# Full wwPDB EM Validation Report

Nov 20, 2022 – 03:36 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 2XRP |
| EMDB ID | : | EMD-1788 |
| Title | : | Human Doublecortin N-DC Repeat (1MJD) and Mammalian Tubulin (1JFF and 3HKE) Docked into the 8-Angstrom Cryo-EM Map of Doublecortin- Stabilised Microtubules |
| Authors | : | Fourniol, F.J.; Sindelar, C.V.; Amigues, B.; Clare, D.K.; Thomas, G.; Perderiset, M.; Francis, F.; Houdusse, A.; Moores, C.A. |
| Deposited on | : | 2010-09-18 |
| Resolution | : | 8.20 Å(reported) |
| Based on initial models | : | 3HKE, 1JFF, 1MJD |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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The following versions of software and data (see references (1)) were used in the production of this report:

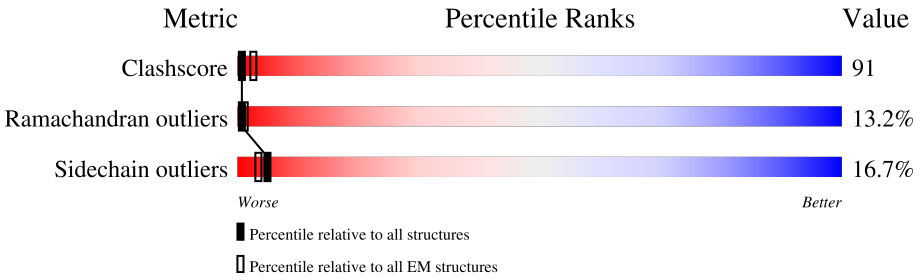
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.20 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) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 445 | 81% 20% 55% 18% |
| 1 | C | 445 | 17% 21% 55% 18% |
| 1 | E | 445 | 82% 22% 54% 18% |
| 1 | G | 445 | 25% 20% 56% 18% |
| 2 | B | 452 | 21% 16% 59% 19% 5% |
| 2 | D | 452 | 81% 17% 59% 18% 5% |
| 2 | F | 452 | 20% 17% 58% 18% 5% |

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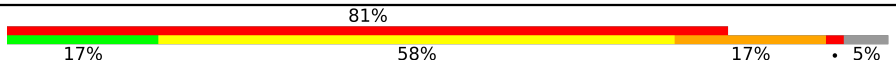
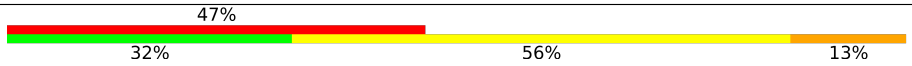
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | H | 452 |   |
| 3 | I | 95 |   |

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28352 atoms, of which 596 are hydrogens and 0 are deuteriums.

In the tables below, 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 TUBULIN BETA-2B CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3351 | 2105 | 575 | 646 | 25 | | |
| 1 | C | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3351 | 2105 | 575 | 646 | 25 | | |
| 1 | E | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3351 | 2105 | 575 | 646 | 25 | | |
| 1 | G | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3351 | 2105 | 575 | 646 | 25 | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 172 | VAL | MET | conflict | UNP Q6B856 |
| A | 318 | VAL | ILE | conflict | UNP Q6B856 |
| C | 172 | VAL | MET | conflict | UNP Q6B856 |
| C | 318 | VAL | ILE | conflict | UNP Q6B856 |
| E | 172 | VAL | MET | conflict | UNP Q6B856 |
| E | 318 | VAL | ILE | conflict | UNP Q6B856 |
| G | 172 | VAL | MET | conflict | UNP Q6B856 |
| G | 318 | VAL | ILE | conflict | UNP Q6B856 |

- Molecule 2 is a protein called TUBULIN ALPHA-1D CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3334 | 2114 | 569 | 630 | 21 | | |
| 2 | D | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3334 | 2114 | 569 | 630 | 21 | | |
| 2 | F | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3334 | 2114 | 569 | 630 | 21 | | |
| 2 | H | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3334 | 2114 | 569 | 630 | 21 | | |

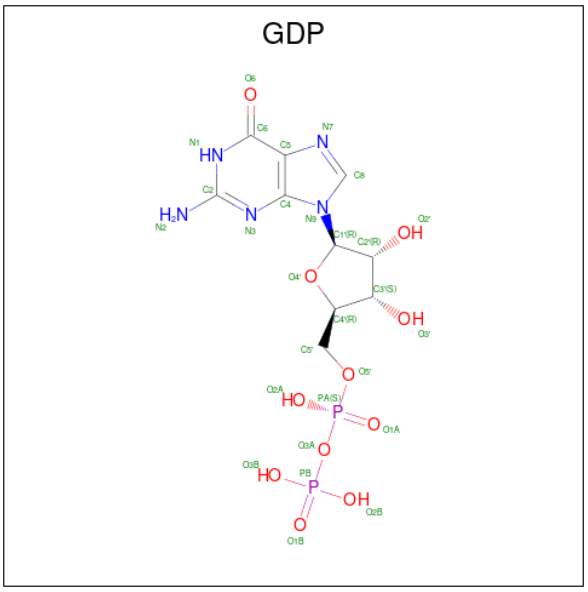
There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 7 | ILE | VAL | conflict | UNP Q2HJ86 |
| B | 114 | ILE | LEU | conflict | UNP Q2HJ86 |
| B | 136 | SER | LEU | conflict | UNP Q2HJ86 |
| B | 358 | GLU | GLN | conflict | UNP Q2HJ86 |
| B | 437 | VAL | MET | conflict | UNP Q2HJ86 |
| B | 450 | GLU | ASP | conflict | UNP Q2HJ86 |
| D | 7 | ILE | VAL | conflict | UNP Q2HJ86 |
| D | 114 | ILE | LEU | conflict | UNP Q2HJ86 |
| D | 136 | SER | LEU | conflict | UNP Q2HJ86 |
| D | 358 | GLU | GLN | conflict | UNP Q2HJ86 |
| D | 437 | VAL | MET | conflict | UNP Q2HJ86 |
| D | 450 | GLU | ASP | conflict | UNP Q2HJ86 |
| F | 7 | ILE | VAL | conflict | UNP Q2HJ86 |
| F | 114 | ILE | LEU | conflict | UNP Q2HJ86 |
| F | 136 | SER | LEU | conflict | UNP Q2HJ86 |
| F | 358 | GLU | GLN | conflict | UNP Q2HJ86 |
| F | 437 | VAL | MET | conflict | UNP Q2HJ86 |
| F | 450 | GLU | ASP | conflict | UNP Q2HJ86 |
| H | 7 | ILE | VAL | conflict | UNP Q2HJ86 |
| H | 114 | ILE | LEU | conflict | UNP Q2HJ86 |
| H | 136 | SER | LEU | conflict | UNP Q2HJ86 |
| H | 358 | GLU | GLN | conflict | UNP Q2HJ86 |
| H | 437 | VAL | MET | conflict | UNP Q2HJ86 |
| H | 450 | GLU | ASP | conflict | UNP Q2HJ86 |

- Molecule 3 is a protein called NEURONAL MIGRATION PROTEIN DOUBLECORTIN.

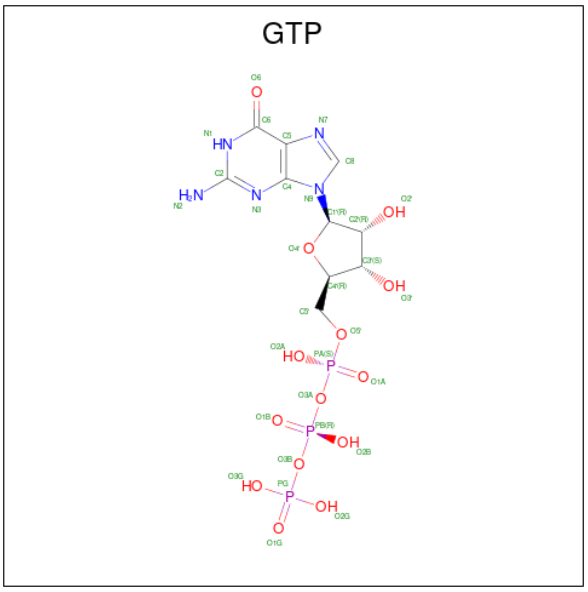
| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | I | 95 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1372 | 490 | 596 | 134 | 150 | 2 | | |

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | A | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 4 | C | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 4 | E | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 4 | G | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



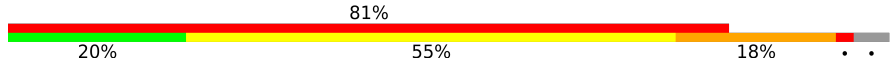
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 5 | B | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 5 | D | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 5 | F | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 5 | H | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

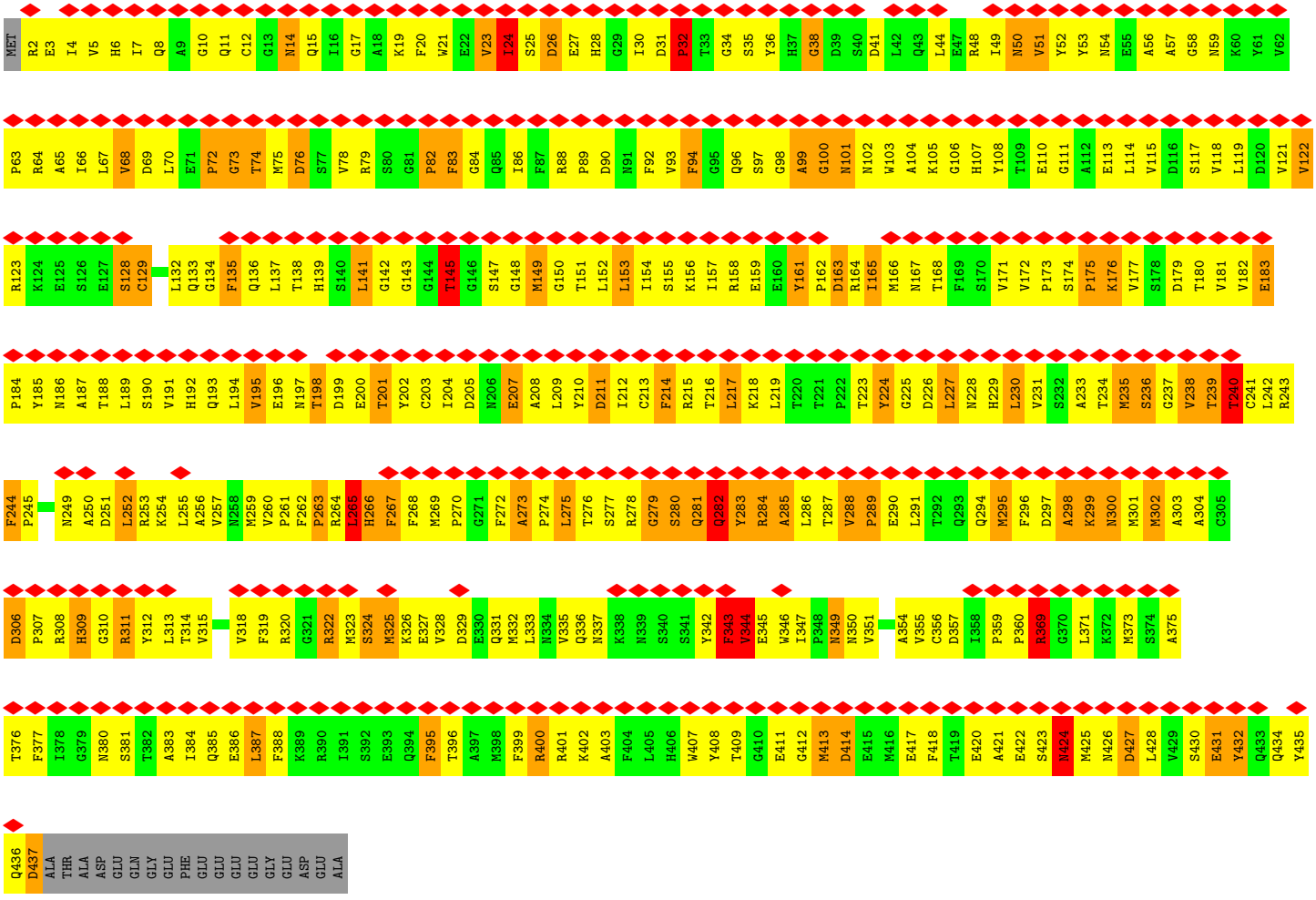
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TUBULIN BETA-2B CHAIN

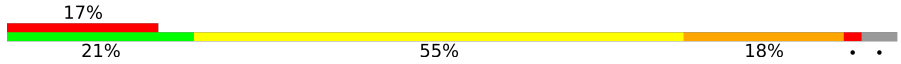
Chain A:

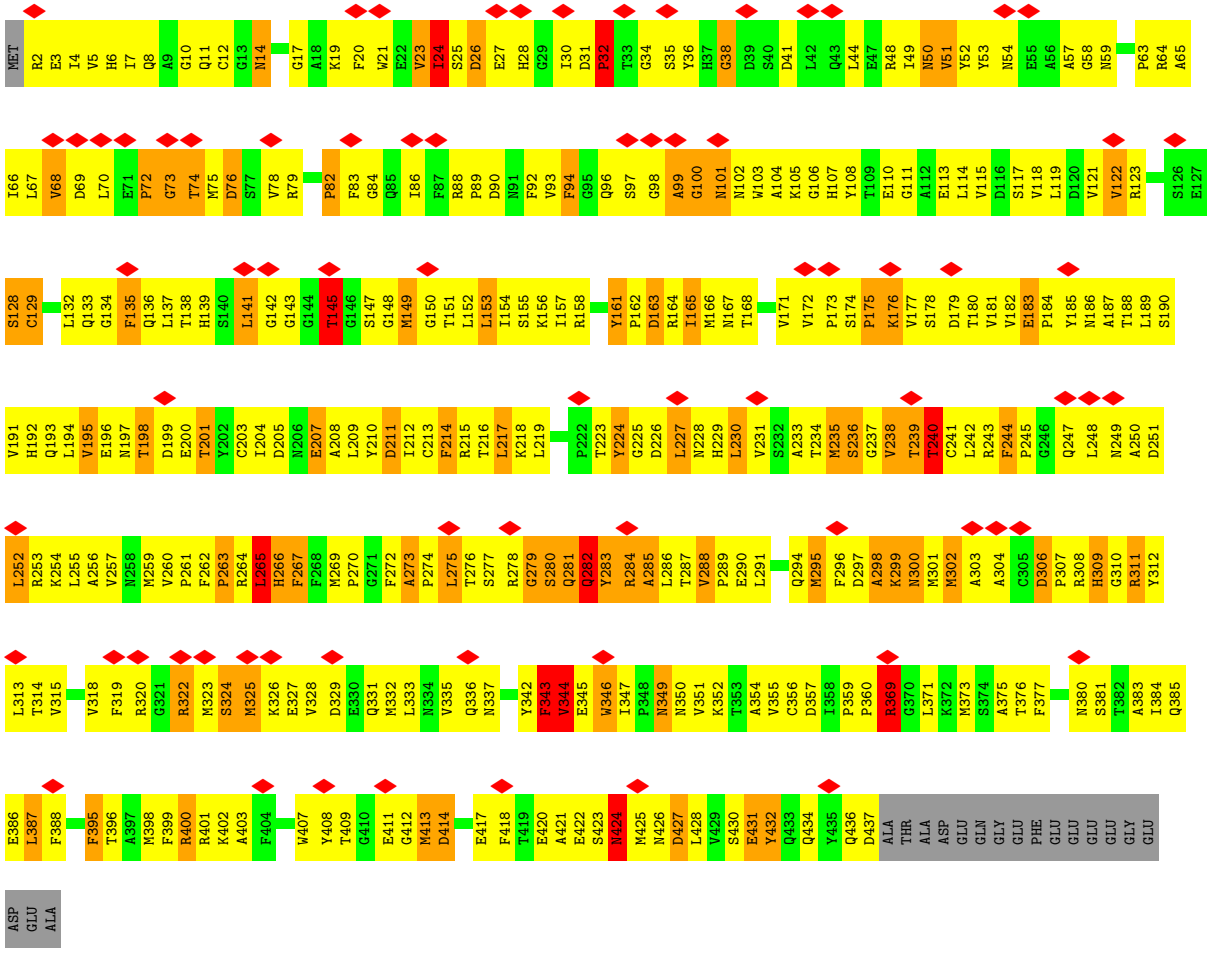



• Molecule 1: TUBULIN BETA-2B CHAIN

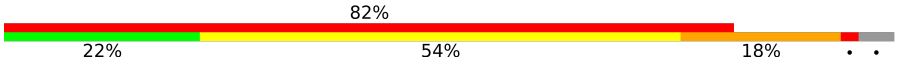
Chain C:

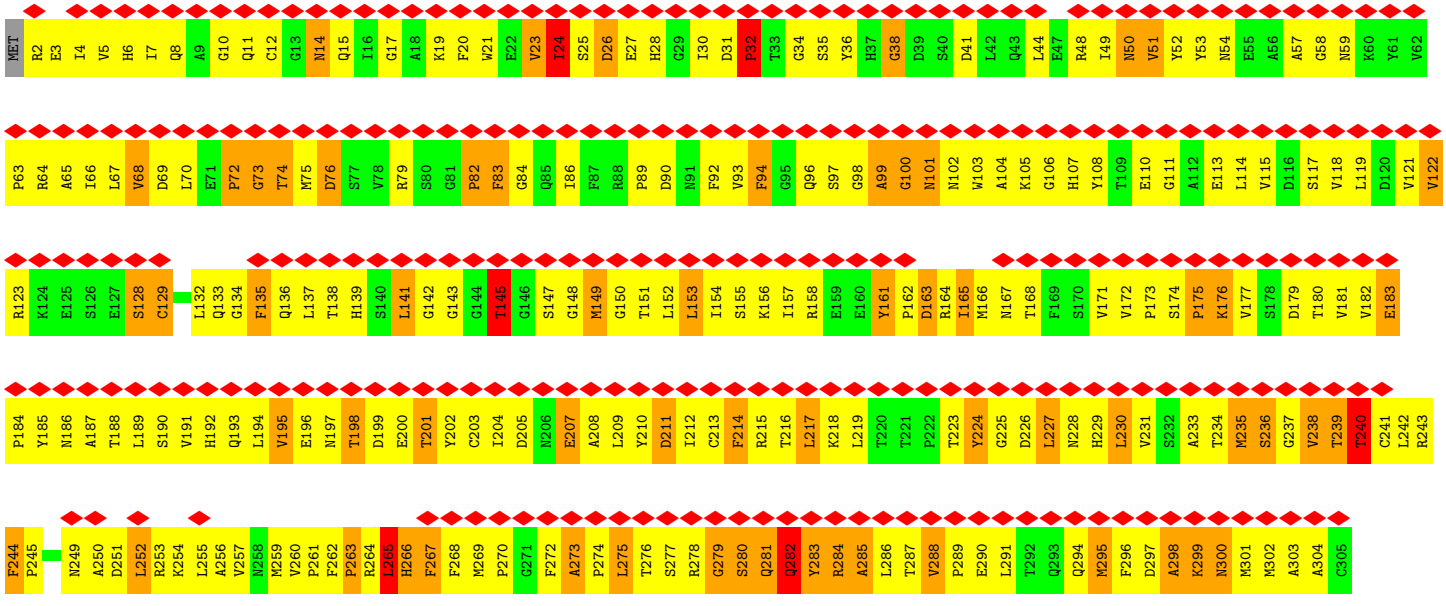


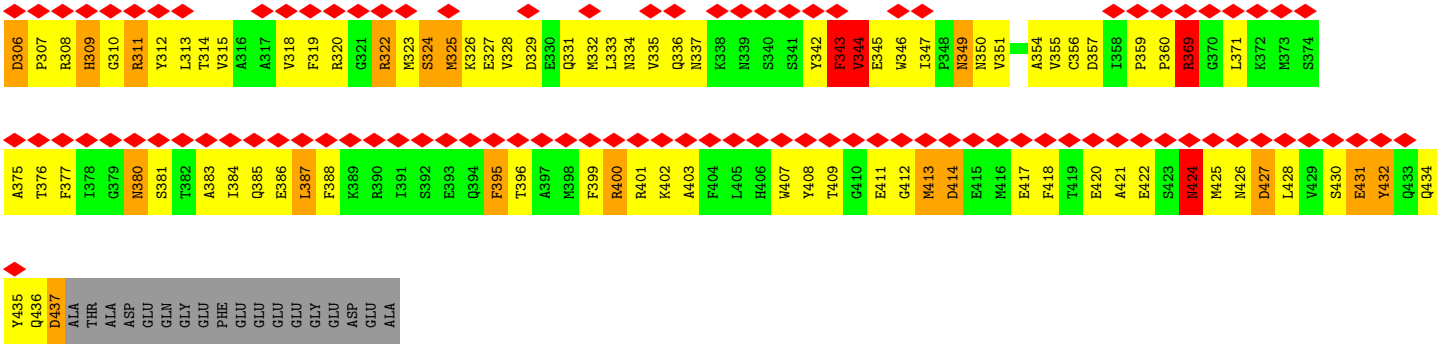


• Molecule 1: TUBULIN BETA-2B CHAIN

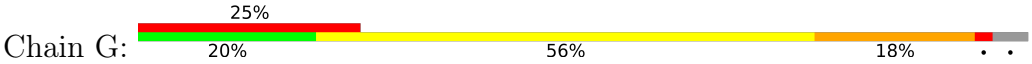
Chain E:

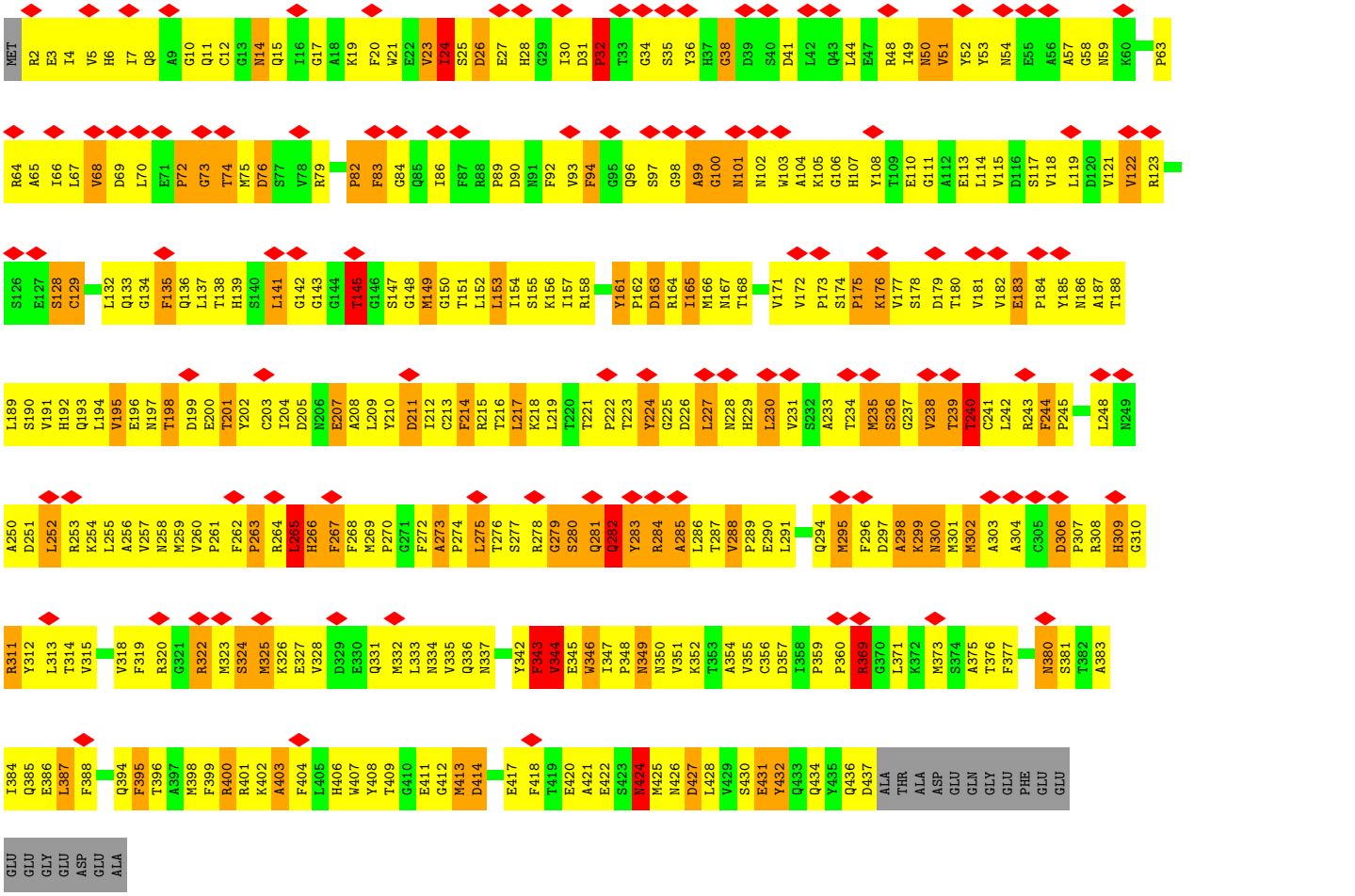


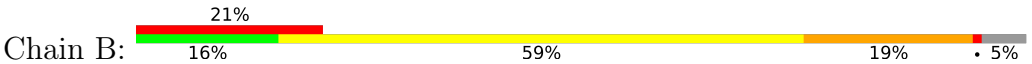


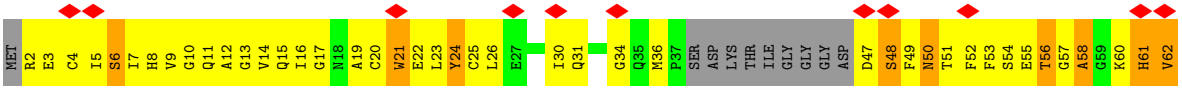

• Molecule 1: TUBULIN BETA-2B CHAIN

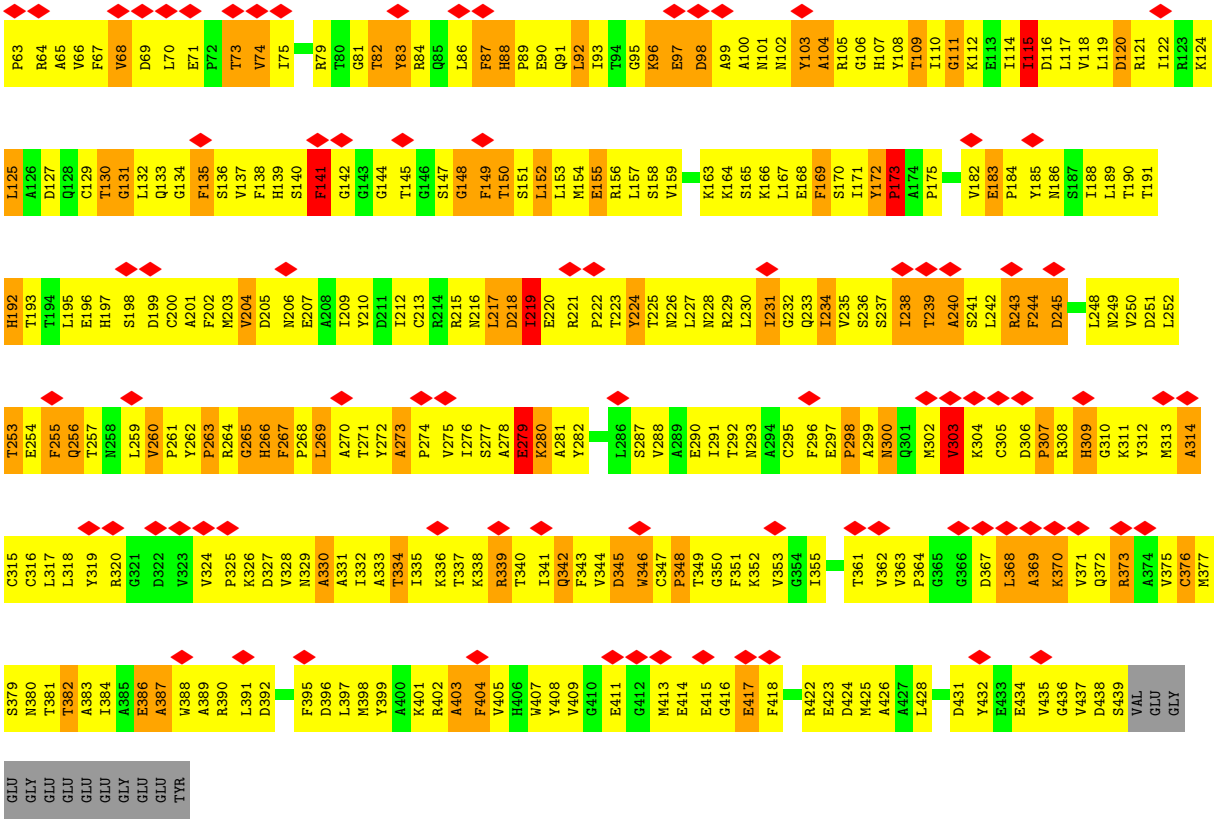



• Molecule 2: TUBULIN ALPHA-1D CHAIN

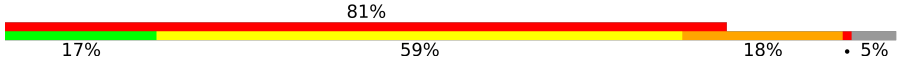


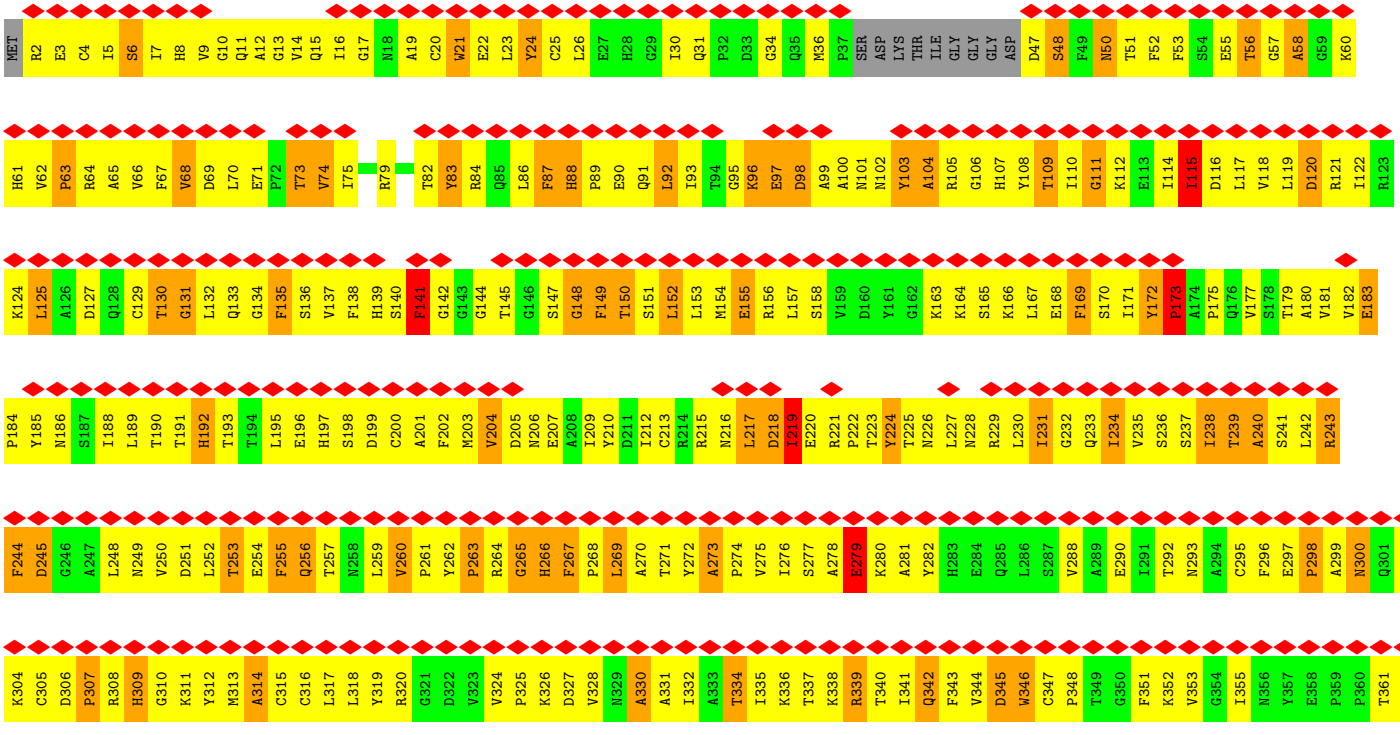



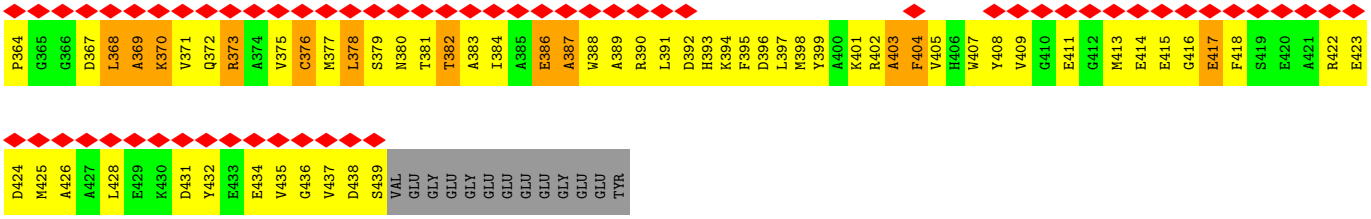


• Molecule 2: TUBULIN ALPHA-1D CHAIN

Chain D:

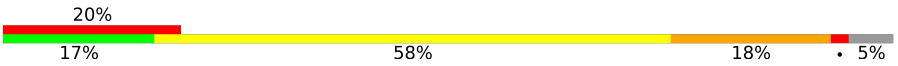


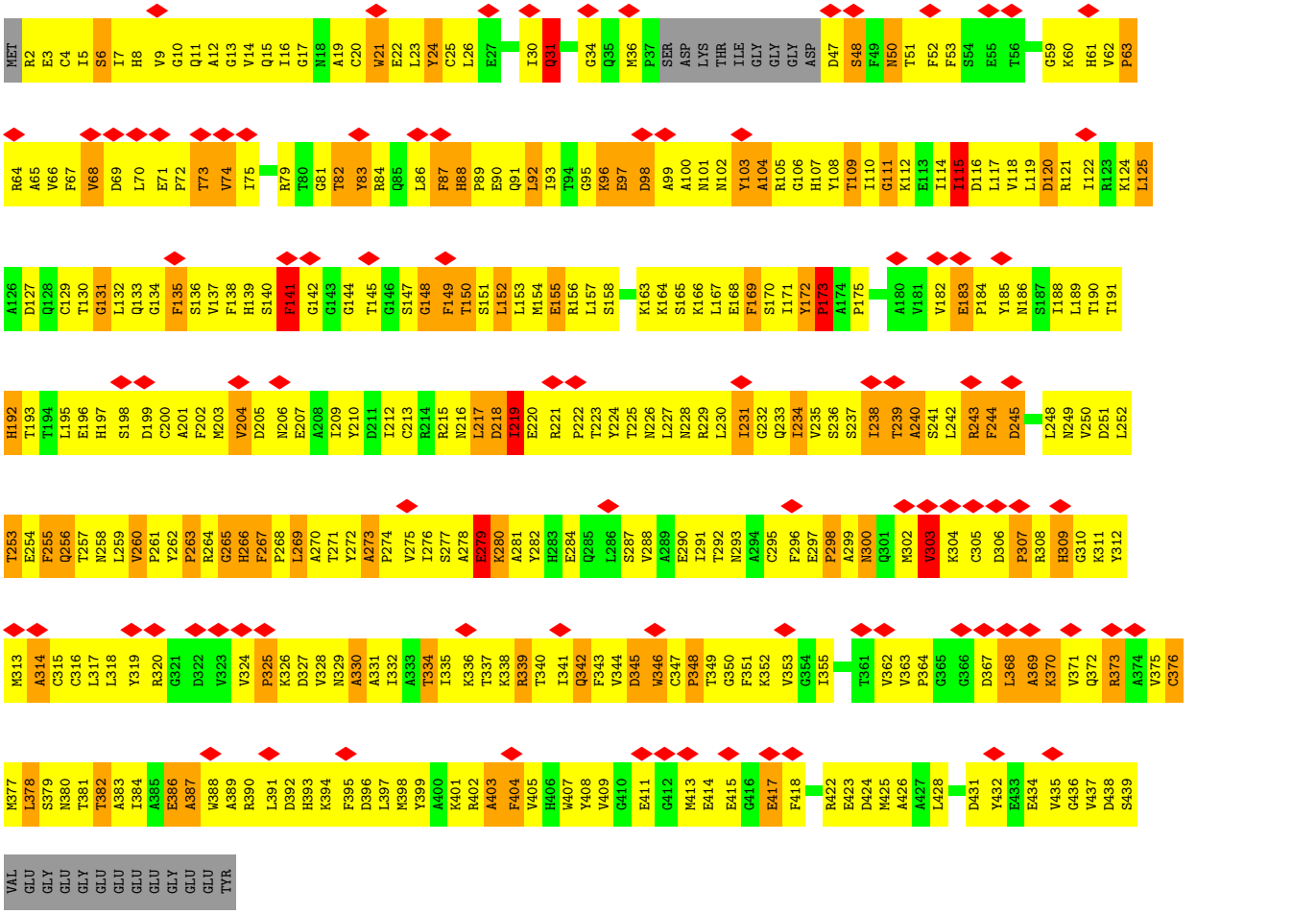






• Molecule 2: TUBULIN ALPHA-1D CHAIN

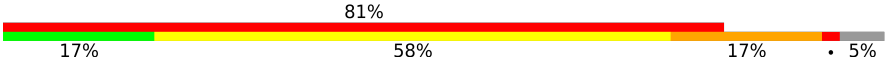
Chain F:

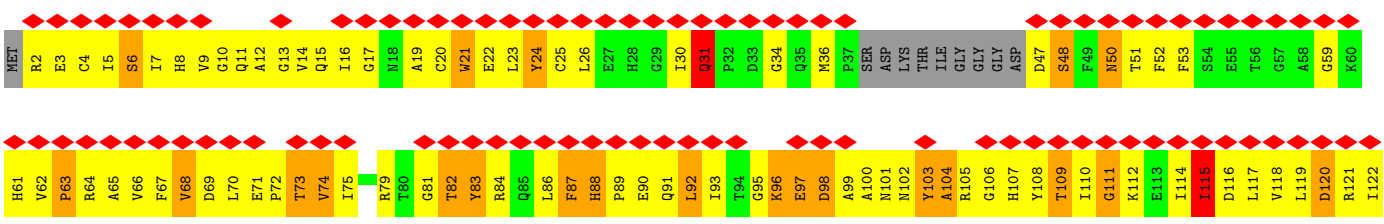


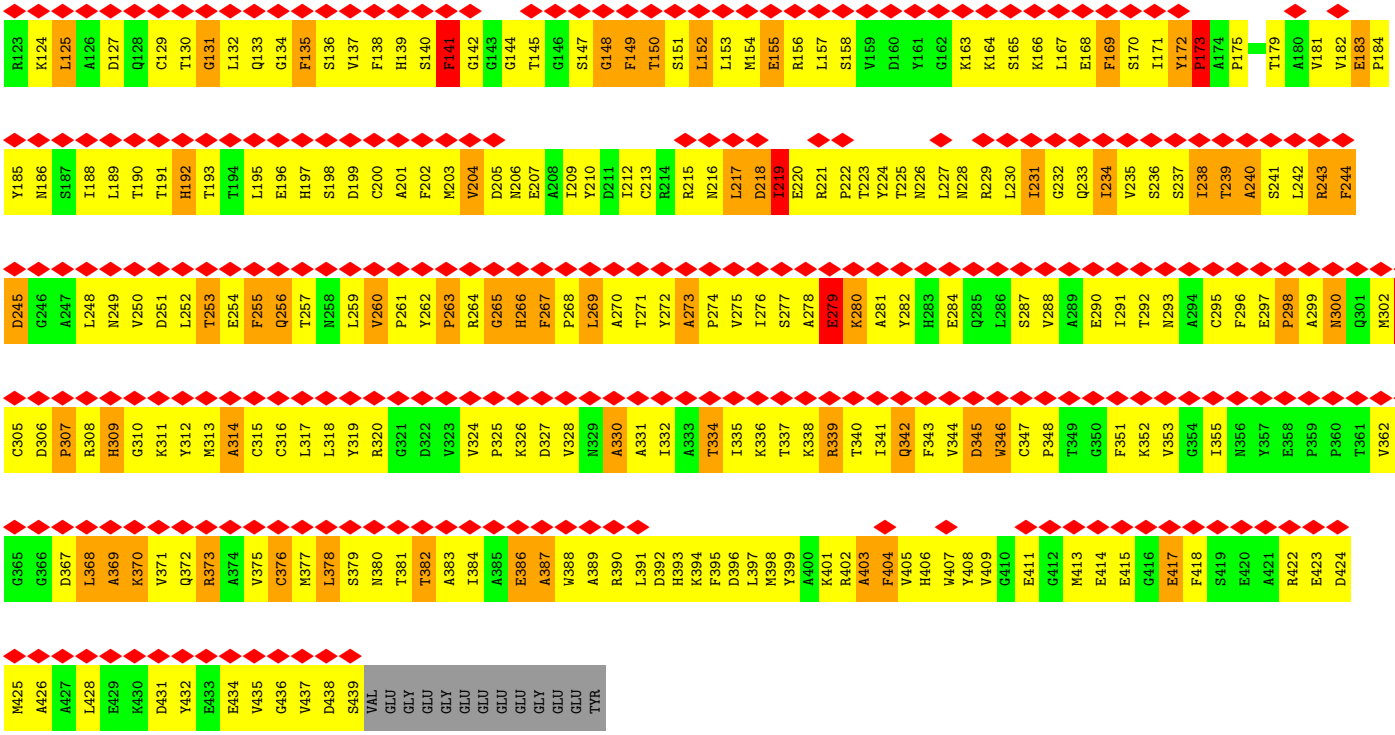




• Molecule 2: TUBULIN ALPHA-1D CHAIN

Chain H:

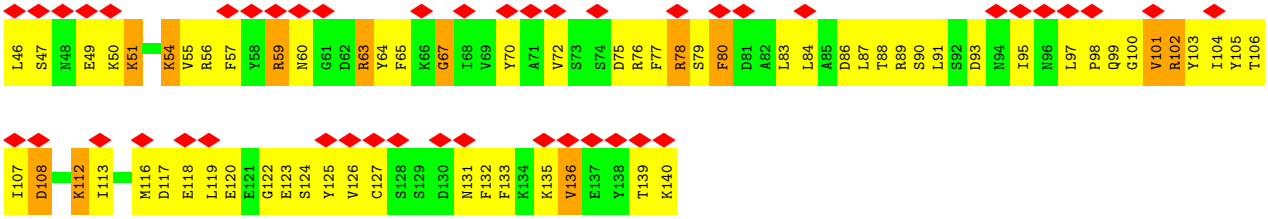





- Molecule 3: NEURONAL MIGRATION PROTEIN DOUBLECORTIN

Chain I:

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided | Depositor |
| Number of particles used | 168000 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | DONE IN FREALIGN | Depositor |
| Microscope | FEI TECNAI F20 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 15 | Depositor |
| Minimum defocus (nm) | 760 | Depositor |
| Maximum defocus (nm) | 2900 | Depositor |
| Magnification | 50000 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |
| Maximum map value | 5.698 | Depositor |
| Minimum map value | -4.734 | Depositor |
| Average map value | 0.106 | Depositor |
| Map value standard deviation | 0.755 | Depositor |
| Recommended contour level | 0.92 | Depositor |
| Map size (Å) | 95.2, 140, 137.2 | wwPDB |
| Map dimensions | 34, 50, 49 | wwPDB |
| Map angles (°) | 90, 90, 90 | wwPDB |
| Pixel spacing (Å) | 2.8, 2.8, 2.8 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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 | 0.51 | 0/3426 | 0.76 | 2/4642 (0.0%) |
| 1 | C | 0.51 | 0/3426 | 0.76 | 2/4642 (0.0%) |
| 1 | E | 0.51 | 0/3426 | 0.76 | 2/4642 (0.0%) |
| 1 | G | 0.51 | 0/3426 | 0.76 | 2/4642 (0.0%) |
| 2 | B | 0.82 | 3/3410 (0.1%) | 0.77 | 3/4629 (0.1%) |
| 2 | D | 0.82 | 3/3410 (0.1%) | 0.78 | 3/4629 (0.1%) |
| 2 | F | 0.82 | 3/3410 (0.1%) | 0.78 | 3/4629 (0.1%) |
| 2 | H | 0.82 | 3/3410 (0.1%) | 0.78 | 3/4629 (0.1%) |
| 3 | I | 0.27 | 0/789 | 0.37 | 0/1055 |
| All | All | 0.67 | 12/28133 (0.0%) | 0.76 | 20/38139 (0.1%) |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | D | 92 | LEU | C-N | 27.99 | 1.98 | 1.34 |
| 2 | B | 92 | LEU | C-N | 27.96 | 1.98 | 1.34 |
| 2 | H | 92 | LEU | C-N | 27.95 | 1.98 | 1.34 |
| 2 | F | 92 | LEU | C-N | 27.95 | 1.98 | 1.34 |
| 2 | F | 298 | PRO | C-N | 17.32 | 1.73 | 1.34 |
| 2 | H | 298 | PRO | C-N | 17.30 | 1.73 | 1.34 |
| 2 | B | 298 | PRO | C-N | 17.29 | 1.73 | 1.34 |
| 2 | D | 298 | PRO | C-N | 17.28 | 1.73 | 1.34 |
| 2 | D | 68 | VAL | C-N | 14.38 | 1.67 | 1.34 |
| 2 | B | 68 | VAL | C-N | 14.35 | 1.67 | 1.34 |
| 2 | H | 68 | VAL | C-N | 14.35 | 1.67 | 1.34 |
| 2 | F | 68 | VAL | C-N | 14.32 | 1.67 | 1.34 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | D | 68 | VAL | O-C-N | -7.14 | 111.27 | 122.70 |
| 2 | B | 68 | VAL | O-C-N | -7.12 | 111.31 | 122.70 |
| 2 | F | 68 | VAL | O-C-N | -7.12 | 111.31 | 122.70 |
| 2 | H | 68 | VAL | O-C-N | -7.10 | 111.34 | 122.70 |
| 2 | F | 298 | PRO | O-C-N | -6.73 | 111.93 | 122.70 |
| 2 | D | 298 | PRO | O-C-N | -6.73 | 111.93 | 122.70 |
| 2 | H | 298 | PRO | O-C-N | -6.72 | 111.95 | 122.70 |
| 2 | B | 298 | PRO | O-C-N | -6.70 | 111.97 | 122.70 |
| 2 | F | 69 | ASP | CB-CG-OD2 | 6.13 | 123.82 | 118.30 |
| 2 | D | 69 | ASP | CB-CG-OD2 | 6.13 | 123.82 | 118.30 |
| 2 | H | 69 | ASP | CB-CG-OD2 | 6.13 | 123.82 | 118.30 |
| 1 | G | 235 | MET | CG-SD-CE | 6.10 | 109.96 | 100.20 |
| 1 | A | 235 | MET | CG-SD-CE | 6.09 | 109.94 | 100.20 |
| 1 | C | 235 | MET | CG-SD-CE | 6.08 | 109.93 | 100.20 |
| 1 | E | 235 | MET | CG-SD-CE | 6.08 | 109.93 | 100.20 |
| 2 | B | 69 | ASP | CB-CG-OD2 | 6.05 | 123.75 | 118.30 |
| 1 | E | 217 | LEU | N-CA-C | -5.40 | 96.43 | 111.00 |
| 1 | G | 217 | LEU | N-CA-C | -5.39 | 96.44 | 111.00 |
| 1 | A | 217 | LEU | N-CA-C | -5.38 | 96.46 | 111.00 |
| 1 | C | 217 | LEU | N-CA-C | -5.38 | 96.47 | 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 | 3351 | 0 | 3229 | 545 | 0 |
| 1 | C | 3351 | 0 | 3229 | 612 | 0 |
| 1 | E | 3351 | 0 | 3229 | 540 | 0 |
| 1 | G | 3351 | 0 | 3229 | 745 | 0 |
| 2 | B | 3334 | 0 | 3223 | 687 | 0 |
| 2 | D | 3334 | 0 | 3223 | 659 | 0 |
| 2 | F | 3334 | 0 | 3223 | 724 | 0 |
| 2 | H | 3334 | 0 | 3223 | 716 | 0 |
| 3 | I | 776 | 596 | 764 | 57 | 0 |
| 4 | A | 28 | 0 | 12 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | C | 28 | 0 | 12 | 1 | 0 |
| 4 | E | 28 | 0 | 12 | 1 | 0 |
| 4 | G | 28 | 0 | 12 | 4 | 0 |
| 5 | B | 32 | 0 | 12 | 5 | 0 |
| 5 | D | 32 | 0 | 12 | 4 | 0 |
| 5 | F | 32 | 0 | 12 | 5 | 0 |
| 5 | H | 32 | 0 | 12 | 5 | 0 |
| All | All | 27756 | 596 | 26668 | 4935 | 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 91.

