H | 1.49 | 0.59 |
| 1:A:434:LEU:HD22 | 1:B:216:LYS:HD3 | 1.84 | 0.59 |
| 1:A:122:VAL:HG11 | 1:A:160:ARG:HB3 | 1.84 | 0.59 |
| 1:B:122:VAL:HG12 | 1:B:122:VAL:O | 2.03 | 0.59 |
| 1:B:86:SER:OG | 1:B:303:GLY:HA3 | 2.03 | 0.59 |
| 1:A:198:LEU:HG | 1:A:410:ILE:CD1 | 2.32 | 0.59 |
| 1:B:71:THR:HB | 1:B:77:LEU:HD23 | 1.85 | 0.59 |
| 1:A:212:LEU:H | 1:A:212:LEU:HD12 | 1.67 | 0.59 |
| 3:F:15:PRO:HD3 | 3:F:105:ILE:HG22 | 1.83 | 0.59 |
| 2:E:49:GLY:HA3 | 2:E:70:ILE:CD1 | 2.33 | 0.59 |
| 3:D:153:GLU:HG3 | 3:D:154:ARG:H | 1.67 | 0.59 |
| 2:E:185:LEU:O | 2:E:185:LEU:HD12 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:451:ARG:HB3 | 1:A:451:ARG:HH11 | 1.66 | 0.59 |
| 1:B:171:ASP:HB2 | 1:B:212:LEU:HD22 | 1.83 | 0.59 |
| 1:B:97:VAL:HG22 | 1:B:104:ALA:HB3 | 1.85 | 0.59 |
| 2:E:121:SER:O | 2:E:122:ALA:O | 2.21 | 0.59 |
| 3:F:58:PRO:C | 3:F:60:ARG:H | 2.05 | 0.59 |
| 1:B:287:ASN:ND2 | 1:B:290:LYS:HG3 | 2.18 | 0.59 |
| 1:A:23:ARG:HG3 | 1:A:23:ARG:HH11 | 1.66 | 0.59 |
| 1:A:60:LEU:O | 1:A:64:ARG:HG3 | 2.02 | 0.59 |
| 2:C:35:SER:HB2 | 2:C:49:GLY:O | 2.02 | 0.59 |
| 1:A:17:ARG:O | 1:A:17:ARG:HD2 | 2.02 | 0.58 |
| 1:A:385:GLU:O | 1:A:387:GLY:N | 2.36 | 0.58 |
| 1:B:252:LEU:HD11 | 1:B:423:LEU:HD23 | 1.84 | 0.58 |
| 1:A:270:ASN:ND2 | 1:A:444:LEU:HD23 | 2.16 | 0.58 |
| 1:B:267:PRO:O | 1:B:270:ASN:HB2 | 2.02 | 0.58 |
| 1:A:356:ILE:O | 1:A:360:MET:HG3 | 2.03 | 0.58 |
| 2:C:127:PRO:HB3 | 2:C:153:TYR:CB | 2.31 | 0.58 |
| 1:B:413:LEU:HD11 | 1:B:419:TYR:HD1 | 1.69 | 0.58 |
| 2:C:146:LEU:HD12 | 2:C:201:VAL:HG11 | 1.86 | 0.58 |
| 1:B:457:GLU:O | 1:B:458:ALA:HB3 | 2.04 | 0.58 |
| 2:C:132:LEU:HD21 | 3:D:132:VAL:HG21 | 1.86 | 0.58 |
| 3:D:95:GLN:H | 3:D:95:GLN:CD | 2.06 | 0.58 |
| 2:E:129:VAL:HG21 | 2:E:214:VAL:HG21 | 1.83 | 0.58 |
| 1:A:266:GLY:N | 1:A:267:PRO:HD2 | 2.18 | 0.58 |
| 1:A:98:ARG:NH1 | 1:A:98:ARG:CB | 2.67 | 0.58 |
| 3:F:72:LEU:HD23 | 3:F:72:LEU:C | 2.24 | 0.58 |
| 1:A:122:VAL:HG12 | 1:A:122:VAL:O | 2.03 | 0.58 |
| 1:B:336:ILE:O | 1:B:340:ARG:HG3 | 2.03 | 0.58 |
| 3:D:158:VAL:O | 3:D:159:LEU:HD23 | 2.03 | 0.58 |
| 3:F:153:GLU:HG3 | 3:F:154:ARG:H | 1.68 | 0.58 |
| 2:E:40:ALA:HA | 2:E:92:ALA:CB | 2.33 | 0.58 |
| 1:B:403:ARG:HH22 | 1:B:437:GLN:CB | 2.16 | 0.58 |
| 1:B:148:GLN:HG3 | 1:B:190:PHE:CZ | 2.39 | 0.58 |
| 1:B:227:ILE:O | 1:B:231:ILE:HG12 | 2.03 | 0.58 |
| 3:F:111:ALA:H | 3:F:199:THR:HG21 | 1.69 | 0.58 |
| 2:E:30:SER:C | 2:E:32:TYR:H | 2.07 | 0.58 |
| 1:A:403:ARG:HH22 | 1:A:437:GLN:CA | 2.17 | 0.58 |
| 2:E:61:THR:HB | 2:E:62:PRO:CD | 2.34 | 0.58 |
| 3:D:189:ASN:ND2 | 3:D:211:ALA:H | 2.01 | 0.58 |
| 1:B:122:VAL:HG11 | 1:B:160:ARG:CB | 2.33 | 0.58 |
| 3:D:117:PHE:N | 3:D:117:PHE:CD1 | 2.72 | 0.58 |
| 2:C:100:TYR:HB3 | 2:C:107:TYR:CE1 | 2.39 | 0.58 |
| 1:B:239:ILE:HD13 | 1:B:394:MET:HE2 | 1.83 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:19:ARG:HG2 | 1:B:19:ARG:HH11 | 1.69 | 0.58 |
| 1:A:305:LEU:HA | 1:A:308:VAL:CG2 | 2.32 | 0.57 |
| 1:A:402:ILE:HD12 | 1:A:445:TYR:CE1 | 2.39 | 0.57 |
| 1:A:336:ILE:O | 1:A:340:ARG:HG3 | 2.04 | 0.57 |
| 1:B:127:VAL:HB | 1:B:157:ASN:ND2 | 2.18 | 0.57 |
| 1:B:63:GLN:C | 1:B:65:MET:H | 2.08 | 0.57 |
| 1:B:99:LYS:HB2 | 1:B:288:ILE:HD11 | 1.86 | 0.57 |
| 1:A:79:LEU:HD22 | 1:A:79:LEU:N | 2.19 | 0.57 |
| 2:C:124:THR:HG22 | 2:C:125:THR:H | 1.68 | 0.57 |
| 1:B:403:ARG:HH22 | 1:B:437:GLN:HB2 | 1.69 | 0.57 |
| 1:A:252:LEU:HD22 | 1:A:427:ILE:CD1 | 2.31 | 0.57 |
| 1:A:23:ARG:HG3 | 1:A:23:ARG:NH1 | 2.19 | 0.57 |
| 3:D:134:PHE:O | 3:D:135:LEU:HD23 | 2.04 | 0.57 |
| 1:B:75:TYR:O | 1:B:79:LEU:HD23 | 2.04 | 0.57 |
| 1:B:90:ALA:O | 1:B:94:TYR:HD1 | 1.87 | 0.57 |
| 1:B:37:PHE:HD2 | 1:B:38:MET:HE2 | 1.69 | 0.57 |
| 1:A:31:THR:H | 1:B:437:GLN:HE22 | 1.52 | 0.57 |
| 2:C:178:LEU:HB2 | 2:C:183:TYR:CE2 | 2.40 | 0.57 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:N | 1.99 | 0.57 |
| 1:A:148:GLN:HB3 | 1:A:190:PHE:HE1 | 1.68 | 0.57 |
| 2:E:91:THR:HG23 | 2:E:118:THR:HA | 1.86 | 0.57 |
| 1:A:170:GLY:O | 1:A:172:GLU:N | 2.37 | 0.57 |
| 2:C:185:LEU:HD12 | 2:C:185:LEU:C | 2.24 | 0.57 |
| 2:C:196:TRP:O | 2:C:197:PRO:C | 2.40 | 0.57 |
| 2:C:200:THR:HG22 | 2:C:200:THR:O | 2.05 | 0.57 |
| 3:D:114:VAL:HG22 | 3:D:135:LEU:CD2 | 2.34 | 0.57 |
| 1:B:266:GLY:N | 1:B:267:PRO:HD2 | 2.20 | 0.57 |
| 1:A:186:LEU:O | 1:A:186:LEU:HG | 2.05 | 0.56 |
| 1:B:318:ASN:HD22 | 1:B:318:ASN:N | 2.02 | 0.56 |
| 2:E:49:GLY:HA3 | 2:E:70:ILE:HD12 | 1.87 | 0.56 |
| 1:A:206:PRO:HG2 | 1:A:211:THR:OG1 | 2.04 | 0.56 |
| 1:A:252:LEU:HD11 | 1:A:423:LEU:HD23 | 1.87 | 0.56 |
| 1:A:148:GLN:HG3 | 1:A:190:PHE:CZ | 2.40 | 0.56 |
| 3:D:190:SER:HA | 3:D:209:ASN:OD1 | 2.06 | 0.56 |
| 1:B:320:ILE:HB | 1:B:321:PRO:HD3 | 1.88 | 0.56 |
| 1:A:437:GLN:HE22 | 1:B:31:THR:H | 1.51 | 0.56 |
| 1:B:357:PHE:CE1 | 1:B:398:LEU:HD22 | 2.40 | 0.56 |
| 1:A:419:TYR:CE1 | 1:B:414:GLU:OE1 | 2.59 | 0.56 |
| 1:B:298:ILE:CG2 | 1:B:346:LEU:HG | 2.35 | 0.56 |
| 3:D:125:THR:O | 3:D:125:THR:HG22 | 2.03 | 0.56 |
| 1:A:200:ILE:CG2 | 1:A:201:ILE:N | 2.67 | 0.56 |
| 2:C:40:ALA:HA | 2:C:92:ALA:HB2 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:E:196:TRP:HB3 | 2:E:197:PRO:HD3 | 1.88 | 0.56 |
| 1:A:239:ILE:HD13 | 1:A:394:MET:HE2 | 1.88 | 0.56 |
| 1:B:170:GLY:O | 1:B:172:GLU:N | 2.39 | 0.56 |
| 2:E:98:ARG:NH1 | 2:E:109:ASP:OD2 | 2.29 | 0.56 |
| 1:B:190:PHE:CE2 | 1:B:411:LEU:HD21 | 2.40 | 0.56 |
| 1:A:75:TYR:O | 1:A:79:LEU:HD23 | 2.05 | 0.56 |
| 1:B:79:LEU:N | 1:B:79:LEU:HD22 | 2.21 | 0.56 |
| 3:F:82:ALA:HB2 | 3:F:105:ILE:CD1 | 2.32 | 0.56 |
| 1:A:333:LEU:HD11 | 1:A:373:MET:HE1 | 1.88 | 0.56 |
| 2:E:107:TYR:HB3 | 3:F:33:HIS:NE2 | 2.21 | 0.56 |
| 2:E:40:ALA:HA | 2:E:92:ALA:HB2 | 1.86 | 0.56 |
| 2:E:146:LEU:HD13 | 2:E:218:ILE:HG21 | 1.87 | 0.56 |
| 1:A:101:ALA:C | 1:A:103:GLU:H | 2.09 | 0.56 |
| 1:B:356:ILE:O | 1:B:360:MET:HG3 | 2.06 | 0.56 |
| 3:D:32:ILE:HG22 | 3:D:33:HIS:N | 2.22 | 0.55 |
| 1:A:18:ARG:HH21 | 1:B:456:GLN:NE2 | 2.03 | 0.55 |
| 2:E:127:PRO:HB3 | 2:E:153:TYR:CB | 2.35 | 0.55 |
| 3:F:114:VAL:HG22 | 3:F:135:LEU:CD2 | 2.35 | 0.55 |
| 1:B:64:ARG:NH1 | 1:B:64:ARG:HB3 | 2.21 | 0.55 |
| 3:D:114:VAL:HG22 | 3:D:135:LEU:HD22 | 1.87 | 0.55 |
| 3:D:192:THR:HA | 3:D:207:SER:CB | 2.30 | 0.55 |
| 1:B:200:ILE:CG2 | 1:B:201:ILE:N | 2.69 | 0.55 |
| 1:A:35:ILE:CG2 | 1:A:176:THR:HG21 | 2.36 | 0.55 |
| 1:A:212:LEU:N | 1:A:212:LEU:HD12 | 2.22 | 0.55 |
| 1:A:452:THR:HG22 | 1:A:452:THR:O | 2.07 | 0.55 |
