



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:06 am GMT

PDB ID : 3E0J
Title : X-ray structure of the complex of regulatory subunits of human DNA polymerase delta
Authors : Baranovskiy, A.G.; Babayeva, N.D.; Pavlov, Y.I.; Vassilyev, D.G.; Tahirov, T.H.
Deposited on : 2008-07-31
Resolution : 3.00 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) | : | 1.9-1692 |
| EDS | : | trunk28620 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

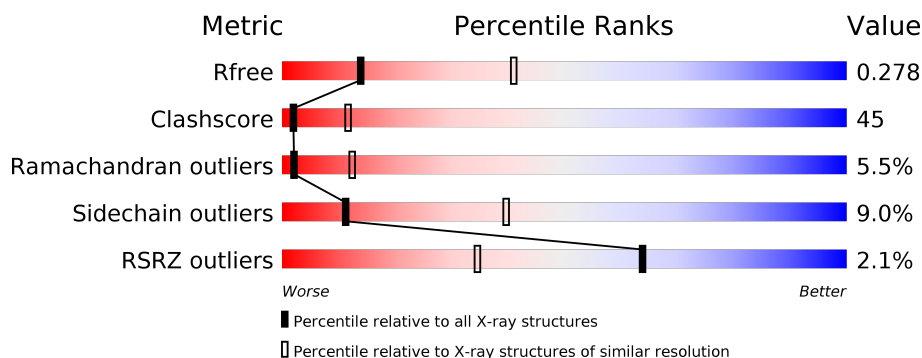
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1692 (3.00-3.00) |
| Clashscore | 112137 | 2037 (3.00-3.00) |
| Ramachandran outliers | 110173 | 1973 (3.00-3.00) |
| Sidechain outliers | 110143 | 1976 (3.00-3.00) |
| RSRZ outliers | 101464 | 1716 (3.00-3.00) |

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.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 476 | <div> <div>31%</div> <div>48%</div> <div>8%</div> <div>13%</div> </div> |
| 1 | C | 476 | <div> <div>29%</div> <div>49%</div> <div>7%</div> <div>14%</div> </div> |
| 1 | E | 476 | <div> <div>30%</div> <div>47%</div> <div>7%</div> <div>14%</div> </div> |
| 1 | G | 476 | <div> <div>34%</div> <div>45%</div> <div>7%</div> <div>14%</div> </div> |
| 2 | B | 144 | <div> <div>42%</div> <div>50%</div> <div>7%</div> </div> |
| 2 | D | 144 | <div> <div>44%</div> <div>49%</div> <div>6%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | F | 144 | <div><div>%</div><div><div></div></div><div>43%51%6% •</div></div> |
| 2 | H | 144 | <div><div>3%</div><div><div></div></div><div>42%52%6% •</div></div> |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA polymerase subunit delta-2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 416 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3185 | 2022 | 537 | 609 | 17 | | | |
| 1 | C | 409 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3133 | 1991 | 530 | 595 | 17 | | | |
| 1 | E | 408 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3125 | 1985 | 529 | 594 | 17 | | | |
| 1 | G | 408 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3125 | 1985 | 529 | 594 | 17 | | | |

There are 28 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -6 | HIS | - | EXPRESSION TAG | UNP P49005 |
| A | -5 | HIS | - | EXPRESSION TAG | UNP P49005 |
| A | -4 | HIS | - | EXPRESSION TAG | UNP P49005 |
| A | -3 | HIS | - | EXPRESSION TAG | UNP P49005 |
| A | -2 | HIS | - | EXPRESSION TAG | UNP P49005 |
| A | -1 | HIS | - | EXPRESSION TAG | UNP P49005 |
| A | 0 | GLY | - | EXPRESSION TAG | UNP P49005 |
| C | -6 | HIS | - | EXPRESSION TAG | UNP P49005 |
| C | -5 | HIS | - | EXPRESSION TAG | UNP P49005 |
| C | -4 | HIS | - | EXPRESSION TAG | UNP P49005 |
| C | -3 | HIS | - | EXPRESSION TAG | UNP P49005 |
| C | -2 | HIS | - | EXPRESSION TAG | UNP P49005 |
| C | -1 | HIS | - | EXPRESSION TAG | UNP P49005 |
| C | 0 | GLY | - | EXPRESSION TAG | UNP P49005 |
| E | -6 | HIS | - | EXPRESSION TAG | UNP P49005 |
| E | -5 | HIS | - | EXPRESSION TAG | UNP P49005 |
| E | -4 | HIS | - | EXPRESSION TAG | UNP P49005 |
| E | -3 | HIS | - | EXPRESSION TAG | UNP P49005 |
| E | -2 | HIS | - | EXPRESSION TAG | UNP P49005 |
| E | -1 | HIS | - | EXPRESSION TAG | UNP P49005 |
| E | 0 | GLY | - | EXPRESSION TAG | UNP P49005 |

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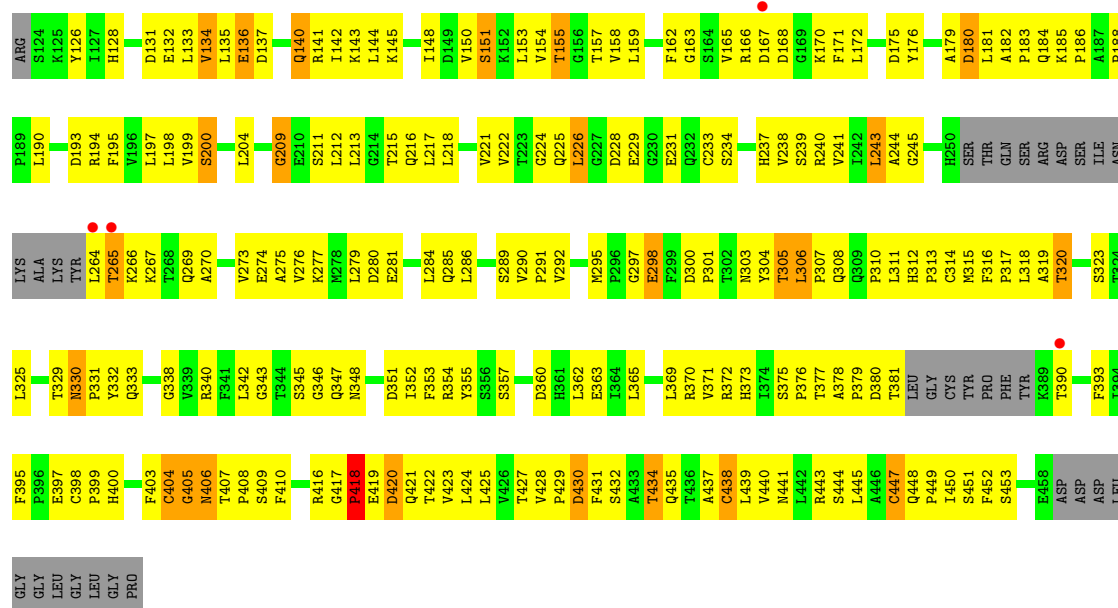
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | -6 | HIS | - | EXPRESSION TAG | UNP P49005 |
| G | -5 | HIS | - | EXPRESSION TAG | UNP P49005 |
| G | -4 | HIS | - | EXPRESSION TAG | UNP P49005 |
| G | -3 | HIS | - | EXPRESSION TAG | UNP P49005 |
| G | -2 | HIS | - | EXPRESSION TAG | UNP P49005 |
| G | -1 | HIS | - | EXPRESSION TAG | UNP P49005 |
| G | 0 | GLY | - | EXPRESSION TAG | UNP P49005 |

- Molecule 2 is a protein called DNA polymerase subunit delta-3.

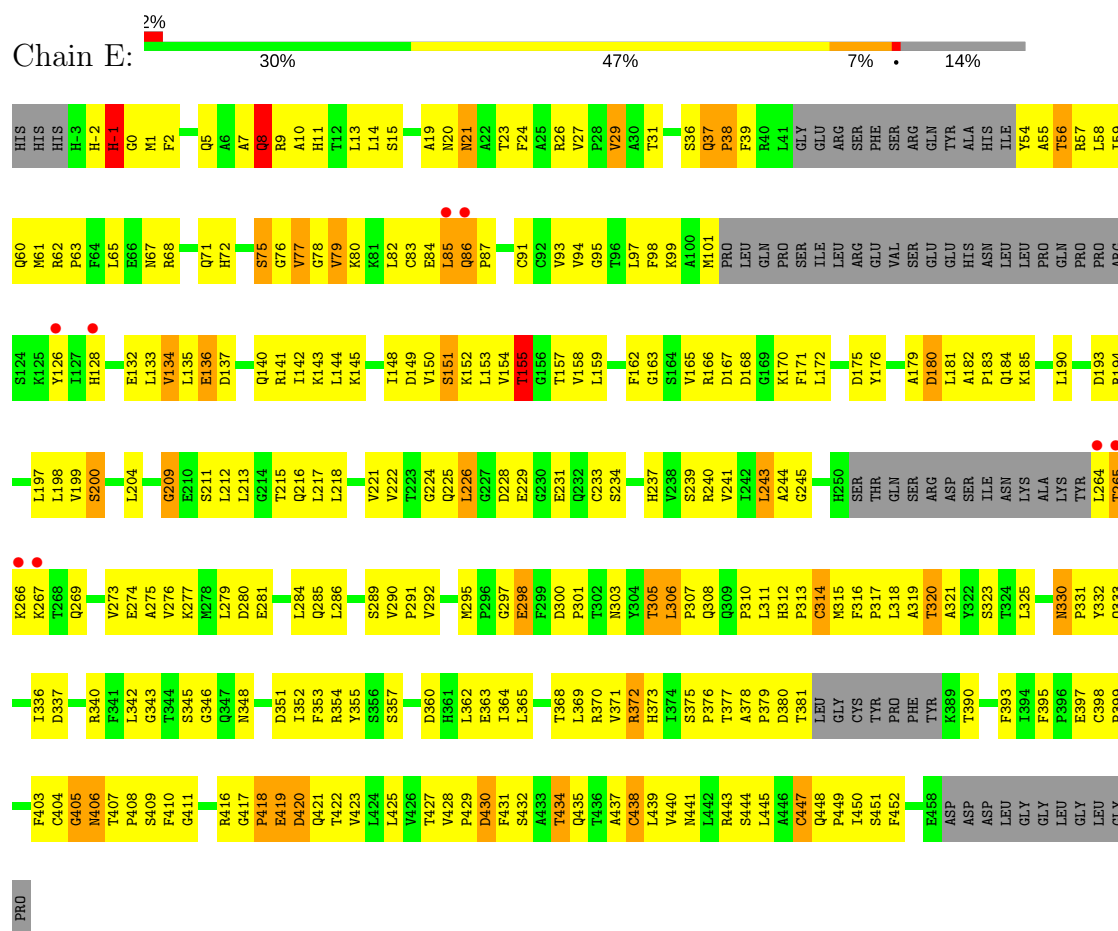
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 715 | 196 | 215 | 5 | | | |
| 2 | D | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 715 | 196 | 215 | 5 | | | |
| 2 | F | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 715 | 196 | 215 | 5 | | | |
| 2 | H | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 715 | 196 | 215 | 5 | | | |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | A | 11 | Total | O | 0 | 0 |
| | | | 11 | 11 | | |
| 3 | B | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 3 | C | 12 | Total | O | 0 | 0 |
| | | | 12 | 12 | | |
| 3 | D | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 3 | E | 15 | Total | O | 0 | 0 |
| | | | 15 | 15 | | |
| 3 | F | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 3 | G | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |
| 3 | H | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

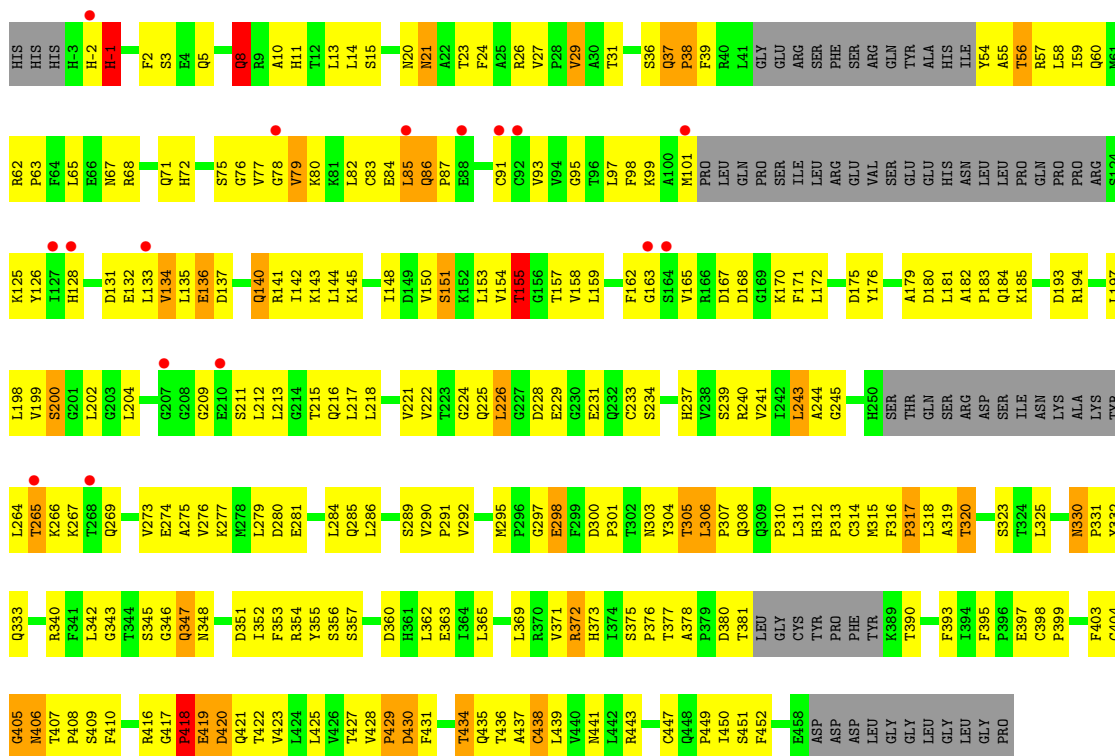


- Molecule 1: DNA polymerase subunit delta-2

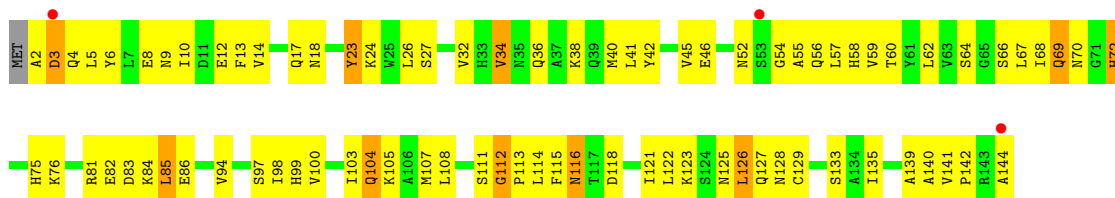


- Molecule 1: DNA polymerase subunit delta-2

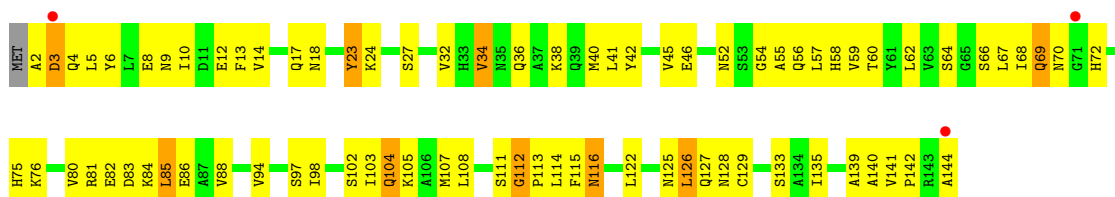
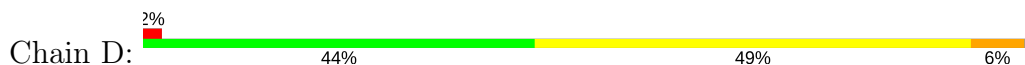




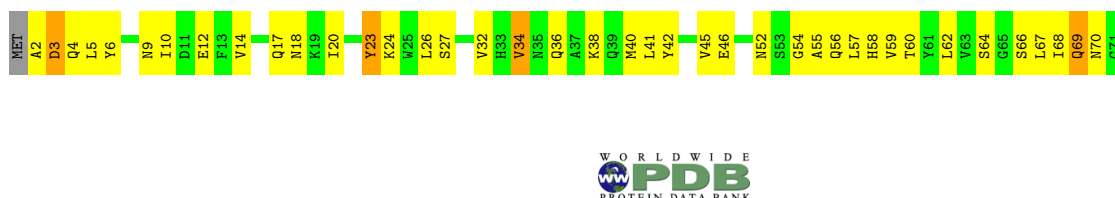
• Molecule 2: DNA polymerase subunit delta-3

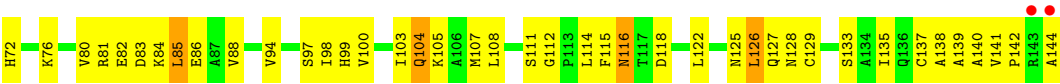


• Molecule 2: DNA polymerase subunit delta-3



• Molecule 2: DNA polymerase subunit delta-3





● Molecule 2: DNA polymerase subunit delta-3



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 95.13Å 248.53Å 103.46Å 90.00° 106.94° 90.00° | Depositor |
| Resolution (Å) | 29.89 – 3.00 38.01 – 2.99 | Depositor EDS |
| % Data completeness (in resolution range) | 91.3 (29.89-3.00) 91.1 (38.01-2.99) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 123.02 (at 3.01Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.257 , 0.281 0.256 , 0.278 | Depositor DCC |
| R_{free} test set | 4224 reflections (5.05%) | DCC |
| Wilson B-factor (Å ²) | 56.1 | Xtriage |
| Anisotropy | 0.055 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 71.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.87 | EDS |
| Total number of atoms | 17153 | wwPDB-VP |
| Average B, all atoms (Å ²) | 60.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 | 0.54 | 1/3254 (0.0%) | 0.78 | 1/4426 (0.0%) |
| 1 | C | 0.56 | 1/3201 (0.0%) | 0.78 | 1/4354 (0.0%) |
| 1 | E | 0.53 | 0/3193 | 0.77 | 0/4343 |
| 1 | G | 0.52 | 0/3193 | 0.77 | 0/4343 |
| 2 | B | 0.56 | 0/1150 | 0.69 | 0/1553 |
| 2 | D | 0.54 | 0/1150 | 0.70 | 0/1553 |
| 2 | F | 0.51 | 0/1150 | 0.67 | 0/1553 |
| 2 | H | 0.47 | 0/1150 | 0.66 | 0/1553 |
| All | All | 0.54 | 2/17441 (0.0%) | 0.75 | 2/23678 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | C | 404 | CYS | CB-SG | -6.43 | 1.71 | 1.82 |
| 1 | A | 404 | CYS | CB-SG | -5.54 | 1.72 | 1.81 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 18 | SER | N-CA-C | -5.32 | 96.64 | 111.00 |
| 1 | C | 18 | SER | N-CA-C | -5.04 | 97.41 | 111.00 |