All (4935) 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:G:257:VAL:HG21 | 2:H:407:TRP:CG | 1.28 | 1.63 |
| 2:D:296:PHE:CE2 | 2:D:341:ILE:HD11 | 1.32 | 1.59 |
| 2:B:296:PHE:CE2 | 2:B:341:ILE:HD11 | 1.32 | 1.59 |
| 2:F:296:PHE:CE2 | 2:F:341:ILE:HD11 | 1.32 | 1.57 |
| 2:H:296:PHE:CE2 | 2:H:341:ILE:HD11 | 1.32 | 1.57 |
| 1:G:352:LYS:CD | 2:H:181:VAL:HG23 | 1.43 | 1.47 |
| 2:F:326:LYS:CB | 1:G:222:PRO:HG2 | 1.42 | 1.45 |
| 2:F:261:PRO:HA | 1:G:404:PHE:CD2 | 1.47 | 1.45 |
| 2:F:349:THR:HG21 | 1:G:178:SER:CA | 1.46 | 1.45 |
| 2:F:349:THR:CB | 1:G:178:SER:HB2 | 1.45 | 1.45 |
| 2:B:5:ILE:HG12 | 2:B:64:ARG:NH1 | 1.27 | 1.43 |
| 1:G:250:ALA:CB | 1:G:254:LYS:HD3 | 1.44 | 1.42 |
| 2:F:298:PRO:C | 2:F:299:ALA:N | 1.73 | 1.42 |
| 2:H:298:PRO:C | 2:H:299:ALA:N | 1.73 | 1.41 |
| 1:G:253:ARG:HB3 | 2:H:407:TRP:CH2 | 1.53 | 1.41 |
| 2:B:298:PRO:C | 2:B:299:ALA:N | 1.73 | 1.41 |
| 2:D:298:PRO:C | 2:D:299:ALA:N | 1.73 | 1.40 |
| 1:G:248:LEU:HD22 | 2:H:179:THR:CG2 | 1.49 | 1.38 |
| 1:A:88:ARG:HD2 | 1:E:283:TYR:CE1 | 1.58 | 1.37 |
| 1:G:257:VAL:CG2 | 2:H:407:TRP:CG | 2.06 | 1.36 |
| 1:G:257:VAL:HG23 | 2:H:407:TRP:CB | 1.57 | 1.34 |
| 1:G:257:VAL:CG2 | 2:H:407:TRP:CB | 2.02 | 1.34 |
| 2:F:3:GLU:CG | 2:F:51:THR:HA | 1.57 | 1.33 |
| 2:D:296:PHE:CE2 | 2:D:341:ILE:CD1 | 2.11 | 1.33 |
| 2:H:3:GLU:CG | 2:H:51:THR:HA | 1.57 | 1.33 |
| 1:G:257:VAL:CG2 | 2:H:407:TRP:HB2 | 1.59 | 1.33 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:3:GLU:CG | 2:D:51:THR:HA | 1.57 | 1.32 |
| 2:F:3:GLU:HG2 | 2:F:51:THR:CA | 1.60 | 1.32 |
| 2:H:3:GLU:HG2 | 2:H:51:THR:CA | 1.60 | 1.32 |
| 2:B:3:GLU:HG2 | 2:B:51:THR:CA | 1.60 | 1.32 |
| 2:B:3:GLU:CG | 2:B:51:THR:HA | 1.57 | 1.32 |
| 2:F:296:PHE:CE2 | 2:F:341:ILE:CD1 | 2.11 | 1.32 |
| 2:B:296:PHE:CE2 | 2:B:341:ILE:CD1 | 2.11 | 1.32 |
| 2:D:3:GLU:HG2 | 2:D:51:THR:CA | 1.60 | 1.31 |
| 2:H:296:PHE:CE2 | 2:H:341:ILE:CD1 | 2.11 | 1.31 |
| 2:B:348:PRO:CD | 1:C:398:MET:HE3 | 1.60 | 1.31 |
| 2:F:329:ASN:HB3 | 1:G:210:TYR:CE1 | 1.66 | 1.31 |
| 2:D:57:GLY:HA3 | 2:D:58:ALA:CB | 1.45 | 1.29 |
| 2:B:63:PRO:HG2 | 2:B:91:GLN:OE1 | 1.29 | 1.29 |
| 1:G:352:LYS:HD3 | 2:H:181:VAL:CG2 | 1.60 | 1.29 |
| 2:D:57:GLY:CA | 2:D:58:ALA:HB2 | 1.63 | 1.29 |
| 2:B:57:GLY:CA | 2:B:58:ALA:HB2 | 1.63 | 1.28 |
| 2:B:57:GLY:HA3 | 2:B:58:ALA:CB | 1.45 | 1.26 |
| 2:B:62:VAL:CG1 | 2:B:63:PRO:HD2 | 1.67 | 1.25 |
| 2:F:349:THR:CG2 | 1:G:178:SER:HB2 | 1.65 | 1.25 |
| 2:F:349:THR:HG21 | 1:G:178:SER:N | 1.50 | 1.25 |
| 2:F:326:LYS:HB2 | 1:G:222:PRO:CG | 1.66 | 1.24 |
| 2:B:348:PRO:CD | 1:C:398:MET:CE | 2.18 | 1.22 |
| 2:F:324:VAL:CG2 | 1:G:221:THR:HB | 1.70 | 1.21 |
| 1:G:257:VAL:HB | 2:H:407:TRP:CE3 | 1.73 | 1.21 |
| 2:F:326:LYS:CB | 1:G:222:PRO:CG | 2.18 | 1.20 |
| 2:F:329:ASN:CG | 1:G:210:TYR:HE1 | 1.44 | 1.19 |
| 2:F:324:VAL:HG21 | 1:G:221:THR:CB | 1.70 | 1.19 |
| 2:D:217:LEU:HD12 | 2:D:277:SER:CB | 1.72 | 1.19 |
| 2:B:5:ILE:CG1 | 2:B:64:ARG:NH1 | 2.05 | 1.18 |
| 2:B:217:LEU:HD12 | 2:B:277:SER:CB | 1.72 | 1.18 |
| 2:F:329:ASN:CB | 1:G:210:TYR:CE1 | 2.26 | 1.18 |
| 2:F:217:LEU:HD12 | 2:F:277:SER:CB | 1.72 | 1.18 |
| 2:H:217:LEU:HD12 | 2:H:277:SER:CB | 1.72 | 1.18 |
| 2:D:30:ILE:HG12 | 2:D:36:MET:HB3 | 1.19 | 1.18 |
| 1:G:2:ARG:CZ | 2:H:98:ASP:HB3 | 1.73 | 1.18 |
| 1:C:88:ARG:HD2 | 1:G:283:TYR:CZ | 1.79 | 1.17 |
| 2:F:349:THR:HG21 | 1:G:178:SER:CB | 1.73 | 1.17 |
| 2:B:92:LEU:C | 2:B:93:ILE:N | 1.98 | 1.16 |
| 1:G:254:LYS:CE | 1:G:352:LYS:HE3 | 1.73 | 1.16 |
| 2:F:262:TYR:OH | 1:G:403:ALA:HA | 1.46 | 1.16 |
| 2:F:92:LEU:C | 2:F:93:ILE:N | 1.98 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:92:LEU:C | 2:H:93:ILE:N | 1.98 | 1.16 |
| 2:B:30:ILE:HG12 | 2:B:36:MET:HB3 | 1.19 | 1.15 |
| 2:B:348:PRO:HD2 | 1:C:398:MET:CE | 1.73 | 1.15 |
| 1:C:88:ARG:HD2 | 1:G:283:TYR:OH | 1.43 | 1.15 |
| 2:D:92:LEU:C | 2:D:93:ILE:N | 1.98 | 1.15 |
| 2:F:261:PRO:HB3 | 1:G:404:PHE:CE2 | 1.81 | 1.15 |
| 2:F:349:THR:HB | 1:G:178:SER:HB2 | 1.16 | 1.15 |
| 2:F:30:ILE:HG12 | 2:F:36:MET:HB3 | 1.17 | 1.15 |
| 2:D:56:THR:O | 2:H:284:GLU:HB3 | 1.46 | 1.15 |
| 1:C:88:ARG:HD3 | 1:G:283:TYR:HE1 | 1.01 | 1.14 |
| 2:B:5:ILE:CD1 | 2:B:64:ARG:HH12 | 1.57 | 1.14 |
| 2:H:30:ILE:HG12 | 2:H:36:MET:HB3 | 1.17 | 1.14 |
| 2:B:243:ARG:NH2 | 2:B:252:LEU:H | 1.45 | 1.14 |
| 2:D:243:ARG:NH2 | 2:D:252:LEU:H | 1.45 | 1.14 |
| 2:B:62:VAL:HG12 | 2:B:63:PRO:CD | 1.76 | 1.14 |
| 2:F:243:ARG:NH2 | 2:F:252:LEU:H | 1.45 | 1.14 |
| 1:G:93:VAL:HG11 | 1:G:118:VAL:HG22 | 1.30 | 1.14 |
| 2:H:243:ARG:NH2 | 2:H:252:LEU:H | 1.45 | 1.14 |
| 1:C:88:ARG:HD3 | 1:G:283:TYR:CE1 | 1.83 | 1.13 |
| 1:G:258:ASN:HA | 2:H:404:PHE:CD2 | 1.84 | 1.13 |
| 2:B:296:PHE:CE1 | 2:B:335:ILE:HG21 | 1.84 | 1.13 |
| 1:C:257:VAL:HG13 | 2:D:407:TRP:CG | 1.83 | 1.13 |
| 2:D:296:PHE:CE1 | 2:D:335:ILE:HG21 | 1.84 | 1.13 |
| 2:H:296:PHE:CE1 | 2:H:335:ILE:HG21 | 1.84 | 1.13 |
| 1:A:88:ARG:CD | 1:E:283:TYR:CE1 | 2.31 | 1.13 |
| 2:F:296:PHE:CE1 | 2:F:335:ILE:HG21 | 1.84 | 1.12 |
| 1:E:93:VAL:HG11 | 1:E:118:VAL:HG22 | 1.30 | 1.12 |
| 1:A:234:THR:HG21 | 1:A:270:PRO:HB2 | 1.23 | 1.12 |
| 2:F:261:PRO:CB | 1:G:404:PHE:CE2 | 2.32 | 1.12 |
| 2:F:261:PRO:CA | 1:G:404:PHE:CD2 | 2.32 | 1.12 |
| 1:A:88:ARG:CD | 1:E:283:TYR:HE1 | 1.63 | 1.12 |
| 1:E:234:THR:HG21 | 1:E:270:PRO:HB2 | 1.23 | 1.11 |
| 2:F:70:LEU:HD13 | 2:F:145:THR:OG1 | 1.49 | 1.11 |
| 1:G:352:LYS:CD | 2:H:181:VAL:CG2 | 2.20 | 1.11 |
| 2:H:70:LEU:HD13 | 2:H:145:THR:OG1 | 1.49 | 1.11 |
| 2:D:67:PHE:HE1 | 2:D:87:PHE:CE1 | 1.68 | 1.10 |
| 2:F:67:PHE:HE1 | 2:F:87:PHE:CE1 | 1.69 | 1.10 |
| 2:B:67:PHE:HE1 | 2:B:87:PHE:CE1 | 1.68 | 1.10 |
| 2:B:70:LEU:HD13 | 2:B:145:THR:OG1 | 1.49 | 1.10 |
| 1:C:88:ARG:CD | 1:G:283:TYR:CE1 | 2.34 | 1.10 |
| 1:C:234:THR:HG21 | 1:C:270:PRO:HB2 | 1.23 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:67:PHE:HE1 | 2:H:87:PHE:CE1 | 1.68 | 1.10 |
| 2:D:70:LEU:HD13 | 2:D:145:THR:OG1 | 1.49 | 1.10 |
| 2:F:349:THR:CG2 | 1:G:178:SER:H | 1.65 | 1.09 |
| 1:G:234:THR:HG21 | 1:G:270:PRO:HB2 | 1.23 | 1.09 |
| 1:G:258:ASN:ND2 | 1:G:352:LYS:HE2 | 1.67 | 1.09 |
| 1:A:93:VAL:HG11 | 1:A:118:VAL:HG22 | 1.30 | 1.08 |
| 2:B:439:SER:C | 1:C:401:ARG:HH21 | 1.58 | 1.08 |
| 2:D:56:THR:O | 2:D:58:ALA:HB3 | 1.54 | 1.08 |
| 1:C:93:VAL:HG11 | 1:C:118:VAL:HG22 | 1.30 | 1.07 |
| 2:F:329:ASN:CB | 1:G:210:TYR:HE1 | 1.66 | 1.07 |
| 1:A:56:ALA:CB | 1:E:283:TYR:CE2 | 2.37 | 1.06 |
| 2:D:274:PRO:C | 2:D:275:VAL:N | 2.09 | 1.06 |
| 2:B:274:PRO:C | 2:B:275:VAL:N | 2.09 | 1.06 |
| 1:G:352:LYS:HD2 | 2:H:181:VAL:HG23 | 1.24 | 1.06 |
| 2:B:11:GLN:HG3 | 2:B:74:VAL:HG11 | 1.34 | 1.06 |
| 2:B:109:THR:HG22 | 2:B:110:ILE:N | 1.71 | 1.06 |
| 2:H:274:PRO:C | 2:H:275:VAL:N | 2.09 | 1.06 |
| 2:B:350:GLY:CA | 1:C:181:VAL:HG13 | 1.86 | 1.05 |
| 2:F:109:THR:HG22 | 2:F:110:ILE:N | 1.71 | 1.05 |
| 2:F:274:PRO:C | 2:F:275:VAL:N | 2.09 | 1.05 |
| 2:F:326:LYS:HG3 | 1:G:222:PRO:HG3 | 1.30 | 1.05 |
| 2:D:5:ILE:HG21 | 2:D:135:PHE:HD2 | 1.18 | 1.05 |
| 2:D:109:THR:HG22 | 2:D:110:ILE:N | 1.70 | 1.05 |
| 2:D:217:LEU:CD1 | 2:D:277:SER:HB3 | 1.87 | 1.05 |
| 2:H:109:THR:HG22 | 2:H:110:ILE:N | 1.70 | 1.05 |
| 2:H:11:GLN:HG3 | 2:H:74:VAL:HG11 | 1.34 | 1.05 |