| 1:B:269:PHE:O | 1:B:273:VAL:HG12 | 2.06 | 0.55 |
| 1:B:318:ASN:HD22 | 1:B:319:LEU:N | 2.04 | 0.55 |
| 3:F:119:PRO:HD3 | 3:F:131:VAL:HG22 | 1.89 | 0.55 |
| 3:F:111:ALA:CA | 3:F:199:THR:HG21 | 2.36 | 0.55 |
| 1:A:318:ASN:HD22 | 1:A:319:LEU:H | 1.55 | 0.55 |
| 1:B:243:LYS:HE2 | 1:B:420:GLN:CG | 2.36 | 0.55 |
| 2:C:156:GLU:HG2 | 2:C:183:TYR:CE1 | 2.41 | 0.55 |
| 2:C:109:ASP:OD2 | 2:C:110:VAL:HG23 | 2.07 | 0.55 |
| 2:E:100:TYR:HB3 | 2:E:107:TYR:CE1 | 2.42 | 0.55 |
| 1:B:294:MET:HG2 | 1:B:294:MET:O | 2.06 | 0.55 |
| 1:A:17:ARG:HH21 | 1:B:119:GLN:NE2 | 2.03 | 0.55 |
| 1:B:123:ARG:HA | 1:B:125:TRP:CH2 | 2.42 | 0.55 |
| 1:A:199:PHE:CD1 | 1:A:407:THR:HG21 | 2.42 | 0.55 |
| 1:A:59:TRP:CZ3 | 1:A:60:LEU:HD23 | 2.42 | 0.55 |
| 1:B:398:LEU:O | 1:B:402:ILE:HG23 | 2.06 | 0.54 |
| 2:C:127:PRO:CB | 2:C:153:TYR:HB3 | 2.32 | 0.54 |
| 2:E:132:LEU:HD21 | 3:F:132:VAL:CG2 | 2.35 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:65:MET:C | 1:B:67:ALA:N | 2.60 | 0.54 |
| 3:D:105:ILE:HB | 3:D:170:SER:OG | 2.07 | 0.54 |
| 1:B:380:PRO:HD2 | 1:B:381:GLN:NE2 | 2.20 | 0.54 |
| 3:F:29:VAL:CG2 | 3:F:32:ILE:HD11 | 2.37 | 0.54 |
| 1:A:457:GLU:HB3 | 1:B:18:ARG:NH1 | 2.22 | 0.54 |
| 1:A:92:PHE:O | 1:A:96:LEU:HD23 | 2.07 | 0.54 |
| 1:A:255:TYR:CG | 1:A:424:PRO:HB3 | 2.43 | 0.54 |
| 1:A:267:PRO:O | 1:A:270:ASN:HB2 | 2.06 | 0.54 |
| 3:F:29:VAL:O | 3:F:67:GLY:HA2 | 2.08 | 0.54 |
| 1:B:332:MET:O | 1:B:336:ILE:HG13 | 2.08 | 0.54 |
| 1:A:243:LYS:HE2 | 1:A:420:GLN:CG | 2.38 | 0.54 |
| 2:E:196:TRP:O | 2:E:197:PRO:C | 2.46 | 0.54 |
| 1:B:212:LEU:HD12 | 1:B:212:LEU:N | 2.23 | 0.54 |
| 2:E:10:GLY:N | 2:E:116:THR:O | 2.41 | 0.54 |
| 2:C:24:ALA:HB1 | 2:C:27:PHE:HE1 | 1.72 | 0.54 |
| 1:A:65:MET:C | 1:A:67:ALA:N | 2.60 | 0.54 |
| 1:B:176:THR:HG22 | 1:B:177:LEU:N | 2.22 | 0.54 |
| 1:B:197:ILE:HG13 | 1:B:222:VAL:HG21 | 1.89 | 0.54 |
| 1:A:457:GLU:O | 1:A:458:ALA:HB3 | 2.08 | 0.54 |
| 1:B:273:VAL:HA | 1:B:345:LEU:HD22 | 1.89 | 0.54 |
| 1:A:90:ALA:O | 1:A:94:TYR:HD1 | 1.91 | 0.54 |
| 3:F:197:HIS:ND1 | 3:F:198:LYS:N | 2.56 | 0.54 |
| 2:E:51:ILE:HD11 | 2:E:55:SER:HB3 | 1.89 | 0.53 |
| 1:A:63:GLN:C | 1:A:65:MET:H | 2.11 | 0.53 |
| 1:A:101:ALA:O | 1:A:103:GLU:N | 2.41 | 0.53 |
| 3:D:197:HIS:ND1 | 3:D:198:LYS:N | 2.55 | 0.53 |
| 3:D:12:SER:HB3 | 3:D:106:LEU:HB2 | 1.90 | 0.53 |
| 2:C:18:LEU:CD2 | 2:C:18:LEU:N | 2.71 | 0.53 |
| 2:C:40:ALA:HA | 2:C:92:ALA:CB | 2.37 | 0.53 |
| 3:F:210:ARG:HG2 | 3:F:210:ARG:HH11 | 1.73 | 0.53 |
| 1:A:21:LEU:HD11 | 1:B:117:GLU:OE1 | 2.09 | 0.53 |
| 3:D:48:TYR:CE1 | 3:D:52:LYS:HD2 | 2.43 | 0.53 |
| 1:B:108:GLY:O | 1:B:153:GLN:HB2 | 2.09 | 0.53 |
| 1:A:318:ASN:ND2 | 1:A:318:ASN:N | 2.55 | 0.53 |
| 1:B:92:PHE:O | 1:B:96:LEU:HD23 | 2.07 | 0.53 |
| 3:D:8:PRO:O | 3:D:101:THR:HG23 | 2.09 | 0.53 |
| 1:A:443:PRO:O | 1:A:446:SER:N | 2.28 | 0.53 |
| 1:A:99:LYS:O | 1:A:99:LYS:HG3 | 2.08 | 0.53 |
| 1:B:59:TRP:CE3 | 1:B:60:LEU:HD23 | 2.43 | 0.53 |
| 2:C:149:LEU:HD12 | 2:C:150:VAL:N | 2.24 | 0.53 |
| 1:B:98:ARG:NH1 | 1:B:98:ARG:CB | 2.72 | 0.53 |
| 1:A:62:ASN:O | 1:A:65:MET:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:C:150:VAL:HG22 | 2:C:205:VAL:HG21 | 1.89 | 0.53 |
| 2:C:91:THR:HG23 | 2:C:118:THR:HA | 1.91 | 0.53 |
| 1:B:198:LEU:HD12 | 1:B:406:LEU:HG | 1.90 | 0.53 |
| 3:F:32:ILE:HG22 | 3:F:33:HIS:N | 2.24 | 0.53 |
| 3:D:3:VAL:HB | 3:D:26:SER:HB3 | 1.90 | 0.53 |
| 1:B:443:PRO:O | 1:B:445:TYR:N | 2.41 | 0.53 |
| 1:B:187:ALA:O | 1:B:189:ALA:N | 2.42 | 0.53 |
| 3:D:22:THR:HG22 | 3:D:23:CYS:H | 1.72 | 0.53 |
| 2:E:39:GLN:C | 2:E:92:ALA:HB1 | 2.29 | 0.53 |
| 1:A:108:GLY:O | 1:A:153:GLN:HB2 | 2.08 | 0.53 |
| 1:B:136:LEU:HD12 | 1:B:136:LEU:H | 1.73 | 0.53 |
| 2:C:39:GLN:C | 2:C:92:ALA:HB1 | 2.29 | 0.53 |
| 1:A:38:MET:HG3 | 1:A:168:LEU:HD21 | 1.91 | 0.53 |
| 2:C:30:SER:O | 2:C:32:TYR:N | 2.42 | 0.53 |
| 3:D:153:GLU:HG3 | 3:D:154:ARG:N | 2.23 | 0.53 |
| 1:B:202:GLU:HG2 | 1:B:202:GLU:O | 2.09 | 0.53 |
| 1:B:148:GLN:NE2 | 1:B:189:ALA:HB1 | 2.24 | 0.52 |
| 1:A:131:LYS:HE2 | 1:A:150:PRO:HA | 1.91 | 0.52 |
| 1:B:75:TYR:HB3 | 1:B:76:PRO:CD | 2.33 | 0.52 |
| 3:F:79:ALA:HA | 3:F:105:ILE:HD13 | 1.90 | 0.52 |
| 1:B:122:VAL:HG11 | 1:B:160:ARG:HB3 | 1.91 | 0.52 |
| 2:E:72:ARG:HG3 | 2:E:74:ASN:OD1 | 2.09 | 0.52 |
| 1:B:74:ASN:CG | 1:B:77:LEU:HB2 | 2.29 | 0.52 |
| 1:B:272:TRP:O | 1:B:276:MET:HB2 | 2.09 | 0.52 |
| 1:A:343:THR:O | 1:A:347:CYS:HB2 | 2.10 | 0.52 |
| 1:A:248:PRO:HG2 | 1:A:251:THR:HG23 | 1.92 | 0.52 |
| 3:D:58:PRO:C | 3:D:60:ARG:H | 2.12 | 0.52 |
| 1:B:171:ASP:CB | 1:B:212:LEU:HD22 | 2.39 | 0.52 |
| 2:E:127:PRO:CB | 2:E:153:TYR:HB3 | 2.37 | 0.52 |
| 1:A:74:ASN:CG | 1:A:77:LEU:HB2 | 2.30 | 0.52 |
| 1:B:109:ILE:CD1 | 1:B:445:TYR:HE2 | 2.17 | 0.52 |
| 1:A:192:ALA:HB1 | 1:A:414:GLU:HG3 | 1.92 | 0.52 |
| 1:A:109:ILE:CD1 | 1:A:445:TYR:HE2 | 2.21 | 0.52 |
| 3:F:115:SER:HB3 | 3:F:117:PHE:CE1 | 2.44 | 0.52 |
| 1:B:101:ALA:O | 1:B:103:GLU:N | 2.43 | 0.52 |
| 3:D:88:GLN:HB2 | 3:D:97:PHE:CD1 | 2.44 | 0.52 |
| 2:C:49:GLY:HA3 | 2:C:70:ILE:CD1 | 2.40 | 0.52 |
| 2:E:67:LYS:HE2 | 2:E:85:LYS:O | 2.10 | 0.52 |
| 1:B:442:LYS:O | 1:B:444:LEU:N | 2.43 | 0.52 |
| 1:B:159:GLY:O | 1:B:162:VAL:HG22 | 2.10 | 0.52 |
| 3:D:107:ARG:NE | 3:D:108:ALA:O | 2.41 | 0.51 |
| 3:F:75:ASN:O | 3:F:76:THR:HB | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:101:ALA:C | 1:B:103:GLU:H | 2.14 | 0.51 |
| 3:F:153:GLU:HG3 | 3:F:154:ARG:N | 2.25 | 0.51 |
| 2:C:120:SER:OG | 2:C:121:SER:N | 2.43 | 0.51 |
| 1:B:333:LEU:HD11 | 1:B:373:MET:HE1 | 1.92 | 0.51 |
| 3:F:158:VAL:O | 3:F:159:LEU:HD23 | 2.11 | 0.51 |
| 1:A:18:ARG:HB2 | 1:B:119:GLN:OE1 | 2.10 | 0.51 |
| 1:B:411:LEU:O | 1:B:414:GLU:HB2 | 2.11 | 0.51 |
| 1:A:201:ILE:HG13 | 1:A:201:ILE:O | 2.10 | 0.51 |
| 1:B:370:ALA:O | 1:B:374:VAL:HG23 | 2.11 | 0.51 |
| 1:A:65:MET:O | 1:A:67:ALA:N | 2.42 | 0.51 |
| 2:E:171:VAL:C | 2:E:172:HIS:HD1 | 2.14 | 0.51 |
| 2:C:32:TYR:CE2 | 2:C:98:ARG:HD3 | 2.45 | 0.51 |
| 1:B:91:MET:O | 1:B:93:GLY:N | 2.44 | 0.51 |
| 1:A:198:LEU:HD12 | 1:A:406:LEU:HG | 1.91 | 0.51 |
| 1:A:119:GLN:O | 1:A:120:ARG:HD2 | 2.11 | 0.51 |
| 2:C:163:ASN:ND2 | 2:C:167:LEU:HD23 | 2.26 | 0.51 |
| 2:E:38:ARG:HE | 2:E:46:LYS:NZ | 2.07 | 0.51 |
| 3:F:29:VAL:HG21 | 3:F:32:ILE:HD11 | 1.93 | 0.51 |
| 1:B:21:LEU:HD22 | 1:B:25:LEU:HG | 1.93 | 0.51 |
| 2:C:30:SER:C | 2:C:32:TYR:N | 2.64 | 0.51 |
| 1:A:59:TRP:CE3 | 1:A:60:LEU:HD23 | 2.44 | 0.51 |