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 | 3185 | 0 | 3150 | 319 | 0 |
| 1 | C | 3133 | 0 | 3112 | 330 | 0 |
| 1 | E | 3125 | 0 | 3101 | 318 | 0 |
| 1 | G | 3125 | 0 | 3101 | 309 | 0 |
| 2 | B | 1131 | 0 | 1138 | 93 | 0 |
| 2 | D | 1131 | 0 | 1138 | 90 | 0 |
| 2 | F | 1131 | 0 | 1138 | 78 | 0 |
| 2 | H | 1131 | 0 | 1138 | 89 | 0 |
| 3 | A | 11 | 0 | 0 | 1 | 0 |
| 3 | B | 6 | 0 | 0 | 0 | 0 |
| 3 | C | 12 | 0 | 0 | 3 | 0 |
| 3 | D | 4 | 0 | 0 | 0 | 0 |
| 3 | E | 15 | 0 | 0 | 2 | 0 |
| 3 | F | 4 | 0 | 0 | 0 | 0 |
| 3 | G | 8 | 0 | 0 | 2 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| All | All | 17153 | 0 | 17016 | 1525 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1525) 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:C:29:VAL:HG11 | 1:C:291:PRO:HG2 | 1.19 | 1.18 |
| 1:C:58:LEU:HD21 | 1:C:95:GLY:HA2 | 1.25 | 1.13 |
| 1:E:58:LEU:HD21 | 1:E:95:GLY:HA2 | 1.25 | 1.09 |
| 1:A:58:LEU:HD21 | 1:A:95:GLY:HA2 | 1.26 | 1.09 |
| 1:G:29:VAL:HG11 | 1:G:291:PRO:HG2 | 1.24 | 1.09 |
| 1:G:58:LEU:HD21 | 1:G:95:GLY:HA2 | 1.29 | 1.09 |
| 1:A:29:VAL:HG11 | 1:A:291:PRO:HG2 | 1.12 | 1.07 |
| 1:E:29:VAL:HG11 | 1:E:291:PRO:HG2 | 1.21 | 1.07 |
| 1:G:193:ASP:HB3 | 1:G:443:ARG:NH1 | 1.74 | 1.00 |
| 1:C:193:ASP:HB3 | 1:C:443:ARG:NH1 | 1.80 | 0.97 |
| 1:A:193:ASP:HB3 | 1:A:443:ARG:NH1 | 1.81 | 0.94 |
| 1:G:330:ASN:HB3 | 1:G:331:PRO:HD3 | 1.50 | 0.94 |
| 1:C:330:ASN:HB3 | 1:C:331:PRO:HD3 | 1.48 | 0.94 |
| 1:G:98:PHE:HB2 | 1:G:134:VAL:HG13 | 1.51 | 0.92 |
| 1:C:193:ASP:HB3 | 1:C:443:ARG:HH11 | 1.33 | 0.91 |
| 1:E:330:ASN:HB3 | 1:E:331:PRO:HD3 | 1.49 | 0.91 |
| 2:B:116:ASN:HD22 | 2:B:116:ASN:H | 1.17 | 0.90 |
| 2:F:116:ASN:H | 2:F:116:ASN:HD22 | 1.20 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:193:ASP:HB3 | 1:E:443:ARG:NH1 | 1.86 | 0.89 |
| 1:A:330:ASN:HB3 | 1:A:331:PRO:HD3 | 1.55 | 0.89 |
| 1:E:99:LYS:H | 1:E:155:THR:HG23 | 1.38 | 0.89 |
| 1:A:340:ARG:HH12 | 1:A:397:GLU:HB3 | 1.38 | 0.89 |
| 1:G:99:LYS:H | 1:G:155:THR:HG23 | 1.39 | 0.88 |
| 1:A:193:ASP:HB3 | 1:A:443:ARG:HH11 | 1.34 | 0.88 |
| 1:A:98:PHE:HB2 | 1:A:134:VAL:HG13 | 1.53 | 0.88 |
| 1:A:407:THR:HG22 | 1:A:409:SER:H | 1.37 | 0.87 |
| 1:C:99:LYS:H | 1:C:155:THR:HG23 | 1.40 | 0.87 |
| 1:C:340:ARG:HH12 | 1:C:397:GLU:HB3 | 1.39 | 0.87 |
| 1:C:98:PHE:HB2 | 1:C:134:VAL:HG13 | 1.56 | 0.87 |
| 2:H:116:ASN:H | 2:H:116:ASN:HD22 | 1.22 | 0.87 |
| 1:G:193:ASP:HB3 | 1:G:443:ARG:HH11 | 1.31 | 0.86 |
| 1:C:407:THR:HG22 | 1:C:409:SER:H | 1.39 | 0.86 |
| 1:E:98:PHE:HB2 | 1:E:134:VAL:HG13 | 1.57 | 0.86 |
| 1:E:182:ALA:HB1 | 1:E:183:PRO:HD2 | 1.58 | 0.86 |
| 1:A:290:VAL:HG22 | 1:A:291:PRO:HD2 | 1.57 | 0.86 |
| 1:A:99:LYS:H | 1:A:155:THR:HG23 | 1.39 | 0.86 |
| 1:A:29:VAL:CG1 | 1:A:291:PRO:HG2 | 2.03 | 0.85 |
| 1:G:340:ARG:HH12 | 1:G:397:GLU:HB3 | 1.39 | 0.85 |
| 1:A:182:ALA:HB1 | 1:A:183:PRO:HD2 | 1.58 | 0.85 |
| 1:C:193:ASP:CB | 1:C:441:ASN:HD21 | 1.90 | 0.85 |
| 1:G:407:THR:HG22 | 1:G:409:SER:H | 1.42 | 0.84 |
| 1:C:182:ALA:HB1 | 1:C:183:PRO:HD2 | 1.56 | 0.84 |
| 2:D:116:ASN:HD22 | 2:D:116:ASN:H | 1.20 | 0.84 |
| 1:G:39:PHE:CE2 | 1:G:331:PRO:HB2 | 2.12 | 0.84 |
| 1:E:340:ARG:HH12 | 1:E:397:GLU:HB3 | 1.40 | 0.83 |
| 1:C:323:SER:HA | 2:D:144:ALA:HB3 | 1.61 | 0.83 |
| 1:G:182:ALA:HB1 | 1:G:183:PRO:HD2 | 1.58 | 0.83 |
| 2:B:116:ASN:N | 2:B:116:ASN:HD22 | 1.72 | 0.83 |
| 1:E:82:LEU:HD11 | 1:E:142:ILE:CG2 | 2.09 | 0.83 |
| 1:E:406:ASN:HD22 | 1:E:406:ASN:N | 1.76 | 0.83 |
| 2:F:116:ASN:N | 2:F:116:ASN:HD22 | 1.75 | 0.82 |
| 1:A:323:SER:HA | 2:B:144:ALA:HB3 | 1.59 | 0.82 |
| 1:E:407:THR:HG22 | 1:E:409:SER:H | 1.44 | 0.82 |
| 1:G:145:LYS:HE3 | 1:G:170:LYS:HB2 | 1.61 | 0.82 |
| 1:E:39:PHE:CE2 | 1:E:331:PRO:HB2 | 2.15 | 0.82 |
| 1:E:193:ASP:CB | 1:E:441:ASN:HD21 | 1.93 | 0.81 |
| 2:D:116:ASN:HD22 | 2:D:116:ASN:N | 1.74 | 0.81 |
| 1:E:145:LYS:HE3 | 1:E:170:LYS:HB2 | 1.63 | 0.81 |
| 1:G:82:LEU:HD21 | 1:G:142:ILE:H | 1.47 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:82:LEU:HD11 | 1:G:142:ILE:CG2 | 2.11 | 0.80 |
| 1:A:56:THR:HA | 1:A:59:ILE:HD12 | 1.64 | 0.80 |
| 1:C:406:ASN:N | 1:C:406:ASN:HD22 | 1.80 | 0.80 |
| 1:C:82:LEU:HD11 | 1:C:142:ILE:CG2 | 2.11 | 0.80 |
| 1:G:406:ASN:HD22 | 1:G:406:ASN:N | 1.79 | 0.80 |
| 1:G:323:SER:HA | 2:H:144:ALA:HB3 | 1.62 | 0.80 |
| 1:G:308:GLN:HB2 | 1:G:330:ASN:HB2 | 1.64 | 0.79 |
| 1:A:82:LEU:HD11 | 1:A:142:ILE:CG2 | 2.11 | 0.79 |
| 1:G:62:ARG:HB3 | 1:G:63:PRO:HD3 | 1.64 | 0.79 |
| 1:E:193:ASP:HB3 | 1:E:443:ARG:HH11 | 1.41 | 0.79 |
| 1:A:148:ILE:HG13 | 1:A:176:TYR:CE2 | 2.17 | 0.79 |
| 1:A:193:ASP:CB | 1:A:441:ASN:HD21 | 1.95 | 0.79 |
| 1:A:308:GLN:HB2 | 1:A:330:ASN:HB2 | 1.62 | 0.79 |
| 1:E:193:ASP:O | 1:E:194:ARG:HD3 | 1.81 | 0.79 |
| 1:A:62:ARG:HB3 | 1:A:63:PRO:HD3 | 1.64 | 0.79 |
| 1:C:308:GLN:HB2 | 1:C:330:ASN:HB2 | 1.63 | 0.79 |
| 1:E:151:SER:HB2 | 1:E:357:SER:HB2 | 1.65 | 0.79 |
| 1:A:306:LEU:HB3 | 1:A:307:PRO:HD3 | 1.65 | 0.79 |
| 1:A:419:GLU:O | 1:A:421:GLN:HG3 | 1.83 | 0.79 |
| 1:G:56:THR:HA | 1:G:59:ILE:HD12 | 1.64 | 0.79 |
| 2:B:116:ASN:H | 2:B:116:ASN:ND2 | 1.82 | 0.78 |
| 1:C:145:LYS:HE3 | 1:C:170:LYS:HB2 | 1.64 | 0.78 |
| 1:C:330:ASN:HB3 | 1:C:331:PRO:CD | 2.12 | 0.78 |
| 1:E:439:LEU:CD1 | 1:E:450:ILE:HD11 | 2.14 | 0.78 |
| 1:G:37:GLN:HE21 | 1:G:38:PRO:HD2 | 1.48 | 0.78 |
| 1:A:193:ASP:O | 1:A:194:ARG:HD3 | 1.84 | 0.78 |
| 1:C:193:ASP:HB3 | 1:C:441:ASN:HD21 | 1.47 | 0.78 |
| 1:C:439:LEU:CD1 | 1:C:450:ILE:HD11 | 2.13 | 0.78 |
| 1:A:193:ASP:HB3 | 1:A:441:ASN:HD21 | 1.48 | 0.78 |
| 1:G:193:ASP:CB | 1:G:441:ASN:HD21 | 1.95 | 0.78 |
| 2:H:116:ASN:N | 2:H:116:ASN:HD22 | 1.78 | 0.78 |
| 1:A:54:TYR:HA | 1:A:380:ASP:OD1 | 1.83 | 0.78 |
| 1:A:226:LEU:HD22 | 2:B:62:LEU:HD11 | 1.64 | 0.78 |
| 1:E:29:VAL:CG1 | 1:E:291:PRO:HG2 | 2.11 | 0.78 |
| 1:E:323:SER:HA | 2:F:144:ALA:HB3 | 1.64 | 0.78 |
| 1:C:56:THR:HA | 1:C:59:ILE:HD12 | 1.66 | 0.78 |
| 1:A:39:PHE:CE2 | 1:A:331:PRO:HB2 | 2.18 | 0.77 |
| 1:E:306:LEU:HB3 | 1:E:307:PRO:HD3 | 1.66 | 0.77 |
| 1:G:330:ASN:HB3 | 1:G:331:PRO:CD | 2.14 | 0.77 |
| 1:G:54:TYR:HA | 1:G:380:ASP:OD1 | 1.85 | 0.77 |
| 1:E:159:LEU:H | 1:E:159:LEU:HD23 | 1.49 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:406:ASN:N | 1:A:406:ASN:HD22 | 1.82 | 0.77 |
| 1:C:62:ARG:HB3 | 1:C:63:PRO:HD3 | 1.65 | 0.77 |
| 1:C:217:LEU:O | 1:C:221:VAL:HG23 | 1.84 | 0.77 |
| 1:A:226:LEU:HD12 | 1:A:226:LEU:C | 2.04 | 0.77 |
| 1:A:145:LYS:HE3 | 1:A:170:LYS:HB2 | 1.67 | 0.77 |
| 1:E:193:ASP:HB3 | 1:E:441:ASN:HD21 | 1.48 | 0.77 |
| 1:C:82:LEU:HD21 | 1:C:142:ILE:H | 1.47 | 0.76 |
| 1:C:148:ILE:HG13 | 1:C:176:TYR:CE2 | 2.20 | 0.76 |
| 1:G:439:LEU:CD1 | 1:G:450:ILE:HD11 | 2.15 | 0.76 |
| 1:A:303:ASN:HD22 | 1:A:305:THR:CG2 | 1.97 | 0.76 |
| 1:C:29:VAL:CG1 | 1:C:291:PRO:HG2 | 2.09 | 0.76 |
| 1:E:82:LEU:HD21 | 1:E:142:ILE:H | 1.51 | 0.76 |
| 1:E:308:GLN:HB2 | 1:E:330:ASN:HB2 | 1.67 | 0.76 |
| 1:G:148:ILE:HG13 | 1:G:176:TYR:CE2 | 2.19 | 0.76 |
| 1:E:226:LEU:HD22 | 2:F:62:LEU:HD11 | 1.66 | 0.76 |
| 1:E:330:ASN:HB3 | 1:E:331:PRO:CD | 2.14 | 0.76 |
| 1:G:290:VAL:HG22 | 1:G:291:PRO:HD2 | 1.67 | 0.76 |
| 1:C:290:VAL:HG22 | 1:C:291:PRO:HD2 | 1.67 | 0.76 |
| 1:G:306:LEU:HB3 | 1:G:307:PRO:HD3 | 1.68 | 0.76 |
| 1:C:419:GLU:O | 1:C:421:GLN:HG3 | 1.85 | 0.75 |
| 2:F:116:ASN:H | 2:F:116:ASN:ND2 | 1.83 | 0.75 |
| 1:G:419:GLU:O | 1:G:421:GLN:HG3 | 1.86 | 0.75 |
| 1:E:148:ILE:HG13 | 1:E:176:TYR:CE2 | 2.22 | 0.75 |
| 1:C:39:PHE:CE2 | 1:C:331:PRO:HB2 | 2.20 | 0.75 |
| 2:D:116:ASN:ND2 | 2:D:116:ASN:H | 1.85 | 0.75 |
| 1:E:56:THR:HA | 1:E:59:ILE:HD12 | 1.67 | 0.75 |
| 1:G:95:GLY:HA3 | 1:G:135:LEU:HD11 | 1.68 | 0.75 |
| 1:A:37:GLN:HE21 | 1:A:38:PRO:HD2 | 1.52 | 0.75 |
| 1:C:193:ASP:O | 1:C:194:ARG:HD3 | 1.87 | 0.75 |
| 1:A:82:LEU:HD21 | 1:A:142:ILE:H | 1.50 | 0.75 |
| 1:E:37:GLN:HE21 | 1:E:38:PRO:HD2 | 1.52 | 0.75 |
| 1:G:217:LEU:O | 1:G:221:VAL:HG23 | 1.87 | 0.75 |
| 1:E:419:GLU:O | 1:E:421:GLN:HG3 | 1.85 | 0.74 |
| 1:G:303:ASN:HD22 | 1:G:305:THR:CG2 | 1.99 | 0.74 |
| 1:E:290:VAL:HG22 | 1:E:291:PRO:HD2 | 1.66 | 0.74 |
| 1:A:151:SER:HB2 | 1:A:357:SER:HB2 | 1.69 | 0.74 |
| 1:C:303:ASN:HD22 | 1:C:305:THR:CG2 | 2.00 | 0.74 |
| 2:B:66:SER:HB3 | 2:B:94:VAL:HG12 | 1.70 | 0.74 |
| 1:A:82:LEU:HD11 | 1:A:142:ILE:HG21 | 1.70 | 0.74 |
| 1:A:330:ASN:HB3 | 1:A:331:PRO:CD | 2.18 | 0.74 |
| 1:C:226:LEU:HD22 | 2:D:62:LEU:HD11 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:193:ASP:O | 1:G:194:ARG:HD3 | 1.86 | 0.74 |
| 1:E:82:LEU:HD11 | 1:E:142:ILE:HG21 | 1.68 | 0.73 |
| 1:C:37:GLN:HE21 | 1:C:38:PRO:HD2 | 1.52 | 0.73 |
| 1:C:82:LEU:HD11 | 1:C:142:ILE:HG21 | 1.70 | 0.73 |
| 1:C:333:GLN:HG2 | 1:C:342:LEU:HD13 | 1.71 | 0.73 |
| 1:A:29:VAL:HG11 | 1:A:291:PRO:CG | 2.07 | 0.73 |
| 1:A:330:ASN:O | 1:A:331:PRO:C | 2.26 | 0.73 |
| 1:E:95:GLY:HA3 | 1:E:135:LEU:HD11 | 1.71 | 0.73 |
| 2:F:85:LEU:O | 2:F:85:LEU:HD12 | 1.88 | 0.73 |
| 1:G:333:GLN:HG2 | 1:G:342:LEU:HD13 | 1.70 | 0.73 |
| 1:A:95:GLY:HA3 | 1:A:135:LEU:HD11 | 1.69 | 0.72 |
| 1:E:62:ARG:HB3 | 1:E:63:PRO:HD3 | 1.70 | 0.72 |
| 1:A:142:ILE:HD13 | 1:A:171:PHE:HB2 | 1.69 | 0.72 |
| 1:G:151:SER:HB2 | 1:G:357:SER:HB2 | 1.71 | 0.72 |
| 1:G:184:GLN:HB2 | 1:G:398:CYS:HB3 | 1.69 | 0.72 |
| 1:A:77:VAL:HG13 | 1:A:79:VAL:HG23 | 1.71 | 0.72 |
| 1:C:151:SER:HB2 | 1:C:357:SER:HB2 | 1.71 | 0.72 |
| 1:G:365:LEU:HD13 | 1:G:404:CYS:HB2 | 1.71 | 0.72 |
| 1:G:82:LEU:HD11 | 1:G:142:ILE:HG21 | 1.70 | 0.72 |
| 1:G:221:VAL:HG22 | 1:G:226:LEU:HD11 | 1.72 | 0.72 |
| 1:G:226:LEU:C | 1:G:226:LEU:HD12 | 2.10 | 0.72 |
| 1:A:439:LEU:CD1 | 1:A:450:ILE:HD11 | 2.20 | 0.72 |
| 1:C:54:TYR:HA | 1:C:380:ASP:OD1 | 1.90 | 0.72 |
| 1:C:159:LEU:HD23 | 1:C:159:LEU:H | 1.54 | 0.71 |
| 1:A:418:PRO:HB2 | 1:A:419:GLU:OE1 | 1.88 | 0.71 |
| 1:G:142:ILE:HD13 | 1:G:171:PHE:HB2 | 1.70 | 0.71 |
| 2:H:116:ASN:H | 2:H:116:ASN:ND2 | 1.87 | 0.71 |
| 1:A:407:THR:HG23 | 1:A:408:PRO:HD2 | 1.71 | 0.71 |
| 1:G:193:ASP:HB3 | 1:G:441:ASN:HD21 | 1.54 | 0.71 |
| 1:A:333:GLN:HG2 | 1:A:342:LEU:HD13 | 1.72 | 0.71 |
| 1:E:221:VAL:HG22 | 1:E:226:LEU:HD11 | 1.72 | 0.71 |
| 1:E:303:ASN:HD22 | 1:E:305:THR:CG2 | 2.03 | 0.71 |
| 1:C:95:GLY:HA3 | 1:C:135:LEU:HD11 | 1.70 | 0.71 |
| 1:C:142:ILE:HD13 | 1:C:171:PHE:HB2 | 1.71 | 0.71 |
| 1:C:365:LEU:HD13 | 1:C:404:CYS:HB2 | 1.73 | 0.71 |
| 1:A:315:MET:O | 1:A:317:PRO:HD3 | 1.92 | 0.70 |
| 1:A:217:LEU:O | 1:A:221:VAL:HG23 | 1.91 | 0.70 |
| 2:B:85:LEU:O | 2:B:85:LEU:HD12 | 1.90 | 0.70 |
| 2:D:70:ASN:H | 2:D:72:HIS:CD2 | 2.08 | 0.70 |
| 1:G:75:SER:O | 1:G:77:VAL:N | 2.23 | 0.70 |
| 1:G:226:LEU:HD22 | 2:H:62:LEU:HD11 | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:75:SER:O | 1:C:77:VAL:N | 2.24 | 0.70 |
| 1:A:159:LEU:H | 1:A:159:LEU:HD23 | 1.57 | 0.70 |
| 1:E:226:LEU:C | 1:E:226:LEU:HD12 | 2.12 | 0.70 |
| 1:C:315:MET:O | 1:C:317:PRO:HD3 | 1.92 | 0.70 |
| 1:A:86:GLN:HA | 1:A:86:GLN:HE21 | 1.57 | 0.69 |
| 3:C:471:HOH:O | 1:E:21:ASN:HB2 | 1.92 | 0.69 |
| 1:G:29:VAL:CG1 | 1:G:291:PRO:HG2 | 2.14 | 0.69 |
| 1:E:418:PRO:HB2 | 1:E:419:GLU:OE1 | 1.92 | 0.69 |
| 1:E:54:TYR:HA | 1:E:380:ASP:OD1 | 1.91 | 0.69 |
| 1:A:303:ASN:HA | 1:C:303:ASN:HA | 1.74 | 0.69 |
| 1:C:329:THR:HG23 | 3:C:476:HOH:O | 1.91 | 0.69 |
| 1:A:80:LYS:HD2 | 1:A:84:GLU:HB2 | 1.74 | 0.69 |
| 1:A:82:LEU:O | 1:A:85:LEU:HD22 | 1.92 | 0.69 |
| 1:G:333:GLN:CG | 1:G:342:LEU:HD13 | 2.22 | 0.69 |
| 1:G:406:ASN:HD22 | 1:G:406:ASN:H | 1.40 | 0.69 |
| 1:C:281:GLU:O | 1:C:285:GLN:HG3 | 1.91 | 0.69 |
| 1:E:75:SER:O | 1:E:77:VAL:N | 2.26 | 0.69 |
| 1:E:142:ILE:HD13 | 1:E:171:PHE:HB2 | 1.73 | 0.69 |
| 1:G:82:LEU:O | 1:G:85:LEU:HD22 | 1.91 | 0.69 |
| 1:E:27:VAL:CG1 | 1:E:237:HIS:HA | 2.22 | 0.69 |
| 1:A:75:SER:O | 1:A:77:VAL:N | 2.25 | 0.69 |
| 1:G:330:ASN:O | 1:G:331:PRO:C | 2.28 | 0.69 |
| 1:G:39:PHE:CD2 | 1:G:331:PRO:HB2 | 2.27 | 0.69 |
| 1:G:340:ARG:NH1 | 1:G:397:GLU:HB3 | 2.08 | 0.69 |
| 1:C:226:LEU:C | 1:C:226:LEU:HD12 | 2.14 | 0.68 |
| 1:A:58:LEU:HD21 | 1:A:95:GLY:CA | 2.17 | 0.68 |
| 2:F:139:ALA:O | 2:F:141:VAL:N | 2.24 | 0.68 |
| 1:G:277:LYS:HE2 | 1:G:281:GLU:OE2 | 1.94 | 0.68 |
| 2:D:85:LEU:O | 2:D:85:LEU:HD12 | 1.93 | 0.68 |
| 1:A:303:ASN:HD22 | 1:A:305:THR:HG23 | 1.59 | 0.68 |
| 1:A:65:LEU:HD21 | 1:A:158:VAL:O | 1.94 | 0.68 |
| 1:E:37:GLN:HE21 | 1:E:38:PRO:CD | 2.06 | 0.68 |
| 1:A:365:LEU:HD13 | 1:A:404:CYS:HB2 | 1.75 | 0.68 |
| 1:G:159:LEU:HD23 | 1:G:159:LEU:H | 1.58 | 0.68 |
| 2:H:85:LEU:O | 2:H:85:LEU:HD12 | 1.93 | 0.68 |
| 1:E:151:SER:HB2 | 1:E:357:SER:CB | 2.24 | 0.68 |
| 1:C:306:LEU:HB3 | 1:C:307:PRO:HD3 | 1.76 | 0.68 |
| 1:E:82:LEU:O | 1:E:85:LEU:HD22 | 1.93 | 0.68 |
| 1:A:340:ARG:NH1 | 1:A:397:GLU:HB3 | 2.09 | 0.67 |
| 1:A:77:VAL:HG13 | 1:A:79:VAL:CG2 | 2.24 | 0.67 |
| 1:C:133:LEU:O | 1:C:144:LEU:HD12 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:340:ARG:NH1 | 1:C:397:GLU:HB3 | 2.07 | 0.67 |
| 1:A:37:GLN:HE21 | 1:A:38:PRO:CD | 2.07 | 0.67 |
| 1:G:82:LEU:HD21 | 1:G:142:ILE:N | 2.09 | 0.67 |
| 1:E:184:GLN:HB2 | 1:E:398:CYS:HB3 | 1.75 | 0.67 |
| 1:C:453:SER:HA | 3:C:473:HOH:O | 1.93 | 0.67 |
| 1:G:315:MET:O | 1:G:317:PRO:HD3 | 1.93 | 0.67 |
| 1:A:80:LYS:CD | 1:A:84:GLU:HB2 | 2.24 | 0.67 |
| 2:B:57:LEU:HD11 | 2:B:103:ILE:HG23 | 1.77 | 0.67 |
| 1:E:148:ILE:HA | 1:E:176:TYR:HE2 | 1.59 | 0.67 |
| 1:C:181:LEU:HD12 | 1:C:417:GLY:HA3 | 1.76 | 0.67 |
| 1:C:82:LEU:O | 1:C:85:LEU:HD22 | 1.95 | 0.67 |
| 1:E:330:ASN:O | 1:E:331:PRO:C | 2.28 | 0.67 |
| 1:E:77:VAL:HG13 | 1:E:79:VAL:HG23 | 1.76 | 0.67 |
| 1:G:97:LEU:HG | 1:G:159:LEU:HD21 | 1.77 | 0.67 |
| 2:B:68:ILE:HD12 | 2:B:68:ILE:N | 2.10 | 0.67 |
| 2:F:68:ILE:N | 2:F:68:ILE:HD12 | 2.09 | 0.66 |
| 1:C:418:PRO:HB2 | 1:C:419:GLU:OE1 | 1.94 | 0.66 |
| 1:G:80:LYS:HD2 | 1:G:84:GLU:HB2 | 1.78 | 0.66 |
| 1:G:86:GLN:HE21 | 1:G:86:GLN:HA | 1.59 | 0.66 |
| 1:C:86:GLN:HE21 | 1:C:86:GLN:HA | 1.60 | 0.66 |
| 1:E:277:LYS:HE2 | 1:E:281:GLU:OE2 | 1.93 | 0.66 |
| 1:E:406:ASN:H | 1:E:406:ASN:HD22 | 1.42 | 0.66 |
| 1:G:37:GLN:HE21 | 1:G:38:PRO:CD | 2.09 | 0.66 |
| 1:G:77:VAL:HG13 | 1:G:79:VAL:HG23 | 1.76 | 0.66 |
| 1:C:303:ASN:HD22 | 1:C:305:THR:HG23 | 1.60 | 0.66 |
| 1:C:330:ASN:O | 1:C:331:PRO:C | 2.30 | 0.66 |
| 1:E:365:LEU:HD13 | 1:E:404:CYS:HB2 | 1.76 | 0.66 |
| 1:A:27:VAL:CG1 | 1:A:237:HIS:HA | 2.25 | 0.66 |
| 1:E:39:PHE:CD2 | 1:E:331:PRO:HB2 | 2.30 | 0.66 |
| 1:G:330:ASN:O | 1:G:332:TYR:N | 2.29 | 0.66 |
| 1:G:418:PRO:HB2 | 1:G:419:GLU:OE1 | 1.95 | 0.66 |
| 1:G:430:ASP:O | 1:G:434:THR:HG23 | 1.95 | 0.66 |
| 1:A:221:VAL:HG22 | 1:A:226:LEU:HD11 | 1.77 | 0.66 |
| 2:D:139:ALA:O | 2:D:141:VAL:N | 2.25 | 0.66 |
| 1:G:417:GLY:HA3 | 1:G:421:GLN:OE1 | 1.96 | 0.66 |
| 1:A:82:LEU:HD21 | 1:A:142:ILE:N | 2.10 | 0.66 |
| 1:C:82:LEU:HD21 | 1:C:142:ILE:N | 2.10 | 0.66 |
| 1:E:226:LEU:HD22 | 2:F:62:LEU:CD1 | 2.26 | 0.66 |
| 1:A:97:LEU:HG | 1:A:159:LEU:HD21 | 1.77 | 0.66 |
| 1:E:410:PHE:HE1 | 1:E:438:CYS:HB2 | 1.61 | 0.66 |
| 2:F:57:LEU:HD11 | 2:F:103:ILE:HG23 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:319:ALA:HB1 | 1:G:325:LEU:HD22 | 1.77 | 0.66 |
| 1:A:410:PHE:HE1 | 1:A:438:CYS:HB2 | 1.61 | 0.65 |
| 1:C:184:GLN:HB2 | 1:C:398:CYS:HB3 | 1.77 | 0.65 |
| 1:E:417:GLY:HA3 | 1:E:421:GLN:OE1 | 1.96 | 0.65 |
| 1:E:430:ASP:O | 1:E:434:THR:HG23 | 1.96 | 0.65 |
| 1:A:330:ASN:O | 1:A:332:TYR:N | 2.30 | 0.65 |
| 1:G:65:LEU:HD21 | 1:G:158:VAL:O | 1.96 | 0.65 |
| 1:G:303:ASN:HD22 | 1:G:305:THR:HG23 | 1.60 | 0.65 |
| 1:A:417:GLY:HA3 | 1:A:421:GLN:OE1 | 1.97 | 0.65 |
| 1:C:37:GLN:HE21 | 1:C:38:PRO:CD | 2.08 | 0.65 |
| 2:D:69:GLN:HB2 | 2:D:72:HIS:CD2 | 2.31 | 0.65 |
| 1:A:27:VAL:HG13 | 1:A:237:HIS:HA | 1.78 | 0.65 |
| 1:C:151:SER:HB2 | 1:C:357:SER:CB | 2.27 | 0.65 |
| 1:C:142:ILE:CD1 | 1:C:171:PHE:HB2 | 2.26 | 0.65 |
| 1:G:133:LEU:O | 1:G:144:LEU:HD12 | 1.96 | 0.65 |
| 1:G:37:GLN:O | 1:G:39:PHE:N | 2.28 | 0.65 |
| 1:G:407:THR:HG23 | 1:G:408:PRO:HD2 | 1.77 | 0.65 |
| 2:H:125:ASN:O | 2:H:127:GLN:N | 2.29 | 0.65 |
| 1:C:126:TYR:HD2 | 1:C:355:TYR:HE1 | 1.44 | 0.65 |
| 1:C:37:GLN:NE2 | 1:C:37:GLN:H | 1.95 | 0.65 |
| 1:C:80:LYS:HD2 | 1:C:84:GLU:HB2 | 1.79 | 0.65 |
| 1:A:142:ILE:CD1 | 1:A:171:PHE:HB2 | 2.27 | 0.65 |
| 1:A:151:SER:HB2 | 1:A:357:SER:CB | 2.27 | 0.65 |
| 1:E:306:LEU:O | 1:E:308:GLN:N | 2.30 | 0.64 |
| 1:G:181:LEU:HD12 | 1:G:417:GLY:HA3 | 1.79 | 0.64 |
| 1:G:439:LEU:HG | 1:G:450:ILE:HD11 | 1.79 | 0.64 |
| 2:B:67:LEU:HD23 | 2:B:76:LYS:HE3 | 1.80 | 0.64 |
| 1:G:145:LYS:CE | 1:G:170:LYS:HB2 | 2.28 | 0.64 |
| 1:G:209:GLY:O | 1:G:212:LEU:HB2 | 1.97 | 0.64 |
| 2:H:57:LEU:HD11 | 2:H:103:ILE:HG23 | 1.77 | 0.64 |
| 1:A:439:LEU:HG | 1:A:450:ILE:HD11 | 1.79 | 0.64 |
| 1:C:410:PHE:HE1 | 1:C:438:CYS:HB2 | 1.63 | 0.64 |
| 1:C:65:LEU:HD21 | 1:C:158:VAL:O | 1.98 | 0.64 |
| 1:E:330:ASN:O | 1:E:332:TYR:N | 2.29 | 0.64 |
| 1:E:54:TYR:N | 3:E:477:HOH:O | 2.31 | 0.64 |
| 2:H:68:ILE:HD12 | 2:H:68:ILE:N | 2.13 | 0.64 |
| 2:H:66:SER:HB3 | 2:H:94:VAL:HG12 | 1.78 | 0.64 |
| 1:C:277:LYS:HE2 | 1:C:281:GLU:OE2 | 1.98 | 0.64 |
| 1:C:406:ASN:H | 1:C:406:ASN:HD22 | 1.45 | 0.64 |
| 1:C:97:LEU:HG | 1:C:159:LEU:HD21 | 1.79 | 0.64 |
| 1:E:154:VAL:HG11 | 1:E:355:TYR:HB2 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:410:PHE:HE1 | 1:G:438:CYS:HB2 | 1.61 | 0.64 |
| 1:A:184:GLN:HB2 | 1:A:398:CYS:HB3 | 1.78 | 0.64 |
| 1:A:406:ASN:HD22 | 1:A:406:ASN:H | 1.45 | 0.64 |
| 1:E:37:GLN:O | 1:E:39:PHE:N | 2.31 | 0.64 |
| 1:G:37:GLN:NE2 | 1:G:37:GLN:H | 1.95 | 0.64 |
| 1:A:277:LYS:HE2 | 1:A:281:GLU:OE2 | 1.98 | 0.64 |
| 1:C:77:VAL:HG13 | 1:C:79:VAL:HG23 | 1.80 | 0.64 |
| 1:C:80:LYS:CD | 1:C:84:GLU:HB2 | 2.28 | 0.64 |
| 1:G:269:GLN:O | 1:G:273:VAL:HG23 | 1.98 | 0.64 |
| 1:G:77:VAL:HG13 | 1:G:79:VAL:CG2 | 2.28 | 0.64 |
| 1:E:77:VAL:HG13 | 1:E:79:VAL:CG2 | 2.28 | 0.64 |
| 1:E:80:LYS:HD2 | 1:E:84:GLU:HB2 | 1.80 | 0.64 |
| 1:E:86:GLN:HA | 1:E:86:GLN:HE21 | 1.62 | 0.64 |
| 1:C:333:GLN:CG | 1:C:342:LEU:HD13 | 2.27 | 0.63 |
| 2:D:57:LEU:HD11 | 2:D:103:ILE:HG23 | 1.80 | 0.63 |
| 1:G:151:SER:HB2 | 1:G:357:SER:CB | 2.28 | 0.63 |
| 1:G:27:VAL:HG13 | 1:G:237:HIS:HA | 1.81 | 0.63 |
| 1:E:55:ALA:O | 1:E:59:ILE:HG13 | 1.98 | 0.63 |
| 1:A:37:GLN:O | 1:A:39:PHE:N | 2.30 | 0.63 |
| 2:B:12:GLU:O | 2:B:17:GLN:HG3 | 1.98 | 0.63 |
| 1:C:193:ASP:HB2 | 1:C:441:ASN:HD21 | 1.63 | 0.63 |
| 1:G:142:ILE:CD1 | 1:G:171:PHE:HB2 | 2.28 | 0.63 |
| 1:G:27:VAL:CG1 | 1:G:237:HIS:HA | 2.28 | 0.63 |
| 1:A:269:GLN:O | 1:A:273:VAL:HG23 | 1.98 | 0.63 |
| 1:E:419:GLU:CD | 1:E:419:GLU:H | 2.01 | 0.63 |
| 1:E:82:LEU:HD21 | 1:E:142:ILE:N | 2.12 | 0.63 |
| 1:A:407:THR:CG2 | 1:A:408:PRO:HD2 | 2.28 | 0.63 |
| 1:C:439:LEU:HG | 1:C:450:ILE:HD11 | 1.80 | 0.63 |
| 2:D:69:GLN:HB2 | 2:D:72:HIS:NE2 | 2.13 | 0.63 |
| 1:E:303:ASN:HD22 | 1:E:305:THR:HG23 | 1.61 | 0.63 |
| 1:C:209:GLY:O | 1:C:212:LEU:HB2 | 1.99 | 0.63 |
| 1:C:231:GLU:HG3 | 2:D:97:SER:OG | 1.98 | 0.63 |
| 1:A:319:ALA:HB1 | 1:A:325:LEU:HD22 | 1.80 | 0.63 |
| 1:C:27:VAL:CG1 | 1:C:237:HIS:HA | 2.28 | 0.63 |
| 2:B:70:ASN:H | 2:B:72:HIS:CD2 | 2.16 | 0.63 |
| 1:C:430:ASP:O | 1:C:434:THR:HG23 | 1.99 | 0.63 |
| 1:E:333:GLN:HG2 | 1:E:342:LEU:HD13 | 1.81 | 0.63 |
| 2:H:139:ALA:O | 2:H:141:VAL:N | 2.30 | 0.63 |
| 1:A:290:VAL:HG22 | 1:A:291:PRO:CD | 2.27 | 0.62 |
| 1:A:333:GLN:CG | 1:A:342:LEU:HD13 | 2.28 | 0.62 |
| 1:A:343:GLY:HA3 | 1:A:403:PHE:CE1 | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:181:LEU:HD12 | 1:A:417:GLY:HA3 | 1.80 | 0.62 |
| 1:C:19:ALA:HB1 | 1:E:193:ASP:H | 1.61 | 0.62 |
| 1:E:319:ALA:HB1 | 1:E:325:LEU:HD22 | 1.80 | 0.62 |
| 2:B:139:ALA:O | 2:B:141:VAL:N | 2.27 | 0.62 |
| 1:C:226:LEU:HD22 | 2:D:62:LEU:CD1 | 2.28 | 0.62 |
| 1:C:330:ASN:O | 1:C:332:TYR:N | 2.31 | 0.62 |
| 1:G:148:ILE:HA | 1:G:176:TYR:HE2 | 1.63 | 0.62 |
| 1:G:281:GLU:O | 1:G:285:GLN:HG3 | 1.99 | 0.62 |
| 1:G:80:LYS:CD | 1:G:84:GLU:HB2 | 2.29 | 0.62 |
| 1:C:193:ASP:HB2 | 1:C:441:ASN:ND2 | 2.14 | 0.62 |
| 2:D:68:ILE:N | 2:D:68:ILE:HD12 | 2.14 | 0.62 |
| 1:E:75:SER:O | 1:E:77:VAL:HG23 | 2.00 | 0.62 |
| 1:E:209:GLY:O | 1:E:212:LEU:HB2 | 2.00 | 0.62 |
| 1:E:27:VAL:HG13 | 1:E:237:HIS:HA | 1.82 | 0.62 |
| 1:E:407:THR:HG23 | 1:E:408:PRO:HD2 | 1.80 | 0.62 |
| 1:G:126:TYR:HD2 | 1:G:355:TYR:HE1 | 1.47 | 0.62 |
| 1:E:37:GLN:NE2 | 1:E:38:PRO:HD2 | 2.15 | 0.62 |
| 1:C:407:THR:OG1 | 1:C:427:THR:HB | 1.99 | 0.62 |
| 1:C:26:ARG:HG3 | 1:C:27:VAL:N | 2.15 | 0.62 |
| 1:E:333:GLN:CG | 1:E:342:LEU:HD13 | 2.30 | 0.62 |
| 2:F:66:SER:HB3 | 2:F:94:VAL:HG12 | 1.81 | 0.62 |
| 1:C:148:ILE:HA | 1:C:176:TYR:HE2 | 1.65 | 0.62 |
| 1:G:243:LEU:HD23 | 1:G:243:LEU:N | 2.14 | 0.62 |