| 2:B:5:ILE:CG1 | 2:B:64:ARG:HH12 | 1.67 | 1.05 |
| 2:B:217:LEU:CD1 | 2:B:277:SER:HB3 | 1.87 | 1.05 |
| 2:B:298:PRO:HB3 | 2:B:307:PRO:HD2 | 1.36 | 1.05 |
| 2:B:350:GLY:HA2 | 1:C:181:VAL:CG1 | 1.86 | 1.05 |
| 2:D:296:PHE:CD2 | 2:D:341:ILE:CD1 | 2.40 | 1.05 |
| 2:F:5:ILE:HG21 | 2:F:135:PHE:HD2 | 1.18 | 1.05 |
| 2:F:11:GLN:HG3 | 2:F:74:VAL:HG11 | 1.34 | 1.05 |
| 2:B:296:PHE:CD2 | 2:B:341:ILE:CD1 | 2.40 | 1.04 |
| 1:G:257:VAL:HG21 | 2:H:407:TRP:CD1 | 1.91 | 1.04 |
| 2:H:5:ILE:HG21 | 2:H:135:PHE:HD2 | 1.17 | 1.04 |
| 2:D:11:GLN:HG3 | 2:D:74:VAL:HG11 | 1.34 | 1.04 |
| 2:D:67:PHE:CE1 | 2:D:87:PHE:CE1 | 2.45 | 1.04 |
| 2:F:296:PHE:CD2 | 2:F:341:ILE:CD1 | 2.40 | 1.04 |
| 2:F:349:THR:CG2 | 1:G:178:SER:CB | 2.32 | 1.04 |
| 2:H:296:PHE:CD2 | 2:H:341:ILE:CD1 | 2.40 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:67:PHE:CE1 | 2:B:87:PHE:CE1 | 2.45 | 1.04 |
| 1:G:250:ALA:HB1 | 1:G:254:LYS:HD3 | 1.39 | 1.04 |
| 1:A:88:ARG:HD2 | 1:E:283:TYR:CZ | 1.91 | 1.04 |
| 2:F:67:PHE:CE1 | 2:F:87:PHE:CE1 | 2.45 | 1.04 |
| 2:F:217:LEU:CD1 | 2:F:277:SER:HB3 | 1.86 | 1.04 |
| 1:G:250:ALA:HB2 | 1:G:254:LYS:CD | 1.88 | 1.04 |
| 1:G:352:LYS:HD3 | 2:H:181:VAL:HG23 | 1.07 | 1.04 |
| 2:H:217:LEU:CD1 | 2:H:277:SER:HB3 | 1.87 | 1.04 |
| 2:H:67:PHE:CE1 | 2:H:87:PHE:CE1 | 2.45 | 1.03 |
| 2:H:298:PRO:HB3 | 2:H:307:PRO:HD2 | 1.36 | 1.03 |
| 2:F:298:PRO:HB3 | 2:F:307:PRO:HD2 | 1.36 | 1.03 |
| 2:F:349:THR:CG2 | 1:G:178:SER:N | 2.21 | 1.03 |
| 1:G:2:ARG:NH2 | 2:H:98:ASP:HB3 | 1.74 | 1.03 |
| 2:D:298:PRO:HB3 | 2:D:307:PRO:HD2 | 1.36 | 1.02 |
| 2:D:243:ARG:HH21 | 2:D:252:LEU:N | 1.57 | 1.02 |
| 2:H:243:ARG:HH21 | 2:H:252:LEU:N | 1.58 | 1.02 |
| 2:B:243:ARG:HH21 | 2:B:252:LEU:N | 1.57 | 1.02 |
| 2:B:348:PRO:CG | 1:C:398:MET:HE3 | 1.90 | 1.02 |
| 2:F:243:ARG:HH21 | 2:F:252:LEU:N | 1.58 | 1.02 |
| 1:G:250:ALA:CB | 1:G:254:LYS:CD | 2.38 | 1.02 |
| 2:F:325:PRO:HD2 | 1:G:223:THR:HA | 1.40 | 1.02 |
| 1:C:172:VAL:HG11 | 1:C:387:LEU:HD21 | 1.37 | 1.02 |
| 1:A:56:ALA:HB2 | 1:E:283:TYR:HE2 | 1.25 | 1.01 |
| 2:F:326:LYS:CG | 1:G:222:PRO:CG | 2.38 | 1.01 |
| 2:B:88:HIS:HB2 | 2:B:91:GLN:HE21 | 1.22 | 1.01 |
| 1:G:248:LEU:CD2 | 2:H:179:THR:CG2 | 2.37 | 1.01 |
| 1:A:172:VAL:HG11 | 1:A:387:LEU:HD21 | 1.37 | 1.01 |
| 1:E:236:SER:O | 1:E:240:THR:HG23 | 1.61 | 1.01 |
| 2:F:329:ASN:CG | 1:G:210:TYR:CE1 | 2.34 | 1.01 |
| 1:G:254:LYS:HE2 | 1:G:352:LYS:CE | 1.90 | 1.01 |
| 1:G:236:SER:O | 1:G:240:THR:HG23 | 1.61 | 1.00 |
| 2:D:88:HIS:HB2 | 2:D:91:GLN:HE21 | 1.22 | 1.00 |
| 1:E:172:VAL:HG11 | 1:E:387:LEU:HD21 | 1.37 | 1.00 |
| 1:G:253:ARG:CB | 2:H:407:TRP:CH2 | 2.43 | 1.00 |
| 1:A:88:ARG:NH1 | 1:E:283:TYR:CE1 | 2.29 | 1.00 |
| 2:B:5:ILE:HG12 | 2:B:64:ARG:CZ | 1.90 | 1.00 |
| 2:B:350:GLY:HA2 | 1:C:181:VAL:HG13 | 1.03 | 1.00 |
| 1:G:172:VAL:HG11 | 1:G:387:LEU:HD21 | 1.37 | 1.00 |
| 1:G:258:ASN:O | 2:H:404:PHE:HE2 | 1.42 | 1.00 |
| 1:G:257:VAL:HG21 | 2:H:407:TRP:CB | 1.77 | 1.00 |
| 1:A:236:SER:O | 1:A:240:THR:HG23 | 1.61 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:30:ILE:HD11 | 2:B:61:HIS:CE1 | 1.97 | 1.00 |
| 2:H:88:HIS:HB2 | 2:H:91:GLN:HE21 | 1.22 | 1.00 |
| 1:C:236:SER:O | 1:C:240:THR:HG23 | 1.61 | 1.00 |
| 2:B:56:THR:O | 2:B:58:ALA:HB3 | 1.59 | 0.99 |
| 1:G:253:ARG:CB | 2:H:407:TRP:HH2 | 1.75 | 0.99 |
| 2:F:349:THR:CB | 1:G:178:SER:CB | 2.40 | 0.99 |
| 2:F:88:HIS:HB2 | 2:F:91:GLN:HE21 | 1.22 | 0.99 |
| 1:C:329:ASP:HB3 | 2:D:177:VAL:CG1 | 1.93 | 0.98 |
| 1:G:250:ALA:HB2 | 1:G:254:LYS:HD3 | 1.01 | 0.98 |
| 1:C:299:LYS:H | 1:C:299:LYS:HD3 | 1.24 | 0.98 |
| 1:G:352:LYS:HA | 2:H:181:VAL:HG22 | 1.44 | 0.98 |
| 1:G:248:LEU:HD22 | 2:H:179:THR:HG22 | 1.43 | 0.98 |
| 2:B:52:PHE:HZ | 2:B:239:THR:HG21 | 1.27 | 0.98 |
| 2:H:276:ILE:HG23 | 2:H:369:ALA:HB2 | 1.43 | 0.98 |
| 1:A:299:LYS:HD3 | 1:A:299:LYS:H | 1.24 | 0.97 |
| 2:B:63:PRO:HG2 | 2:B:91:GLN:CD | 1.84 | 0.97 |
| 1:G:248:LEU:HD22 | 2:H:179:THR:HG21 | 1.46 | 0.97 |
| 2:B:276:ILE:HG23 | 2:B:369:ALA:HB2 | 1.43 | 0.97 |
| 2:F:276:ILE:HG23 | 2:F:369:ALA:HB2 | 1.43 | 0.97 |
| 2:D:276:ILE:HG23 | 2:D:369:ALA:HB2 | 1.43 | 0.97 |
| 2:F:349:THR:CG2 | 1:G:178:SER:CA | 2.42 | 0.97 |
| 1:G:254:LYS:HE2 | 1:G:352:LYS:HE3 | 0.97 | 0.97 |
| 2:B:348:PRO:HD3 | 1:C:398:MET:HE3 | 1.47 | 0.96 |
| 1:E:299:LYS:H | 1:E:299:LYS:HD3 | 1.24 | 0.96 |
| 2:D:259:LEU:HD11 | 2:D:378:LEU:HD13 | 1.47 | 0.96 |
| 2:F:259:LEU:HD11 | 2:F:378:LEU:HD13 | 1.47 | 0.96 |
| 2:F:326:LYS:HG3 | 1:G:222:PRO:CG | 1.96 | 0.96 |
| 2:B:62:VAL:HG12 | 2:B:63:PRO:HD2 | 0.97 | 0.96 |
| 2:B:278:ALA:O | 2:B:279:GLU:HB3 | 1.66 | 0.96 |
| 2:F:326:LYS:CG | 1:G:222:PRO:HG3 | 1.94 | 0.96 |
| 2:H:259:LEU:HD11 | 2:H:378:LEU:HD13 | 1.47 | 0.96 |
| 1:G:299:LYS:HD3 | 1:G:299:LYS:H | 1.24 | 0.96 |
| 2:D:278:ALA:O | 2:D:279:GLU:HB3 | 1.66 | 0.96 |
| 1:A:56:ALA:HB2 | 1:E:283:TYR:CE2 | 2.00 | 0.96 |
| 2:H:98:ASP:HB2 | 2:H:105:ARG:HH21 | 1.31 | 0.96 |
| 2:F:324:VAL:HG21 | 1:G:221:THR:HB | 0.97 | 0.96 |
| 2:B:98:ASP:HB2 | 2:B:105:ARG:HH21 | 1.31 | 0.95 |
| 2:B:259:LEU:HD11 | 2:B:378:LEU:HD13 | 1.47 | 0.95 |
| 1:C:273:ALA:HB3 | 1:C:274:PRO:HD3 | 1.48 | 0.95 |
| 2:F:98:ASP:HB2 | 2:F:105:ARG:HH21 | 1.31 | 0.95 |
| 2:B:251:ASP:N | 2:B:254:GLU:HG3 | 1.82 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:98:ASP:HB2 | 2:D:105:ARG:HH21 | 1.31 | 0.95 |
| 2:H:5:ILE:CG2 | 2:H:135:PHE:HD2 | 1.78 | 0.95 |
| 1:G:257:VAL:HB | 2:H:407:TRP:CD2 | 2.01 | 0.95 |
| 2:D:251:ASP:N | 2:D:254:GLU:HG3 | 1.82 | 0.95 |
| 2:F:5:ILE:CG2 | 2:F:135:PHE:HD2 | 1.78 | 0.95 |
| 1:A:273:ALA:HB3 | 1:A:274:PRO:HD3 | 1.48 | 0.95 |
| 2:D:5:ILE:CG2 | 2:D:135:PHE:HD2 | 1.78 | 0.95 |
| 2:H:251:ASP:N | 2:H:254:GLU:HG3 | 1.82 | 0.95 |
| 2:F:251:ASP:N | 2:F:254:GLU:HG3 | 1.82 | 0.95 |
| 2:D:56:THR:CB | 2:H:284:GLU:CD | 2.34 | 0.95 |
| 1:C:248:LEU:HD22 | 2:D:179:THR:HG21 | 1.47 | 0.95 |
| 2:D:52:PHE:CZ | 2:D:239:THR:HB | 2.02 | 0.94 |
| 2:D:217:LEU:HD12 | 2:D:277:SER:HB3 | 0.95 | 0.94 |
| 1:G:273:ALA:HB3 | 1:G:274:PRO:HD3 | 1.48 | 0.94 |
| 2:H:278:ALA:O | 2:H:279:GLU:HB3 | 1.66 | 0.94 |
| 1:C:88:ARG:CD | 1:G:283:TYR:OH | 2.13 | 0.94 |
| 2:F:278:ALA:O | 2:F:279:GLU:HB3 | 1.66 | 0.94 |
| 2:B:217:LEU:HD12 | 2:B:277:SER:HB3 | 0.95 | 0.94 |
| 2:F:30:ILE:CG1 | 2:F:36:MET:HB3 | 1.96 | 0.94 |
| 2:H:30:ILE:CG1 | 2:H:36:MET:HB3 | 1.96 | 0.94 |
| 2:H:251:ASP:H | 2:H:254:GLU:HG3 | 1.33 | 0.94 |
| 2:B:316:CYS:HB3 | 2:B:378:LEU:HD11 | 1.49 | 0.94 |
| 1:E:273:ALA:HB3 | 1:E:274:PRO:HD3 | 1.48 | 0.94 |
| 2:F:251:ASP:H | 2:F:254:GLU:HG3 | 1.33 | 0.94 |
| 2:H:217:LEU:HD12 | 2:H:277:SER:HB3 | 0.95 | 0.94 |
| 2:D:109:THR:HG22 | 2:D:110:ILE:H | 1.33 | 0.94 |
| 1:A:70:LEU:H | 1:A:145:THR:HG21 | 1.33 | 0.93 |
| 1:C:70:LEU:H | 1:C:145:THR:HG21 | 1.33 | 0.93 |
| 2:F:217:LEU:HD12 | 2:F:277:SER:HB3 | 0.95 | 0.93 |
| 2:F:151:SER:HB3 | 2:F:193:THR:HG21 | 1.51 | 0.93 |
| 2:D:237:SER:HB2 | 2:D:376:CYS:SG | 2.08 | 0.93 |
| 1:E:281:GLN:O | 1:E:283:TYR:N | 2.00 | 0.93 |
| 2:F:109:THR:HG22 | 2:F:110:ILE:H | 1.33 | 0.93 |
| 2:H:151:SER:HB3 | 2:H:193:THR:HG21 | 1.51 | 0.93 |
| 2:D:62:VAL:HG21 | 2:D:88:HIS:CE1 | 2.04 | 0.93 |
| 1:A:132:LEU:HD23 | 1:A:164:ARG:HG3 | 1.50 | 0.93 |