| 1:A:64:ARG:HB3 | 1:A:64:ARG:NH1 | 2.25 | 0.51 |
| 1:A:28:ARG:CD | 1:B:207:GLN:HG2 | 2.28 | 0.51 |
| 1:A:220:ILE:HG12 | 1:B:430:LEU:CD2 | 2.36 | 0.51 |
| 2:E:24:ALA:HB1 | 2:E:27:PHE:CE1 | 2.44 | 0.51 |
| 2:C:156:GLU:OE2 | 2:C:176:ALA:HB3 | 2.11 | 0.51 |
| 1:A:128:LEU:HB2 | 1:A:129:PRO:CD | 2.41 | 0.51 |
| 3:D:7:SER:CB | 3:D:8:PRO:CD | 2.88 | 0.51 |
| 1:B:128:LEU:HB2 | 1:B:129:PRO:CD | 2.41 | 0.51 |
| 2:C:67:LYS:HE2 | 2:C:85:LYS:O | 2.10 | 0.51 |
| 1:A:18:ARG:NH1 | 1:B:457:GLU:CB | 2.71 | 0.51 |
| 1:A:357:PHE:CZ | 1:A:398:LEU:HD13 | 2.46 | 0.51 |
| 1:B:255:TYR:CD2 | 1:B:424:PRO:HB3 | 2.46 | 0.51 |
| 3:D:210:ARG:HH11 | 3:D:210:ARG:HG2 | 1.74 | 0.51 |
| 1:A:459:GLU:O | 1:A:459:GLU:HG2 | 2.10 | 0.50 |
| 1:A:191:ASN:O | 1:A:191:ASN:ND2 | 2.44 | 0.50 |
| 3:F:205:VAL:O | 3:F:206:LYS:HG2 | 2.11 | 0.50 |
| 1:A:123:ARG:HD2 | 1:A:125:TRP:CZ2 | 2.46 | 0.50 |
| 1:B:95:PHE:O | 1:B:97:VAL:N | 2.44 | 0.50 |
| 3:D:86:TYR:CE2 | 3:D:100:GLY:HA3 | 2.46 | 0.50 |
| 1:B:284:HIS:HA | 1:B:290:LYS:CB | 2.40 | 0.50 |
| 1:A:197:ILE:HG13 | 1:A:222:VAL:HG21 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:430:LEU:C | 1:A:432:ALA:N | 2.64 | 0.50 |
| 3:F:116:ILE:CD1 | 3:F:193:CYS:HB2 | 2.41 | 0.50 |
| 3:F:114:VAL:HG13 | 3:F:135:LEU:HD23 | 1.92 | 0.50 |
| 3:F:116:ILE:HD13 | 3:F:193:CYS:CB | 2.42 | 0.50 |
| 3:D:7:SER:HB2 | 3:D:22:THR:HB | 1.92 | 0.50 |
| 1:B:413:LEU:CD1 | 1:B:422:ILE:HD13 | 2.41 | 0.50 |
| 1:B:53:PHE:HE2 | 1:B:147:ARG:HB2 | 1.77 | 0.50 |
| 1:A:298:ILE:HG21 | 1:A:346:LEU:HG | 1.92 | 0.50 |
| 2:C:34:MET:HB3 | 2:C:79:LEU:HD22 | 1.93 | 0.50 |
| 1:B:358:ALA:N | 1:B:359:PRO:HD2 | 2.27 | 0.50 |
| 2:C:12:VAL:CG2 | 2:C:119:VAL:HG22 | 2.40 | 0.50 |
| 1:A:139:LEU:HD13 | 1:A:147:ARG:HB3 | 1.93 | 0.50 |
| 2:E:200:THR:O | 2:E:200:THR:HG22 | 2.11 | 0.50 |
| 1:B:65:MET:O | 1:B:67:ALA:N | 2.44 | 0.50 |
| 1:B:212:LEU:HD12 | 1:B:212:LEU:H | 1.77 | 0.50 |
| 1:B:197:ILE:HD13 | 1:B:219:PHE:CD1 | 2.46 | 0.50 |
| 3:D:110:ALA:C | 3:D:199:THR:HG21 | 2.33 | 0.50 |
| 1:A:255:TYR:HB3 | 1:A:428:THR:OG1 | 2.12 | 0.49 |
| 1:A:190:PHE:H | 1:A:190:PHE:HD1 | 1.59 | 0.49 |
| 1:A:320:ILE:HB | 1:A:321:PRO:HD3 | 1.94 | 0.49 |
| 1:A:361:LEU:HD23 | 1:A:394:MET:O | 2.13 | 0.49 |
| 1:A:123:ARG:HA | 1:A:125:TRP:CZ3 | 2.47 | 0.49 |
| 1:B:35:ILE:CG2 | 1:B:176:THR:HG21 | 2.42 | 0.49 |
| 1:A:138:THR:O | 1:A:143:MET:HG3 | 2.13 | 0.49 |
| 1:B:412:VAL:O | 1:B:416:THR:HG23 | 2.12 | 0.49 |
| 2:E:132:LEU:CD2 | 3:F:132:VAL:HG21 | 2.40 | 0.49 |
| 1:A:176:THR:HG22 | 1:A:177:LEU:N | 2.27 | 0.49 |
| 2:C:111:TRP:N | 2:C:111:TRP:CD1 | 2.80 | 0.49 |
| 1:A:33:LEU:C | 1:A:33:LEU:HD23 | 2.32 | 0.49 |
| 1:A:17:ARG:C | 1:A:19:ARG:H | 2.16 | 0.49 |
| 1:A:274:LEU:CA | 1:A:277:GLN:HE21 | 2.18 | 0.49 |
| 1:B:241:VAL:HG12 | 1:B:244:LEU:HD21 | 1.95 | 0.49 |
| 2:E:207:HIS:CE1 | 2:E:210:SER:H | 2.30 | 0.49 |
| 1:A:356:ILE:HG12 | 1:A:356:ILE:O | 2.13 | 0.49 |
| 3:D:194:GLU:CG | 3:D:205:VAL:HG12 | 2.29 | 0.49 |
| 2:E:30:SER:O | 2:E:32:TYR:N | 2.46 | 0.49 |
| 3:D:77:MET:SD | 3:D:103:LEU:HD21 | 2.52 | 0.49 |
| 2:E:108:PHE:CD1 | 3:F:88:GLN:NE2 | 2.79 | 0.49 |
| 2:E:79:LEU:HD23 | 2:E:96:CYS:HB2 | 1.94 | 0.49 |
| 3:D:107:ARG:NH2 | 3:D:108:ALA:O | 2.43 | 0.49 |
| 1:B:357:PHE:CZ | 1:B:398:LEU:HD13 | 2.47 | 0.49 |
| 1:B:148:GLN:HE22 | 1:B:189:ALA:HB1 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:223:ILE:O | 1:B:227:ILE:HD13 | 2.12 | 0.49 |
| 2:C:124:THR:CG2 | 2:C:125:THR:N | 2.74 | 0.49 |
| 3:D:19:VAL:HG12 | 3:D:74:ILE:HB | 1.94 | 0.49 |
| 1:B:144:VAL:HG11 | 1:B:344:THR:OG1 | 2.12 | 0.49 |
| 1:A:176:THR:O | 1:A:180:THR:HG23 | 2.11 | 0.49 |
| 2:C:196:TRP:O | 2:C:199:GLU:N | 2.45 | 0.49 |
| 1:A:284:HIS:HA | 1:A:290:LYS:CB | 2.43 | 0.49 |
| 2:E:72:ARG:HH11 | 2:E:72:ARG:HG3 | 1.78 | 0.49 |
| 1:B:403:ARG:HH22 | 1:B:437:GLN:CA | 2.26 | 0.49 |
| 1:B:318:ASN:N | 1:B:318:ASN:ND2 | 2.60 | 0.49 |
| 2:C:29:TYR:OH | 2:C:34:MET:HG3 | 2.13 | 0.49 |
| 2:E:178:LEU:HD12 | 2:E:182:LEU:O | 2.12 | 0.49 |
| 1:A:380:PRO:HD2 | 1:A:381:GLN:NE2 | 2.26 | 0.49 |
| 3:D:29:VAL:CG2 | 3:D:32:ILE:HD11 | 2.43 | 0.49 |
| 1:A:171:ASP:HB2 | 1:A:212:LEU:HD22 | 1.94 | 0.49 |
| 1:A:84:LEU:O | 1:A:88:VAL:HG23 | 2.12 | 0.49 |
| 1:B:148:GLN:HB3 | 1:B:190:PHE:HE1 | 1.77 | 0.49 |
| 1:A:241:VAL:HG12 | 1:A:244:LEU:HD21 | 1.95 | 0.49 |
| 2:C:126:PRO:HB3 | 2:C:210:SER:HG | 1.75 | 0.49 |
| 1:B:320:ILE:HD13 | 1:B:394:MET:HE2 | 1.94 | 0.49 |
| 1:A:294:MET:O | 1:A:298:ILE:HG13 | 2.13 | 0.49 |
| 2:C:24:ALA:HB1 | 2:C:27:PHE:CE1 | 2.46 | 0.49 |
| 1:B:59:TRP:CZ3 | 1:B:60:LEU:HD23 | 2.48 | 0.49 |
| 1:B:385:GLU:O | 1:B:386:ALA:C | 2.51 | 0.49 |
| 1:A:18:ARG:CZ | 1:B:456:GLN:HE21 | 2.25 | 0.48 |
| 1:B:220:ILE:O | 1:B:224:MET:HG2 | 2.12 | 0.48 |
| 1:A:337:PHE:CE1 | 1:A:363:LEU:HD12 | 2.48 | 0.48 |
| 1:A:402:ILE:HD12 | 1:A:445:TYR:CD1 | 2.48 | 0.48 |
| 2:C:72:ARG:HG2 | 2:C:72:ARG:O | 2.12 | 0.48 |
| 3:F:153:GLU:O | 3:F:154:ARG:HB2 | 2.12 | 0.48 |
| 1:B:100:TYR:O | 1:B:101:ALA:HB2 | 2.12 | 0.48 |
| 2:E:163:ASN:ND2 | 2:E:167:LEU:HD23 | 2.28 | 0.48 |
| 1:B:183:ALA:O | 1:B:184:ALA:C | 2.51 | 0.48 |
| 1:A:383:HIS:HD2 | 2:C:33:TRP:CE3 | 2.31 | 0.48 |
| 1:B:23:ARG:HH11 | 1:B:23:ARG:HG3 | 1.78 | 0.48 |
| 2:E:98:ARG:O | 2:E:109:ASP:HB3 | 2.13 | 0.48 |
| 3:F:8:PRO:O | 3:F:101:THR:HG23 | 2.13 | 0.48 |
| 3:F:189:ASN:ND2 | 3:F:211:ALA:H | 2.05 | 0.48 |
| 1:A:270:ASN:HA | 1:A:273:VAL:CG1 | 2.43 | 0.48 |
| 1:A:202:GLU:O | 1:A:202:GLU:HG2 | 2.13 | 0.48 |
| 1:A:109:ILE:HG21 | 1:A:445:TYR:CD2 | 2.48 | 0.48 |
| 2:C:107:TYR:HB3 | 3:D:33:HIS:NE2 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:D:153:GLU:O | 3:D:154:ARG:HB2 | 2.12 | 0.48 |
| 1:B:262:PHE:CZ | 1:B:367:LEU:HD23 | 2.48 | 0.48 |
| 3:D:178:LEU:HD12 | 3:D:179:THR:N | 2.29 | 0.48 |
| 1:B:78:LEU:HD13 | 1:B:307:PHE:CZ | 2.49 | 0.48 |
| 2:C:37:VAL:HG22 | 2:C:47:TRP:HA | 1.96 | 0.48 |
| 2:E:16:GLY:O | 2:E:86:VAL:HG13 | 2.14 | 0.48 |
| 1:B:33:LEU:HD23 | 1:B:33:LEU:C | 2.34 | 0.48 |
| 1:B:131:LYS:HE2 | 1:B:150:PRO:HA | 1.95 | 0.48 |
| 1:A:320:ILE:HG21 | 1:A:394:MET:HE3 | 1.95 | 0.48 |
| 3:F:79:ALA:O | 3:F:105:ILE:HD11 | 2.14 | 0.48 |
| 2:E:144:VAL:O | 2:E:144:VAL:HG13 | 2.14 | 0.48 |
| 1:B:305:LEU:C | 1:B:307:PHE:H | 2.16 | 0.48 |
| 1:A:414:GLU:OE1 | 1:B:419:TYR:CE1 | 2.67 | 0.48 |
| 1:B:250:ASN:ND2 | 2:E:105:TYR:CD1 | 2.80 | 0.48 |
| 1:A:128:LEU:CB | 1:A:129:PRO:CD | 2.91 | 0.48 |
| 2:E:69:ILE:O | 2:E:69:ILE:HG22 | 2.14 | 0.48 |