| 1:A:419:GLU:CD | 1:A:419:GLU:H | 2.03 | 0.61 |
| 2:F:70:ASN:C | 2:F:72:HIS:H | 2.04 | 0.61 |
| 1:A:55:ALA:O | 1:A:59:ILE:HG13 | 2.00 | 0.61 |
| 1:C:65:LEU:CD2 | 1:C:158:VAL:HG12 | 2.30 | 0.61 |
| 1:E:281:GLU:O | 1:E:285:GLN:HG3 | 2.00 | 0.61 |
| 1:G:13:LEU:HD13 | 2:H:38:LYS:HD2 | 1.82 | 0.61 |
| 1:A:281:GLU:O | 1:A:285:GLN:HG3 | 2.00 | 0.61 |
| 1:C:417:GLY:HA3 | 1:C:421:GLN:OE1 | 1.99 | 0.61 |
| 1:A:37:GLN:NE2 | 1:A:37:GLN:H | 1.99 | 0.61 |
| 1:C:132:GLU:OE2 | 1:C:143:LYS:HE2 | 2.00 | 0.61 |
| 1:C:27:VAL:HG13 | 1:C:237:HIS:HA | 1.81 | 0.61 |
| 1:E:133:LEU:O | 1:E:144:LEU:HD12 | 2.00 | 0.61 |
| 1:E:65:LEU:HD21 | 1:E:158:VAL:O | 2.00 | 0.61 |
| 1:E:340:ARG:NH1 | 1:E:397:GLU:HB3 | 2.11 | 0.61 |
| 1:G:65:LEU:CD2 | 1:G:158:VAL:HG12 | 2.31 | 0.61 |
| 1:G:226:LEU:HB2 | 2:H:62:LEU:CD1 | 2.30 | 0.61 |
| 1:G:343:GLY:HA3 | 1:G:403:PHE:CE1 | 2.36 | 0.61 |
| 1:C:55:ALA:O | 1:C:59:ILE:HG13 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:65:LEU:HD23 | 1:G:159:LEU:O | 1.99 | 0.61 |
| 1:A:226:LEU:HD22 | 2:B:62:LEU:CD1 | 2.29 | 0.61 |
| 1:C:193:ASP:H | 1:E:19:ALA:HB1 | 1.65 | 0.61 |
| 1:C:319:ALA:HB1 | 1:C:325:LEU:HD22 | 1.83 | 0.61 |
| 2:D:116:ASN:ND2 | 2:D:116:ASN:N | 2.45 | 0.61 |
| 1:G:439:LEU:CG | 1:G:450:ILE:HD11 | 2.31 | 0.61 |
| 1:C:439:LEU:CG | 1:C:450:ILE:HD11 | 2.30 | 0.61 |
| 1:G:37:GLN:NE2 | 1:G:38:PRO:HD2 | 2.16 | 0.61 |
| 1:G:55:ALA:O | 1:G:59:ILE:HG13 | 2.01 | 0.61 |
| 2:D:125:ASN:O | 2:D:127:GLN:N | 2.33 | 0.61 |
| 1:G:133:LEU:HD21 | 1:G:150:VAL:HG13 | 1.83 | 0.61 |
| 2:B:111:SER:O | 2:B:114:LEU:HB2 | 2.00 | 0.61 |
| 1:G:290:VAL:HG22 | 1:G:291:PRO:CD | 2.31 | 0.61 |
| 1:C:221:VAL:HG22 | 1:C:226:LEU:HD11 | 1.83 | 0.60 |
| 1:C:39:PHE:CD2 | 1:C:331:PRO:HB2 | 2.36 | 0.60 |
| 1:C:97:LEU:HD22 | 1:C:133:LEU:HB3 | 1.83 | 0.60 |
| 1:G:154:VAL:HG11 | 1:G:355:TYR:HB2 | 1.83 | 0.60 |
| 1:A:209:GLY:O | 1:A:212:LEU:HB2 | 2.00 | 0.60 |
| 1:E:145:LYS:CE | 1:E:170:LYS:HB2 | 2.31 | 0.60 |
| 1:G:406:ASN:ND2 | 1:G:406:ASN:N | 2.50 | 0.60 |
| 2:H:67:LEU:HD23 | 2:H:76:LYS:HE3 | 1.82 | 0.60 |
| 1:A:290:VAL:CG2 | 1:A:291:PRO:HD2 | 2.31 | 0.60 |
| 1:A:39:PHE:CD2 | 1:A:331:PRO:HB2 | 2.37 | 0.60 |
| 1:E:97:LEU:HG | 1:E:159:LEU:HD21 | 1.83 | 0.60 |
| 1:G:193:ASP:HB2 | 1:G:441:ASN:ND2 | 2.17 | 0.60 |
| 1:C:58:LEU:HD21 | 1:C:95:GLY:CA | 2.17 | 0.60 |
| 1:E:315:MET:O | 1:E:317:PRO:HD3 | 2.02 | 0.60 |
| 1:E:343:GLY:HA3 | 1:E:403:PHE:CE1 | 2.36 | 0.60 |
| 1:E:142:ILE:CD1 | 1:E:171:PHE:HB2 | 2.32 | 0.60 |
| 1:G:37:GLN:C | 1:G:39:PHE:H | 2.05 | 0.60 |
| 1:A:148:ILE:HA | 1:A:176:TYR:HE2 | 1.66 | 0.60 |
| 1:A:126:TYR:HD2 | 1:A:355:TYR:HE1 | 1.49 | 0.60 |
| 1:E:68:ARG:HG3 | 1:E:179:ALA:HA | 1.84 | 0.60 |
| 1:G:193:ASP:HB2 | 1:G:441:ASN:HD21 | 1.66 | 0.60 |
| 2:D:66:SER:HB3 | 2:D:94:VAL:HG12 | 1.83 | 0.60 |
| 1:A:-1:HIS:ND1 | 1:A:0:GLY:N | 2.50 | 0.60 |
| 1:E:58:LEU:HD21 | 1:E:95:GLY:CA | 2.17 | 0.60 |
| 1:G:226:LEU:HD22 | 2:H:62:LEU:CD1 | 2.32 | 0.60 |
| 1:G:306:LEU:O | 1:G:308:GLN:N | 2.35 | 0.60 |
| 2:H:116:ASN:N | 2:H:116:ASN:ND2 | 2.48 | 0.60 |
| 1:C:286:LEU:HB3 | 1:C:292:VAL:HG21 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:65:LEU:HD23 | 1:E:159:LEU:O | 2.02 | 0.60 |
| 1:A:5:GLN:O | 1:A:8:GLN:HB2 | 2.02 | 0.59 |
| 1:G:439:LEU:HG | 1:G:450:ILE:CD1 | 2.32 | 0.59 |
| 1:A:226:LEU:CD1 | 1:A:226:LEU:C | 2.70 | 0.59 |
| 1:C:133:LEU:HD21 | 1:C:150:VAL:HG13 | 1.84 | 0.59 |
| 1:A:314:CYS:SG | 1:C:315:MET:HG2 | 2.42 | 0.59 |
| 1:E:193:ASP:OD2 | 1:E:193:ASP:N | 2.34 | 0.59 |
| 1:E:231:GLU:HG3 | 2:F:97:SER:OG | 2.03 | 0.59 |
| 1:E:193:ASP:HB2 | 1:E:441:ASN:ND2 | 2.17 | 0.59 |
| 2:D:70:ASN:C | 2:D:72:HIS:H | 2.05 | 0.59 |
| 1:G:380:ASP:O | 1:G:381:THR:HG23 | 2.03 | 0.59 |
| 1:A:133:LEU:O | 1:A:144:LEU:HD12 | 2.02 | 0.59 |
| 1:A:154:VAL:HG11 | 1:A:355:TYR:HB2 | 1.84 | 0.59 |
| 1:A:37:GLN:C | 1:A:39:PHE:H | 2.06 | 0.59 |
| 1:C:13:LEU:HD13 | 2:D:38:LYS:HD2 | 1.84 | 0.59 |
| 1:E:37:GLN:H | 1:E:37:GLN:NE2 | 2.00 | 0.59 |
| 1:G:68:ARG:HG3 | 1:G:179:ALA:HA | 1.85 | 0.59 |
| 2:B:66:SER:HB3 | 2:B:94:VAL:CG1 | 2.32 | 0.59 |
| 1:C:101:MET:HB2 | 1:C:128:HIS:CG | 2.38 | 0.59 |
| 1:E:80:LYS:CD | 1:E:84:GLU:HB2 | 2.32 | 0.59 |
| 1:A:430:ASP:O | 1:A:434:THR:HG23 | 2.03 | 0.58 |
| 1:A:439:LEU:HG | 1:A:450:ILE:CD1 | 2.33 | 0.58 |
| 2:B:125:ASN:O | 2:B:127:GLN:N | 2.36 | 0.58 |
| 1:E:82:LEU:HD11 | 1:E:142:ILE:HG22 | 1.83 | 0.58 |
| 1:A:348:ASN:CB | 1:A:375:SER:HB2 | 2.32 | 0.58 |
| 1:A:439:LEU:CG | 1:A:450:ILE:HD11 | 2.33 | 0.58 |
| 1:C:193:ASP:N | 1:C:193:ASP:OD2 | 2.36 | 0.58 |
| 1:G:419:GLU:CD | 1:G:419:GLU:H | 2.06 | 0.58 |
| 1:C:407:THR:O | 1:C:429:PRO:HA | 2.03 | 0.58 |
| 1:C:77:VAL:HG13 | 1:C:79:VAL:CG2 | 2.33 | 0.58 |
| 1:E:217:LEU:O | 1:E:221:VAL:HG23 | 2.03 | 0.58 |
| 2:F:64:SER:OG | 2:F:97:SER:HB2 | 2.03 | 0.58 |
| 1:G:407:THR:CG2 | 1:G:408:PRO:HD2 | 2.33 | 0.58 |
| 1:A:407:THR:OG1 | 1:A:427:THR:HB | 2.03 | 0.58 |
| 1:C:406:ASN:N | 1:C:406:ASN:ND2 | 2.51 | 0.58 |
| 1:E:133:LEU:HD21 | 1:E:150:VAL:HG13 | 1.85 | 0.58 |
| 1:A:185:LYS:HE3 | 1:A:397:GLU:OE2 | 2.04 | 0.58 |
| 1:G:274:GLU:O | 1:G:277:LYS:HB3 | 2.03 | 0.58 |
| 1:C:269:GLN:O | 1:C:273:VAL:HG23 | 2.04 | 0.58 |
| 1:E:286:LEU:HB3 | 1:E:292:VAL:HG21 | 1.86 | 0.58 |
| 1:E:193:ASP:HB2 | 1:E:441:ASN:HD21 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:97:LEU:HD22 | 1:E:133:LEU:HB3 | 1.85 | 0.58 |
| 1:A:97:LEU:HD22 | 1:A:133:LEU:HB3 | 1.84 | 0.58 |
| 1:G:26:ARG:HG3 | 1:G:27:VAL:N | 2.18 | 0.58 |
| 1:G:82:LEU:HD11 | 1:G:142:ILE:HG22 | 1.85 | 0.58 |
| 2:F:125:ASN:O | 2:F:127:GLN:N | 2.37 | 0.58 |
| 1:A:101:MET:HB2 | 1:A:128:HIS:CG | 2.39 | 0.58 |
| 1:A:226:LEU:HB2 | 2:B:62:LEU:CD1 | 2.34 | 0.58 |
| 1:E:274:GLU:O | 1:E:277:LYS:HB3 | 2.04 | 0.58 |
| 1:E:343:GLY:HA3 | 1:E:403:PHE:CD1 | 2.39 | 0.58 |
| 1:A:193:ASP:HB2 | 1:A:441:ASN:ND2 | 2.19 | 0.58 |
| 1:C:306:LEU:HD12 | 1:C:306:LEU:O | 2.03 | 0.58 |
| 1:C:419:GLU:H | 1:C:419:GLU:CD | 2.07 | 0.58 |
| 1:E:226:LEU:HB2 | 2:F:62:LEU:CD1 | 2.34 | 0.58 |
| 1:A:132:GLU:OE2 | 1:A:143:LYS:HE2 | 2.04 | 0.57 |
| 1:C:145:LYS:CE | 1:C:170:LYS:HB2 | 2.34 | 0.57 |
| 1:C:154:VAL:HG11 | 1:C:355:TYR:HB2 | 1.85 | 0.57 |
| 1:G:297:GLY:N | 1:G:300:ASP:OD2 | 2.37 | 0.57 |
| 1:G:371:VAL:O | 1:G:371:VAL:HG12 | 2.04 | 0.57 |
| 1:A:37:GLN:NE2 | 1:A:38:PRO:HD2 | 2.17 | 0.57 |
| 1:A:83:CYS:HA | 1:A:140:GLN:HE22 | 1.70 | 0.57 |
| 1:E:290:VAL:HG22 | 1:E:291:PRO:CD | 2.34 | 0.57 |
| 1:G:154:VAL:HG12 | 1:G:155:THR:N | 2.19 | 0.57 |
| 1:G:286:LEU:HB3 | 1:G:292:VAL:HG21 | 1.85 | 0.57 |
| 1:C:330:ASN:CB | 1:C:331:PRO:HD3 | 2.29 | 0.57 |
| 1:E:407:THR:O | 1:E:429:PRO:HA | 2.05 | 0.57 |
| 1:E:181:LEU:HD12 | 1:E:417:GLY:HA3 | 1.86 | 0.57 |
| 1:C:290:VAL:HG22 | 1:C:291:PRO:CD | 2.34 | 0.57 |
| 1:C:65:LEU:HD21 | 1:C:158:VAL:HG12 | 1.87 | 0.57 |
| 1:G:101:MET:HB2 | 1:G:128:HIS:CG | 2.40 | 0.57 |
| 1:G:200:SER:HB3 | 1:G:428:VAL:HG12 | 1.86 | 0.57 |
| 1:A:193:ASP:OD2 | 1:A:193:ASP:N | 2.38 | 0.57 |
| 1:A:193:ASP:HB2 | 1:A:441:ASN:HD21 | 1.69 | 0.57 |
| 1:G:343:GLY:HA3 | 1:G:403:PHE:CD1 | 2.39 | 0.57 |
| 1:C:297:GLY:N | 1:C:300:ASP:OD2 | 2.37 | 0.57 |
| 1:C:439:LEU:HG | 1:C:450:ILE:CD1 | 2.34 | 0.57 |
| 1:A:226:LEU:HD12 | 1:A:226:LEU:O | 2.03 | 0.57 |
| 1:A:24:PHE:CZ | 1:A:233:CYS:HB2 | 2.40 | 0.57 |
| 1:A:36:SER:HB3 | 1:A:333:GLN:H | 1.69 | 0.57 |
| 1:C:343:GLY:HA3 | 1:C:403:PHE:CE1 | 2.40 | 0.57 |
| 1:E:126:TYR:HD2 | 1:E:355:TYR:HE1 | 1.51 | 0.57 |
| 1:E:224:GLY:HA3 | 2:F:135:ILE:HG13 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:37:GLN:C | 1:E:39:PHE:H | 2.09 | 0.57 |
| 1:E:65:LEU:CD2 | 1:E:158:VAL:HG12 | 2.34 | 0.57 |
| 2:H:70:ASN:C | 2:H:72:HIS:H | 2.09 | 0.57 |
| 1:A:343:GLY:HA3 | 1:A:403:PHE:CD1 | 2.40 | 0.56 |
| 2:B:70:ASN:HB2 | 2:B:72:HIS:CE1 | 2.40 | 0.56 |
| 1:C:37:GLN:N | 1:C:38:PRO:HD2 | 2.20 | 0.56 |
| 1:C:82:LEU:HD11 | 1:C:142:ILE:HG22 | 1.85 | 0.56 |
| 1:E:26:ARG:HG3 | 1:E:27:VAL:N | 2.20 | 0.56 |
| 1:A:231:GLU:HG3 | 2:B:97:SER:OG | 2.04 | 0.56 |
| 1:A:303:ASN:HD22 | 1:A:305:THR:HG22 | 1.70 | 0.56 |
| 1:A:407:THR:O | 1:A:429:PRO:HA | 2.05 | 0.56 |
| 1:A:65:LEU:CD2 | 1:A:158:VAL:HG12 | 2.35 | 0.56 |
| 1:G:97:LEU:HD22 | 1:G:133:LEU:HB3 | 1.87 | 0.56 |
| 1:E:269:GLN:O | 1:E:273:VAL:HG23 | 2.04 | 0.56 |
| 1:C:145:LYS:HE2 | 1:C:168:ASP:OD1 | 2.05 | 0.56 |
| 1:E:360:ASP:OD2 | 1:E:362:LEU:HB3 | 2.05 | 0.56 |
| 2:F:111:SER:O | 2:F:114:LEU:HB2 | 2.04 | 0.56 |
| 1:A:65:LEU:HD23 | 1:A:159:LEU:O | 2.04 | 0.56 |
| 1:C:348:ASN:HB2 | 1:C:375:SER:HB2 | 1.86 | 0.56 |
| 1:E:36:SER:HB3 | 1:E:333:GLN:H | 1.71 | 0.56 |
| 2:B:6:TYR:HA | 2:B:9:ASN:HD22 | 1.71 | 0.56 |
| 1:C:37:GLN:O | 1:C:39:PHE:N | 2.38 | 0.56 |
| 1:E:243:LEU:N | 1:E:243:LEU:HD23 | 2.20 | 0.56 |
| 1:E:313:PRO:HB2 | 1:G:273:VAL:HG22 | 1.88 | 0.56 |
| 1:G:348:ASN:CB | 1:G:375:SER:HB2 | 2.35 | 0.56 |
| 2:H:12:GLU:O | 2:H:17:GLN:HG3 | 2.06 | 0.56 |
| 1:C:37:GLN:C | 1:C:39:PHE:H | 2.09 | 0.56 |
| 2:D:111:SER:O | 2:D:114:LEU:HB2 | 2.06 | 0.56 |
| 1:G:193:ASP:OD2 | 1:G:193:ASP:N | 2.39 | 0.56 |
| 1:C:14:LEU:HD11 | 2:D:98:ILE:CG2 | 2.36 | 0.56 |
| 2:D:64:SER:OG | 2:D:97:SER:HB2 | 2.06 | 0.56 |
| 2:F:67:LEU:HD23 | 2:F:76:LYS:HE3 | 1.86 | 0.56 |
| 1:A:348:ASN:HB2 | 1:A:375:SER:HB2 | 1.87 | 0.56 |
| 1:A:75:SER:O | 1:A:77:VAL:HG23 | 2.06 | 0.56 |
| 1:C:393:PHE:N | 1:C:393:PHE:CD2 | 2.72 | 0.56 |
| 2:D:45:VAL:HG23 | 2:D:46:GLU:N | 2.21 | 0.56 |
| 2:F:66:SER:HB3 | 2:F:94:VAL:CG1 | 2.36 | 0.56 |
| 1:G:99:LYS:N | 1:G:155:THR:HG23 | 2.16 | 0.56 |
| 1:G:407:THR:O | 1:G:429:PRO:HA | 2.06 | 0.56 |
| 1:A:77:VAL:CG1 | 1:A:79:VAL:HB | 2.36 | 0.55 |
| 1:A:82:LEU:HD11 | 1:A:142:ILE:HG22 | 1.85 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:407:THR:HG23 | 1:C:408:PRO:HD2 | 1.87 | 0.55 |
| 1:A:145:LYS:CE | 1:A:170:LYS:HB2 | 2.35 | 0.55 |
| 1:E:410:PHE:CE1 | 1:E:438:CYS:HB2 | 2.41 | 0.55 |
| 1:E:419:GLU:CD | 1:E:419:GLU:N | 2.59 | 0.55 |
| 1:G:132:GLU:OE2 | 1:G:143:LYS:HE2 | 2.06 | 0.55 |
| 1:A:306:LEU:O | 1:A:306:LEU:HD12 | 2.06 | 0.55 |
| 2:B:6:TYR:CD1 | 2:B:40:MET:HG2 | 2.40 | 0.55 |
| 1:C:199:VAL:HG12 | 1:C:200:SER:N | 2.22 | 0.55 |
| 1:C:348:ASN:CB | 1:C:375:SER:HB2 | 2.36 | 0.55 |
| 1:A:193:ASP:C | 1:A:194:ARG:HD3 | 2.26 | 0.55 |
| 1:A:26:ARG:HG3 | 1:A:27:VAL:N | 2.21 | 0.55 |
| 1:C:26:ARG:HG3 | 1:C:27:VAL:H | 1.71 | 0.55 |
| 2:F:58:HIS:CE1 | 2:F:107:MET:HB2 | 2.41 | 0.55 |
| 1:G:410:PHE:CE1 | 1:G:438:CYS:HB2 | 2.41 | 0.55 |
| 1:G:65:LEU:HD21 | 1:G:158:VAL:HG12 | 1.86 | 0.55 |
| 2:H:58:HIS:CE1 | 2:H:107:MET:HB2 | 2.41 | 0.55 |
| 1:A:306:LEU:O | 1:A:308:GLN:N | 2.38 | 0.55 |
| 1:C:99:LYS:N | 1:C:155:THR:HG23 | 2.18 | 0.55 |
| 1:C:37:GLN:NE2 | 1:C:38:PRO:HD2 | 2.18 | 0.55 |
| 2:D:2:ALA:O | 2:D:5:LEU:HB3 | 2.06 | 0.55 |
| 1:E:37:GLN:N | 1:E:38:PRO:HD2 | 2.21 | 0.55 |
| 1:G:185:LYS:HE3 | 1:G:397:GLU:OE2 | 2.07 | 0.55 |
| 1:G:330:ASN:CB | 1:G:331:PRO:HD3 | 2.32 | 0.55 |
| 1:A:68:ARG:HG3 | 1:A:179:ALA:HA | 1.89 | 0.55 |
| 1:C:284:LEU:HD22 | 1:C:318:LEU:HB3 | 1.89 | 0.55 |
| 1:C:330:ASN:CB | 1:C:331:PRO:CD | 2.84 | 0.55 |
| 1:C:5:GLN:O | 1:C:8:GLN:HB2 | 2.07 | 0.55 |
| 1:C:19:ALA:HB2 | 1:E:443:ARG:CZ | 2.37 | 0.55 |
| 2:F:24:LYS:O | 2:F:27:SER:HB3 | 2.06 | 0.55 |
| 1:C:14:LEU:HD11 | 2:D:98:ILE:HG22 | 1.89 | 0.55 |
| 1:A:274:GLU:O | 1:A:277:LYS:HB3 | 2.07 | 0.55 |
| 1:A:37:GLN:N | 1:A:38:PRO:HD2 | 2.21 | 0.55 |
| 1:C:99:LYS:HE2 | 1:C:150:VAL:HG12 | 1.89 | 0.55 |
| 1:C:154:VAL:HG12 | 1:C:155:THR:N | 2.20 | 0.55 |
| 1:C:226:LEU:HB2 | 2:D:62:LEU:CD1 | 2.37 | 0.55 |
| 2:D:67:LEU:HD23 | 2:D:76:LYS:HE3 | 1.89 | 0.55 |
| 2:D:70:ASN:HB2 | 2:D:72:HIS:CE1 | 2.42 | 0.55 |
| 1:E:279:LEU:HD12 | 1:E:279:LEU:O | 2.07 | 0.55 |
| 1:E:393:PHE:CD2 | 1:E:393:PHE:N | 2.73 | 0.55 |
| 1:G:77:VAL:CG1 | 1:G:79:VAL:HB | 2.36 | 0.55 |
| 1:G:451:SER:HB2 | 2:H:76:LYS:HD3 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:199:VAL:HG12 | 1:G:200:SER:N | 2.22 | 0.55 |
| 1:E:13:LEU:HD13 | 2:F:38:LYS:HD2 | 1.89 | 0.54 |
| 1:E:5:GLN:O | 1:E:8:GLN:HB2 | 2.07 | 0.54 |
| 1:C:21:ASN:H | 1:E:237:HIS:CE1 | 2.24 | 0.54 |
| 1:C:343:GLY:HA3 | 1:C:403:PHE:CD1 | 2.42 | 0.54 |
| 1:C:360:ASP:OD2 | 1:C:362:LEU:HB3 | 2.07 | 0.54 |
| 2:D:6:TYR:HA | 2:D:9:ASN:HD22 | 1.72 | 0.54 |
| 1:E:204:LEU:HD12 | 1:E:279:LEU:HB2 | 1.89 | 0.54 |
| 1:E:373:HIS:HA | 1:E:393:PHE:O | 2.07 | 0.54 |
| 1:E:77:VAL:CG1 | 1:E:79:VAL:HB | 2.37 | 0.54 |
| 1:G:226:LEU:C | 1:G:226:LEU:CD1 | 2.76 | 0.54 |
| 1:G:290:VAL:CG2 | 1:G:291:PRO:HD2 | 2.34 | 0.54 |
| 1:A:133:LEU:HD21 | 1:A:150:VAL:HG13 | 1.88 | 0.54 |
| 1:C:279:LEU:O | 1:C:279:LEU:HD12 | 2.06 | 0.54 |
| 1:C:226:LEU:HD13 | 2:D:62:LEU:HD11 | 1.89 | 0.54 |
| 1:C:36:SER:HB3 | 1:C:333:GLN:H | 1.72 | 0.54 |
| 1:E:228:ASP:OD1 | 1:E:229:GLU:N | 2.39 | 0.54 |
| 1:E:303:ASN:HB2 | 1:E:305:THR:HG22 | 1.90 | 0.54 |
| 1:E:380:ASP:O | 1:E:381:THR:HG23 | 2.08 | 0.54 |
| 1:E:68:ARG:O | 1:E:72:HIS:HB2 | 2.07 | 0.54 |
| 1:G:68:ARG:O | 1:G:72:HIS:HB2 | 2.07 | 0.54 |
| 1:A:145:LYS:HE2 | 1:A:168:ASP:OD1 | 2.07 | 0.54 |
| 1:A:68:ARG:O | 1:A:72:HIS:HB2 | 2.07 | 0.54 |
| 2:B:58:HIS:CE1 | 2:B:107:MET:HB2 | 2.42 | 0.54 |
| 1:E:410:PHE:HA | 1:E:429:PRO:HD3 | 1.90 | 0.54 |
| 1:G:279:LEU:O | 1:G:279:LEU:HD12 | 2.08 | 0.54 |
| 1:G:303:ASN:HD22 | 1:G:305:THR:HG22 | 1.73 | 0.54 |
| 1:A:286:LEU:HB3 | 1:A:292:VAL:HG21 | 1.90 | 0.54 |
| 1:A:297:GLY:N | 1:A:300:ASP:OD2 | 2.41 | 0.54 |
| 1:A:380:ASP:O | 1:A:381:THR:HG23 | 2.07 | 0.54 |
| 1:A:65:LEU:HD21 | 1:A:158:VAL:C | 2.27 | 0.54 |
| 1:E:290:VAL:CG2 | 1:E:291:PRO:HD2 | 2.37 | 0.54 |
| 1:E:371:VAL:HG12 | 1:E:371:VAL:O | 2.07 | 0.54 |
| 1:A:154:VAL:HG12 | 1:A:155:THR:N | 2.23 | 0.54 |
| 1:A:243:LEU:N | 1:A:243:LEU:HD23 | 2.23 | 0.54 |
| 1:C:380:ASP:O | 1:C:381:THR:HG23 | 2.06 | 0.54 |
| 1:E:407:THR:CG2 | 1:E:408:PRO:HD2 | 2.38 | 0.54 |
| 1:A:360:ASP:OD2 | 1:A:362:LEU:HB3 | 2.08 | 0.54 |
| 1:A:373:HIS:HA | 1:A:393:PHE:O | 2.07 | 0.54 |
| 1:C:303:ASN:HB2 | 1:C:305:THR:HG22 | 1.89 | 0.54 |
| 2:D:58:HIS:CE1 | 2:D:107:MET:HB2 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:399:PRO:O | 1:E:423:VAL:HG22 | 2.06 | 0.54 |
| 1:G:82:LEU:HD13 | 1:G:93:VAL:HG11 | 1.89 | 0.54 |
| 2:H:6:TYR:CD1 | 2:H:40:MET:HG2 | 2.43 | 0.54 |
| 1:C:224:GLY:HA3 | 2:D:135:ILE:HG13 | 1.90 | 0.54 |
| 1:E:193:ASP:C | 1:E:194:ARG:HD3 | 2.27 | 0.54 |
| 1:G:-2:HIS:O | 1:G:-1:HIS:HB2 | 2.08 | 0.54 |
| 1:C:306:LEU:O | 1:C:308:GLN:N | 2.39 | 0.54 |
| 1:E:98:PHE:HA | 1:E:155:THR:HG22 | 1.88 | 0.54 |
| 1:E:163:GLY:HA3 | 1:E:172:LEU:O | 2.08 | 0.54 |
| 1:E:303:ASN:HA | 1:G:303:ASN:HA | 1.90 | 0.54 |
| 1:G:224:GLY:HA3 | 2:H:135:ILE:HG13 | 1.90 | 0.54 |
| 1:A:406:ASN:N | 1:A:406:ASN:ND2 | 2.53 | 0.53 |
| 1:C:68:ARG:HG3 | 1:C:179:ALA:HA | 1.90 | 0.53 |
| 1:C:26:ARG:NH1 | 1:C:289:SER:O | 2.40 | 0.53 |
| 1:C:57:ARG:NH2 | 1:C:378:ALA:O | 2.41 | 0.53 |
| 1:E:101:MET:HB2 | 1:E:128:HIS:CG | 2.42 | 0.53 |
| 2:F:12:GLU:O | 2:F:17:GLN:HG3 | 2.07 | 0.53 |
| 1:G:360:ASP:OD2 | 1:G:362:LEU:HB3 | 2.08 | 0.53 |
| 1:C:61:MET:HE3 | 1:C:158:VAL:HB | 1.89 | 0.53 |
| 1:C:243:LEU:N | 1:C:243:LEU:HD23 | 2.24 | 0.53 |
| 1:G:393:PHE:N | 1:G:393:PHE:CD2 | 2.73 | 0.53 |
| 2:H:111:SER:O | 2:H:114:LEU:HB2 | 2.08 | 0.53 |
| 1:A:419:GLU:CD | 1:A:419:GLU:N | 2.61 | 0.53 |
| 1:A:82:LEU:HD13 | 1:A:93:VAL:HG11 | 1.89 | 0.53 |
| 1:C:346:GLY:CA | 1:C:405:GLY:HA3 | 2.39 | 0.53 |
| 1:E:407:THR:OG1 | 1:E:427:THR:HB | 2.07 | 0.53 |
| 1:G:65:LEU:HD21 | 1:G:158:VAL:C | 2.29 | 0.53 |
| 1:G:307:PRO:HG3 | 1:G:393:PHE:CZ | 2.43 | 0.53 |
| 1:A:303:ASN:ND2 | 1:A:308:GLN:HA | 2.22 | 0.53 |
| 1:C:26:ARG:CG | 1:C:27:VAL:N | 2.72 | 0.53 |
| 1:C:98:PHE:HA | 1:C:155:THR:HG22 | 1.91 | 0.53 |
| 1:E:83:CYS:HA | 1:E:140:GLN:HE22 | 1.72 | 0.53 |
| 1:G:29:VAL:HG11 | 1:G:291:PRO:CG | 2.18 | 0.53 |
| 2:H:45:VAL:HG23 | 2:H:46:GLU:N | 2.22 | 0.53 |
| 1:C:163:GLY:HA3 | 1:C:172:LEU:O | 2.08 | 0.53 |
| 1:C:266:LYS:HG3 | 1:C:267:LYS:HG3 | 1.91 | 0.53 |
| 1:C:77:VAL:CG1 | 1:C:79:VAL:HB | 2.38 | 0.53 |
| 2:F:6:TYR:HA | 2:F:9:ASN:HD22 | 1.74 | 0.53 |
| 1:G:83:CYS:HA | 1:G:140:GLN:HE22 | 1.73 | 0.53 |
| 1:G:99:LYS:HE2 | 1:G:150:VAL:HG12 | 1.90 | 0.53 |
| 2:H:52:ASN:CB | 2:H:55:ALA:HB2 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:57:ARG:NH2 | 1:A:378:ALA:O | 2.42 | 0.53 |
| 1:C:290:VAL:CG2 | 1:C:291:PRO:HD2 | 2.38 | 0.53 |
| 1:C:371:VAL:O | 1:C:371:VAL:HG12 | 2.08 | 0.53 |
| 1:C:83:CYS:HA | 1:C:140:GLN:HE22 | 1.73 | 0.53 |
| 1:E:226:LEU:C | 1:E:226:LEU:CD1 | 2.76 | 0.53 |
| 2:F:23:TYR:CD1 | 2:F:38:LYS:HE2 | 2.44 | 0.53 |
| 1:A:212:LEU:O | 1:A:215:THR:N | 2.42 | 0.53 |
| 1:E:65:LEU:HD21 | 1:E:158:VAL:HG12 | 1.90 | 0.53 |
| 2:F:2:ALA:O | 2:F:5:LEU:HB3 | 2.09 | 0.53 |
| 1:A:438:CYS:SG | 1:A:439:LEU:N | 2.82 | 0.53 |
| 1:C:439:LEU:HD12 | 1:C:450:ILE:HD11 | 1.91 | 0.53 |
| 1:G:330:ASN:CB | 1:G:331:PRO:CD | 2.87 | 0.53 |
| 2:H:125:ASN:C | 2:H:127:GLN:N | 2.62 | 0.53 |
| 1:A:351:ASP:HA | 1:A:354:ARG:HD2 | 1.90 | 0.53 |
| 2:B:52:ASN:CB | 2:B:55:ALA:HB2 | 2.39 | 0.53 |
| 1:C:75:SER:O | 1:C:77:VAL:HG23 | 2.09 | 0.53 |
| 1:E:193:ASP:CB | 1:E:441:ASN:ND2 | 2.67 | 0.53 |
| 1:A:199:VAL:HG12 | 1:A:200:SER:N | 2.23 | 0.52 |
| 1:A:266:LYS:HG3 | 1:A:267:LYS:HG3 | 1.91 | 0.52 |
| 1:A:279:LEU:HD12 | 1:A:279:LEU:O | 2.08 | 0.52 |
| 1:E:197:LEU:HD21 | 1:E:218:LEU:HD11 | 1.90 | 0.52 |
| 1:E:212:LEU:O | 1:E:215:THR:N | 2.42 | 0.52 |
| 1:E:269:GLN:NE2 | 1:G:320:THR:HB | 2.24 | 0.52 |
| 2:H:66:SER:HB3 | 2:H:94:VAL:CG1 | 2.40 | 0.52 |
| 1:A:99:LYS:N | 1:A:155:THR:HG23 | 2.17 | 0.52 |
| 1:A:303:ASN:HB2 | 1:A:305:THR:HG22 | 1.91 | 0.52 |
| 2:B:23:TYR:CD2 | 2:B:24:LYS:N | 2.77 | 0.52 |
| 1:A:193:ASP:CB | 1:A:441:ASN:ND2 | 2.69 | 0.52 |
| 1:C:419:GLU:N | 1:C:419:GLU:CD | 2.63 | 0.52 |
| 1:C:200:SER:HB3 | 1:C:428:VAL:HG12 | 1.92 | 0.52 |
| 1:E:297:GLY:N | 1:E:300:ASP:OD2 | 2.43 | 0.52 |
| 1:E:439:LEU:HD12 | 1:E:450:ILE:HD11 | 1.89 | 0.52 |
| 1:E:98:PHE:HA | 1:E:155:THR:CG2 | 2.39 | 0.52 |
| 2:D:12:GLU:O | 2:D:17:GLN:HG3 | 2.10 | 0.52 |
| 1:G:37:GLN:N | 1:G:38:PRO:HD2 | 2.24 | 0.52 |
| 1:E:303:ASN:ND2 | 1:E:308:GLN:HA | 2.24 | 0.52 |
| 1:E:315:MET:HG2 | 1:G:314:CYS:SG | 2.49 | 0.52 |
| 2:F:10:ILE:O | 2:F:14:VAL:HG23 | 2.10 | 0.52 |
| 1:G:303:ASN:HB2 | 1:G:305:THR:HG22 | 1.90 | 0.52 |
| 1:G:407:THR:OG1 | 1:G:427:THR:HB | 2.09 | 0.52 |
| 1:G:58:LEU:HD21 | 1:G:95:GLY:CA | 2.19 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:122:LEU:O | 2:B:125:ASN:N | 2.38 | 0.52 |
| 1:C:274:GLU:O | 1:C:277:LYS:HB3 | 2.09 | 0.52 |
| 1:C:82:LEU:HD13 | 1:C:93:VAL:HG11 | 1.91 | 0.52 |
| 1:E:148:ILE:HA | 1:E:176:TYR:CE2 | 2.42 | 0.52 |
| 1:E:395:PHE:H | 1:E:395:PHE:HD1 | 1.58 | 0.52 |
| 1:G:395:PHE:HD1 | 1:G:395:PHE:H | 1.58 | 0.52 |
| 1:A:212:LEU:O | 1:A:213:LEU:C | 2.46 | 0.52 |
| 1:A:371:VAL:O | 1:A:371:VAL:HG12 | 2.09 | 0.52 |
| 1:C:193:ASP:C | 1:C:194:ARG:HD3 | 2.30 | 0.52 |
| 1:C:68:ARG:O | 1:C:72:HIS:HB2 | 2.09 | 0.52 |
| 1:E:348:ASN:CB | 1:E:375:SER:HB2 | 2.40 | 0.52 |
| 2:F:41:LEU:HD22 | 2:F:103:ILE:HD12 | 1.90 | 0.52 |
| 1:G:21:ASN:OD1 | 2:H:36:GLN:HB2 | 2.10 | 0.52 |
| 1:A:200:SER:HB3 | 1:A:428:VAL:HG12 | 1.91 | 0.52 |
| 1:A:14:LEU:HD11 | 2:B:98:ILE:HG22 | 1.92 | 0.52 |
| 1:C:225:GLN:HE21 | 2:D:133:SER:HB2 | 1.74 | 0.52 |
| 1:E:99:LYS:N | 1:E:155:THR:HG23 | 2.17 | 0.52 |
| 1:A:26:ARG:HD3 | 1:A:290:VAL:HG23 | 1.91 | 0.52 |
| 1:A:459:ASP:C | 1:A:461:ASP:H | 2.11 | 0.52 |
| 1:C:82:LEU:HB2 | 1:C:137:ASP:HB2 | 1.92 | 0.52 |
| 1:C:264:LEU:HD23 | 1:C:265:THR:N | 2.25 | 0.52 |
| 1:C:303:ASN:ND2 | 1:C:308:GLN:HA | 2.24 | 0.52 |
| 1:C:393:PHE:HD2 | 1:C:393:PHE:N | 2.08 | 0.52 |
| 1:E:330:ASN:CB | 1:E:331:PRO:HD3 | 2.33 | 0.52 |
| 1:E:393:PHE:HD2 | 1:E:393:PHE:N | 2.08 | 0.52 |
| 1:G:98:PHE:HA | 1:G:155:THR:HG22 | 1.91 | 0.52 |
| 1:G:197:LEU:HD21 | 1:G:218:LEU:HD11 | 1.92 | 0.52 |
| 1:A:393:PHE:CD2 | 1:A:393:PHE:N | 2.75 | 0.51 |
| 2:B:68:ILE:CD1 | 2:B:68:ILE:N | 2.72 | 0.51 |
| 2:D:10:ILE:O | 2:D:14:VAL:HG23 | 2.10 | 0.51 |
| 1:E:199:VAL:HG12 | 1:E:200:SER:N | 2.24 | 0.51 |
| 1:E:330:ASN:CB | 1:E:331:PRO:CD | 2.87 | 0.51 |
| 1:E:351:ASP:O | 1:E:352:ILE:C | 2.49 | 0.51 |
| 2:F:68:ILE:N | 2:F:68:ILE:CD1 | 2.73 | 0.51 |
| 2:H:6:TYR:HA | 2:H:9:ASN:HD22 | 1.75 | 0.51 |
| 1:E:197:LEU:HB3 | 1:E:241:VAL:HG22 | 1.91 | 0.51 |
| 2:H:62:LEU:HD23 | 2:H:62:LEU:C | 2.30 | 0.51 |
| 1:C:65:LEU:HD21 | 1:C:158:VAL:C | 2.31 | 0.51 |
| 2:D:86:GLU:OE2 | 2:D:86:GLU:HA | 2.10 | 0.51 |
| 1:G:348:ASN:HB3 | 1:G:375:SER:HB2 | 1.92 | 0.51 |
| 1:A:14:LEU:HD11 | 2:B:98:ILE:CG2 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:41:LEU:HD22 | 2:B:103:ILE:HD12 | 1.92 | 0.51 |