| 2:B:237:SER:HB2 | 2:B:376:CYS:SG | 2.08 | 0.93 |
| 1:G:264:ARG:O | 1:G:265:LEU:HB3 | 1.69 | 0.93 |
| 2:H:316:CYS:HB3 | 2:H:378:LEU:HD11 | 1.48 | 0.93 |
| 2:B:151:SER:HB3 | 2:B:193:THR:HG21 | 1.51 | 0.93 |
| 1:E:264:ARG:O | 1:E:265:LEU:HB3 | 1.69 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:281:GLN:O | 1:G:283:TYR:N | 2.00 | 0.93 |
| 1:C:88:ARG:HD2 | 1:G:283:TYR:CE1 | 2.02 | 0.93 |
| 1:C:132:LEU:HD23 | 1:C:164:ARG:HG3 | 1.50 | 0.93 |
| 1:C:281:GLN:O | 1:C:283:TYR:N | 2.00 | 0.93 |
| 1:E:132:LEU:HD23 | 1:E:164:ARG:HG3 | 1.50 | 0.93 |
| 2:F:316:CYS:HB3 | 2:F:378:LEU:HD11 | 1.48 | 0.93 |
| 2:B:109:THR:HG22 | 2:B:110:ILE:H | 1.33 | 0.93 |
| 2:D:316:CYS:HB3 | 2:D:378:LEU:HD11 | 1.49 | 0.93 |
| 2:F:62:VAL:HG21 | 2:F:88:HIS:CE1 | 2.03 | 0.93 |
| 2:H:109:THR:HG22 | 2:H:110:ILE:H | 1.33 | 0.93 |
| 1:A:281:GLN:O | 1:A:283:TYR:N | 2.00 | 0.93 |
| 2:F:237:SER:HB2 | 2:F:376:CYS:SG | 2.08 | 0.93 |
| 2:H:237:SER:HB2 | 2:H:376:CYS:SG | 2.08 | 0.93 |
| 1:G:132:LEU:HD23 | 1:G:164:ARG:HG3 | 1.50 | 0.92 |
| 2:H:52:PHE:CZ | 2:H:239:THR:HB | 2.04 | 0.92 |
| 2:H:62:VAL:HG21 | 2:H:88:HIS:CE1 | 2.04 | 0.92 |
| 2:D:151:SER:HB3 | 2:D:193:THR:HG21 | 1.51 | 0.92 |
| 1:A:264:ARG:O | 1:A:265:LEU:HB3 | 1.69 | 0.92 |
| 1:C:264:ARG:O | 1:C:265:LEU:HB3 | 1.69 | 0.92 |
| 2:B:251:ASP:H | 2:B:254:GLU:HG3 | 1.33 | 0.92 |
| 2:F:52:PHE:CZ | 2:F:239:THR:HB | 2.05 | 0.92 |
| 2:H:52:PHE:HZ | 2:H:239:THR:HG21 | 1.35 | 0.92 |
| 1:E:70:LEU:H | 1:E:145:THR:HG21 | 1.33 | 0.91 |
| 2:B:30:ILE:CD1 | 2:B:61:HIS:ND1 | 2.34 | 0.91 |
| 1:C:88:ARG:CD | 1:G:283:TYR:HE1 | 1.73 | 0.91 |
| 1:G:70:LEU:H | 1:G:145:THR:HG21 | 1.33 | 0.91 |
| 2:B:57:GLY:CA | 2:B:58:ALA:CB | 2.30 | 0.91 |
| 1:C:88:ARG:CD | 1:G:283:TYR:CZ | 2.52 | 0.91 |
| 2:D:251:ASP:H | 2:D:254:GLU:HG3 | 1.33 | 0.91 |
| 2:F:52:PHE:HZ | 2:F:239:THR:HG21 | 1.35 | 0.91 |
| 2:H:184:PRO:HG2 | 2:H:398:MET:HE1 | 1.51 | 0.91 |
| 2:F:296:PHE:CD2 | 2:F:341:ILE:HD11 | 2.03 | 0.91 |
| 2:F:337:THR:HG22 | 3:I:99:GLN:OE1 | 1.69 | 0.91 |
| 2:H:296:PHE:CD2 | 2:H:341:ILE:HD11 | 2.03 | 0.91 |
| 1:G:254:LYS:CE | 1:G:352:LYS:CE | 2.49 | 0.91 |
| 2:H:296:PHE:HE2 | 2:H:341:ILE:HD11 | 1.21 | 0.91 |
| 2:B:55:GLU:O | 2:B:57:GLY:N | 2.04 | 0.91 |
| 1:A:88:ARG:HH11 | 1:E:283:TYR:HE1 | 1.09 | 0.90 |
| 2:F:261:PRO:HG3 | 1:G:404:PHE:HE2 | 1.35 | 0.90 |
| 2:D:5:ILE:CG2 | 2:D:135:PHE:CD2 | 2.54 | 0.90 |
| 2:D:70:LEU:CD1 | 2:D:145:THR:OG1 | 2.18 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:352:LYS:HB2 | 2:H:181:VAL:HG21 | 1.52 | 0.90 |
| 2:B:70:LEU:CD1 | 2:B:145:THR:OG1 | 2.18 | 0.90 |
| 2:D:119:LEU:HD23 | 2:D:122:ILE:HD11 | 1.53 | 0.90 |
| 2:D:52:PHE:HZ | 2:D:239:THR:HG21 | 1.34 | 0.90 |
| 1:E:147:SER:O | 1:E:151:THR:HB | 1.71 | 0.90 |
| 1:G:253:ARG:HB3 | 2:H:407:TRP:HH2 | 1.10 | 0.90 |
| 2:F:70:LEU:CD1 | 2:F:145:THR:OG1 | 2.18 | 0.90 |
| 2:F:296:PHE:HE2 | 2:F:341:ILE:HD11 | 1.21 | 0.90 |
| 2:H:5:ILE:CG2 | 2:H:135:PHE:CD2 | 2.54 | 0.90 |
| 2:B:119:LEU:HD23 | 2:B:122:ILE:HD11 | 1.53 | 0.89 |
| 2:F:119:LEU:HD23 | 2:F:122:ILE:HD11 | 1.53 | 0.89 |
| 2:F:262:TYR:CE2 | 1:G:403:ALA:O | 2.24 | 0.89 |
| 1:G:257:VAL:HG21 | 2:H:407:TRP:CD2 | 2.08 | 0.89 |
| 2:D:296:PHE:HE2 | 2:D:341:ILE:HD11 | 1.21 | 0.89 |
| 2:F:5:ILE:CG2 | 2:F:135:PHE:CD2 | 2.54 | 0.89 |
| 1:G:147:SER:O | 1:G:151:THR:HB | 1.71 | 0.89 |
| 2:H:119:LEU:HD23 | 2:H:122:ILE:HD11 | 1.53 | 0.89 |
| 1:A:8:GLN:OE1 | 1:A:67:LEU:HD22 | 1.72 | 0.89 |
| 1:A:102:ASN:HD21 | 1:A:408:TYR:HA | 1.38 | 0.89 |
| 1:C:8:GLN:OE1 | 1:C:67:LEU:HD22 | 1.73 | 0.89 |
| 1:C:102:ASN:HD21 | 1:C:408:TYR:HA | 1.38 | 0.89 |
| 2:H:70:LEU:CD1 | 2:H:145:THR:OG1 | 2.18 | 0.89 |
| 1:A:93:VAL:HG11 | 1:A:118:VAL:CG2 | 2.03 | 0.89 |
| 1:A:147:SER:O | 1:A:151:THR:HB | 1.71 | 0.89 |
| 1:E:102:ASN:HD21 | 1:E:408:TYR:HA | 1.38 | 0.89 |
| 1:G:93:VAL:HG11 | 1:G:118:VAL:CG2 | 2.03 | 0.89 |
| 1:G:102:ASN:HD21 | 1:G:408:TYR:HA | 1.38 | 0.89 |
| 1:G:264:ARG:HB2 | 1:G:266:HIS:CD2 | 2.08 | 0.89 |
| 1:E:93:VAL:HG11 | 1:E:118:VAL:CG2 | 2.03 | 0.89 |
| 1:E:264:ARG:HB2 | 1:E:266:HIS:CD2 | 2.08 | 0.89 |
| 2:B:52:PHE:CE1 | 2:B:239:THR:HB | 2.07 | 0.89 |
| 1:C:93:VAL:HG11 | 1:C:118:VAL:CG2 | 2.03 | 0.89 |
| 2:D:56:THR:O | 2:H:284:GLU:CB | 2.21 | 0.89 |
| 1:G:258:ASN:HA | 2:H:404:PHE:CE2 | 2.08 | 0.89 |
| 2:B:296:PHE:HE2 | 2:B:341:ILE:HD11 | 1.21 | 0.89 |
| 1:C:264:ARG:HB2 | 1:C:266:HIS:CD2 | 2.08 | 0.89 |
| 2:F:257:THR:HG21 | 1:G:101:ASN:HB3 | 1.54 | 0.89 |
| 2:B:343:PHE:CZ | 2:B:351:PHE:CE1 | 2.61 | 0.88 |
| 1:A:101:ASN:HD21 | 1:A:143:GLY:HA2 | 1.38 | 0.88 |
| 1:A:264:ARG:HB2 | 1:A:266:HIS:CD2 | 2.08 | 0.88 |
| 2:B:110:ILE:HG23 | 2:B:111:GLY:H | 1.38 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:63:PRO:CD | 2:B:87:PHE:HA | 2.03 | 0.88 |
| 1:C:147:SER:O | 1:C:151:THR:HB | 1.71 | 0.88 |
| 2:D:343:PHE:CZ | 2:D:351:PHE:CE1 | 2.61 | 0.88 |
| 2:F:343:PHE:CZ | 2:F:351:PHE:CE1 | 2.60 | 0.88 |
| 2:H:343:PHE:CZ | 2:H:351:PHE:CE1 | 2.60 | 0.88 |
| 2:D:122:ILE:HD12 | 2:D:157:LEU:HD21 | 1.54 | 0.88 |
| 2:F:110:ILE:HG23 | 2:F:111:GLY:H | 1.38 | 0.88 |
| 2:F:261:PRO:HA | 1:G:404:PHE:HD2 | 0.87 | 0.88 |
| 1:C:101:ASN:HD21 | 1:C:143:GLY:HA2 | 1.38 | 0.88 |
| 2:H:110:ILE:HG23 | 2:H:111:GLY:H | 1.38 | 0.88 |
| 2:B:349:THR:HG21 | 1:C:178:SER:OG | 1.74 | 0.88 |
| 1:C:311:ARG:HD3 | 1:C:342:TYR:HA | 1.56 | 0.88 |
| 2:F:296:PHE:CD2 | 2:F:341:ILE:HD12 | 2.08 | 0.88 |
| 2:F:349:THR:HB | 1:G:178:SER:CB | 2.02 | 0.88 |
| 1:G:8:GLN:OE1 | 1:G:67:LEU:HD22 | 1.73 | 0.88 |
| 1:E:8:GLN:OE1 | 1:E:67:LEU:HD22 | 1.73 | 0.88 |
| 2:F:261:PRO:CA | 1:G:404:PHE:CE2 | 2.56 | 0.88 |
| 1:G:10:GLY:HA2 | 1:G:145:THR:HB | 1.55 | 0.88 |
| 1:A:311:ARG:HD3 | 1:A:342:TYR:HA | 1.56 | 0.88 |
| 2:D:110:ILE:HG23 | 2:D:111:GLY:H | 1.38 | 0.88 |
| 2:B:296:PHE:CD2 | 2:B:341:ILE:HD12 | 2.08 | 0.87 |
| 2:B:439:SER:C | 1:C:401:ARG:NH2 | 2.28 | 0.87 |
| 2:D:30:ILE:CG1 | 2:D:36:MET:HB3 | 2.02 | 0.87 |
| 1:G:2:ARG:CZ | 2:H:98:ASP:CB | 2.52 | 0.87 |
| 1:G:248:LEU:CD2 | 2:H:179:THR:HG22 | 2.03 | 0.87 |
| 1:A:10:GLY:HA2 | 1:A:145:THR:HB | 1.55 | 0.87 |
| 1:E:10:GLY:HA2 | 1:E:145:THR:HB | 1.55 | 0.87 |
| 2:H:296:PHE:CD2 | 2:H:341:ILE:HD12 | 2.08 | 0.87 |
| 1:C:346:TRP:HB2 | 2:D:401:LYS:HD2 | 1.56 | 0.87 |
| 2:F:147:SER:HB2 | 2:F:190:THR:OG1 | 1.73 | 0.87 |
| 2:H:147:SER:HB2 | 2:H:190:THR:OG1 | 1.73 | 0.87 |
| 2:B:30:ILE:CD1 | 2:B:61:HIS:CE1 | 2.57 | 0.87 |
| 2:B:122:ILE:HD12 | 2:B:157:LEU:HD21 | 1.54 | 0.87 |
| 2:D:52:PHE:HZ | 2:D:239:THR:CG2 | 1.88 | 0.87 |
| 1:E:311:ARG:HD3 | 1:E:342:TYR:HA | 1.56 | 0.87 |
| 1:G:311:ARG:HD3 | 1:G:342:TYR:HA | 1.56 | 0.87 |
| 2:B:30:ILE:CG1 | 2:B:36:MET:HB3 | 2.02 | 0.87 |
| 2:D:147:SER:HB2 | 2:D:190:THR:OG1 | 1.73 | 0.87 |
| 1:G:360:PRO:HG2 | 1:G:371:LEU:HB3 | 1.56 | 0.87 |
| 1:E:360:PRO:HG2 | 1:E:371:LEU:HB3 | 1.56 | 0.87 |
| 2:D:5:ILE:HG21 | 2:D:135:PHE:CD2 | 2.08 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:122:ILE:HD12 | 2:F:157:LEU:HD21 | 1.54 | 0.87 |
| 2:H:122:ILE:HD12 | 2:H:157:LEU:HD21 | 1.54 | 0.87 |
| 2:D:57:GLY:CA | 2:D:58:ALA:CB | 2.30 | 0.86 |
| 2:H:52:PHE:HZ | 2:H:239:THR:CG2 | 1.88 | 0.86 |
| 1:A:360:PRO:HG2 | 1:A:371:LEU:HB3 | 1.56 | 0.86 |