| 1:A:228:MET:O | 1:A:232:PHE:HD1 | 1.97 | 0.48 |
| 1:B:124:TRP:HA | 1:B:157:ASN:ND2 | 2.19 | 0.48 |
| 1:B:270:ASN:ND2 | 1:B:444:LEU:CD2 | 2.77 | 0.48 |
| 2:C:38:ARG:HE | 2:C:46:LYS:NZ | 2.12 | 0.48 |
| 1:B:402:ILE:HD12 | 1:B:445:TYR:CD1 | 2.49 | 0.48 |
| 2:E:30:SER:C | 2:E:32:TYR:N | 2.67 | 0.48 |
| 1:A:100:TYR:O | 1:A:101:ALA:HB2 | 2.14 | 0.48 |
| 1:B:74:ASN:HB3 | 1:B:77:LEU:HB3 | 1.96 | 0.48 |
| 2:E:106:TRP:HD1 | 2:E:106:TRP:H | 1.61 | 0.48 |
| 3:D:6:GLN:OE1 | 3:D:86:TYR:HA | 2.14 | 0.47 |
| 1:A:35:ILE:HG23 | 1:A:176:THR:HG21 | 1.96 | 0.47 |
| 2:C:49:GLY:HA3 | 2:C:70:ILE:HD12 | 1.96 | 0.47 |
| 2:C:196:TRP:HB3 | 2:C:197:PRO:HD3 | 1.95 | 0.47 |
| 1:A:91:MET:C | 1:A:93:GLY:N | 2.67 | 0.47 |
| 1:B:84:LEU:O | 1:B:88:VAL:HG23 | 2.13 | 0.47 |
| 1:B:312:THR:HG22 | 1:B:339:ALA:HB3 | 1.96 | 0.47 |
| 1:B:402:ILE:HD12 | 1:B:445:TYR:CE1 | 2.49 | 0.47 |
| 1:A:279:LEU:HA | 1:A:282:ARG:NH1 | 2.22 | 0.47 |
| 1:A:308:VAL:O | 1:A:309:ALA:HB2 | 2.14 | 0.47 |
| 1:B:23:ARG:NH1 | 1:B:23:ARG:HG3 | 2.29 | 0.47 |
| 1:B:441:GLY:O | 1:B:442:LYS:HG3 | 2.14 | 0.47 |
| 1:B:99:LYS:HG3 | 1:B:99:LYS:O | 2.13 | 0.47 |
| 3:F:164:ASP:O | 3:F:165:GLN:C | 2.52 | 0.47 |
| 1:A:127:VAL:HB | 1:A:157:ASN:ND2 | 2.29 | 0.47 |
| 1:B:25:LEU:C | 1:B:27:GLU:H | 2.18 | 0.47 |
| 2:C:6:GLU:CD | 2:C:114:GLY:HA2 | 2.35 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:128:LEU:CB | 1:B:129:PRO:CD | 2.92 | 0.47 |
| 1:A:293:LEU:C | 1:A:295:GLY:N | 2.67 | 0.47 |
| 2:E:5:LEU:HD13 | 2:E:5:LEU:C | 2.34 | 0.47 |
| 2:C:22:CYS:O | 2:C:78:THR:HG23 | 2.13 | 0.47 |
| 1:B:294:MET:O | 1:B:298:ILE:HG13 | 2.15 | 0.47 |
| 2:E:87:ARG:HG3 | 2:E:89:GLU:OE2 | 2.15 | 0.47 |
| 1:B:241:VAL:O | 1:B:241:VAL:HG12 | 2.13 | 0.47 |
| 1:B:38:MET:HG3 | 1:B:168:LEU:HD21 | 1.95 | 0.47 |
| 2:E:185:LEU:C | 2:E:185:LEU:HD12 | 2.35 | 0.47 |
| 2:C:63:SER:HG | 2:C:68:PHE:HE1 | 1.61 | 0.47 |
| 1:A:370:ALA:O | 1:A:374:VAL:HG23 | 2.15 | 0.47 |
| 2:C:126:PRO:CB | 2:C:210:SER:OG | 2.59 | 0.47 |
| 2:E:18:LEU:CD2 | 2:E:18:LEU:N | 2.78 | 0.47 |
| 2:C:221:ARG:CZ | 3:D:118:PRO:HG2 | 2.44 | 0.47 |
| 1:A:241:VAL:HG12 | 1:A:241:VAL:O | 2.14 | 0.47 |
| 1:A:200:ILE:HA | 1:A:204:MET:HB2 | 1.95 | 0.47 |
| 1:B:138:THR:HG21 | 1:B:352:ALA:HB1 | 1.96 | 0.47 |
| 1:B:385:GLU:O | 1:B:387:GLY:N | 2.48 | 0.47 |
| 1:A:422:ILE:HG23 | 1:A:423:LEU:N | 2.29 | 0.47 |
| 1:A:150:PRO:CG | 1:A:354:GLY:HA2 | 2.45 | 0.47 |
| 3:F:34:TRP:CE2 | 3:F:72:LEU:HB2 | 2.50 | 0.47 |
| 1:A:122:VAL:HG21 | 1:A:178:LEU:HD11 | 1.96 | 0.47 |
| 2:E:36:TRP:CE2 | 2:E:81:LEU:HB2 | 2.50 | 0.47 |
| 1:A:160:ARG:HD3 | 1:A:163:LEU:HD23 | 1.97 | 0.47 |
| 3:F:3:VAL:HB | 3:F:26:SER:HB3 | 1.97 | 0.47 |
| 2:C:12:VAL:O | 2:C:119:VAL:HA | 2.14 | 0.47 |
| 3:F:73:THR:HG22 | 3:F:74:ILE:N | 2.29 | 0.47 |
| 1:A:284:HIS:C | 1:A:286:GLY:H | 2.19 | 0.46 |
| 1:A:109:ILE:HG21 | 1:A:445:TYR:HD2 | 1.80 | 0.46 |
| 1:A:451:ARG:O | 1:A:455:LYS:HB2 | 2.16 | 0.46 |
| 3:D:106:LEU:HD23 | 3:D:107:ARG:N | 2.30 | 0.46 |
| 3:F:36:GLN:HG3 | 3:F:85:TYR:CE2 | 2.50 | 0.46 |
| 2:C:103:TYR:HD2 | 3:D:31:TYR:CE2 | 2.33 | 0.46 |
| 1:A:150:PRO:HG2 | 1:A:354:GLY:HA2 | 1.97 | 0.46 |
| 1:A:144:VAL:O | 1:A:145:LEU:HD23 | 2.15 | 0.46 |
| 1:A:22:ILE:HD13 | 1:B:454:ALA:CB | 2.44 | 0.46 |
| 1:B:318:ASN:ND2 | 1:B:319:LEU:N | 2.64 | 0.46 |
| 1:A:28:ARG:NH2 | 1:B:443:PRO:HB3 | 2.31 | 0.46 |
| 3:F:88:GLN:HB2 | 3:F:97:PHE:HD1 | 1.78 | 0.46 |
| 1:B:94:TYR:CZ | 1:B:352:ALA:HB2 | 2.50 | 0.46 |
| 1:A:293:LEU:C | 1:A:295:GLY:H | 2.18 | 0.46 |
| 2:C:144:VAL:HG13 | 2:C:144:VAL:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:198:LEU:HG | 1:B:410:ILE:CD1 | 2.38 | 0.46 |
| 3:F:49:ASP:O | 3:F:50:THR:HB | 2.16 | 0.46 |
| 1:A:109:ILE:HG12 | 1:A:152:VAL:HG11 | 1.97 | 0.46 |
| 1:A:437:GLN:C | 1:A:439:THR:H | 2.18 | 0.46 |
| 1:A:270:ASN:ND2 | 1:A:444:LEU:HG | 2.31 | 0.46 |
| 1:B:331:GLY:O | 1:B:333:LEU:N | 2.48 | 0.46 |
| 1:B:91:MET:C | 1:B:93:GLY:N | 2.66 | 0.46 |
| 2:C:4:LEU:HD12 | 2:C:4:LEU:HA | 1.72 | 0.46 |
| 3:F:7:SER:CB | 3:F:8:PRO:CD | 2.85 | 0.46 |
| 1:A:272:TRP:O | 1:A:276:MET:HB2 | 2.15 | 0.46 |
| 3:D:73:THR:HG22 | 3:D:74:ILE:N | 2.30 | 0.46 |
| 1:A:444:LEU:HD13 | 1:A:444:LEU:O | 2.16 | 0.46 |
| 1:A:248:PRO:HG2 | 1:A:251:THR:CG2 | 2.46 | 0.46 |
| 1:A:25:LEU:C | 1:A:27:GLU:H | 2.19 | 0.46 |
| 3:F:116:ILE:HD12 | 3:F:133:CYS:HB2 | 1.98 | 0.46 |
| 2:C:38:ARG:HH21 | 2:C:46:LYS:HZ2 | 1.63 | 0.46 |
| 3:D:46:TRP:HA | 3:D:46:TRP:CE3 | 2.51 | 0.46 |
| 1:B:452:THR:O | 1:B:452:THR:HG22 | 2.15 | 0.46 |
| 1:B:282:ARG:O | 1:B:285:GLY:N | 2.49 | 0.46 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:CG | 2.25 | 0.46 |
| 2:E:72:ARG:O | 2:E:72:ARG:HG2 | 2.16 | 0.46 |
| 1:B:138:THR:HG22 | 1:B:143:MET:SD | 2.54 | 0.46 |
| 2:C:210:SER:O | 2:C:212:THR:HG23 | 2.15 | 0.46 |
| 2:C:189:VAL:O | 2:C:189:VAL:CG1 | 2.59 | 0.46 |
| 1:B:35:ILE:HG23 | 1:B:176:THR:HG21 | 1.97 | 0.46 |
| 1:B:440:GLY:O | 1:B:441:GLY:O | 2.34 | 0.46 |
| 2:E:162:TRP:CZ3 | 2:E:203:CYS:HB3 | 2.51 | 0.46 |
| 1:A:358:ALA:N | 1:A:359:PRO:HD2 | 2.30 | 0.46 |
| 3:F:29:VAL:HG23 | 3:F:70:TYR:CE1 | 2.50 | 0.46 |
| 2:E:48:ILE:HG22 | 2:E:49:GLY:N | 2.31 | 0.46 |
| 1:B:99:LYS:C | 1:B:100:TYR:CD1 | 2.90 | 0.46 |
| 2:E:66:ASP:O | 2:E:67:LYS:C | 2.54 | 0.46 |
| 1:A:358:ALA:HB3 | 1:A:359:PRO:CD | 2.46 | 0.46 |
| 3:F:82:ALA:HB2 | 3:F:105:ILE:CG1 | 2.45 | 0.46 |
| 1:B:139:LEU:HD13 | 1:B:147:ARG:HB3 | 1.97 | 0.46 |
| 1:A:294:MET:HG2 | 1:A:294:MET:O | 2.16 | 0.46 |
| 3:D:105:ILE:HD12 | 3:D:170:SER:OG | 2.16 | 0.46 |
| 1:A:136:LEU:HD12 | 1:A:136:LEU:N | 2.31 | 0.46 |
| 1:A:203:GLU:CD | 1:B:28:ARG:HH22 | 2.20 | 0.45 |
| 1:B:305:LEU:HA | 1:B:308:VAL:CG2 | 2.37 | 0.45 |
| 3:F:79:ALA:CA | 3:F:105:ILE:HD13 | 2.46 | 0.45 |
| 3:F:64:SER:OG | 3:F:65:GLY:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:94:TYR:HE2 | 1:B:350:SER:O | 1.99 | 0.45 |
| 1:B:312:THR:HG22 | 1:B:339:ALA:CB | 2.46 | 0.45 |
| 2:E:4:LEU:HD12 | 2:E:4:LEU:HA | 1.73 | 0.45 |
| 1:B:109:ILE:HB | 1:B:445:TYR:CE2 | 2.51 | 0.45 |
| 1:A:359:PRO:O | 1:A:363:LEU:HD23 | 2.17 | 0.45 |
| 3:D:29:VAL:HG23 | 3:D:70:TYR:CE1 | 2.50 | 0.45 |
| 2:C:196:TRP:HD1 | 2:C:201:VAL:HG23 | 1.81 | 0.45 |
| 1:A:97:VAL:HG12 | 1:A:98:ARG:N | 2.31 | 0.45 |
| 1:A:430:LEU:HD21 | 1:B:220:ILE:CG1 | 2.38 | 0.45 |
| 3:F:19:VAL:HG12 | 3:F:74:ILE:HB | 1.99 | 0.45 |
| 1:A:74:ASN:HB3 | 1:A:77:LEU:HB3 | 1.97 | 0.45 |
| 2:C:45:LEU:H | 2:C:45:LEU:CD1 | 2.07 | 0.45 |