| 1:E:61:MET:HE3 | 1:E:158:VAL:HB | 1.92 | 0.51 |
| 2:F:122:LEU:O | 2:F:125:ASN:N | 2.42 | 0.51 |
| 2:H:10:ILE:O | 2:H:14:VAL:HG23 | 2.10 | 0.51 |
| 1:C:5:GLN:HG3 | 1:C:193:ASP:OD1 | 2.11 | 0.51 |
| 1:E:154:VAL:HG12 | 1:E:155:THR:N | 2.26 | 0.51 |
| 1:A:65:LEU:HD21 | 1:A:158:VAL:HG12 | 1.93 | 0.51 |
| 1:G:226:LEU:HD12 | 1:G:226:LEU:O | 2.10 | 0.51 |
| 1:G:57:ARG:NH2 | 1:G:378:ALA:O | 2.44 | 0.51 |
| 1:A:5:GLN:HG3 | 1:A:193:ASP:OD1 | 2.10 | 0.51 |
| 1:C:65:LEU:HD23 | 1:C:159:LEU:O | 2.10 | 0.51 |
| 1:C:239:SER:O | 1:C:240:ARG:HG2 | 2.10 | 0.51 |
| 1:C:303:ASN:HD22 | 1:C:305:THR:HG22 | 1.74 | 0.51 |
| 2:D:6:TYR:CD1 | 2:D:40:MET:HG2 | 2.46 | 0.51 |
| 1:G:204:LEU:HD12 | 1:G:279:LEU:HB2 | 1.93 | 0.51 |
| 1:G:212:LEU:O | 1:G:215:THR:N | 2.44 | 0.51 |
| 1:G:351:ASP:HA | 1:G:354:ARG:HD2 | 1.93 | 0.51 |
| 1:A:264:LEU:HD23 | 1:A:265:THR:N | 2.25 | 0.51 |
| 1:A:225:GLN:NE2 | 2:B:133:SER:HB2 | 2.26 | 0.51 |
| 2:B:64:SER:OG | 2:B:97:SER:HB2 | 2.11 | 0.51 |
| 2:B:81:ARG:NH1 | 2:B:108:LEU:O | 2.44 | 0.51 |
| 1:C:53:ILE:HG22 | 1:C:55:ALA:H | 1.76 | 0.51 |
| 1:C:216:GLN:HE21 | 2:D:115:PHE:HD1 | 1.57 | 0.51 |
| 1:G:345:SER:C | 1:G:405:GLY:HA3 | 2.31 | 0.51 |
| 1:A:224:GLY:HA3 | 2:B:135:ILE:HG13 | 1.93 | 0.51 |
| 1:E:264:LEU:HD23 | 1:E:265:THR:N | 2.26 | 0.51 |
| 1:E:82:LEU:HD13 | 1:E:93:VAL:HG11 | 1.91 | 0.51 |
| 1:G:231:GLU:HG3 | 2:H:97:SER:OG | 2.11 | 0.51 |
| 1:C:410:PHE:HA | 1:C:429:PRO:HD3 | 1.93 | 0.51 |
| 1:E:439:LEU:CG | 1:E:450:ILE:HD11 | 2.41 | 0.51 |
| 1:E:99:LYS:HE2 | 1:E:150:VAL:HG12 | 1.93 | 0.51 |
| 2:F:42:TYR:O | 2:F:45:VAL:HG22 | 2.11 | 0.51 |
| 1:G:239:SER:O | 1:G:240:ARG:HG2 | 2.10 | 0.51 |
| 1:G:284:LEU:HD22 | 1:G:318:LEU:HB3 | 1.92 | 0.51 |
| 1:G:36:SER:HB3 | 1:G:333:GLN:H | 1.76 | 0.51 |
| 1:G:5:GLN:O | 1:G:8:GLN:HB2 | 2.10 | 0.51 |
| 1:C:19:ALA:HB1 | 1:E:193:ASP:OD2 | 2.11 | 0.50 |
| 1:E:65:LEU:HD21 | 1:E:158:VAL:C | 2.32 | 0.50 |
| 1:E:307:PRO:HG3 | 1:E:393:PHE:CZ | 2.46 | 0.50 |
| 1:E:351:ASP:HA | 1:E:354:ARG:HD2 | 1.93 | 0.50 |
| 1:A:225:GLN:HE21 | 2:B:133:SER:HB2 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:23:TYR:CD1 | 2:B:38:LYS:HE2 | 2.46 | 0.50 |
| 1:A:13:LEU:HD13 | 2:B:38:LYS:HD2 | 1.92 | 0.50 |
| 1:C:410:PHE:CE1 | 1:C:438:CYS:HB2 | 2.45 | 0.50 |
| 2:D:41:LEU:HD22 | 2:D:103:ILE:HD12 | 1.92 | 0.50 |
| 1:E:200:SER:HB3 | 1:E:428:VAL:HG12 | 1.92 | 0.50 |
| 1:G:5:GLN:HG3 | 1:G:193:ASP:OD1 | 2.11 | 0.50 |
| 2:H:2:ALA:O | 2:H:5:LEU:HB3 | 2.12 | 0.50 |
| 1:A:211:SER:HA | 1:A:435:GLN:NE2 | 2.27 | 0.50 |
| 1:E:225:GLN:NE2 | 2:F:133:SER:HB2 | 2.26 | 0.50 |
| 2:H:23:TYR:CD2 | 2:H:24:LYS:N | 2.79 | 0.50 |
| 2:H:24:LYS:O | 2:H:27:SER:HB3 | 2.10 | 0.50 |
| 1:C:423:VAL:HG12 | 1:C:425:LEU:HD23 | 1.93 | 0.50 |
| 1:E:154:VAL:HG11 | 1:E:355:TYR:CB | 2.41 | 0.50 |
| 1:G:393:PHE:N | 1:G:393:PHE:HD2 | 2.10 | 0.50 |
| 2:B:2:ALA:O | 2:B:5:LEU:HB3 | 2.12 | 0.50 |
| 1:C:373:HIS:HA | 1:C:393:PHE:O | 2.11 | 0.50 |
| 1:C:231:GLU:CG | 2:D:97:SER:OG | 2.60 | 0.50 |
| 1:C:29:VAL:HG11 | 1:C:291:PRO:CG | 2.13 | 0.50 |
| 1:C:315:MET:C | 1:C:317:PRO:HD3 | 2.33 | 0.50 |
| 1:E:132:GLU:OE2 | 1:E:143:LYS:HE2 | 2.12 | 0.50 |
| 2:F:52:ASN:CB | 2:F:55:ALA:HB2 | 2.42 | 0.50 |
| 1:G:351:ASP:O | 1:G:352:ILE:C | 2.50 | 0.50 |
| 1:A:26:ARG:CD | 1:A:290:VAL:HG23 | 2.42 | 0.50 |
| 2:B:72:HIS:HD2 | 2:B:72:HIS:O | 1.94 | 0.50 |
| 1:C:65:LEU:HD12 | 1:C:179:ALA:HB2 | 1.94 | 0.50 |
| 1:G:266:LYS:HG3 | 1:G:267:LYS:HG3 | 1.94 | 0.50 |
| 1:G:306:LEU:HD12 | 1:G:306:LEU:O | 2.11 | 0.50 |
| 1:A:330:ASN:CB | 1:A:331:PRO:CD | 2.89 | 0.50 |
| 1:E:266:LYS:HG3 | 1:E:267:LYS:HG3 | 1.94 | 0.50 |
| 1:E:439:LEU:HG | 1:E:450:ILE:HD11 | 1.94 | 0.50 |
| 1:G:419:GLU:N | 1:G:419:GLU:CD | 2.64 | 0.50 |
| 1:A:459:ASP:O | 1:A:462:LEU:HG | 2.13 | 0.49 |
| 2:B:99:HIS:ND1 | 2:B:100:VAL:O | 2.40 | 0.49 |
| 2:D:125:ASN:C | 2:D:127:GLN:N | 2.64 | 0.49 |
| 1:E:212:LEU:O | 1:E:213:LEU:C | 2.48 | 0.49 |
| 1:E:26:ARG:HD3 | 1:E:290:VAL:HG23 | 1.94 | 0.49 |
| 1:G:172:LEU:HD22 | 3:G:474:HOH:O | 2.11 | 0.49 |
| 2:B:86:GLU:HA | 2:B:86:GLU:OE2 | 2.11 | 0.49 |
| 1:C:151:SER:O | 1:C:357:SER:N | 2.45 | 0.49 |
| 1:C:225:GLN:NE2 | 2:D:133:SER:HB2 | 2.27 | 0.49 |
| 1:E:221:VAL:HG21 | 1:E:452:PHE:HE2 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:154:VAL:HG11 | 1:G:355:TYR:CB | 2.41 | 0.49 |
| 1:A:190:LEU:HB2 | 1:A:443:ARG:HB2 | 1.94 | 0.49 |
| 1:A:303:ASN:HD21 | 1:A:308:GLN:HA | 1.77 | 0.49 |
| 1:A:307:PRO:HG3 | 1:A:393:PHE:CZ | 2.47 | 0.49 |
| 1:A:410:PHE:HA | 1:A:429:PRO:HD3 | 1.94 | 0.49 |
| 1:A:98:PHE:HA | 1:A:155:THR:HG22 | 1.93 | 0.49 |
| 2:B:52:ASN:HB3 | 2:B:55:ALA:HB2 | 1.95 | 0.49 |
| 1:C:399:PRO:O | 1:C:423:VAL:HG22 | 2.12 | 0.49 |
| 1:E:303:ASN:HB3 | 1:G:304:TYR:CD1 | 2.47 | 0.49 |
| 2:F:32:VAL:HG11 | 2:F:40:MET:HE1 | 1.94 | 0.49 |
| 1:G:67:ASN:O | 1:G:71:GLN:HG2 | 2.12 | 0.49 |
| 1:A:410:PHE:CE1 | 1:A:438:CYS:HB2 | 2.44 | 0.49 |
| 1:C:226:LEU:C | 1:C:226:LEU:CD1 | 2.81 | 0.49 |
| 2:F:45:VAL:HG23 | 2:F:46:GLU:N | 2.27 | 0.49 |
| 1:G:218:LEU:HD22 | 1:G:431:PHE:CE2 | 2.48 | 0.49 |
| 2:D:66:SER:HB3 | 2:D:94:VAL:CG1 | 2.42 | 0.49 |
| 2:D:81:ARG:NH1 | 2:D:108:LEU:O | 2.45 | 0.49 |
| 1:E:11:HIS:N | 1:E:11:HIS:CD2 | 2.81 | 0.49 |
| 1:E:275:ALA:O | 1:E:276:VAL:C | 2.51 | 0.49 |
| 1:E:14:LEU:HD11 | 2:F:98:ILE:CG2 | 2.42 | 0.49 |
| 2:B:103:ILE:N | 2:B:104:GLN:HE21 | 2.10 | 0.49 |
| 2:B:62:LEU:C | 2:B:62:LEU:HD23 | 2.33 | 0.49 |
| 1:C:157:THR:HG23 | 1:C:371:VAL:HG11 | 1.93 | 0.49 |
| 1:C:67:ASN:O | 1:C:71:GLN:HG2 | 2.12 | 0.49 |
| 1:E:159:LEU:N | 1:E:159:LEU:HD23 | 2.25 | 0.49 |
| 1:C:185:LYS:HE3 | 1:C:397:GLU:OE2 | 2.12 | 0.49 |
| 1:E:5:GLN:HG3 | 1:E:193:ASP:OD1 | 2.12 | 0.49 |
| 1:E:345:SER:C | 1:E:405:GLY:HA3 | 2.33 | 0.49 |
| 1:G:439:LEU:HD12 | 1:G:450:ILE:HD11 | 1.94 | 0.49 |
| 1:A:348:ASN:HB3 | 1:A:375:SER:HB2 | 1.95 | 0.49 |
| 1:A:395:PHE:H | 1:A:395:PHE:HD1 | 1.58 | 0.49 |
| 2:B:125:ASN:C | 2:B:127:GLN:N | 2.66 | 0.49 |
| 1:C:351:ASP:O | 1:C:352:ILE:C | 2.50 | 0.49 |
| 1:C:407:THR:CG2 | 1:C:408:PRO:HD2 | 2.41 | 0.49 |
| 2:D:62:LEU:C | 2:D:62:LEU:HD23 | 2.33 | 0.49 |
| 1:E:60:GLN:O | 1:E:63:PRO:HD2 | 2.13 | 0.49 |
| 2:F:81:ARG:NH1 | 2:F:108:LEU:O | 2.46 | 0.49 |
| 1:G:82:LEU:HB2 | 1:G:137:ASP:HB2 | 1.95 | 0.49 |
| 1:G:264:LEU:HD23 | 1:G:265:THR:N | 2.27 | 0.49 |
| 1:G:98:PHE:HA | 1:G:155:THR:CG2 | 2.43 | 0.49 |
| 1:A:26:ARG:NH1 | 1:A:289:SER:O | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:360:ASP:O | 1:C:363:GLU:HB3 | 2.13 | 0.49 |
| 1:E:151:SER:O | 1:E:357:SER:N | 2.46 | 0.49 |
| 1:G:75:SER:O | 1:G:77:VAL:HG23 | 2.13 | 0.49 |
| 1:A:204:LEU:HD12 | 1:A:279:LEU:HB2 | 1.94 | 0.49 |
| 1:A:26:ARG:HG3 | 1:A:27:VAL:H | 1.77 | 0.49 |
| 1:A:444:SER:O | 1:A:445:LEU:HB2 | 2.12 | 0.49 |
| 1:C:351:ASP:HA | 1:C:354:ARG:HD2 | 1.94 | 0.49 |
| 1:C:218:LEU:HD22 | 1:C:431:PHE:CE2 | 2.47 | 0.49 |
| 1:C:237:HIS:CE1 | 1:E:21:ASN:H | 2.31 | 0.49 |
| 1:E:185:LYS:HE3 | 1:E:397:GLU:OE2 | 2.12 | 0.49 |
| 1:A:346:GLY:CA | 1:A:405:GLY:HA3 | 2.43 | 0.48 |
| 2:B:10:ILE:O | 2:B:14:VAL:HG23 | 2.13 | 0.48 |
| 2:D:45:VAL:CG2 | 2:D:46:GLU:N | 2.76 | 0.48 |
| 1:A:221:VAL:HG21 | 1:A:452:PHE:HE2 | 1.78 | 0.48 |
| 1:A:3:SER:OG | 2:B:75:HIS:ND1 | 2.34 | 0.48 |
| 1:E:406:ASN:ND2 | 1:E:406:ASN:N | 2.47 | 0.48 |
| 1:G:95:GLY:CA | 1:G:135:LEU:HD11 | 2.42 | 0.48 |
| 1:G:275:ALA:O | 1:G:276:VAL:C | 2.51 | 0.48 |
| 1:G:423:VAL:HG12 | 1:G:425:LEU:HD23 | 1.96 | 0.48 |
| 2:H:64:SER:OG | 2:H:97:SER:HB2 | 2.12 | 0.48 |
| 1:A:2:PHE:CG | 1:A:439:LEU:HD12 | 2.48 | 0.48 |
| 1:A:7:ALA:O | 1:A:9:ARG:N | 2.47 | 0.48 |
| 1:E:57:ARG:NH2 | 1:E:378:ALA:O | 2.47 | 0.48 |
| 1:G:148:ILE:HA | 1:G:176:TYR:CE2 | 2.46 | 0.48 |
| 1:G:410:PHE:HA | 1:G:429:PRO:HD3 | 1.94 | 0.48 |
| 1:A:11:HIS:CD2 | 1:A:11:HIS:N | 2.81 | 0.48 |
| 1:C:98:PHE:HA | 1:C:155:THR:CG2 | 2.43 | 0.48 |
| 1:C:182:ALA:HB1 | 1:C:183:PRO:CD | 2.37 | 0.48 |
| 1:C:373:HIS:O | 1:C:376:PRO:HD3 | 2.13 | 0.48 |
| 2:D:24:LYS:O | 2:D:27:SER:HB3 | 2.13 | 0.48 |
| 1:E:452:PHE:N | 1:E:452:PHE:CD1 | 2.81 | 0.48 |
| 2:H:41:LEU:HD22 | 2:H:103:ILE:HD12 | 1.94 | 0.48 |
| 1:A:351:ASP:O | 1:A:352:ILE:C | 2.51 | 0.48 |
| 2:B:32:VAL:HG11 | 2:B:40:MET:HE1 | 1.95 | 0.48 |
| 2:B:45:VAL:HG23 | 2:B:46:GLU:N | 2.27 | 0.48 |
| 1:E:430:ASP:OD1 | 1:E:432:SER:HB3 | 2.13 | 0.48 |
| 1:G:24:PHE:CZ | 1:G:233:CYS:HB2 | 2.49 | 0.48 |
| 1:G:319:ALA:CB | 1:G:325:LEU:HD22 | 2.42 | 0.48 |
| 1:A:269:GLN:NE2 | 1:C:320:THR:HB | 2.29 | 0.48 |
| 1:A:67:ASN:O | 1:A:71:GLN:HG2 | 2.14 | 0.48 |
| 1:C:443:ARG:CZ | 1:E:19:ALA:HB2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:319:ALA:O | 1:E:321:ALA:N | 2.47 | 0.48 |
| 1:E:37:GLN:H | 1:E:37:GLN:CD | 2.17 | 0.48 |
| 1:E:94:VAL:HB | 3:E:484:HOH:O | 2.12 | 0.48 |
| 1:G:60:GLN:O | 1:G:63:PRO:HD2 | 2.14 | 0.48 |
| 2:B:24:LYS:O | 2:B:27:SER:HB3 | 2.12 | 0.48 |
| 1:G:348:ASN:HB2 | 1:G:375:SER:HB2 | 1.95 | 0.48 |
| 2:H:42:TYR:O | 2:H:45:VAL:HG22 | 2.13 | 0.48 |
| 2:H:68:ILE:CD1 | 2:H:68:ILE:N | 2.77 | 0.48 |
| 1:G:14:LEU:HD11 | 2:H:98:ILE:CG2 | 2.44 | 0.48 |
| 1:A:37:GLN:CD | 1:A:37:GLN:H | 2.17 | 0.48 |
| 2:B:23:TYR:CG | 2:B:24:LYS:N | 2.82 | 0.48 |
| 2:B:42:TYR:O | 2:B:45:VAL:HG22 | 2.14 | 0.48 |
| 1:E:419:GLU:O | 1:E:420:ASP:C | 2.52 | 0.48 |
| 1:G:11:HIS:N | 1:G:11:HIS:CD2 | 2.80 | 0.48 |
| 1:G:162:PHE:HB3 | 1:G:175:ASP:O | 2.14 | 0.48 |
| 1:G:151:SER:O | 1:G:357:SER:N | 2.45 | 0.48 |
| 1:C:21:ASN:OD1 | 2:D:36:GLN:HB2 | 2.14 | 0.48 |
| 1:E:244:ALA:HA | 1:E:295:MET:HB2 | 1.96 | 0.48 |
| 1:E:218:LEU:HD22 | 1:E:431:PHE:CE2 | 2.49 | 0.48 |
| 1:E:225:GLN:HE21 | 2:F:133:SER:HB2 | 1.78 | 0.48 |
| 1:G:311:LEU:HA | 1:G:311:LEU:HD23 | 1.63 | 0.48 |
| 1:G:419:GLU:O | 1:G:420:ASP:C | 2.52 | 0.48 |
| 1:A:163:GLY:HA3 | 1:A:172:LEU:O | 2.13 | 0.48 |
| 1:A:284:LEU:HD22 | 1:A:318:LEU:HB3 | 1.96 | 0.48 |
| 2:D:52:ASN:HB3 | 2:D:55:ALA:HB2 | 1.96 | 0.48 |
| 1:E:82:LEU:HB2 | 1:E:137:ASP:HB2 | 1.96 | 0.48 |
| 1:E:157:THR:HG23 | 1:E:371:VAL:HG11 | 1.95 | 0.48 |
| 1:A:378:ALA:HA | 1:A:379:PRO:HD3 | 1.75 | 0.47 |
| 1:A:97:LEU:CD2 | 1:A:133:LEU:HB3 | 2.44 | 0.47 |
| 1:E:136:GLU:HG2 | 1:E:141:ARG:HB3 | 1.96 | 0.47 |
| 1:E:29:VAL:HG11 | 1:E:291:PRO:CG | 2.16 | 0.47 |
| 1:E:319:ALA:CB | 1:E:325:LEU:HD22 | 2.44 | 0.47 |
| 1:G:163:GLY:HA3 | 1:G:172:LEU:O | 2.14 | 0.47 |
| 1:G:193:ASP:CB | 1:G:443:ARG:NH1 | 2.64 | 0.47 |
| 2:H:103:ILE:N | 2:H:104:GLN:HE21 | 2.12 | 0.47 |
| 1:A:151:SER:O | 1:A:357:SER:N | 2.47 | 0.47 |
| 1:C:204:LEU:HD12 | 1:C:279:LEU:HB2 | 1.96 | 0.47 |
| 1:C:307:PRO:HG3 | 1:C:393:PHE:CZ | 2.48 | 0.47 |
| 2:D:52:ASN:CB | 2:D:55:ALA:HB2 | 2.43 | 0.47 |
| 1:E:355:TYR:N | 1:E:355:TYR:CD1 | 2.82 | 0.47 |
| 1:E:198:LEU:HB3 | 1:E:428:VAL:HG21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:216:GLN:HE21 | 2:F:115:PHE:HD1 | 1.61 | 0.47 |
| 1:G:373:HIS:HA | 1:G:393:PHE:O | 2.14 | 0.47 |
| 1:A:83:CYS:HA | 1:A:140:GLN:NE2 | 2.28 | 0.47 |
| 2:B:72:HIS:O | 2:B:72:HIS:CD2 | 2.68 | 0.47 |
| 1:C:228:ASP:OD1 | 1:C:229:GLU:N | 2.45 | 0.47 |
| 1:C:195:PHE:HB2 | 1:C:238:VAL:HG22 | 1.96 | 0.47 |
| 1:C:86:GLN:O | 1:C:87:PRO:C | 2.53 | 0.47 |
| 1:E:97:LEU:CD2 | 1:E:133:LEU:HB3 | 2.43 | 0.47 |
| 1:G:65:LEU:HD12 | 1:G:179:ALA:HB2 | 1.95 | 0.47 |
| 1:G:37:GLN:H | 1:G:37:GLN:CD | 2.18 | 0.47 |
| 1:A:416:ARG:HA | 1:A:421:GLN:O | 2.14 | 0.47 |
| 1:C:19:ALA:CB | 1:E:193:ASP:OD2 | 2.63 | 0.47 |
| 1:G:145:LYS:HE2 | 1:G:168:ASP:OD1 | 2.15 | 0.47 |
| 1:G:315:MET:C | 1:G:317:PRO:HD3 | 2.33 | 0.47 |
| 1:G:157:THR:HG23 | 1:G:371:VAL:HG11 | 1.96 | 0.47 |
| 1:C:37:GLN:CD | 1:C:37:GLN:H | 2.17 | 0.47 |
| 2:D:23:TYR:CD1 | 2:D:38:LYS:HE2 | 2.50 | 0.47 |
| 2:D:72:HIS:O | 2:D:72:HIS:HD2 | 1.97 | 0.47 |
| 1:E:99:LYS:HE2 | 1:E:150:VAL:CG1 | 2.44 | 0.47 |
| 1:E:153:LEU:HD12 | 1:E:153:LEU:N | 2.30 | 0.47 |
| 1:E:398:CYS:SG | 1:E:423:VAL:HG21 | 2.54 | 0.47 |
| 2:F:125:ASN:C | 2:F:127:GLN:N | 2.67 | 0.47 |
| 2:F:62:LEU:C | 2:F:62:LEU:HD23 | 2.33 | 0.47 |
| 1:G:136:GLU:HG2 | 1:G:141:ARG:HB3 | 1.96 | 0.47 |
| 1:G:239:SER:O | 1:G:240:ARG:CG | 2.62 | 0.47 |
| 1:C:-2:HIS:O | 1:C:-1:HIS:HB2 | 2.15 | 0.47 |
| 1:C:395:PHE:HD1 | 1:C:395:PHE:H | 1.57 | 0.47 |
| 2:D:122:LEU:O | 2:D:125:ASN:N | 2.46 | 0.47 |
| 1:E:423:VAL:HG12 | 1:E:425:LEU:HD23 | 1.97 | 0.47 |
| 1:E:439:LEU:HG | 1:E:450:ILE:CD1 | 2.44 | 0.47 |
| 1:G:228:ASP:OD1 | 1:G:229:GLU:N | 2.43 | 0.47 |
| 1:G:221:VAL:HG21 | 1:G:452:PHE:HE2 | 1.80 | 0.47 |
| 1:C:65:LEU:HD22 | 1:C:158:VAL:HG12 | 1.96 | 0.47 |
| 2:D:68:ILE:N | 2:D:68:ILE:CD1 | 2.77 | 0.47 |
| 1:E:65:LEU:HD23 | 1:E:159:LEU:C | 2.34 | 0.47 |
| 1:E:306:LEU:HD12 | 1:E:306:LEU:O | 2.14 | 0.47 |
| 1:E:37:GLN:HB2 | 1:E:38:PRO:CD | 2.45 | 0.47 |
| 1:A:226:LEU:HB3 | 2:B:23:TYR:OH | 2.15 | 0.47 |
| 2:B:59:VAL:HG12 | 2:B:60:THR:N | 2.29 | 0.47 |
| 1:C:212:LEU:O | 1:C:215:THR:N | 2.48 | 0.47 |
| 1:A:303:ASN:HB3 | 1:C:304:TYR:CD1 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:23:TYR:CD2 | 2:D:24:LYS:N | 2.81 | 0.47 |
| 2:D:70:ASN:O | 2:D:72:HIS:N | 2.46 | 0.47 |
| 1:E:303:ASN:HD21 | 1:E:308:GLN:HA | 1.80 | 0.47 |
| 1:E:416:ARG:HA | 1:E:421:GLN:O | 2.15 | 0.47 |
| 1:G:346:GLY:CA | 1:G:405:GLY:HA3 | 2.45 | 0.47 |
| 1:A:393:PHE:HD2 | 1:A:393:PHE:N | 2.13 | 0.47 |
| 1:A:65:LEU:HD12 | 1:A:179:ALA:HB2 | 1.97 | 0.47 |
| 1:A:82:LEU:HB2 | 1:A:137:ASP:HB2 | 1.96 | 0.47 |
| 1:A:86:GLN:O | 1:A:87:PRO:C | 2.53 | 0.47 |
| 1:C:83:CYS:HA | 1:C:140:GLN:NE2 | 2.30 | 0.47 |
| 1:E:395:PHE:N | 1:E:395:PHE:CD1 | 2.82 | 0.47 |
| 1:A:26:ARG:CG | 1:A:27:VAL:N | 2.77 | 0.47 |
| 1:A:315:MET:C | 1:A:317:PRO:HD3 | 2.35 | 0.47 |
| 1:A:418:PRO:CB | 1:A:419:GLU:OE1 | 2.62 | 0.47 |
| 1:A:423:VAL:HG12 | 1:A:425:LEU:HD23 | 1.97 | 0.47 |
| 1:C:11:HIS:CD2 | 1:C:11:HIS:N | 2.82 | 0.47 |
| 1:E:145:LYS:HE2 | 1:E:168:ASP:OD1 | 2.15 | 0.47 |
| 1:E:348:ASN:HB2 | 1:E:375:SER:HB2 | 1.97 | 0.47 |
| 2:F:38:LYS:HD3 | 2:F:99:HIS:CE1 | 2.50 | 0.47 |
| 1:G:193:ASP:C | 1:G:194:ARG:HD3 | 2.35 | 0.47 |
| 1:G:198:LEU:HB3 | 1:G:428:VAL:HG21 | 1.97 | 0.47 |
| 1:G:86:GLN:NE2 | 1:G:86:GLN:HA | 2.29 | 0.47 |
| 1:A:78:GLY:O | 1:A:91:CYS:HB2 | 2.15 | 0.46 |
| 1:C:419:GLU:O | 1:C:420:ASP:C | 2.53 | 0.46 |
| 1:C:211:SER:HA | 1:C:435:GLN:NE2 | 2.30 | 0.46 |
| 1:C:438:CYS:SG | 1:C:439:LEU:N | 2.88 | 0.46 |
| 1:G:226:LEU:HD13 | 2:H:62:LEU:HD11 | 1.96 | 0.46 |
| 2:H:52:ASN:HB3 | 2:H:55:ALA:HB2 | 1.95 | 0.46 |
| 1:A:153:LEU:HD12 | 1:A:153:LEU:N | 2.30 | 0.46 |
| 1:A:65:LEU:HD23 | 1:A:159:LEU:C | 2.36 | 0.46 |
| 2:F:23:TYR:CD2 | 2:F:24:LYS:N | 2.81 | 0.46 |
| 1:A:395:PHE:CD1 | 1:A:395:PHE:N | 2.83 | 0.46 |
| 1:A:73:TRP:HZ3 | 1:A:92:CYS:SG | 2.38 | 0.46 |
| 1:C:95:GLY:CA | 1:C:135:LEU:HD11 | 2.41 | 0.46 |
| 1:C:145:LYS:NZ | 1:C:168:ASP:HB2 | 2.30 | 0.46 |
| 1:C:428:VAL:HA | 1:C:429:PRO:HD2 | 1.72 | 0.46 |
| 1:E:226:LEU:O | 1:E:226:LEU:HD12 | 2.14 | 0.46 |
| 1:G:65:LEU:HD22 | 1:G:158:VAL:HG12 | 1.98 | 0.46 |
| 1:A:98:PHE:HA | 1:A:155:THR:CG2 | 2.45 | 0.46 |
| 1:A:208:GLY:N | 3:A:474:HOH:O | 2.48 | 0.46 |
| 1:A:216:GLN:HE21 | 2:B:115:PHE:HD1 | 1.62 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:430:ASP:OD1 | 1:A:432:SER:HB3 | 2.15 | 0.46 |
| 2:D:23:TYR:CG | 2:D:24:LYS:N | 2.84 | 0.46 |
| 1:E:315:MET:C | 1:E:317:PRO:HD3 | 2.35 | 0.46 |
| 2:F:59:VAL:HG12 | 2:F:60:THR:N | 2.30 | 0.46 |
| 1:A:182:ALA:HB1 | 1:A:183:PRO:CD | 2.39 | 0.46 |
| 2:B:116:ASN:N | 2:B:116:ASN:ND2 | 2.44 | 0.46 |
| 1:C:197:LEU:HD21 | 1:C:218:LEU:HD11 | 1.97 | 0.46 |
| 1:C:378:ALA:HA | 1:C:379:PRO:HD3 | 1.75 | 0.46 |
| 1:C:410:PHE:CD2 | 1:C:449:PRO:HG3 | 2.51 | 0.46 |
| 1:E:67:ASN:O | 1:E:71:GLN:HG2 | 2.16 | 0.46 |
| 1:E:78:GLY:O | 1:E:91:CYS:HB2 | 2.16 | 0.46 |
| 2:F:23:TYR:CE1 | 2:F:38:LYS:HE2 | 2.50 | 0.46 |
| 1:A:369:LEU:CD2 | 1:A:423:VAL:HG11 | 2.46 | 0.46 |
| 1:E:83:CYS:HA | 1:E:140:GLN:NE2 | 2.31 | 0.46 |
| 1:E:360:ASP:O | 1:E:363:GLU:HB3 | 2.16 | 0.46 |
| 2:F:103:ILE:N | 2:F:104:GLN:HE21 | 2.14 | 0.46 |
| 1:G:145:LYS:NZ | 1:G:168:ASP:HB2 | 2.30 | 0.46 |
| 1:G:333:GLN:HG3 | 1:G:342:LEU:HD13 | 1.95 | 0.46 |
| 1:G:399:PRO:O | 1:G:423:VAL:HG22 | 2.15 | 0.46 |
| 1:G:86:GLN:O | 1:G:87:PRO:C | 2.54 | 0.46 |
| 1:G:97:LEU:HG | 1:G:159:LEU:CD2 | 2.45 | 0.46 |
| 1:C:-1:HIS:ND1 | 1:C:0:GLY:N | 2.63 | 0.46 |
| 1:E:306:LEU:HD23 | 1:E:393:PHE:HE1 | 1.79 | 0.46 |
| 2:F:52:ASN:HB3 | 2:F:55:ALA:HB2 | 1.97 | 0.46 |
| 1:G:26:ARG:HD3 | 1:G:290:VAL:HG23 | 1.97 | 0.46 |
| 1:G:99:LYS:HE2 | 1:G:150:VAL:CG1 | 2.45 | 0.46 |
| 2:H:23:TYR:CD1 | 2:H:38:LYS:HE2 | 2.50 | 0.46 |
| 1:A:228:ASP:OD1 | 1:A:229:GLU:N | 2.47 | 0.46 |
| 2:D:115:PHE:O | 2:D:116:ASN:C | 2.55 | 0.46 |
| 2:D:59:VAL:O | 2:D:82:GLU:HB2 | 2.15 | 0.46 |
| 1:G:277:LYS:HE2 | 1:G:281:GLU:CD | 2.36 | 0.46 |
| 1:G:452:PHE:N | 1:G:452:PHE:CD1 | 2.84 | 0.46 |
| 2:H:23:TYR:CG | 2:H:24:LYS:N | 2.83 | 0.46 |
| 2:H:85:LEU:C | 2:H:85:LEU:HD12 | 2.36 | 0.46 |
| 1:A:373:HIS:O | 1:A:376:PRO:HD3 | 2.16 | 0.46 |
| 1:C:97:LEU:CD2 | 1:C:133:LEU:HB3 | 2.43 | 0.46 |
| 1:C:440:VAL:HG22 | 1:C:447:CYS:SG | 2.56 | 0.46 |
| 1:C:60:GLN:O | 1:C:63:PRO:HD2 | 2.16 | 0.46 |
| 1:E:333:GLN:HG3 | 1:E:342:LEU:HD13 | 1.98 | 0.46 |
| 2:F:99:HIS:ND1 | 2:F:100:VAL:O | 2.45 | 0.46 |
| 2:F:23:TYR:CD1 | 2:F:34:VAL:HG22 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:86:GLU:HA | 2:F:86:GLU:OE2 | 2.15 | 0.46 |
| 2:H:23:TYR:CD1 | 2:H:34:VAL:HG22 | 2.50 | 0.46 |
| 1:A:372:ARG:NH1 | 1:A:395:PHE:O | 2.49 | 0.46 |
| 1:C:60:GLN:OE1 | 1:C:390:THR:HG23 | 2.16 | 0.46 |
| 1:E:194:ARG:HG3 | 1:E:194:ARG:NH1 | 2.31 | 0.46 |
| 1:G:216:GLN:HE21 | 2:H:115:PHE:HD1 | 1.63 | 0.46 |
| 2:H:45:VAL:CG2 | 2:H:46:GLU:N | 2.79 | 0.46 |
| 1:A:198:LEU:HB3 | 1:A:428:VAL:HG21 | 1.97 | 0.45 |
| 1:A:80:LYS:HD3 | 1:A:84:GLU:HB2 | 1.98 | 0.45 |
| 2:B:3:ASP:CG | 2:B:4:GLN:N | 2.69 | 0.45 |
| 1:C:239:SER:O | 1:C:240:ARG:CG | 2.64 | 0.45 |
| 1:E:180:ASP:HA | 1:E:370:ARG:O | 2.17 | 0.45 |
| 1:G:65:LEU:HD23 | 1:G:159:LEU:C | 2.36 | 0.45 |
| 1:A:157:THR:HG23 | 1:A:371:VAL:HG11 | 1.97 | 0.45 |
| 1:A:60:GLN:O | 1:A:63:PRO:HD2 | 2.16 | 0.45 |
| 1:A:225:GLN:O | 2:B:23:TYR:HE1 | 2.00 | 0.45 |
| 1:C:148:ILE:HG13 | 1:C:176:TYR:CZ | 2.51 | 0.45 |
| 1:C:162:PHE:HB3 | 1:C:175:ASP:O | 2.15 | 0.45 |
| 1:E:95:GLY:CA | 1:E:135:LEU:HD11 | 2.44 | 0.45 |
| 1:A:355:TYR:CD1 | 1:A:355:TYR:N | 2.83 | 0.45 |
| 1:C:154:VAL:HG11 | 1:C:355:TYR:CB | 2.46 | 0.45 |
| 1:C:226:LEU:HB3 | 2:D:23:TYR:OH | 2.17 | 0.45 |
| 1:C:78:GLY:O | 1:C:91:CYS:HB2 | 2.16 | 0.45 |
| 1:E:162:PHE:HB3 | 1:E:175:ASP:O | 2.15 | 0.45 |
| 1:E:60:GLN:OE1 | 1:E:390:THR:HG23 | 2.16 | 0.45 |
| 1:G:153:LEU:N | 1:G:153:LEU:HD12 | 2.31 | 0.45 |
| 1:A:21:ASN:OD1 | 2:B:36:GLN:HB2 | 2.16 | 0.45 |
| 1:C:395:PHE:CD1 | 1:C:395:PHE:N | 2.83 | 0.45 |
| 2:D:72:HIS:CD2 | 2:D:72:HIS:O | 2.70 | 0.45 |
| 1:G:290:VAL:CG2 | 1:G:291:PRO:CD | 2.94 | 0.45 |
| 2:H:26:LEU:HD22 | 2:H:41:LEU:HD21 | 1.98 | 0.45 |
| 1:A:86:GLN:HA | 1:A:86:GLN:NE2 | 2.29 | 0.45 |
| 2:B:112:GLY:O | 2:B:113:PRO:C | 2.55 | 0.45 |
| 1:G:436:THR:HA | 1:G:450:ILE:O | 2.17 | 0.45 |
| 2:H:59:VAL:HG12 | 2:H:60:THR:N | 2.31 | 0.45 |
| 1:A:304:TYR:CD1 | 1:C:303:ASN:HB3 | 2.52 | 0.45 |
| 1:A:37:GLN:C | 1:A:39:PHE:N | 2.70 | 0.45 |
| 2:B:10:ILE:O | 2:B:13:PHE:HB2 | 2.17 | 0.45 |
| 2:D:3:ASP:C | 2:D:5:LEU:N | 2.69 | 0.45 |
| 2:D:85:LEU:C | 2:D:85:LEU:HD12 | 2.36 | 0.45 |
| 1:E:438:CYS:SG | 1:E:439:LEU:N | 2.89 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:231:GLU:CG | 2:F:97:SER:OG | 2.64 | 0.45 |
| 1:G:303:ASN:ND2 | 1:G:308:GLN:HA | 2.32 | 0.45 |
| 1:G:351:ASP:HB2 | 1:G:377:THR:HG21 | 1.99 | 0.45 |
| 1:G:428:VAL:HA | 1:G:429:PRO:HD2 | 1.77 | 0.45 |
| 2:H:86:GLU:OE2 | 2:H:86:GLU:HA | 2.16 | 0.45 |
| 1:A:24:PHE:O | 2:B:135:ILE:HA | 2.16 | 0.45 |
| 1:A:356:SER:OG | 1:A:357:SER:N | 2.50 | 0.45 |
| 1:A:86:GLN:CA | 1:A:86:GLN:HE21 | 2.23 | 0.45 |
| 1:C:99:LYS:HE2 | 1:C:150:VAL:CG1 | 2.46 | 0.45 |
| 1:C:65:LEU:HD23 | 1:C:159:LEU:C | 2.37 | 0.45 |
| 1:C:3:SER:OG | 2:D:75:HIS:ND1 | 2.35 | 0.45 |
| 1:G:355:TYR:CD1 | 1:G:355:TYR:N | 2.84 | 0.45 |
| 1:G:60:GLN:OE1 | 1:G:390:THR:HG23 | 2.16 | 0.45 |
| 1:A:148:ILE:HA | 1:A:176:TYR:CE2 | 2.50 | 0.45 |
| 1:A:65:LEU:HD22 | 1:A:158:VAL:HG12 | 1.99 | 0.45 |
| 1:A:60:GLN:OE1 | 1:A:390:THR:HG23 | 2.16 | 0.45 |
| 1:A:451:SER:HB2 | 2:B:76:LYS:HD3 | 1.99 | 0.45 |
| 1:E:198:LEU:O | 1:E:437:ALA:HB1 | 2.16 | 0.45 |
| 2:F:23:TYR:CG | 2:F:24:LYS:N | 2.84 | 0.45 |
| 1:G:212:LEU:O | 1:G:213:LEU:C | 2.53 | 0.45 |
| 1:G:37:GLN:C | 1:G:39:PHE:N | 2.69 | 0.45 |
| 1:A:360:ASP:O | 1:A:363:GLU:HB3 | 2.16 | 0.45 |