| 3:D:22:THR:CG2 | 3:D:23:CYS:N | 2.77 | 0.45 |
| 1:A:192:ALA:HB1 | 1:A:414:GLU:CG | 2.46 | 0.45 |
| 3:F:90:TRP:CZ2 | 3:F:95:GLN:NE2 | 2.84 | 0.45 |
| 1:A:270:ASN:HA | 1:A:273:VAL:HG12 | 1.97 | 0.45 |
| 2:C:196:TRP:CG | 2:C:197:PRO:N | 2.84 | 0.45 |
| 2:E:196:TRP:CG | 2:E:197:PRO:N | 2.85 | 0.45 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:CG | 2.30 | 0.45 |
| 3:D:65:GLY:CA | 3:D:70:TYR:HA | 2.44 | 0.45 |
| 1:A:200:ILE:HG22 | 1:A:201:ILE:H | 1.80 | 0.45 |
| 1:A:318:ASN:HD22 | 1:A:319:LEU:N | 2.13 | 0.45 |
| 1:A:385:GLU:O | 1:A:386:ALA:C | 2.55 | 0.45 |
| 2:C:109:ASP:CG | 2:C:110:VAL:HG23 | 2.37 | 0.45 |
| 1:B:136:LEU:N | 1:B:136:LEU:HD12 | 2.31 | 0.45 |
| 3:F:22:THR:CG2 | 3:F:23:CYS:N | 2.78 | 0.45 |
| 1:A:413:LEU:CD1 | 1:A:422:ILE:HD13 | 2.46 | 0.45 |
| 2:E:207:HIS:ND1 | 2:E:210:SER:CB | 2.79 | 0.45 |
| 1:B:270:ASN:ND2 | 1:B:444:LEU:CG | 2.79 | 0.45 |
| 1:A:94:TYR:CZ | 1:A:352:ALA:HB2 | 2.51 | 0.45 |
| 2:E:64:LEU:O | 2:E:65:LYS:C | 2.55 | 0.45 |
| 2:C:64:LEU:HD23 | 2:C:64:LEU:N | 2.32 | 0.45 |
| 1:B:402:ILE:HG12 | 1:B:402:ILE:O | 2.16 | 0.45 |
| 2:E:45:LEU:HD11 | 3:F:86:TYR:CE1 | 2.51 | 0.45 |
| 1:B:116:LEU:HD23 | 1:B:178:LEU:HD23 | 1.99 | 0.45 |
| 1:A:423:LEU:HB3 | 1:A:424:PRO:CD | 2.44 | 0.45 |
| 1:A:123:ARG:HD2 | 1:A:125:TRP:HZ2 | 1.82 | 0.45 |
| 1:B:123:ARG:HD2 | 1:B:125:TRP:CZ2 | 2.52 | 0.45 |
| 2:C:2:VAL:HG13 | 2:C:2:VAL:O | 2.16 | 0.45 |
| 1:B:270:ASN:ND2 | 1:B:444:LEU:HG | 2.31 | 0.45 |
| 1:A:298:ILE:HG23 | 1:A:346:LEU:HG | 1.98 | 0.45 |
| 1:A:116:LEU:HD23 | 1:A:178:LEU:HD23 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:90:ALA:CB | 1:B:299:GLY:HA3 | 2.46 | 0.45 |
| 1:B:298:ILE:HG21 | 1:B:346:LEU:HG | 1.98 | 0.45 |
| 1:B:183:ALA:C | 1:B:185:GLY:N | 2.68 | 0.45 |
| 3:D:201:THR:CG2 | 3:D:202:SER:N | 2.79 | 0.45 |
| 2:E:149:LEU:HD12 | 2:E:150:VAL:N | 2.32 | 0.45 |
| 1:B:359:PRO:O | 1:B:363:LEU:HD23 | 2.17 | 0.45 |
| 1:B:343:THR:O | 1:B:347:CYS:HB2 | 2.17 | 0.45 |
| 1:A:399:ALA:O | 1:A:403:ARG:HA | 2.17 | 0.45 |
| 1:A:420:GLN:HG3 | 1:A:420:GLN:H | 1.49 | 0.45 |
| 2:C:146:LEU:HD13 | 2:C:218:ILE:HG21 | 1.98 | 0.45 |
| 3:F:48:TYR:CE1 | 3:F:52:LYS:HD2 | 2.52 | 0.45 |
| 3:F:149:ILE:HG12 | 3:F:191:TYR:CE2 | 2.52 | 0.45 |
| 2:E:131:PRO:HB3 | 2:E:216:LYS:HG3 | 1.99 | 0.45 |
| 3:D:32:ILE:HG12 | 3:D:70:TYR:CE2 | 2.52 | 0.44 |
| 1:B:421:LEU:O | 1:B:424:PRO:CD | 2.59 | 0.44 |
| 1:B:37:PHE:O | 1:B:37:PHE:CD2 | 2.71 | 0.44 |
| 1:A:270:ASN:ND2 | 1:A:444:LEU:CD2 | 2.79 | 0.44 |
| 1:B:135:GLY:O | 1:B:136:LEU:C | 2.54 | 0.44 |
| 1:A:208:PHE:O | 1:A:209:ARG:HB3 | 2.17 | 0.44 |
| 1:A:167:ARG:HG2 | 1:A:167:ARG:HH11 | 1.82 | 0.44 |
| 2:C:99:LEU:HD21 | 2:C:108:PHE:CD2 | 2.52 | 0.44 |
| 1:A:219:PHE:HB3 | 1:B:430:LEU:HD13 | 1.99 | 0.44 |
| 1:A:357:PHE:HE1 | 1:A:398:LEU:HD22 | 1.78 | 0.44 |
| 1:B:182:ALA:HB3 | 1:B:200:ILE:HD11 | 1.98 | 0.44 |
| 1:B:437:GLN:C | 1:B:439:THR:H | 2.21 | 0.44 |
| 2:C:156:GLU:OE1 | 2:C:157:PRO:HA | 2.17 | 0.44 |
| 2:E:162:TRP:CZ3 | 2:E:203:CYS:CB | 3.00 | 0.44 |
| 1:A:210:TYR:CE1 | 1:B:208:PHE:HA | 2.52 | 0.44 |
| 3:F:189:ASN:ND2 | 3:F:210:ARG:N | 2.65 | 0.44 |
| 3:F:58:PRO:C | 3:F:60:ARG:N | 2.70 | 0.44 |
| 1:B:63:GLN:C | 1:B:65:MET:N | 2.71 | 0.44 |
| 1:A:21:LEU:HD22 | 1:A:25:LEU:HG | 1.99 | 0.44 |
| 1:B:272:TRP:CD1 | 1:B:272:TRP:N | 2.83 | 0.44 |
| 2:E:178:LEU:HD12 | 2:E:179:GLN:H | 1.82 | 0.44 |
| 2:E:167:LEU:HD21 | 2:E:191:VAL:HG11 | 1.97 | 0.44 |
| 2:E:69:ILE:HB | 2:E:82:GLN:HB2 | 1.99 | 0.44 |
| 3:F:187:ARG:HG3 | 3:F:187:ARG:O | 2.17 | 0.44 |
| 1:B:411:LEU:O | 1:B:415:MET:HG2 | 2.17 | 0.44 |
| 3:F:33:HIS:CE1 | 3:F:49:ASP:H | 2.35 | 0.44 |
| 1:B:218:VAL:O | 1:B:221:GLY:N | 2.50 | 0.44 |
| 1:A:160:ARG:CD | 1:A:163:LEU:HD23 | 2.47 | 0.44 |
| 1:A:442:LYS:O | 1:A:444:LEU:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:163:LEU:CD2 | 1:B:174:ARG:HA | 2.47 | 0.44 |
| 3:F:86:TYR:HE2 | 3:F:100:GLY:HA3 | 1.83 | 0.44 |
| 1:A:437:GLN:O | 1:A:439:THR:N | 2.51 | 0.44 |
| 2:C:29:TYR:CZ | 2:C:34:MET:HG3 | 2.52 | 0.44 |
| 2:C:60:TYR:CD1 | 2:C:60:TYR:N | 2.85 | 0.44 |
| 1:B:383:HIS:HD2 | 2:E:33:TRP:CE3 | 2.36 | 0.44 |
| 1:A:37:PHE:HD2 | 1:A:38:MET:CE | 2.28 | 0.44 |
| 3:F:119:PRO:CD | 3:F:131:VAL:HG22 | 2.48 | 0.44 |
| 1:A:91:MET:HG3 | 1:A:296:GLY:HA3 | 1.99 | 0.44 |
| 1:A:382:TYR:HB3 | 1:A:384:LEU:HD21 | 1.99 | 0.44 |
| 3:F:35:TYR:N | 3:F:35:TYR:CD1 | 2.85 | 0.44 |
| 3:D:7:SER:CB | 3:D:22:THR:HB | 2.47 | 0.44 |
| 1:A:150:PRO:HD3 | 1:A:355:GLY:N | 2.33 | 0.44 |
| 1:A:109:ILE:HB | 1:A:445:TYR:CE2 | 2.53 | 0.44 |
| 1:B:369:THR:HG22 | 1:B:373:MET:HE3 | 2.00 | 0.44 |
| 3:D:53:LEU:HB3 | 3:D:57:VAL:HB | 1.99 | 0.44 |
| 1:B:148:GLN:O | 1:B:149:GLY:C | 2.56 | 0.44 |
| 1:A:270:ASN:ND2 | 1:A:444:LEU:CG | 2.81 | 0.44 |
| 1:B:248:PRO:HG2 | 1:B:251:THR:HG23 | 2.00 | 0.44 |
| 1:B:437:GLN:C | 1:B:439:THR:N | 2.71 | 0.44 |
| 2:E:61:THR:HB | 2:E:62:PRO:HD2 | 1.99 | 0.44 |
| 2:C:121:SER:O | 2:C:122:ALA:C | 2.56 | 0.44 |
| 2:C:67:LYS:HA | 2:C:67:LYS:HD3 | 1.77 | 0.44 |
| 3:D:162:TRP:CD1 | 3:D:174:MET:HB2 | 2.53 | 0.44 |
| 3:D:6:GLN:HG3 | 3:D:100:GLY:H | 1.82 | 0.43 |
| 1:A:280:LEU:O | 1:A:284:HIS:CE1 | 2.71 | 0.43 |
| 1:A:307:PHE:O | 1:A:307:PHE:CG | 2.71 | 0.43 |
| 2:C:40:ALA:HB3 | 2:C:43:LYS:HB2 | 2.00 | 0.43 |
| 1:A:211:THR:HG22 | 1:A:212:LEU:N | 2.33 | 0.43 |
| 1:B:64:ARG:HH11 | 1:B:64:ARG:HB3 | 1.82 | 0.43 |
| 1:A:69:VAL:CG1 | 1:A:70:HIS:N | 2.81 | 0.43 |
| 1:A:155:GLY:HA3 | 1:A:181:GLY:O | 2.17 | 0.43 |
| 1:B:224:MET:O | 1:B:228:MET:HG2 | 2.18 | 0.43 |
| 2:C:210:SER:OG | 2:C:212:THR:HG23 | 2.17 | 0.43 |
| 3:F:60:ARG:NH1 | 3:F:81:ASP:OD1 | 2.51 | 0.43 |
| 2:E:38:ARG:HE | 2:E:46:LYS:HZ1 | 1.64 | 0.43 |
| 1:B:109:ILE:HG21 | 1:B:445:TYR:CD2 | 2.53 | 0.43 |
| 1:B:215:ILE:HG22 | 1:B:216:LYS:N | 2.32 | 0.43 |
| 1:A:454:ALA:O | 1:A:458:ALA:HB3 | 2.18 | 0.43 |
| 1:A:138:THR:HG21 | 1:A:352:ALA:HB1 | 2.00 | 0.43 |
| 2:E:67:LYS:HA | 2:E:67:LYS:HD3 | 1.65 | 0.43 |
| 2:C:162:TRP:C | 2:C:164:SER:N | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:446:SER:O | 1:B:449:LEU:N | 2.51 | 0.43 |
| 1:B:148:GLN:HG2 | 1:B:358:ALA:HB2 | 1.99 | 0.43 |
| 1:A:398:LEU:O | 1:A:402:ILE:HG23 | 2.18 | 0.43 |
| 2:C:185:LEU:CD1 | 2:C:185:LEU:C | 2.87 | 0.43 |
| 1:A:128:LEU:HB2 | 1:A:129:PRO:HD2 | 2.00 | 0.43 |
| 1:A:136:LEU:HD12 | 1:A:136:LEU:H | 1.82 | 0.43 |
| 1:B:337:PHE:CE1 | 1:B:363:LEU:HD12 | 2.54 | 0.43 |
| 1:A:266:GLY:HA3 | 1:A:400:ALA:CB | 2.47 | 0.43 |
| 1:A:250:ASN:ND2 | 2:C:105:TYR:CD1 | 2.82 | 0.43 |
| 1:B:136:LEU:H | 1:B:136:LEU:CD1 | 2.31 | 0.43 |
| 1:B:116:LEU:CD2 | 1:B:178:LEU:HD23 | 2.48 | 0.43 |
| 1:A:372:GLY:O | 1:A:376:VAL:HG23 | 2.18 | 0.43 |
| 1:B:187:ALA:C | 1:B:189:ALA:N | 2.72 | 0.43 |
| 1:A:279:LEU:O | 1:A:279:LEU:HD23 | 2.18 | 0.43 |
| 1:B:126:ARG:O | 1:B:130:VAL:HG23 | 2.19 | 0.43 |
| 1:A:148:GLN:HB3 | 1:A:190:PHE:CE1 | 2.51 | 0.43 |
| 1:A:182:ALA:HB1 | 1:A:204:MET:HE2 | 2.00 | 0.43 |
| 1:A:90:ALA:CB | 1:A:299:GLY:HA3 | 2.49 | 0.43 |
| 1:A:136:LEU:O | 1:A:140:GLY:N | 2.51 | 0.43 |
| 1:A:28:ARG:HH22 | 1:B:203:GLU:CD | 2.22 | 0.43 |
| 1:B:457:GLU:O | 1:B:458:ALA:CB | 2.66 | 0.43 |
| 1:A:305:LEU:C | 1:A:307:PHE:H | 2.22 | 0.43 |
| 3:F:82:ALA:CB | 3:F:105:ILE:HD11 | 2.41 | 0.43 |
| 1:B:21:LEU:CD2 | 1:B:25:LEU:HG | 2.49 | 0.43 |
| 1:A:99:LYS:C | 1:A:100:TYR:CD1 | 2.91 | 0.43 |
| 1:B:298:ILE:HG23 | 1:B:346:LEU:HG | 1.99 | 0.43 |
| 2:C:167:LEU:HD21 | 2:C:191:VAL:HG11 | 2.00 | 0.43 |
| 2:E:4:LEU:HB3 | 2:E:112:GLY:CA | 2.48 | 0.43 |
| 1:A:380:PRO:CD | 1:A:381:GLN:HE22 | 2.30 | 0.43 |
| 1:B:223:ILE:HG22 | 1:B:227:ILE:HD13 | 2.01 | 0.43 |
| 3:F:79:ALA:O | 3:F:105:ILE:CD1 | 2.66 | 0.43 |
| 2:E:125:THR:HA | 2:E:126:PRO:HD2 | 1.94 | 0.43 |
| 1:B:250:ASN:HD22 | 2:E:105:TYR:HE1 | 1.62 | 0.43 |
| 1:B:264:ILE:HG13 | 1:B:265:PHE:N | 2.33 | 0.43 |
| 2:C:16:GLY:O | 2:C:86:VAL:HG13 | 2.18 | 0.43 |
| 1:A:367:LEU:O | 1:A:367:LEU:HD12 | 2.19 | 0.43 |
| 1:B:284:HIS:C | 1:B:286:GLY:H | 2.21 | 0.43 |
| 1:B:308:VAL:O | 1:B:309:ALA:HB2 | 2.19 | 0.43 |
| 1:B:78:LEU:HD13 | 1:B:307:PHE:CE2 | 2.54 | 0.43 |
| 1:B:92:PHE:C | 1:B:92:PHE:CD1 | 2.93 | 0.43 |
| 2:E:178:LEU:HB2 | 2:E:183:TYR:CE2 | 2.54 | 0.43 |
| 1:A:210:TYR:HB2 | 1:B:210:TYR:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:208:PHE:O | 1:B:209:ARG:HB3 | 2.19 | 0.42 |
| 1:A:210:TYR:N | 1:B:210:TYR:HB2 | 2.34 | 0.42 |
| 1:A:430:LEU:O | 1:A:432:ALA:N | 2.52 | 0.42 |
| 1:B:307:PHE:CG | 1:B:307:PHE:O | 2.71 | 0.42 |
| 1:B:394:MET:O | 1:B:394:MET:HG2 | 2.19 | 0.42 |
| 2:E:29:TYR:OH | 2:E:34:MET:HG3 | 2.18 | 0.42 |
| 1:B:293:LEU:C | 1:B:295:GLY:H | 2.22 | 0.42 |
| 2:E:51:ILE:CD1 | 2:E:72:ARG:HD2 | 2.49 | 0.42 |
| 1:A:295:GLY:C | 1:A:297:ALA:N | 2.73 | 0.42 |
| 2:C:131:PRO:HB3 | 2:C:216:LYS:HG3 | 2.01 | 0.42 |
| 1:A:256:LEU:HD12 | 1:A:256:LEU:HA | 1.86 | 0.42 |
| 1:A:78:LEU:HD13 | 1:A:307:PHE:CZ | 2.55 | 0.42 |
| 2:C:107:TYR:CD1 | 2:C:107:TYR:C | 2.93 | 0.42 |
| 1:B:320:ILE:HD13 | 1:B:394:MET:CE | 2.49 | 0.42 |
| 1:B:444:LEU:HD13 | 1:B:444:LEU:O | 2.20 | 0.42 |
| 1:B:89:LEU:HA | 1:B:89:LEU:HD23 | 1.92 | 0.42 |
| 1:A:282:ARG:O | 1:A:285:GLY:N | 2.52 | 0.42 |
| 2:E:27:PHE:HE2 | 2:E:98:ARG:HG3 | 1.85 | 0.42 |
| 3:F:84:THR:OG1 | 3:F:102:LYS:HG3 | 2.19 | 0.42 |
| 1:A:17:ARG:C | 1:A:19:ARG:N | 2.73 | 0.42 |
| 1:A:190:PHE:HE2 | 1:A:361:LEU:HD11 | 1.84 | 0.42 |
| 3:D:118:PRO:HB3 | 3:D:208:PHE:CE1 | 2.55 | 0.42 |
| 1:A:234:HIS:NE2 | 3:F:52:LYS:NZ | 2.67 | 0.42 |
| 2:E:33:TRP:CE2 | 2:E:52:ASN:HB2 | 2.55 | 0.42 |
| 3:D:112:PRO:HB3 | 3:D:138:PHE:HB3 | 2.01 | 0.42 |
| 1:A:317:PHE:HA | 1:A:317:PHE:HD2 | 1.71 | 0.42 |
| 1:B:207:GLN:HB3 | 1:B:208:PHE:CE1 | 2.54 | 0.42 |
| 2:E:126:PRO:CB | 2:E:210:SER:OG | 2.62 | 0.42 |
| 1:A:171:ASP:CB | 1:A:212:LEU:HD22 | 2.49 | 0.42 |
| 1:B:276:MET:O | 1:B:280:LEU:HB2 | 2.20 | 0.42 |
| 1:B:128:LEU:HB2 | 1:B:129:PRO:HD2 | 2.02 | 0.42 |
| 1:B:155:GLY:O | 1:B:158:ILE:N | 2.50 | 0.42 |
| 1:A:434:LEU:HA | 1:A:434:LEU:HD22 | 1.92 | 0.42 |
| 3:F:90:TRP:CH2 | 3:F:95:GLN:NE2 | 2.88 | 0.42 |
| 2:E:38:ARG:HH21 | 2:E:46:LYS:HZ2 | 1.66 | 0.42 |
| 3:F:162:TRP:CD2 | 3:F:174:MET:HG3 | 2.54 | 0.42 |
| 1:A:95:PHE:O | 1:A:97:VAL:N | 2.53 | 0.42 |
| 1:A:422:ILE:CG2 | 1:A:423:LEU:N | 2.83 | 0.42 |
| 1:A:395:GLY:O | 1:A:398:LEU:HB2 | 2.20 | 0.42 |
| 1:A:437:GLN:C | 1:A:439:THR:N | 2.73 | 0.42 |
| 2:E:64:LEU:HD23 | 2:E:64:LEU:N | 2.34 | 0.42 |
| 1:A:159:GLY:O | 1:A:162:VAL:HG22 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:D:116:ILE:HD12 | 3:D:193:CYS:HB2 | 2.02 | 0.42 |
| 3:D:89:GLN:C | 3:D:89:GLN:CD | 2.78 | 0.42 |
| 3:F:192:THR:CB | 3:F:207:SER:HB3 | 2.48 | 0.42 |
| 1:B:228:MET:O | 1:B:232:PHE:HD1 | 2.03 | 0.42 |
| 3:F:82:ALA:O | 3:F:83:ALA:HB2 | 2.19 | 0.42 |
| 1:A:116:LEU:HD23 | 1:A:178:LEU:CD2 | 2.50 | 0.42 |
| 3:F:114:VAL:CG1 | 3:F:115:SER:N | 2.83 | 0.42 |
| 1:A:191:ASN:HB2 | 1:A:229:TYR:CE2 | 2.55 | 0.42 |
| 1:A:380:PRO:CD | 1:A:381:GLN:NE2 | 2.83 | 0.42 |
| 1:B:190:PHE:HE2 | 1:B:361:LEU:HD11 | 1.85 | 0.42 |
| 1:A:276:MET:O | 1:A:280:LEU:HB2 | 2.20 | 0.42 |
| 1:A:190:PHE:CD1 | 1:A:190:PHE:N | 2.87 | 0.42 |
| 1:A:190:PHE:HD2 | 1:A:415:MET:SD | 2.42 | 0.42 |
| 1:A:270:ASN:HD22 | 1:A:270:ASN:HA | 1.58 | 0.42 |
| 3:F:117:PHE:HA | 3:F:118:PRO:HD3 | 1.79 | 0.42 |
| 1:B:95:PHE:O | 1:B:96:LEU:C | 2.58 | 0.42 |
| 2:E:179:GLN:O | 2:E:180:ALA:HB3 | 2.20 | 0.42 |
| 1:A:91:MET:O | 1:A:93:GLY:N | 2.53 | 0.42 |
| 2:E:76:LYS:O | 2:E:77:ASP:C | 2.58 | 0.42 |
| 1:B:69:VAL:CG1 | 1:B:70:HIS:N | 2.83 | 0.42 |
| 1:B:80:THR:O | 1:B:83:PHE:HB3 | 2.20 | 0.42 |
| 1:B:98:ARG:HH11 | 1:B:98:ARG:CB | 2.15 | 0.41 |
| 1:B:172:GLU:HG2 | 1:B:212:LEU:O | 2.20 | 0.41 |
| 2:C:181:ALA:O | 2:C:182:LEU:HD23 | 2.20 | 0.41 |
| 1:A:215:ILE:HG22 | 1:A:216:LYS:N | 2.35 | 0.41 |
| 2:E:99:LEU:HD21 | 2:E:108:PHE:CD2 | 2.55 | 0.41 |
| 2:C:176:ALA:HA | 2:C:185:LEU:HB3 | 2.02 | 0.41 |
| 3:D:35:TYR:HE1 | 3:D:88:GLN:HB3 | 1.86 | 0.41 |
| 2:C:29:TYR:CD2 | 2:C:77:ASP:HA | 2.56 | 0.41 |
| 2:E:131:PRO:HD3 | 2:E:216:LYS:HG2 | 2.01 | 0.41 |
| 1:B:258:LEU:O | 1:B:258:LEU:HG | 2.20 | 0.41 |
| 3:F:6:GLN:HE21 | 3:F:6:GLN:HB3 | 1.64 | 0.41 |
| 1:B:283:VAL:HG12 | 1:B:283:VAL:O | 2.19 | 0.41 |
| 1:A:427:ILE:HG22 | 1:A:427:ILE:O | 2.20 | 0.41 |
| 1:A:337:PHE:HE1 | 1:A:363:LEU:HD12 | 1.84 | 0.41 |
| 2:E:107:TYR:CB | 3:F:33:HIS:CD2 | 2.95 | 0.41 |
| 2:E:32:TYR:O | 2:E:72:ARG:NH2 | 2.53 | 0.41 |
| 1:B:255:TYR:CG | 1:B:424:PRO:HB3 | 2.55 | 0.41 |
| 3:F:73:THR:CG2 | 3:F:74:ILE:N | 2.83 | 0.41 |
| 2:C:196:TRP:O | 2:C:198:SER:N | 2.52 | 0.41 |
| 2:E:151:LYS:HB2 | 2:E:151:LYS:HE3 | 1.78 | 0.41 |
| 1:A:223:ILE:CG2 | 1:A:227:ILE:HD13 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:D:22:THR:CG2 | 3:D:23:CYS:H | 2.32 | 0.41 |
| 1:A:78:LEU:O | 1:A:79:LEU:C | 2.59 | 0.41 |
| 3:F:33:HIS:O | 3:F:87:CYS:HA | 2.20 | 0.41 |
| 2:C:132:LEU:HD21 | 3:D:132:VAL:CG2 | 2.50 | 0.41 |