| 1:C:221:VAL:HG21 | 1:C:452:PHE:HE2 | 1.81 | 0.45 |
| 2:H:59:VAL:O | 2:H:82:GLU:HB2 | 2.17 | 0.45 |
| 1:A:277:LYS:HE2 | 1:A:281:GLU:CD | 2.37 | 0.45 |
| 1:A:319:ALA:CB | 1:A:325:LEU:HD22 | 2.46 | 0.45 |
| 2:B:23:TYR:CE1 | 2:B:38:LYS:HE2 | 2.52 | 0.45 |
| 1:C:316:PHE:O | 1:C:320:THR:HG23 | 2.16 | 0.45 |
| 2:D:32:VAL:HG11 | 2:D:40:MET:HE1 | 1.98 | 0.45 |
| 1:C:13:LEU:HD13 | 2:D:38:LYS:CD | 2.46 | 0.45 |
| 1:E:451:SER:HB2 | 2:F:76:LYS:HD3 | 1.99 | 0.45 |
| 1:G:280:ASP:OD1 | 1:G:317:PRO:HD2 | 2.17 | 0.45 |
| 1:A:136:GLU:HG2 | 1:A:141:ARG:HB3 | 1.98 | 0.44 |
| 1:A:218:LEU:HD22 | 1:A:431:PHE:CE2 | 2.52 | 0.44 |
| 1:G:373:HIS:O | 1:G:376:PRO:HD3 | 2.17 | 0.44 |
| 1:A:419:GLU:O | 1:A:420:ASP:C | 2.55 | 0.44 |
| 2:B:18:ASN:OD1 | 2:B:105:LYS:HE2 | 2.17 | 0.44 |
| 1:C:244:ALA:HA | 1:C:295:MET:HB2 | 1.98 | 0.44 |
| 1:C:303:ASN:HD21 | 1:C:308:GLN:HA | 1.82 | 0.44 |
| 1:C:280:ASP:OD1 | 1:C:317:PRO:HD2 | 2.16 | 0.44 |
| 1:C:351:ASP:HB2 | 1:C:377:THR:HG21 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:86:GLN:NE2 | 1:C:86:GLN:HA | 2.31 | 0.44 |
| 1:G:360:ASP:O | 1:G:363:GLU:HB3 | 2.17 | 0.44 |
| 1:A:95:GLY:CA | 1:A:135:LEU:HD11 | 2.43 | 0.44 |
| 1:A:440:VAL:HG22 | 1:A:447:CYS:SG | 2.57 | 0.44 |
| 1:C:198:LEU:HB3 | 1:C:428:VAL:HG21 | 1.99 | 0.44 |
| 2:D:103:ILE:N | 2:D:104:GLN:HE21 | 2.14 | 0.44 |
| 1:E:24:PHE:CZ | 1:E:233:CYS:HB2 | 2.52 | 0.44 |
| 2:F:59:VAL:O | 2:F:82:GLU:HB2 | 2.17 | 0.44 |
| 1:G:26:ARG:HG3 | 1:G:27:VAL:H | 1.81 | 0.44 |
| 1:G:26:ARG:NH1 | 1:G:289:SER:O | 2.48 | 0.44 |
| 1:A:61:MET:HE3 | 1:A:158:VAL:HB | 2.00 | 0.44 |
| 1:A:351:ASP:HB2 | 1:A:377:THR:HG21 | 1.99 | 0.44 |
| 1:C:444:SER:O | 1:C:445:LEU:HB2 | 2.17 | 0.44 |
| 1:E:311:LEU:HA | 1:E:311:LEU:HD23 | 1.75 | 0.44 |
| 1:E:418:PRO:CB | 1:E:419:GLU:OE1 | 2.64 | 0.44 |
| 2:F:6:TYR:CD1 | 2:F:40:MET:HG2 | 2.52 | 0.44 |
| 1:G:83:CYS:HA | 1:G:140:GLN:NE2 | 2.32 | 0.44 |
| 1:G:2:PHE:CG | 1:G:439:LEU:HD12 | 2.52 | 0.44 |
| 1:A:99:LYS:HE2 | 1:A:150:VAL:HG12 | 1.98 | 0.44 |
| 1:C:37:GLN:N | 1:C:37:GLN:NE2 | 2.64 | 0.44 |
| 1:C:345:SER:C | 1:C:405:GLY:HA3 | 2.37 | 0.44 |
| 1:E:351:ASP:HB2 | 1:E:377:THR:HG21 | 1.98 | 0.44 |
| 1:G:97:LEU:CD2 | 1:G:133:LEU:HB3 | 2.47 | 0.44 |
| 1:G:398:CYS:SG | 1:G:423:VAL:HG21 | 2.57 | 0.44 |
| 1:G:78:GLY:O | 1:G:91:CYS:HB2 | 2.17 | 0.44 |
| 1:A:197:LEU:HB3 | 1:A:241:VAL:HG22 | 1.99 | 0.44 |
| 1:A:226:LEU:HB2 | 2:B:62:LEU:HD13 | 1.99 | 0.44 |
| 1:C:151:SER:CB | 1:C:357:SER:HB2 | 2.45 | 0.44 |
| 1:E:61:MET:CE | 1:E:158:VAL:HB | 2.47 | 0.44 |
| 1:E:211:SER:HA | 1:E:435:GLN:NE2 | 2.32 | 0.44 |
| 1:G:438:CYS:SG | 1:G:439:LEU:N | 2.91 | 0.44 |
| 2:H:125:ASN:C | 2:H:127:GLN:H | 2.20 | 0.44 |
| 1:A:398:CYS:SG | 1:A:423:VAL:HG21 | 2.58 | 0.44 |
| 2:B:85:LEU:HD12 | 2:B:85:LEU:C | 2.37 | 0.44 |
| 1:C:128:HIS:ND1 | 1:C:131:ASP:OD1 | 2.51 | 0.44 |
| 1:C:194:ARG:HG3 | 1:C:194:ARG:NH1 | 2.32 | 0.44 |
| 1:C:354:ARG:C | 1:C:355:TYR:HD1 | 2.21 | 0.44 |
| 1:E:239:SER:O | 1:E:240:ARG:HG2 | 2.18 | 0.44 |
| 1:E:303:ASN:HD22 | 1:E:305:THR:HG22 | 1.79 | 0.44 |
| 2:F:85:LEU:C | 2:F:85:LEU:HD12 | 2.37 | 0.44 |
| 1:C:2:PHE:CG | 1:C:439:LEU:HD12 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:193:ASP:CB | 1:C:443:ARG:NH1 | 2.68 | 0.44 |
| 2:D:3:ASP:CG | 2:D:4:GLN:N | 2.71 | 0.44 |
| 2:F:122:LEU:O | 2:F:126:LEU:N | 2.51 | 0.44 |
| 2:F:70:ASN:C | 2:F:72:HIS:N | 2.69 | 0.44 |
| 1:G:354:ARG:C | 1:G:355:TYR:HD1 | 2.21 | 0.44 |
| 1:A:197:LEU:HD21 | 1:A:218:LEU:HD11 | 2.00 | 0.44 |
| 2:B:70:ASN:C | 2:B:72:HIS:H | 2.21 | 0.44 |
| 1:E:151:SER:CB | 1:E:357:SER:HB2 | 2.42 | 0.44 |
| 1:E:65:LEU:HD22 | 1:E:158:VAL:HG12 | 2.00 | 0.44 |
| 1:G:26:ARG:CG | 1:G:27:VAL:N | 2.81 | 0.44 |
| 1:A:148:ILE:HG13 | 1:A:176:TYR:CZ | 2.51 | 0.43 |
| 1:A:185:LYS:HA | 1:A:186:PRO:HD3 | 1.79 | 0.43 |
| 1:A:452:PHE:CD1 | 1:A:452:PHE:N | 2.85 | 0.43 |
| 1:C:24:PHE:O | 2:D:135:ILE:HA | 2.18 | 0.43 |
| 1:C:26:ARG:HD3 | 1:C:290:VAL:HG23 | 1.98 | 0.43 |
| 1:E:26:ARG:CD | 1:E:290:VAL:HG23 | 2.48 | 0.43 |
| 1:E:348:ASN:HB3 | 1:E:375:SER:HB2 | 1.99 | 0.43 |
| 1:E:440:VAL:HG22 | 1:E:447:CYS:SG | 2.58 | 0.43 |
| 1:G:244:ALA:HA | 1:G:295:MET:HB2 | 1.99 | 0.43 |
| 1:E:269:GLN:HE22 | 1:G:320:THR:HB | 1.83 | 0.43 |
| 2:H:81:ARG:NH1 | 2:H:108:LEU:O | 2.51 | 0.43 |
| 1:A:145:LYS:NZ | 1:A:168:ASP:HB2 | 2.33 | 0.43 |
| 1:A:-1:HIS:ND1 | 1:A:-1:HIS:C | 2.72 | 0.43 |
| 1:A:330:ASN:CB | 1:A:331:PRO:HD3 | 2.35 | 0.43 |
| 1:A:284:LEU:HD23 | 2:B:126:LEU:HD11 | 2.00 | 0.43 |
| 1:C:308:GLN:OE1 | 1:C:330:ASN:ND2 | 2.39 | 0.43 |
| 1:C:342:LEU:HD12 | 1:C:343:GLY:H | 1.83 | 0.43 |
| 1:C:418:PRO:CB | 1:C:419:GLU:OE1 | 2.65 | 0.43 |
| 1:E:372:ARG:NH1 | 1:E:395:PHE:O | 2.51 | 0.43 |
| 2:F:3:ASP:C | 2:F:5:LEU:N | 2.70 | 0.43 |
| 1:E:14:LEU:HD11 | 2:F:98:ILE:HG22 | 1.99 | 0.43 |
| 1:G:197:LEU:HB3 | 1:G:241:VAL:HG22 | 2.00 | 0.43 |
| 1:G:243:LEU:CD2 | 1:G:243:LEU:N | 2.81 | 0.43 |
| 1:G:-2:HIS:O | 1:G:-1:HIS:CB | 2.66 | 0.43 |
| 1:G:37:GLN:HB2 | 1:G:38:PRO:CD | 2.48 | 0.43 |
| 1:G:395:PHE:CD1 | 1:G:395:PHE:N | 2.83 | 0.43 |
| 2:H:103:ILE:CA | 2:H:104:GLN:HE21 | 2.31 | 0.43 |
| 1:A:162:PHE:HB3 | 1:A:175:ASP:O | 2.17 | 0.43 |
| 1:A:298:GLU:OE1 | 1:A:298:GLU:HA | 2.18 | 0.43 |
| 2:B:32:VAL:CG1 | 2:B:36:GLN:OE1 | 2.65 | 0.43 |
| 2:B:59:VAL:CG1 | 2:B:60:THR:N | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:61:MET:CE | 1:C:158:VAL:HB | 2.48 | 0.43 |
| 1:A:315:MET:HG2 | 1:C:314:CYS:SG | 2.58 | 0.43 |
| 1:G:148:ILE:HG13 | 1:G:176:TYR:CZ | 2.52 | 0.43 |
| 1:G:416:ARG:HA | 1:G:421:GLN:O | 2.18 | 0.43 |
| 1:G:443:ARG:HG2 | 1:G:443:ARG:HH11 | 1.83 | 0.43 |
| 1:A:85:LEU:CG | 1:A:165:VAL:HG21 | 2.48 | 0.43 |
| 1:C:148:ILE:HA | 1:C:176:TYR:CE2 | 2.49 | 0.43 |
| 2:D:23:TYR:CD1 | 2:D:34:VAL:HG22 | 2.53 | 0.43 |
| 1:E:280:ASP:CG | 1:E:318:LEU:HB2 | 2.39 | 0.43 |
| 1:E:82:LEU:HD21 | 1:E:142:ILE:HG22 | 2.00 | 0.43 |
| 2:F:3:ASP:CG | 2:F:4:GLN:N | 2.72 | 0.43 |
| 1:G:24:PHE:O | 2:H:135:ILE:HA | 2.18 | 0.43 |
| 2:H:18:ASN:OD1 | 2:H:105:LYS:HE2 | 2.18 | 0.43 |
| 2:H:55:ALA:O | 2:H:57:LEU:N | 2.52 | 0.43 |
| 1:A:280:ASP:CG | 1:A:318:LEU:HB2 | 2.38 | 0.43 |
| 1:A:62:ARG:CB | 1:A:63:PRO:HD3 | 2.44 | 0.43 |
| 1:C:185:LYS:HG2 | 1:C:185:LYS:H | 1.69 | 0.43 |
| 1:C:269:GLN:O | 1:C:270:ALA:C | 2.57 | 0.43 |
| 2:D:32:VAL:CG1 | 2:D:36:GLN:OE1 | 2.65 | 0.43 |
| 1:E:373:HIS:O | 1:E:376:PRO:HD3 | 2.17 | 0.43 |
| 2:F:24:LYS:HB3 | 2:F:118:ASP:OD1 | 2.19 | 0.43 |
| 2:F:26:LEU:HD22 | 2:F:41:LEU:HD21 | 2.00 | 0.43 |
| 1:G:346:GLY:N | 1:G:405:GLY:HA3 | 2.34 | 0.43 |
| 1:G:82:LEU:HD21 | 1:G:142:ILE:HG22 | 2.01 | 0.43 |
| 1:G:231:GLU:CG | 2:H:97:SER:OG | 2.66 | 0.43 |
| 1:A:154:VAL:HG11 | 1:A:355:TYR:CB | 2.46 | 0.43 |
| 2:B:23:TYR:CD1 | 2:B:34:VAL:HG22 | 2.53 | 0.43 |
| 2:D:3:ASP:O | 2:D:5:LEU:N | 2.52 | 0.43 |
| 2:H:34:VAL:O | 2:H:38:LYS:HG3 | 2.18 | 0.43 |
| 2:B:59:VAL:O | 2:B:82:GLU:HB2 | 2.18 | 0.43 |
| 1:C:194:ARG:HG3 | 1:C:194:ARG:HH11 | 1.84 | 0.43 |
| 1:G:298:GLU:OE1 | 1:G:298:GLU:HA | 2.18 | 0.43 |
| 2:H:103:ILE:C | 2:H:104:GLN:HE21 | 2.22 | 0.43 |
| 1:A:239:SER:O | 1:A:240:ARG:HG2 | 2.19 | 0.43 |
| 2:B:103:ILE:CA | 2:B:104:GLN:HE21 | 2.32 | 0.43 |
| 2:B:17:GLN:O | 2:B:18:ASN:HB2 | 2.18 | 0.43 |
| 2:B:55:ALA:O | 2:B:57:LEU:N | 2.52 | 0.43 |
| 1:C:346:GLY:N | 1:C:405:GLY:HA3 | 2.34 | 0.43 |
| 1:C:365:LEU:CD1 | 1:C:404:CYS:HB2 | 2.47 | 0.43 |
| 1:C:80:LYS:HD3 | 1:C:84:GLU:HB2 | 2.01 | 0.43 |
| 2:D:4:GLN:O | 2:D:8:GLU:HG3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:280:ASP:OD1 | 1:E:317:PRO:HD2 | 2.19 | 0.43 |
| 1:A:399:PRO:O | 1:A:423:VAL:HG22 | 2.19 | 0.43 |
| 1:C:136:GLU:HG2 | 1:C:141:ARG:HB3 | 2.01 | 0.43 |
| 2:F:20:ILE:HG23 | 2:F:104:GLN:HG3 | 2.01 | 0.43 |
| 1:G:306:LEU:HD23 | 1:G:393:PHE:HE1 | 1.82 | 0.43 |
| 1:A:369:LEU:HD21 | 1:A:423:VAL:HG11 | 2.01 | 0.43 |
| 1:C:275:ALA:O | 1:C:276:VAL:C | 2.55 | 0.43 |
| 1:E:194:ARG:HH11 | 1:E:194:ARG:HG3 | 1.83 | 0.43 |
| 1:E:346:GLY:CA | 1:E:405:GLY:HA3 | 2.48 | 0.43 |
| 1:G:226:LEU:HB3 | 2:H:23:TYR:OH | 2.19 | 0.43 |
| 1:A:-3:HIS:CD2 | 1:A:-3:HIS:H1 | 2.37 | 0.42 |
| 2:B:125:ASN:C | 2:B:127:GLN:H | 2.22 | 0.42 |
| 2:B:3:ASP:C | 2:B:5:LEU:N | 2.72 | 0.42 |
| 1:A:231:GLU:CG | 2:B:97:SER:OG | 2.66 | 0.42 |
| 1:C:101:MET:HB2 | 1:C:128:HIS:CD2 | 2.54 | 0.42 |
| 1:C:451:SER:HB2 | 2:D:76:LYS:HD3 | 2.01 | 0.42 |
| 2:D:10:ILE:O | 2:D:13:PHE:HB2 | 2.19 | 0.42 |
| 2:D:60:THR:OG1 | 2:D:102:SER:OG | 2.27 | 0.42 |
| 1:E:86:GLN:O | 1:E:87:PRO:C | 2.56 | 0.42 |
| 1:G:128:HIS:ND1 | 1:G:131:ASP:OD1 | 2.52 | 0.42 |
| 1:G:145:LYS:CE | 1:G:168:ASP:HB3 | 2.49 | 0.42 |
| 1:G:182:ALA:HB1 | 1:G:183:PRO:CD | 2.39 | 0.42 |
| 1:G:151:SER:CB | 1:G:357:SER:HB2 | 2.45 | 0.42 |
| 2:H:3:ASP:CG | 2:H:4:GLN:N | 2.72 | 0.42 |
| 1:A:151:SER:CB | 1:A:357:SER:HB2 | 2.45 | 0.42 |
| 1:C:355:TYR:N | 1:C:355:TYR:CD1 | 2.86 | 0.42 |
| 2:D:34:VAL:O | 2:D:38:LYS:HG3 | 2.19 | 0.42 |
| 1:E:336:ILE:O | 1:E:337:ASP:C | 2.58 | 0.42 |
| 1:C:188:PRO:HD2 | 1:C:338:GLY:O | 2.19 | 0.42 |
| 1:C:197:LEU:HB3 | 1:C:241:VAL:HG22 | 2.01 | 0.42 |
| 1:E:26:ARG:NH1 | 1:E:289:SER:O | 2.51 | 0.42 |
| 2:F:18:ASN:OD1 | 2:F:105:LYS:HE2 | 2.20 | 0.42 |
| 1:G:125:LYS:NZ | 1:G:356:SER:O | 2.51 | 0.42 |
| 2:H:32:VAL:HG11 | 2:H:40:MET:HE1 | 2.00 | 0.42 |
| 2:H:59:VAL:CG1 | 2:H:60:THR:N | 2.82 | 0.42 |
| 1:A:37:GLN:HB2 | 1:A:38:PRO:CD | 2.50 | 0.42 |
| 1:A:395:PHE:HA | 1:A:396:PRO:HD3 | 1.87 | 0.42 |
| 2:B:103:ILE:C | 2:B:104:GLN:HE21 | 2.23 | 0.42 |
| 2:D:42:TYR:O | 2:D:45:VAL:HG22 | 2.20 | 0.42 |
| 1:E:312:HIS:ND1 | 1:E:313:PRO:HD2 | 2.33 | 0.42 |
| 1:E:354:ARG:C | 1:E:355:TYR:HD1 | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:439:LEU:HD11 | 1:E:450:ILE:HD11 | 2.00 | 0.42 |
| 1:C:14:LEU:HA | 1:C:14:LEU:HD23 | 1.90 | 0.42 |
| 1:C:190:LEU:HB2 | 1:C:443:ARG:HB2 | 2.01 | 0.42 |
| 1:C:312:HIS:ND1 | 1:C:313:PRO:HD2 | 2.34 | 0.42 |
| 1:C:342:LEU:HD12 | 1:C:343:GLY:N | 2.34 | 0.42 |
| 1:E:-1:HIS:ND1 | 1:E:0:GLY:N | 2.67 | 0.42 |
| 1:E:182:ALA:HB1 | 1:E:183:PRO:CD | 2.38 | 0.42 |
| 1:E:209:GLY:HA2 | 1:E:212:LEU:HD12 | 2.01 | 0.42 |
| 1:E:277:LYS:O | 1:E:280:ASP:HB3 | 2.20 | 0.42 |
| 1:E:411:GLY:HA3 | 1:E:427:THR:OG1 | 2.19 | 0.42 |
| 1:E:443:ARG:HH11 | 1:E:443:ARG:HG2 | 1.84 | 0.42 |
| 2:F:59:VAL:CG1 | 2:F:60:THR:N | 2.81 | 0.42 |
| 1:G:211:SER:HA | 1:G:435:GLN:NE2 | 2.34 | 0.42 |
| 1:G:307:PRO:HG3 | 1:G:393:PHE:HZ | 1.83 | 0.42 |
| 1:G:346:GLY:O | 1:G:347:GLN:C | 2.58 | 0.42 |
| 1:C:145:LYS:NZ | 1:C:168:ASP:CB | 2.82 | 0.42 |
| 1:C:148:ILE:O | 1:C:148:ILE:HG23 | 2.19 | 0.42 |
| 1:E:65:LEU:HD12 | 1:E:179:ALA:HB2 | 2.01 | 0.42 |
| 1:E:284:LEU:HD22 | 1:E:318:LEU:HB3 | 2.01 | 0.42 |
| 1:G:145:LYS:NZ | 1:G:168:ASP:CB | 2.82 | 0.42 |
| 1:G:86:GLN:HE21 | 1:G:86:GLN:CA | 2.24 | 0.42 |
| 1:A:275:ALA:O | 1:A:276:VAL:C | 2.57 | 0.42 |
| 2:B:69:GLN:HE21 | 2:B:69:GLN:HB2 | 1.60 | 0.42 |
| 1:E:185:LYS:HG2 | 1:E:185:LYS:H | 1.70 | 0.42 |
| 1:E:314:CYS:SG | 1:G:315:MET:HG2 | 2.59 | 0.42 |
| 1:G:37:GLN:NE2 | 1:G:37:GLN:N | 2.63 | 0.42 |
| 1:G:369:LEU:CD2 | 1:G:423:VAL:HG11 | 2.50 | 0.42 |
| 2:H:6:TYR:O | 2:H:10:ILE:HG13 | 2.20 | 0.42 |
| 1:A:354:ARG:C | 1:A:355:TYR:HD1 | 2.23 | 0.42 |
| 1:C:180:ASP:HA | 1:C:370:ARG:O | 2.20 | 0.42 |
| 1:C:37:GLN:HB2 | 1:C:38:PRO:CD | 2.50 | 0.42 |
| 1:E:-2:HIS:O | 1:E:-1:HIS:HB2 | 2.19 | 0.42 |
| 1:G:365:LEU:CD1 | 1:G:404:CYS:HB2 | 2.46 | 0.42 |
| 1:G:225:GLN:HE21 | 2:H:133:SER:HB2 | 1.85 | 0.42 |
| 2:H:21:VAL:O | 2:H:102:SER:HA | 2.20 | 0.42 |
| 1:A:101:MET:HB2 | 1:A:128:HIS:CD2 | 2.54 | 0.42 |
| 1:A:280:ASP:OD1 | 1:A:317:PRO:HD2 | 2.19 | 0.42 |
| 2:B:115:PHE:O | 2:B:116:ASN:C | 2.58 | 0.42 |
| 1:C:85:LEU:CG | 1:C:165:VAL:HG21 | 2.50 | 0.42 |
| 1:C:1:MET:SD | 1:C:448:GLN:HB2 | 2.59 | 0.42 |
| 2:D:103:ILE:C | 2:D:104:GLN:HE21 | 2.23 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:70:ASN:C | 2:D:72:HIS:N | 2.72 | 0.42 |
| 2:D:80:VAL:HG11 | 2:D:88:VAL:HG21 | 2.01 | 0.42 |
| 1:E:24:PHE:O | 2:F:135:ILE:HA | 2.19 | 0.42 |
| 1:G:198:LEU:O | 1:G:437:ALA:HB1 | 2.20 | 0.42 |
| 2:H:99:HIS:ND1 | 2:H:100:VAL:O | 2.45 | 0.42 |
| 1:A:345:SER:C | 1:A:405:GLY:HA3 | 2.41 | 0.42 |
| 1:A:82:LEU:HA | 1:A:82:LEU:HD12 | 1.87 | 0.42 |
| 1:C:298:GLU:HA | 1:C:298:GLU:OE1 | 2.20 | 0.42 |
| 1:C:416:ARG:HA | 1:C:421:GLN:O | 2.19 | 0.42 |
| 2:D:59:VAL:HG12 | 2:D:60:THR:N | 2.33 | 0.42 |
| 1:E:149:ASP:OD2 | 1:E:152:LYS:HB2 | 2.20 | 0.42 |
| 2:F:69:GLN:HE21 | 2:F:69:GLN:HB2 | 1.59 | 0.42 |
| 1:G:101:MET:HB2 | 1:G:128:HIS:CD2 | 2.55 | 0.42 |
| 1:G:225:GLN:OE1 | 2:H:24:LYS:HE3 | 2.20 | 0.42 |
| 1:A:85:LEU:HD12 | 1:A:165:VAL:CG2 | 2.50 | 0.41 |
| 1:A:97:LEU:HG | 1:A:159:LEU:CD2 | 2.47 | 0.41 |
| 2:B:24:LYS:HB3 | 2:B:118:ASP:OD1 | 2.20 | 0.41 |
| 1:C:277:LYS:HE2 | 1:C:281:GLU:CD | 2.40 | 0.41 |
| 1:C:340:ARG:HB2 | 1:C:400:HIS:ND1 | 2.35 | 0.41 |
| 1:C:424:LEU:HD12 | 1:C:425:LEU:N | 2.35 | 0.41 |
| 2:F:32:VAL:CG1 | 2:F:36:GLN:OE1 | 2.68 | 0.41 |
| 1:G:372:ARG:NH1 | 1:G:395:PHE:O | 2.51 | 0.41 |
| 1:G:85:LEU:CG | 1:G:165:VAL:HG21 | 2.50 | 0.41 |
| 2:H:64:SER:HA | 2:H:76:LYS:O | 2.20 | 0.41 |
| 1:C:153:LEU:HD12 | 1:C:153:LEU:N | 2.35 | 0.41 |
| 1:C:213:LEU:O | 1:C:217:LEU:HG | 2.20 | 0.41 |
| 2:D:64:SER:HA | 2:D:76:LYS:O | 2.20 | 0.41 |
| 2:F:17:GLN:O | 2:F:18:ASN:HB2 | 2.20 | 0.41 |
| 2:B:122:LEU:O | 2:B:123:LYS:C | 2.59 | 0.41 |
| 2:B:122:LEU:O | 2:B:126:LEU:N | 2.53 | 0.41 |
| 1:C:212:LEU:O | 1:C:213:LEU:C | 2.56 | 0.41 |
| 2:D:59:VAL:CG1 | 2:D:60:THR:N | 2.82 | 0.41 |
| 1:E:298:GLU:HA | 1:E:298:GLU:OE1 | 2.20 | 0.41 |
| 1:E:410:PHE:CD2 | 1:E:449:PRO:HG3 | 2.55 | 0.41 |
| 1:E:369:LEU:CD2 | 1:E:423:VAL:HG11 | 2.50 | 0.41 |
| 1:E:197:LEU:HA | 1:E:439:LEU:HD23 | 2.03 | 0.41 |
| 1:G:14:LEU:HD11 | 2:H:98:ILE:HG22 | 2.01 | 0.41 |
| 1:A:410:PHE:CD2 | 1:A:449:PRO:HG3 | 2.55 | 0.41 |
| 1:A:77:VAL:HG13 | 1:A:79:VAL:CB | 2.50 | 0.41 |
| 2:B:26:LEU:HD22 | 2:B:41:LEU:HD21 | 2.01 | 0.41 |
| 1:E:26:ARG:CG | 1:E:27:VAL:N | 2.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:1:MET:SD | 1:E:448:GLN:HB2 | 2.60 | 0.41 |
| 2:F:45:VAL:CG2 | 2:F:46:GLU:N | 2.82 | 0.41 |
| 1:G:185:LYS:H | 1:G:185:LYS:HG2 | 1.73 | 0.41 |
| 2:H:3:ASP:O | 2:H:5:LEU:N | 2.54 | 0.41 |
| 2:H:38:LYS:HD3 | 2:H:99:HIS:CE1 | 2.56 | 0.41 |
| 1:A:290:VAL:CG2 | 1:A:291:PRO:CD | 2.94 | 0.41 |
| 1:A:351:ASP:C | 1:A:353:PHE:N | 2.74 | 0.41 |
| 1:A:180:ASP:HA | 1:A:370:ARG:O | 2.20 | 0.41 |
| 1:A:-3:HIS:H3 | 1:A:414:ILE:HD12 | 1.86 | 0.41 |
| 1:A:405:GLY:O | 1:A:428:VAL:O | 2.38 | 0.41 |
| 2:B:62:LEU:O | 2:B:98:ILE:HA | 2.20 | 0.41 |
| 2:F:3:ASP:O | 2:F:5:LEU:N | 2.54 | 0.41 |
| 2:H:115:PHE:O | 2:H:116:ASN:C | 2.58 | 0.41 |
| 2:H:122:LEU:O | 2:H:126:LEU:N | 2.54 | 0.41 |
| 2:H:80:VAL:HG11 | 2:H:88:VAL:HG21 | 2.03 | 0.41 |
| 1:A:99:LYS:HE2 | 1:A:150:VAL:CG1 | 2.50 | 0.41 |
| 2:D:18:ASN:OD1 | 2:D:105:LYS:HE2 | 2.20 | 0.41 |
| 1:E:342:LEU:HD12 | 1:E:343:GLY:N | 2.35 | 0.41 |
| 1:E:37:GLN:N | 1:E:37:GLN:NE2 | 2.67 | 0.41 |
| 1:G:172:LEU:CD2 | 3:G:474:HOH:O | 2.66 | 0.41 |
| 1:G:410:PHE:CD2 | 1:G:449:PRO:HG3 | 2.55 | 0.41 |
| 2:H:32:VAL:CG1 | 2:H:36:GLN:OE1 | 2.69 | 0.41 |
| 2:H:23:TYR:CE1 | 2:H:38:LYS:HE2 | 2.55 | 0.41 |
| 2:H:3:ASP:C | 2:H:5:LEU:N | 2.72 | 0.41 |
| 1:G:3:SER:OG | 2:H:75:HIS:ND1 | 2.37 | 0.41 |
| 1:A:277:LYS:O | 1:A:280:ASP:HB3 | 2.20 | 0.41 |
| 1:A:391:ASP:HA | 1:A:392:PRO:HD3 | 1.80 | 0.41 |
| 1:C:83:CYS:HB3 | 1:C:140:GLN:OE1 | 2.20 | 0.41 |
| 1:C:351:ASP:C | 1:C:353:PHE:N | 2.73 | 0.41 |
| 2:D:112:GLY:O | 2:D:113:PRO:C | 2.56 | 0.41 |
| 1:E:330:ASN:ND2 | 1:E:345:SER:OG | 2.53 | 0.41 |
| 1:E:364:ILE:O | 1:E:368:THR:HG23 | 2.20 | 0.41 |
| 1:G:316:PHE:O | 1:G:320:THR:HG23 | 2.21 | 0.41 |
| 1:C:37:GLN:C | 1:C:39:PHE:N | 2.73 | 0.41 |
| 1:E:2:PHE:CG | 1:E:439:LEU:HD12 | 2.56 | 0.41 |
| 2:F:20:ILE:HG23 | 2:F:104:GLN:CG | 2.51 | 0.41 |
| 1:A:342:LEU:HD12 | 1:A:343:GLY:N | 2.36 | 0.41 |
| 1:A:84:GLU:H | 1:A:84:GLU:HG3 | 1.63 | 0.41 |
| 2:B:3:ASP:O | 2:B:5:LEU:N | 2.53 | 0.41 |
| 1:C:135:LEU:HB2 | 1:C:144:LEU:HD11 | 2.03 | 0.41 |
| 1:C:24:PHE:CZ | 1:C:233:CYS:HB2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:280:ASP:CG | 1:C:318:LEU:HB2 | 2.40 | 0.41 |
| 1:G:225:GLN:NE2 | 2:H:133:SER:HB2 | 2.35 | 0.41 |
| 1:A:82:LEU:HD21 | 1:A:142:ILE:HG22 | 2.02 | 0.41 |
| 1:A:346:GLY:N | 1:A:405:GLY:HA3 | 2.36 | 0.41 |
| 1:A:364:ILE:O | 1:A:367:TRP:HB3 | 2.20 | 0.41 |
| 1:C:229:GLU:OE2 | 1:E:9:ARG:NH1 | 2.52 | 0.41 |
| 1:C:333:GLN:HG3 | 1:C:342:LEU:HD13 | 2.02 | 0.41 |
| 1:E:353:PHE:CD1 | 1:E:353:PHE:C | 2.94 | 0.41 |
| 1:E:378:ALA:HA | 1:E:379:PRO:HD3 | 1.77 | 0.41 |
| 1:E:226:LEU:HB3 | 2:F:23:TYR:OH | 2.21 | 0.41 |
| 2:F:80:VAL:HG11 | 2:F:88:VAL:HG21 | 2.03 | 0.41 |
| 1:G:77:VAL:HG13 | 1:G:79:VAL:CB | 2.51 | 0.41 |
| 1:A:269:GLN:O | 1:A:270:ALA:C | 2.60 | 0.41 |
| 1:C:145:LYS:CE | 1:C:168:ASP:HB3 | 2.51 | 0.41 |
| 1:C:348:ASN:HB3 | 1:C:375:SER:HB2 | 2.03 | 0.41 |
| 1:G:14:LEU:HA | 1:G:14:LEU:HD23 | 1.88 | 0.41 |
| 1:G:145:LYS:HZ1 | 1:G:168:ASP:CB | 2.33 | 0.41 |
| 1:A:197:LEU:HD13 | 1:A:439:LEU:HD23 | 2.03 | 0.40 |
| 2:B:45:VAL:CG2 | 2:B:46:GLU:N | 2.84 | 0.40 |
| 2:B:4:GLN:O | 2:B:8:GLU:HG3 | 2.21 | 0.40 |
| 1:C:185:LYS:HA | 1:C:186:PRO:HD3 | 1.80 | 0.40 |
| 1:C:311:LEU:HA | 1:C:311:LEU:HD23 | 1.73 | 0.40 |
| 1:C:430:ASP:OD1 | 1:C:432:SER:HB3 | 2.21 | 0.40 |
| 1:C:82:LEU:HD21 | 1:C:142:ILE:HG22 | 2.03 | 0.40 |
| 2:D:125:ASN:O | 2:D:126:LEU:C | 2.58 | 0.40 |
| 1:E:159:LEU:CD2 | 1:E:159:LEU:H | 2.27 | 0.40 |
| 1:G:277:LYS:O | 1:G:281:GLU:HG3 | 2.21 | 0.40 |
| 2:H:70:ASN:O | 2:H:72:HIS:N | 2.54 | 0.40 |
| 1:A:195:PHE:HB2 | 1:A:238:VAL:HG22 | 2.03 | 0.40 |
| 1:A:458:GLU:HG2 | 1:A:459:ASP:N | 2.36 | 0.40 |
| 1:C:369:LEU:CD2 | 1:C:423:VAL:HG11 | 2.51 | 0.40 |
| 1:C:198:LEU:O | 1:C:437:ALA:HB1 | 2.21 | 0.40 |
| 1:C:61:MET:O | 1:C:62:ARG:C | 2.58 | 0.40 |
| 1:C:80:LYS:HD2 | 1:C:84:GLU:O | 2.21 | 0.40 |
| 2:D:3:ASP:C | 2:D:5:LEU:H | 2.25 | 0.40 |
| 1:E:61:MET:O | 1:E:62:ARG:C | 2.60 | 0.40 |
| 1:E:21:ASN:OD1 | 2:F:36:GLN:HB2 | 2.21 | 0.40 |
| 1:G:126:TYR:HD2 | 1:G:355:TYR:CE1 | 2.34 | 0.40 |
| 1:A:312:HIS:ND1 | 1:A:313:PRO:HD2 | 2.36 | 0.40 |
| 1:A:340:ARG:HB2 | 1:A:400:HIS:ND1 | 2.36 | 0.40 |
| 1:A:342:LEU:O | 1:A:402:TYR:HA | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:424:LEU:C | 1:C:424:LEU:HD12 | 2.41 | 0.40 |
| 1:C:197:LEU:HA | 1:C:439:LEU:HD23 | 2.03 | 0.40 |
| 1:E:277:LYS:HE2 | 1:E:281:GLU:CD | 2.40 | 0.40 |
| 1:E:85:LEU:CG | 1:E:165:VAL:HG21 | 2.52 | 0.40 |
| 1:G:148:ILE:HG23 | 1:G:148:ILE:O | 2.20 | 0.40 |
| 1:G:202:LEU:HA | 1:G:202:LEU:HD23 | 1.89 | 0.40 |
| 1:G:312:HIS:ND1 | 1:G:313:PRO:HD2 | 2.36 | 0.40 |
| 1:G:353:PHE:CD1 | 1:G:353:PHE:C | 2.95 | 0.40 |
| 1:G:82:LEU:HA | 1:G:82:LEU:HD12 | 1.83 | 0.40 |
| 2:H:125:ASN:O | 2:H:126:LEU:C | 2.59 | 0.40 |
| 1:A:197:LEU:HD13 | 1:A:439:LEU:CD2 | 2.51 | 0.40 |
| 1:A:410:PHE:CG | 1:A:449:PRO:HG3 | 2.57 | 0.40 |
| 2:B:121:ILE:HD12 | 2:B:121:ILE:HA | 1.92 | 0.40 |
| 2:D:125:ASN:C | 2:D:127:GLN:H | 2.24 | 0.40 |
| 1:E:274:GLU:O | 1:E:275:ALA:C | 2.60 | 0.40 |
| 1:E:37:GLN:C | 1:E:39:PHE:N | 2.72 | 0.40 |
| 2:H:112:GLY:O | 2:H:113:PRO:C | 2.60 | 0.40 |
| 2:H:70:ASN:C | 2:H:72:HIS:N | 2.73 | 0.40 |
| 2:H:4:GLN:O | 2:H:8:GLU:HG3 | 2.21 | 0.40 |
| 1:A:14:LEU:HA | 1:A:14:LEU:HD23 | 1.95 | 0.40 |
| 2:B:5:LEU:O | 2:B:9:ASN:ND2 | 2.54 | 0.40 |
| 1:C:11:HIS:C | 1:C:12:THR:CG2 | 2.89 | 0.40 |
| 1:C:274:GLU:O | 1:C:275:ALA:C | 2.59 | 0.40 |
| 1:C:226:LEU:HB2 | 2:D:62:LEU:HD13 | 2.03 | 0.40 |
| 1:E:190:LEU:HB2 | 1:E:443:ARG:HB2 | 2.02 | 0.40 |
| 1:E:316:PHE:O | 1:E:320:THR:HG23 | 2.22 | 0.40 |
| 1:E:444:SER:O | 1:E:445:LEU:HB2 | 2.22 | 0.40 |
| 1:E:7:ALA:O | 1:E:9:ARG:N | 2.55 | 0.40 |
| 2:F:137:CYS:O | 2:F:138:ALA:C | 2.59 | 0.40 |
| 1:G:306:LEU:HB3 | 1:G:307:PRO:CD | 2.47 | 0.40 |
| 2:H:41:LEU:HD13 | 2:H:103:ILE:HD12 | 2.04 | 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 | 406/476 (85%) | 321 (79%) | 63 (16%) | 22 (5%) | 2 | 13 |
| 1 | C | 399/476 (84%) | 317 (79%) | 60 (15%) | 22 (6%) | 2 | 12 |
| 1 | E | 398/476 (84%) | 325 (82%) | 50 (13%) | 23 (6%) | 2 | 11 |
| 1 | G | 398/476 (84%) | 319 (80%) | 56 (14%) | 23 (6%) | 2 | 11 |
| 2 | B | 141/144 (98%) | 110 (78%) | 24 (17%) | 7 (5%) | 2 | 15 |
| 2 | D | 141/144 (98%) | 115 (82%) | 19 (14%) | 7 (5%) | 2 | 15 |
| 2 | F | 141/144 (98%) | 113 (80%) | 21 (15%) | 7 (5%) | 2 | 15 |
| 2 | H | 141/144 (98%) | 114 (81%) | 19 (14%) | 8 (6%) | 2 | 12 |
| All | All | 2165/2480 (87%) | 1734 (80%) | 312 (14%) | 119 (6%) | 2 | 12 |