| 1:B:167:ARG:HH11 | 1:B:167:ARG:HG2 | 1.85 | 0.41 |
| 1:B:218:VAL:O | 1:B:219:PHE:C | 2.58 | 0.41 |
| 3:F:115:SER:CB | 3:F:117:PHE:HE1 | 2.34 | 0.41 |
| 2:C:66:ASP:O | 2:C:67:LYS:C | 2.58 | 0.41 |
| 3:F:47:ILE:HG22 | 3:F:48:TYR:N | 2.35 | 0.41 |
| 3:F:86:TYR:CE2 | 3:F:100:GLY:HA3 | 2.54 | 0.41 |
| 1:B:198:LEU:CD1 | 1:B:406:LEU:HG | 2.51 | 0.41 |
| 1:A:443:PRO:O | 1:A:445:TYR:N | 2.54 | 0.41 |
| 2:E:72:ARG:NH1 | 2:E:72:ARG:HG3 | 2.35 | 0.41 |
| 3:F:95:GLN:N | 3:F:95:GLN:CD | 2.71 | 0.41 |
| 1:B:199:PHE:CD1 | 1:B:407:THR:HG21 | 2.55 | 0.41 |
| 2:E:38:ARG:NE | 2:E:46:LYS:HZ1 | 2.18 | 0.41 |
| 1:B:110:PRO:HG2 | 1:B:448:ILE:HG21 | 2.02 | 0.41 |
| 1:B:148:GLN:HB3 | 1:B:190:PHE:CE1 | 2.56 | 0.41 |
| 1:A:430:LEU:O | 1:A:431:GLY:C | 2.57 | 0.41 |
| 1:A:148:GLN:O | 1:A:149:GLY:C | 2.59 | 0.41 |
| 3:D:189:ASN:ND2 | 3:D:210:ARG:N | 2.68 | 0.41 |
| 1:A:250:ASN:ND2 | 2:C:105:TYR:HD1 | 2.17 | 0.41 |
| 1:A:30:LYS:NZ | 1:B:442:LYS:HE2 | 2.35 | 0.41 |
| 1:B:420:GLN:HB2 | 1:B:420:GLN:HE21 | 1.62 | 0.41 |
| 1:A:96:LEU:O | 1:A:100:TYR:HB2 | 2.20 | 0.41 |
| 1:A:369:THR:HG22 | 1:A:373:MET:HE3 | 2.01 | 0.41 |
| 3:F:4:LEU:HD11 | 3:F:89:GLN:HG3 | 2.03 | 0.41 |
| 1:B:380:PRO:CD | 1:B:381:GLN:NE2 | 2.82 | 0.41 |
| 1:A:250:ASN:HD22 | 2:C:105:TYR:HD1 | 1.61 | 0.41 |
| 2:E:109:ASP:OD2 | 2:E:110:VAL:HG23 | 2.21 | 0.41 |
| 1:B:293:LEU:C | 1:B:295:GLY:N | 2.72 | 0.41 |
| 1:A:47:GLY:O | 1:A:48:LEU:C | 2.58 | 0.41 |
| 3:D:127:GLY:HA2 | 3:D:182:LYS:HB2 | 2.02 | 0.41 |
| 2:E:134:PRO:HD3 | 2:E:146:LEU:CD2 | 2.51 | 0.41 |
| 1:B:267:PRO:O | 1:B:270:ASN:N | 2.53 | 0.41 |
| 1:B:273:VAL:HG11 | 1:B:444:LEU:HD21 | 2.03 | 0.41 |
| 3:F:57:VAL:HA | 3:F:58:PRO:HD3 | 1.95 | 0.41 |
| 2:C:99:LEU:HD21 | 2:C:108:PHE:CE2 | 2.55 | 0.41 |
| 1:B:191:ASN:ND2 | 1:B:191:ASN:O | 2.53 | 0.41 |
| 1:B:402:ILE:CG1 | 1:B:402:ILE:O | 2.69 | 0.41 |
| 3:D:86:TYR:HE2 | 3:D:100:GLY:HA3 | 1.83 | 0.41 |
| 1:A:394:MET:O | 1:A:394:MET:HG2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:F:90:TRP:CG | 3:F:95:GLN:HB3 | 2.56 | 0.41 |
| 1:A:63:GLN:N | 1:A:63:GLN:OE1 | 2.53 | 0.41 |
| 2:C:124:THR:CG2 | 2:C:125:THR:H | 2.32 | 0.41 |
| 2:E:18:LEU:HD11 | 2:E:117:VAL:CG1 | 2.51 | 0.41 |
| 1:B:247:ALA:HA | 1:B:248:PRO:HD2 | 1.76 | 0.41 |
| 1:A:86:SER:HB2 | 1:A:300:GLY:HA2 | 2.02 | 0.41 |
| 1:A:205:ARG:HA | 1:A:206:PRO:HD2 | 1.92 | 0.41 |
| 1:B:91:MET:HG3 | 1:B:296:GLY:HA3 | 2.02 | 0.41 |
| 2:E:38:ARG:HE | 2:E:46:LYS:HE3 | 1.86 | 0.41 |
| 3:F:202:SER:HA | 3:F:203:PRO:HD2 | 1.92 | 0.41 |
| 1:B:287:ASN:HB3 | 1:B:290:LYS:HB2 | 2.02 | 0.41 |
| 1:A:75:TYR:CB | 1:A:76:PRO:HD3 | 2.37 | 0.41 |
| 1:A:63:GLN:C | 1:A:65:MET:N | 2.74 | 0.41 |
| 1:B:270:ASN:HA | 1:B:273:VAL:CG1 | 2.51 | 0.41 |
| 1:A:21:LEU:CD2 | 1:A:25:LEU:HG | 2.51 | 0.41 |
| 1:B:331:GLY:C | 1:B:333:LEU:N | 2.75 | 0.41 |
| 3:F:125:THR:O | 3:F:125:THR:HG22 | 2.21 | 0.41 |
| 1:B:337:PHE:O | 1:B:341:VAL:HG23 | 2.21 | 0.40 |
| 1:B:150:PRO:CG | 1:B:354:GLY:HA2 | 2.51 | 0.40 |
| 1:A:198:LEU:CD1 | 1:A:406:LEU:HG | 2.51 | 0.40 |
| 1:B:270:ASN:HA | 1:B:273:VAL:HG12 | 2.02 | 0.40 |
| 2:E:33:TRP:CZ2 | 2:E:52:ASN:HB2 | 2.57 | 0.40 |
| 3:D:66:SER:O | 3:D:68:THR:N | 2.54 | 0.40 |
| 3:D:149:ILE:HG12 | 3:D:191:TYR:CE2 | 2.56 | 0.40 |
| 1:A:210:TYR:H | 1:B:210:TYR:HB2 | 1.87 | 0.40 |
| 1:B:166:PHE:C | 1:B:167:ARG:HG2 | 2.42 | 0.40 |
| 1:B:211:THR:HG22 | 1:B:212:LEU:H | 1.86 | 0.40 |
| 1:B:437:GLN:O | 1:B:439:THR:N | 2.54 | 0.40 |
| 3:F:178:LEU:HD12 | 3:F:179:THR:N | 2.36 | 0.40 |
| 3:D:58:PRO:C | 3:D:60:ARG:N | 2.74 | 0.40 |
| 1:A:33:LEU:O | 1:A:33:LEU:HD23 | 2.21 | 0.40 |
| 2:C:103:TYR:CD2 | 3:D:31:TYR:CE2 | 3.09 | 0.40 |
| 3:F:125:THR:O | 3:F:126:SER:HB3 | 2.22 | 0.40 |
| 3:F:59:VAL:HG12 | 3:F:59:VAL:O | 2.21 | 0.40 |
| 1:A:312:THR:HG22 | 1:A:339:ALA:HB3 | 2.02 | 0.40 |
| 2:E:174:PHE:HA | 2:E:175:PRO:HD3 | 1.96 | 0.40 |
| 1:B:109:ILE:HG21 | 1:B:445:TYR:HD2 | 1.85 | 0.40 |
| 1:B:279:LEU:HD23 | 1:B:279:LEU:C | 2.41 | 0.40 |
| 1:B:148:GLN:O | 1:B:151:THR:N | 2.51 | 0.40 |
| 1:A:282:ARG:C | 1:A:284:HIS:H | 2.25 | 0.40 |
| 1:A:193:PRO:HA | 1:A:222:VAL:CG1 | 2.52 | 0.40 |
| 2:E:51:ILE:HD13 | 2:E:72:ARG:HD2 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:D:74:ILE:CG2 | 3:D:77:MET:HA | 2.51 | 0.40 |
| 3:D:184:GLU:O | 3:D:187:ARG:HG2 | 2.22 | 0.40 |
| 3:F:113:THR:HG22 | 3:F:113:THR:O | 2.21 | 0.40 |
| 1:A:223:ILE:HG22 | 1:A:227:ILE:HD13 | 2.02 | 0.40 |
| 2:E:107:TYR:C | 2:E:107:TYR:CD1 | 2.95 | 0.40 |
| 3:D:64:SER:OG | 3:D:65:GLY:N | 2.54 | 0.40 |
| 1:B:197:ILE:CG1 | 1:B:222:VAL:HG21 | 2.51 | 0.40 |
| 1:B:250:ASN:ND2 | 2:E:105:TYR:HD1 | 2.19 | 0.40 |
| 1:B:270:ASN:HD22 | 1:B:270:ASN:HA | 1.57 | 0.40 |
| 1:A:109:ILE:CG2 | 1:A:445:TYR:HD2 | 2.34 | 0.40 |
| 1:B:451:ARG:O | 1:B:455:LYS:HB2 | 2.21 | 0.40 |
| 1:B:139:LEU:O | 1:B:142:GLY:N | 2.50 | 0.40 |
| 1:A:136:LEU:H | 1:A:136:LEU:CD1 | 2.34 | 0.40 |
| 1:A:89:LEU:HA | 1:A:89:LEU:HD23 | 1.86 | 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 | 442/473 (93%) | 311 (70%) | 103 (23%) | 28 (6%) | 2 | 16 |
| 1 | B | 439/473 (93%) | 296 (67%) | 111 (25%) | 32 (7%) | 2 | 12 |
| 2 | C | 219/222 (99%) | 174 (80%) | 35 (16%) | 10 (5%) | 4 | 24 |
| 2 | E | 219/222 (99%) | 180 (82%) | 28 (13%) | 11 (5%) | 3 | 22 |
| 3 | D | 209/211 (99%) | 169 (81%) | 27 (13%) | 13 (6%) | 2 | 16 |
| 3 | F | 209/211 (99%) | 165 (79%) | 36 (17%) | 8 (4%) | 5 | 30 |
| All | All | 1737/1812 (96%) | 1295 (75%) | 340 (20%) | 102 (6%) | 2 | 17 |

All (102) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 132 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 171 | ASP |
| 1 | A | 201 | ILE |
| 1 | A | 283 | VAL |
| 1 | A | 307 | PHE |
| 1 | A | 309 | ALA |
| 1 | A | 386 | ALA |
| 1 | B | 132 | PHE |
| 1 | B | 171 | ASP |
| 1 | B | 201 | ILE |
| 1 | B | 283 | VAL |
| 1 | B | 309 | ALA |
| 1 | B | 441 | GLY |
| 1 | B | 444 | LEU |
| 2 | C | 65 | LYS |
| 2 | C | 106 | TRP |
| 2 | C | 140 | ALA |
| 3 | D | 7 | SER |
| 3 | D | 67 | GLY |
| 3 | D | 126 | SER |
| 3 | D | 153 | GLU |
| 2 | E | 65 | LYS |
| 2 | E | 106 | TRP |
| 2 | E | 122 | ALA |
| 2 | E | 140 | ALA |
| 3 | F | 7 | SER |
| 3 | F | 67 | GLY |
| 3 | F | 112 | PRO |
| 3 | F | 126 | SER |
| 1 | A | 102 | PRO |
| 1 | A | 314 | GLY |
| 1 | A | 441 | GLY |
| 1 | A | 444 | LEU |
| 1 | B | 102 | PRO |
| 1 | B | 307 | PHE |
| 1 | B | 314 | GLY |
| 1 | B | 332 | MET |
| 1 | B | 351 | GLY |