All (119) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | ALA |
| 1 | A | 76 | GLY |
| 1 | A | 79 | VAL |
| 1 | A | 330 | ASN |
| 1 | A | 405 | GLY |
| 2 | B | 140 | ALA |
| 1 | C | -1 | HIS |
| 1 | C | 10 | ALA |
| 1 | C | 76 | GLY |
| 1 | C | 79 | VAL |
| 1 | C | 330 | ASN |
| 1 | C | 405 | GLY |
| 2 | D | 140 | ALA |
| 1 | E | -1 | HIS |
| 1 | E | 76 | GLY |
| 1 | E | 79 | VAL |
| 1 | E | 330 | ASN |
| 1 | E | 405 | GLY |
| 2 | F | 140 | ALA |
| 1 | G | -1 | HIS |
| 1 | G | 76 | GLY |
| 1 | G | 79 | VAL |
| 1 | G | 330 | ASN |
| 1 | G | 405 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | H | 126 | LEU |
| 2 | H | 140 | ALA |
| 1 | A | -1 | HIS |
| 1 | A | 8 | GLN |
| 1 | A | 310 | PRO |
| 1 | A | 420 | ASP |
| 2 | B | 56 | GLN |
| 2 | B | 84 | LYS |
| 2 | B | 126 | LEU |
| 1 | C | 8 | GLN |
| 1 | C | 310 | PRO |
| 1 | C | 420 | ASP |
| 2 | D | 84 | LYS |
| 2 | D | 126 | LEU |
| 1 | E | 8 | GLN |
| 1 | E | 10 | ALA |
| 1 | E | 320 | THR |
| 1 | E | 420 | ASP |
| 2 | F | 84 | LYS |
| 2 | F | 126 | LEU |
| 1 | G | 8 | GLN |
| 1 | G | 10 | ALA |
| 1 | G | 310 | PRO |
| 1 | G | 420 | ASP |
| 2 | H | 56 | GLN |
| 2 | H | 84 | LYS |
| 1 | A | 38 | PRO |
| 1 | A | 180 | ASP |
| 1 | A | 265 | THR |
| 1 | A | 298 | GLU |
| 1 | A | 305 | THR |
| 1 | A | 320 | THR |
| 1 | C | 298 | GLU |
| 1 | C | 305 | THR |
| 1 | C | 320 | THR |
| 2 | D | 56 | GLN |
| 1 | E | 38 | PRO |
| 1 | E | 75 | SER |
| 1 | E | 298 | GLU |
| 1 | E | 305 | THR |
| 1 | E | 310 | PRO |
| 2 | F | 56 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 38 | PRO |
| 1 | G | 298 | GLU |
| 1 | G | 305 | THR |
| 1 | G | 320 | THR |
| 1 | A | 209 | GLY |
| 1 | A | 347 | GLN |
| 1 | C | 38 | PRO |
| 1 | C | 265 | THR |
| 1 | C | 301 | PRO |
| 1 | C | 347 | GLN |
| 1 | E | 180 | ASP |
| 1 | E | 301 | PRO |
| 1 | G | 155 | THR |
| 1 | G | 180 | ASP |
| 1 | G | 265 | THR |
| 1 | G | 301 | PRO |
| 1 | A | 155 | THR |
| 1 | A | 301 | PRO |
| 2 | B | 142 | PRO |
| 1 | C | 180 | ASP |
| 1 | C | 209 | GLY |
| 1 | E | 155 | THR |
| 1 | E | 209 | GLY |
| 1 | E | 265 | THR |
| 1 | E | 418 | PRO |
| 2 | F | 142 | PRO |
| 1 | G | 347 | GLN |
| 1 | A | 29 | VAL |
| 1 | A | 418 | PRO |
| 2 | B | 112 | GLY |
| 1 | C | 75 | SER |
| 1 | C | 418 | PRO |
| 2 | D | 142 | PRO |
| 1 | E | 245 | GLY |
| 1 | G | 29 | VAL |
| 1 | G | 418 | PRO |
| 2 | H | 142 | PRO |
| 2 | B | 54 | GLY |
| 1 | C | 29 | VAL |
| 2 | F | 54 | GLY |
| 1 | G | 245 | GLY |
| 2 | H | 54 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 54 | GLY |
| 2 | D | 112 | GLY |
| 1 | E | 29 | VAL |
| 1 | C | 245 | GLY |
| 1 | E | 77 | VAL |
| 2 | F | 112 | GLY |
| 2 | H | 71 | GLY |
| 1 | A | 317 | PRO |
| 1 | G | 317 | PRO |
| 1 | G | 429 | PRO |
| 2 | H | 112 | GLY |