| 1 | B | 386 | ALA |
| 1 | B | 443 | PRO |
| 2 | C | 9 | GLY |
| 3 | D | 105 | ILE |
| 2 | E | 9 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | F | 153 | GLU |
| 1 | A | 96 | LEU |
| 1 | A | 189 | ALA |
| 1 | A | 337 | PHE |
| 1 | A | 438 | PHE |
| 1 | A | 443 | PRO |
| 1 | A | 447 | ALA |
| 1 | B | 92 | PHE |
| 1 | B | 96 | LEU |
| 1 | B | 188 | ALA |
| 2 | C | 31 | ARG |
| 2 | C | 53 | PRO |
| 2 | C | 109 | ASP |
| 2 | C | 196 | TRP |
| 3 | D | 154 | ARG |
| 3 | F | 113 | THR |
| 3 | F | 154 | ARG |
| 1 | A | 107 | SER |
| 1 | A | 419 | TYR |
| 1 | B | 95 | PHE |
| 1 | B | 107 | SER |
| 1 | B | 128 | LEU |
| 1 | B | 447 | ALA |
| 2 | C | 157 | PRO |
| 3 | D | 15 | PRO |
| 3 | D | 55 | SER |
| 3 | D | 83 | ALA |
| 3 | D | 199 | THR |
| 2 | E | 31 | ARG |
| 2 | E | 64 | LEU |
| 1 | A | 95 | PHE |
| 1 | A | 128 | LEU |
| 1 | B | 26 | LEU |
| 1 | B | 64 | ARG |
| 1 | B | 285 | GLY |
| 1 | B | 337 | PHE |
| 1 | B | 405 | PRO |
| 3 | D | 51 | SER |
| 3 | D | 137 | ASN |
| 2 | E | 53 | PRO |
| 2 | E | 196 | TRP |
| 1 | A | 242 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 412 | VAL |
| 1 | B | 59 | TRP |
| 1 | B | 101 | ALA |
| 1 | B | 422 | ILE |
| 3 | D | 80 | GLU |
| 3 | F | 15 | PRO |
| 1 | A | 376 | VAL |
| 1 | B | 200 | ILE |
| 2 | C | 54 | VAL |
| 1 | A | 200 | ILE |
| 1 | B | 121 | PRO |
| 1 | A | 101 | ALA |
| 1 | A | 285 | GLY |
| 2 | E | 14 | PRO |
| 1 | A | 405 | PRO |
| 1 | B | 338 | VAL |
| 2 | E | 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 | 335/358 (94%) | 305 (91%) | 30 (9%) | 14 | 47 |
| 1 | B | 332/358 (93%) | 304 (92%) | 28 (8%) | 16 | 52 |
| 2 | C | 181/182 (100%) | 163 (90%) | 18 (10%) | 11 | 39 |
| 2 | E | 181/182 (100%) | 162 (90%) | 19 (10%) | 10 | 35 |
| 3 | D | 185/185 (100%) | 177 (96%) | 8 (4%) | 40 | 80 |
| 3 | F | 185/185 (100%) | 173 (94%) | 12 (6%) | 24 | 65 |
| All | All | 1399/1450 (96%) | 1284 (92%) | 115 (8%) | 17 | 53 |

All (115) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 18 | ARG |
| 1 | A | 21 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 48 | LEU |
| 1 | A | 63 | GLN |
| 1 | A | 98 | ARG |
| 1 | A | 120 | ARG |
| 1 | A | 138 | THR |
| 1 | A | 167 | ARG |
| 1 | A | 171 | ASP |
| 1 | A | 172 | GLU |
| 1 | A | 178 | LEU |
| 1 | A | 180 | THR |
| 1 | A | 207 | GLN |
| 1 | A | 208 | PHE |
| 1 | A | 212 | LEU |
| 1 | A | 215 | ILE |
| 1 | A | 230 | ARG |
| 1 | A | 274 | LEU |
| 1 | A | 304 | LEU |
| 1 | A | 317 | PHE |
| 1 | A | 318 | ASN |
| 1 | A | 340 | ARG |
| 1 | A | 347 | CYS |
| 1 | A | 379 | PHE |
| 1 | A | 381 | GLN |
| 1 | A | 391 | ILE |
| 1 | A | 397 | LEU |
| 1 | A | 420 | GLN |
| 1 | A | 434 | LEU |
| 1 | A | 451 | ARG |
| 1 | B | 21 | LEU |
| 1 | B | 48 | LEU |
| 1 | B | 63 | GLN |
| 1 | B | 98 | ARG |
| 1 | B | 120 | ARG |
| 1 | B | 138 | THR |
| 1 | B | 167 | ARG |
| 1 | B | 171 | ASP |
| 1 | B | 172 | GLU |
| 1 | B | 180 | THR |
| 1 | B | 198 | LEU |
| 1 | B | 207 | GLN |
| 1 | B | 208 | PHE |
| 1 | B | 212 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 215 | ILE |
| 1 | B | 230 | ARG |
| 1 | B | 274 | LEU |
| 1 | B | 304 | LEU |
| 1 | B | 317 | PHE |
| 1 | B | 318 | ASN |
| 1 | B | 340 | ARG |
| 1 | B | 347 | CYS |
| 1 | B | 379 | PHE |
| 1 | B | 381 | GLN |
| 1 | B | 397 | LEU |
| 1 | B | 420 | GLN |
| 1 | B | 434 | LEU |
| 1 | B | 451 | ARG |
| 2 | C | 4 | LEU |
| 2 | C | 18 | LEU |
| 2 | C | 27 | PHE |
| 2 | C | 41 | PRO |
| 2 | C | 45 | LEU |
| 2 | C | 61 | THR |
| 2 | C | 67 | LYS |
| 2 | C | 72 | ARG |
| 2 | C | 77 | ASP |
| 2 | C | 107 | TYR |
| 2 | C | 115 | THR |
| 2 | C | 157 | PRO |
| 2 | C | 172 | HIS |
| 2 | C | 185 | LEU |
| 2 | C | 200 | THR |
| 2 | C | 203 | CYS |
| 2 | C | 204 | ASN |
| 2 | C | 221 | ARG |
| 3 | D | 28 | SER |
| 3 | D | 46 | TRP |
| 3 | D | 75 | ASN |
| 3 | D | 77 | MET |
| 3 | D | 88 | GLN |
| 3 | D | 117 | PHE |
| 3 | D | 146 | LYS |
| 3 | D | 189 | ASN |
| 2 | E | 4 | LEU |
| 2 | E | 27 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 45 | LEU |
| 2 | E | 61 | THR |
| 2 | E | 67 | LYS |
| 2 | E | 72 | ARG |
| 2 | E | 77 | ASP |
| 2 | E | 98 | ARG |
| 2 | E | 107 | TYR |
| 2 | E | 124 | THR |
| 2 | E | 127 | PRO |
| 2 | E | 157 | PRO |
| 2 | E | 167 | LEU |
| 2 | E | 172 | HIS |
| 2 | E | 185 | LEU |
| 2 | E | 186 | SER |
| 2 | E | 200 | THR |
| 2 | E | 203 | CYS |
| 2 | E | 204 | ASN |
| 3 | F | 1 | ASP |
| 3 | F | 15 | PRO |
| 3 | F | 28 | SER |
| 3 | F | 46 | TRP |
| 3 | F | 75 | ASN |
| 3 | F | 77 | MET |
| 3 | F | 88 | GLN |
| 3 | F | 102 | LYS |
| 3 | F | 119 | PRO |
| 3 | F | 146 | LYS |
| 3 | F | 189 | ASN |
| 3 | F | 201 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 62 | ASN |
| 1 | A | 148 | GLN |
| 1 | A | 157 | ASN |
| 1 | A | 207 | GLN |
| 1 | A | 270 | ASN |
| 1 | A | 277 | GLN |
| 1 | A | 287 | ASN |
| 1 | A | 318 | ASN |
| 1 | A | 327 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 381 | GLN |
| 1 | A | 383 | HIS |
| 1 | A | 437 | GLN |
| 1 | A | 456 | GLN |
| 1 | A | 460 | GLN |
| 1 | B | 62 | ASN |
| 1 | B | 119 | GLN |
| 1 | B | 148 | GLN |
| 1 | B | 157 | ASN |
| 1 | B | 207 | GLN |
| 1 | B | 270 | ASN |
| 1 | B | 277 | GLN |
| 1 | B | 287 | ASN |
| 1 | B | 318 | ASN |
| 1 | B | 327 | ASN |
| 1 | B | 381 | GLN |
| 1 | B | 383 | HIS |
| 1 | B | 437 | GLN |
| 1 | B | 456 | GLN |
| 3 | D | 93 | HIS |
| 3 | D | 136 | ASN |
| 3 | D | 137 | ASN |
| 3 | D | 155 | GLN |
| 3 | D | 189 | ASN |
| 2 | E | 163 | ASN |
| 3 | F | 136 | ASN |
| 3 | F | 137 | ASN |
| 3 | F | 155 | GLN |
| 3 | F | 189 | ASN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1 | A | 444/473 (93%) | -0.11 | 2 (0%) 88 39 | 50, 77, 100, 111 | 0 |
| 1 | B | 441/473 (93%) | -0.09 | 1 (0%) 93 61 | 46, 76, 103, 121 | 0 |
| 2 | C | 221/222 (99%) | 0.00 | 0 100 100 | 43, 74, 94, 125 | 0 |
| 2 | E | 221/222 (99%) | 0.02 | 0 100 100 | 40, 75, 95, 116 | 0 |
| 3 | D | 211/211 (100%) | 0.04 | 0 100 100 | 57, 85, 98, 103 | 0 |
| 3 | F | 211/211 (100%) | 0.00 | 1 (0%) 88 39 | 40, 71, 99, 110 | 0 |
| All | All | 1749/1812 (96%) | -0.04 | 4 (0%) 93 61 | 40, 77, 99, 125 | 0 |

All (4) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 72 | ALA | 2.9 |
| 3 | F | 153 | GLU | 2.9 |
| 1 | B | 235 | GLU | 2.4 |
| 1 | A | 235 | GLU | 2.3 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.