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 | 355/409 (87%) | 320 (90%) | 35 (10%) | 9 | 34 |
| 1 | C | 350/409 (86%) | 318 (91%) | 32 (9%) | 11 | 39 |
| 1 | E | 349/409 (85%) | 317 (91%) | 32 (9%) | 11 | 38 |
| 1 | G | 349/409 (85%) | 317 (91%) | 32 (9%) | 11 | 38 |
| 2 | B | 125/126 (99%) | 114 (91%) | 11 (9%) | 12 | 41 |
| 2 | D | 125/126 (99%) | 115 (92%) | 10 (8%) | 14 | 45 |
| 2 | F | 125/126 (99%) | 115 (92%) | 10 (8%) | 14 | 45 |
| 2 | H | 125/126 (99%) | 115 (92%) | 10 (8%) | 14 | 45 |
| All | All | 1903/2140 (89%) | 1731 (91%) | 172 (9%) | 11 | 40 |

All (172) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | -1 | HIS |
| 1 | A | 8 | GLN |
| 1 | A | 15 | SER |
| 1 | A | 20 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 21 | ASN |
| 1 | A | 23 | THR |
| 1 | A | 31 | THR |
| 1 | A | 37 | GLN |
| 1 | A | 56 | THR |
| 1 | A | 85 | LEU |
| 1 | A | 86 | GLN |
| 1 | A | 134 | VAL |
| 1 | A | 136 | GLU |
| 1 | A | 140 | GLN |
| 1 | A | 151 | SER |
| 1 | A | 155 | THR |
| 1 | A | 167 | ASP |
| 1 | A | 200 | SER |
| 1 | A | 222 | VAL |
| 1 | A | 226 | LEU |
| 1 | A | 234 | SER |
| 1 | A | 243 | LEU |
| 1 | A | 306 | LEU |
| 1 | A | 314 | CYS |
| 1 | A | 372 | ARG |
| 1 | A | 406 | ASN |
| 1 | A | 419 | GLU |
| 1 | A | 422 | THR |
| 1 | A | 430 | ASP |
| 1 | A | 434 | THR |
| 1 | A | 438 | CYS |
| 1 | A | 447 | CYS |
| 1 | A | 459 | ASP |
| 1 | A | 460 | ASP |
| 1 | A | 462 | LEU |
| 2 | B | 3 | ASP |
| 2 | B | 23 | TYR |
| 2 | B | 34 | VAL |
| 2 | B | 69 | GLN |
| 2 | B | 72 | HIS |
| 2 | B | 83 | ASP |
| 2 | B | 85 | LEU |
| 2 | B | 104 | GLN |
| 2 | B | 116 | ASN |
| 2 | B | 128 | ASN |
| 2 | B | 129 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | -1 | HIS |
| 1 | C | 8 | GLN |
| 1 | C | 15 | SER |
| 1 | C | 20 | ASN |
| 1 | C | 21 | ASN |
| 1 | C | 23 | THR |
| 1 | C | 31 | THR |
| 1 | C | 37 | GLN |
| 1 | C | 56 | THR |
| 1 | C | 85 | LEU |
| 1 | C | 86 | GLN |
| 1 | C | 134 | VAL |
| 1 | C | 136 | GLU |
| 1 | C | 140 | GLN |
| 1 | C | 151 | SER |
| 1 | C | 155 | THR |
| 1 | C | 166 | ARG |
| 1 | C | 167 | ASP |
| 1 | C | 200 | SER |
| 1 | C | 222 | VAL |
| 1 | C | 226 | LEU |
| 1 | C | 234 | SER |
| 1 | C | 243 | LEU |
| 1 | C | 306 | LEU |
| 1 | C | 372 | ARG |
| 1 | C | 406 | ASN |
| 1 | C | 418 | PRO |
| 1 | C | 422 | THR |
| 1 | C | 430 | ASP |
| 1 | C | 434 | THR |
| 1 | C | 438 | CYS |
| 1 | C | 447 | CYS |
| 2 | D | 3 | ASP |
| 2 | D | 23 | TYR |
| 2 | D | 34 | VAL |
| 2 | D | 69 | GLN |
| 2 | D | 83 | ASP |
| 2 | D | 85 | LEU |
| 2 | D | 104 | GLN |
| 2 | D | 116 | ASN |
| 2 | D | 128 | ASN |
| 2 | D | 129 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | -1 | HIS |
| 1 | E | 8 | GLN |
| 1 | E | 15 | SER |
| 1 | E | 20 | ASN |
| 1 | E | 21 | ASN |
| 1 | E | 23 | THR |
| 1 | E | 31 | THR |
| 1 | E | 37 | GLN |
| 1 | E | 56 | THR |
| 1 | E | 85 | LEU |
| 1 | E | 86 | GLN |
| 1 | E | 134 | VAL |
| 1 | E | 136 | GLU |
| 1 | E | 151 | SER |
| 1 | E | 155 | THR |
| 1 | E | 166 | ARG |
| 1 | E | 167 | ASP |
| 1 | E | 200 | SER |
| 1 | E | 222 | VAL |
| 1 | E | 226 | LEU |
| 1 | E | 234 | SER |
| 1 | E | 243 | LEU |
| 1 | E | 306 | LEU |
| 1 | E | 314 | CYS |
| 1 | E | 372 | ARG |
| 1 | E | 406 | ASN |
| 1 | E | 419 | GLU |
| 1 | E | 422 | THR |
| 1 | E | 430 | ASP |
| 1 | E | 434 | THR |
| 1 | E | 438 | CYS |
| 1 | E | 447 | CYS |
| 2 | F | 3 | ASP |
| 2 | F | 23 | TYR |
| 2 | F | 34 | VAL |
| 2 | F | 69 | GLN |
| 2 | F | 83 | ASP |
| 2 | F | 85 | LEU |
| 2 | F | 104 | GLN |
| 2 | F | 116 | ASN |
| 2 | F | 128 | ASN |
| 2 | F | 129 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | -1 | HIS |
| 1 | G | 8 | GLN |
| 1 | G | 15 | SER |
| 1 | G | 20 | ASN |
| 1 | G | 21 | ASN |
| 1 | G | 23 | THR |
| 1 | G | 31 | THR |
| 1 | G | 37 | GLN |
| 1 | G | 56 | THR |
| 1 | G | 85 | LEU |
| 1 | G | 86 | GLN |
| 1 | G | 134 | VAL |
| 1 | G | 136 | GLU |
| 1 | G | 140 | GLN |
| 1 | G | 151 | SER |
| 1 | G | 155 | THR |
| 1 | G | 167 | ASP |
| 1 | G | 200 | SER |
| 1 | G | 222 | VAL |
| 1 | G | 226 | LEU |
| 1 | G | 234 | SER |
| 1 | G | 243 | LEU |
| 1 | G | 306 | LEU |
| 1 | G | 372 | ARG |
| 1 | G | 406 | ASN |
| 1 | G | 418 | PRO |
| 1 | G | 419 | GLU |
| 1 | G | 422 | THR |
| 1 | G | 430 | ASP |
| 1 | G | 434 | THR |
| 1 | G | 438 | CYS |
| 1 | G | 447 | CYS |
| 2 | H | 3 | ASP |
| 2 | H | 23 | TYR |
| 2 | H | 34 | VAL |
| 2 | H | 69 | GLN |
| 2 | H | 83 | ASP |
| 2 | H | 85 | LEU |
| 2 | H | 104 | GLN |
| 2 | H | 116 | ASN |
| 2 | H | 128 | ASN |
| 2 | H | 129 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | -3 | HIS |
| 1 | A | 20 | ASN |
| 1 | A | 37 | GLN |
| 1 | A | 70 | GLN |
| 1 | A | 86 | GLN |
| 1 | A | 216 | GLN |
| 1 | A | 269 | GLN |
| 1 | A | 333 | GLN |
| 1 | A | 406 | ASN |
| 1 | A | 435 | GLN |
| 2 | B | 9 | ASN |
| 2 | B | 69 | GLN |
| 2 | B | 72 | HIS |
| 2 | B | 104 | GLN |
| 2 | B | 116 | ASN |
| 2 | B | 127 | GLN |
| 2 | B | 128 | ASN |
| 1 | C | -3 | HIS |
| 1 | C | 20 | ASN |
| 1 | C | 37 | GLN |
| 1 | C | 70 | GLN |
| 1 | C | 86 | GLN |
| 1 | C | 216 | GLN |
| 1 | C | 269 | GLN |
| 1 | C | 285 | GLN |
| 1 | C | 333 | GLN |
| 1 | C | 406 | ASN |
| 2 | D | 9 | ASN |
| 2 | D | 69 | GLN |
| 2 | D | 72 | HIS |
| 2 | D | 104 | GLN |
| 2 | D | 116 | ASN |
| 2 | D | 127 | GLN |
| 2 | D | 128 | ASN |
| 1 | E | -3 | HIS |
| 1 | E | 5 | GLN |
| 1 | E | 11 | HIS |
| 1 | E | 37 | GLN |
| 1 | E | 70 | GLN |
| 1 | E | 86 | GLN |
| 1 | E | 216 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 269 | GLN |
| 1 | E | 326 | GLN |
| 1 | E | 333 | GLN |
| 1 | E | 406 | ASN |
| 1 | E | 435 | GLN |
| 2 | F | 9 | ASN |
| 2 | F | 69 | GLN |
| 2 | F | 104 | GLN |
| 2 | F | 116 | ASN |
| 2 | F | 127 | GLN |
| 2 | F | 128 | ASN |
| 1 | G | -3 | HIS |
| 1 | G | 11 | HIS |
| 1 | G | 37 | GLN |
| 1 | G | 70 | GLN |
| 1 | G | 86 | GLN |
| 1 | G | 216 | GLN |
| 1 | G | 333 | GLN |
| 1 | G | 406 | ASN |
| 1 | G | 435 | GLN |
| 2 | H | 9 | ASN |
| 2 | H | 69 | GLN |
| 2 | H | 104 | GLN |
| 2 | H | 116 | ASN |
| 2 | H | 127 | GLN |
| 2 | H | 128 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 416/476 (87%) | -0.26 | 4 (0%) 82 58 | 21, 54, 104, 113 | 0 |
| 1 | C | 409/476 (85%) | -0.35 | 6 (1%) 74 47 | 20, 50, 98, 108 | 0 |
| 1 | E | 408/476 (85%) | -0.29 | 8 (1%) 65 36 | 24, 53, 94, 107 | 0 |
| 1 | G | 408/476 (85%) | -0.16 | 16 (3%) 40 16 | 27, 58, 103, 114 | 0 |
| 2 | B | 143/144 (99%) | -0.36 | 3 (2%) 64 34 | 29, 52, 90, 113 | 0 |
| 2 | D | 143/144 (99%) | -0.41 | 3 (2%) 64 34 | 32, 49, 83, 102 | 0 |
| 2 | F | 143/144 (99%) | -0.17 | 2 (1%) 75 49 | 38, 64, 88, 116 | 0 |
| 2 | H | 143/144 (99%) | -0.12 | 4 (2%) 53 25 | 34, 68, 93, 111 | 0 |
| All | All | 2213/2480 (89%) | -0.26 | 46 (2%) 64 34 | 20, 56, 100, 116 | 0 |

All (46) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 144 | ALA | 5.0 |
| 2 | H | 144 | ALA | 4.2 |
| 1 | A | 388 | TYR | 3.8 |
| 1 | G | 265 | THR | 3.7 |
| 2 | F | 144 | ALA | 3.6 |
| 2 | D | 3 | ASP | 3.4 |
| 1 | G | 91 | CYS | 3.3 |
| 1 | C | 265 | THR | 3.2 |
| 2 | H | 53 | SER | 3.2 |
| 1 | G | -2 | HIS | 3.2 |
| 1 | E | 128 | HIS | 3.2 |
| 1 | G | 128 | HIS | 3.1 |
| 2 | H | 4 | GLN | 3.1 |
| 2 | F | 143 | ARG | 2.8 |
| 2 | D | 71 | GLY | 2.8 |
| 1 | E | 86 | GLN | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 53 | SER | 2.8 |
| 1 | A | 264 | LEU | 2.7 |
| 1 | C | 264 | LEU | 2.6 |
| 1 | G | 268 | THR | 2.6 |
| 1 | G | 88 | GLU | 2.6 |
| 1 | A | 265 | THR | 2.5 |
| 1 | G | 210 | GLU | 2.4 |
| 1 | E | 85 | LEU | 2.4 |
| 1 | E | 264 | LEU | 2.4 |
| 1 | G | 163 | GLY | 2.4 |
| 1 | C | 101 | MET | 2.3 |
| 1 | G | 92 | CYS | 2.3 |
| 2 | D | 144 | ALA | 2.3 |
| 2 | H | 55 | ALA | 2.3 |
| 1 | A | 131 | ASP | 2.2 |
| 1 | C | -2 | HIS | 2.2 |
| 1 | G | 78 | GLY | 2.2 |
| 1 | G | 164 | SER | 2.2 |
| 1 | E | 265 | THR | 2.1 |
| 1 | E | 266 | LYS | 2.1 |
| 1 | G | 85 | LEU | 2.1 |
| 1 | C | 167 | ASP | 2.1 |
| 1 | E | 267 | LYS | 2.1 |
| 1 | G | 133 | LEU | 2.1 |
| 1 | G | 207 | GLY | 2.1 |
| 1 | C | 390 | THR | 2.1 |
| 1 | G | 127 | ILE | 2.0 |
| 2 | B | 3 | ASP | 2.0 |
| 1 | E | 126 | TYR | 2.0 |
| 1 | G | 101 | MET | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.