| 1:C:10:GLY:HA2 | 1:C:145:THR:HB | 1.55 | 0.86 |
| 1:E:6:HIS:CE1 | 1:E:8:GLN:HG2 | 2.10 | 0.86 |
| 1:G:257:VAL:CB | 2:H:407:TRP:CD2 | 2.57 | 0.86 |
| 1:G:153:LEU:O | 1:G:157:ILE:HG12 | 1.76 | 0.86 |
| 1:G:248:LEU:HD22 | 2:H:179:THR:HG23 | 1.56 | 0.86 |
| 2:B:63:PRO:CG | 2:B:91:GLN:OE1 | 2.19 | 0.86 |
| 1:C:19:LYS:HG3 | 1:C:228:ASN:HB3 | 1.57 | 0.86 |
| 1:G:6:HIS:CE1 | 1:G:8:GLN:HG2 | 2.10 | 0.86 |
| 1:A:6:HIS:CE1 | 1:A:8:GLN:HG2 | 2.10 | 0.86 |
| 1:A:153:LEU:O | 1:A:157:ILE:HG12 | 1.75 | 0.86 |
| 2:B:147:SER:HB2 | 2:B:190:THR:OG1 | 1.73 | 0.86 |
| 1:E:153:LEU:O | 1:E:157:ILE:HG12 | 1.75 | 0.86 |
| 1:E:195:VAL:HG13 | 1:E:196:GLU:HG2 | 1.57 | 0.86 |
| 1:A:276:THR:HB | 1:A:281:GLN:HG3 | 1.56 | 0.86 |
| 2:B:333:ALA:HA | 1:C:177:VAL:CG2 | 2.05 | 0.86 |
| 2:F:52:PHE:HZ | 2:F:239:THR:CG2 | 1.89 | 0.86 |
| 1:G:276:THR:HB | 1:G:281:GLN:HG3 | 1.56 | 0.86 |
| 2:B:63:PRO:HD3 | 2:B:87:PHE:HA | 1.56 | 0.86 |
| 2:D:296:PHE:CD2 | 2:D:341:ILE:HD12 | 2.08 | 0.86 |
| 1:G:19:LYS:HG3 | 1:G:228:ASN:HB3 | 1.57 | 0.86 |
| 1:C:360:PRO:HG2 | 1:C:371:LEU:HB3 | 1.56 | 0.86 |
| 2:F:324:VAL:HG11 | 1:G:221:THR:CA | 2.06 | 0.86 |
| 1:C:276:THR:HB | 1:C:281:GLN:HG3 | 1.56 | 0.86 |
| 1:C:6:HIS:CE1 | 1:C:8:GLN:HG2 | 2.10 | 0.85 |
| 1:E:276:THR:HB | 1:E:281:GLN:HG3 | 1.56 | 0.85 |
| 1:A:19:LYS:HG3 | 1:A:228:ASN:HB3 | 1.57 | 0.85 |
| 1:C:153:LEU:O | 1:C:157:ILE:HG12 | 1.75 | 0.85 |
| 1:E:19:LYS:HG3 | 1:E:228:ASN:HB3 | 1.57 | 0.85 |
| 1:E:101:ASN:HD21 | 1:E:143:GLY:HA2 | 1.38 | 0.85 |
| 1:G:101:ASN:HD21 | 1:G:143:GLY:HA2 | 1.38 | 0.85 |
| 1:G:195:VAL:HG13 | 1:G:196:GLU:HG2 | 1.57 | 0.85 |
| 2:F:5:ILE:HG21 | 2:F:135:PHE:CD2 | 2.08 | 0.85 |
| 2:H:5:ILE:HG21 | 2:H:135:PHE:CD2 | 2.08 | 0.85 |
| 1:C:257:VAL:HG13 | 2:D:407:TRP:CD2 | 2.11 | 0.85 |
| 1:G:257:VAL:CG2 | 2:H:407:TRP:CD2 | 2.59 | 0.85 |
| 2:D:56:THR:C | 2:H:284:GLU:CB | 2.44 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:261:PRO:CG | 1:G:404:PHE:HE2 | 1.88 | 0.85 |
| 1:G:352:LYS:HA | 2:H:181:VAL:CG2 | 2.06 | 0.85 |
| 1:A:195:VAL:HG13 | 1:A:196:GLU:HG2 | 1.57 | 0.85 |
| 2:D:234:ILE:HG13 | 2:D:270:ALA:HB1 | 1.59 | 0.85 |
| 2:B:234:ILE:HG13 | 2:B:270:ALA:HB1 | 1.59 | 0.85 |
| 1:C:195:VAL:HG13 | 1:C:196:GLU:HG2 | 1.57 | 0.85 |
| 2:D:204:VAL:HG11 | 2:D:231:ILE:HD12 | 1.59 | 0.85 |
| 2:F:234:ILE:HG13 | 2:F:270:ALA:HB1 | 1.59 | 0.84 |
| 2:F:264:ARG:O | 2:F:266:HIS:N | 2.09 | 0.84 |
| 2:H:264:ARG:O | 2:H:266:HIS:N | 2.09 | 0.84 |
| 1:E:234:THR:HG21 | 1:E:270:PRO:CB | 2.06 | 0.84 |
| 2:F:204:VAL:HG11 | 2:F:231:ILE:HD12 | 1.59 | 0.84 |
| 1:G:179:ASP:HB2 | 4:G:600:GDP:H3' | 1.58 | 0.84 |
| 2:H:234:ILE:HG13 | 2:H:270:ALA:HB1 | 1.59 | 0.84 |
| 2:D:52:PHE:CZ | 2:D:239:THR:CB | 2.60 | 0.84 |
| 2:F:184:PRO:HG2 | 2:F:398:MET:HE1 | 1.57 | 0.84 |
| 2:F:263:PRO:HD3 | 1:G:406:HIS:CD2 | 2.12 | 0.84 |
| 2:B:204:VAL:HG11 | 2:B:231:ILE:HD12 | 1.59 | 0.84 |
| 1:C:209:LEU:HB3 | 1:C:227:LEU:HD22 | 1.59 | 0.84 |
| 2:B:52:PHE:CZ | 2:B:239:THR:HG21 | 2.11 | 0.84 |
| 1:C:150:GLY:HA2 | 1:C:153:LEU:HD22 | 1.60 | 0.84 |
| 1:C:242:LEU:HD22 | 1:C:250:ALA:H | 1.41 | 0.84 |
| 2:H:204:VAL:HG11 | 2:H:231:ILE:HD12 | 1.59 | 0.84 |
| 1:A:150:GLY:HA2 | 1:A:153:LEU:HD22 | 1.60 | 0.84 |
| 2:B:264:ARG:O | 2:B:266:HIS:N | 2.09 | 0.84 |
| 2:D:106:GLY:O | 2:D:111:GLY:HA3 | 1.78 | 0.84 |
| 2:D:264:ARG:HB2 | 2:D:266:HIS:CD2 | 2.13 | 0.84 |
| 2:F:324:VAL:HG21 | 1:G:221:THR:CG2 | 2.06 | 0.84 |
| 1:G:209:LEU:HB3 | 1:G:227:LEU:HD22 | 1.59 | 0.84 |
| 1:G:234:THR:HG21 | 1:G:270:PRO:CB | 2.06 | 0.84 |
| 2:B:106:GLY:O | 2:B:111:GLY:HA3 | 1.78 | 0.84 |
| 1:G:242:LEU:HD22 | 1:G:250:ALA:H | 1.41 | 0.84 |
| 1:A:20:PHE:CD2 | 1:A:235:MET:SD | 2.71 | 0.84 |
| 1:A:56:ALA:HB1 | 1:E:283:TYR:CD2 | 2.13 | 0.84 |
| 1:A:242:LEU:HD22 | 1:A:250:ALA:H | 1.41 | 0.84 |
| 1:C:3:GLU:O | 1:C:133:GLN:HB3 | 1.78 | 0.84 |
| 1:C:248:LEU:CD2 | 2:D:179:THR:HG21 | 2.08 | 0.84 |
| 2:D:52:PHE:CE1 | 2:D:239:THR:HB | 2.12 | 0.84 |
| 2:D:264:ARG:O | 2:D:266:HIS:N | 2.09 | 0.84 |
| 2:F:316:CYS:HB3 | 2:F:378:LEU:CD1 | 2.08 | 0.84 |
| 1:G:150:GLY:HA2 | 1:G:153:LEU:HD22 | 1.60 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:4:ILE:HD13 | 1:A:136:GLN:HE21 | 1.42 | 0.84 |
| 1:A:209:LEU:HB3 | 1:A:227:LEU:HD22 | 1.59 | 0.84 |
| 1:C:191:VAL:HG11 | 1:C:425:MET:HG3 | 1.60 | 0.84 |
| 1:E:3:GLU:O | 1:E:133:GLN:HB3 | 1.78 | 0.84 |
| 1:E:4:ILE:HD13 | 1:E:136:GLN:HE21 | 1.42 | 0.84 |
| 1:G:3:GLU:O | 1:G:133:GLN:HB3 | 1.78 | 0.84 |
| 1:G:4:ILE:HD13 | 1:G:136:GLN:HE21 | 1.42 | 0.84 |
| 2:H:217:LEU:CD1 | 2:H:277:SER:CA | 2.56 | 0.84 |
| 1:A:324:SER:HB3 | 1:A:327:GLU:HG2 | 1.60 | 0.83 |
| 1:C:20:PHE:CD2 | 1:C:235:MET:SD | 2.71 | 0.83 |
| 2:D:316:CYS:HB3 | 2:D:378:LEU:CD1 | 2.08 | 0.83 |
| 2:B:264:ARG:HB2 | 2:B:266:HIS:CD2 | 2.13 | 0.83 |
| 1:E:20:PHE:CD2 | 1:E:235:MET:SD | 2.71 | 0.83 |
| 2:F:217:LEU:CD1 | 2:F:277:SER:CA | 2.56 | 0.83 |
| 2:H:316:CYS:HB3 | 2:H:378:LEU:CD1 | 2.08 | 0.83 |
| 1:A:3:GLU:O | 1:A:133:GLN:HB3 | 1.78 | 0.83 |
| 1:C:4:ILE:HD13 | 1:C:136:GLN:HE21 | 1.42 | 0.83 |
| 2:D:56:THR:CB | 2:H:284:GLU:CG | 2.56 | 0.83 |
| 1:A:191:VAL:HG11 | 1:A:425:MET:HG3 | 1.60 | 0.83 |
| 2:B:151:SER:CB | 2:B:193:THR:HG21 | 2.09 | 0.83 |
| 1:E:150:GLY:HA2 | 1:E:153:LEU:HD22 | 1.60 | 0.83 |
| 1:E:209:LEU:HB3 | 1:E:227:LEU:HD22 | 1.59 | 0.83 |
| 2:F:151:SER:CB | 2:F:193:THR:HG21 | 2.09 | 0.83 |
| 1:G:20:PHE:CD2 | 1:G:235:MET:SD | 2.71 | 0.83 |
| 1:C:324:SER:HB3 | 1:C:327:GLU:HG2 | 1.60 | 0.83 |
| 2:F:106:GLY:O | 2:F:111:GLY:HA3 | 1.78 | 0.83 |
| 2:H:106:GLY:O | 2:H:111:GLY:HA3 | 1.78 | 0.83 |
| 2:H:151:SER:CB | 2:H:193:THR:HG21 | 2.09 | 0.83 |
| 1:A:148:GLY:O | 1:A:151:THR:HG22 | 1.79 | 0.83 |
| 2:B:217:LEU:CD1 | 2:B:277:SER:CA | 2.56 | 0.83 |
| 2:B:316:CYS:HB3 | 2:B:378:LEU:CD1 | 2.08 | 0.83 |
| 2:F:67:PHE:CE1 | 2:F:87:PHE:HE1 | 1.96 | 0.83 |
| 2:F:349:THR:HG21 | 1:G:178:SER:C | 1.98 | 0.83 |
| 1:G:148:GLY:O | 1:G:151:THR:HG22 | 1.79 | 0.83 |
| 2:D:151:SER:CB | 2:D:193:THR:HG21 | 2.09 | 0.83 |
| 2:H:67:PHE:CE1 | 2:H:87:PHE:HE1 | 1.96 | 0.83 |
| 2:H:264:ARG:HB2 | 2:H:266:HIS:CD2 | 2.13 | 0.83 |
| 1:A:234:THR:HG21 | 1:A:270:PRO:CB | 2.06 | 0.83 |
| 2:D:217:LEU:CD1 | 2:D:277:SER:CA | 2.56 | 0.83 |
| 1:E:242:LEU:HD22 | 1:E:250:ALA:H | 1.41 | 0.83 |
| 1:A:287:THR:O | 1:A:288:VAL:HG23 | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:148:GLY:O | 1:C:151:THR:HG22 | 1.79 | 0.83 |
| 1:C:234:THR:HG21 | 1:C:270:PRO:CB | 2.06 | 0.83 |
| 1:C:287:THR:O | 1:C:288:VAL:HG23 | 1.78 | 0.83 |
| 2:F:264:ARG:HB2 | 2:F:266:HIS:CD2 | 2.13 | 0.83 |
| 2:H:52:PHE:CZ | 2:H:239:THR:CB | 2.62 | 0.83 |
| 1:E:110:GLU:O | 1:E:113:GLU:HG2 | 1.79 | 0.83 |
| 1:E:148:GLY:O | 1:E:151:THR:HG22 | 1.79 | 0.83 |
| 1:E:324:SER:HB3 | 1:E:327:GLU:HG2 | 1.60 | 0.82 |
| 1:G:110:GLU:O | 1:G:113:GLU:HG2 | 1.79 | 0.82 |
| 2:H:52:PHE:CE1 | 2:H:239:THR:HB | 2.13 | 0.82 |
| 1:C:110:GLU:O | 1:C:113:GLU:HG2 | 1.79 | 0.82 |
| 1:G:324:SER:HB3 | 1:G:327:GLU:HG2 | 1.60 | 0.82 |
| 1:A:110:GLU:O | 1:A:113:GLU:HG2 | 1.80 | 0.82 |
| 1:G:287:THR:O | 1:G:288:VAL:HG23 | 1.78 | 0.82 |
| 2:F:52:PHE:CE1 | 2:F:239:THR:HB | 2.14 | 0.82 |
| 2:F:52:PHE:CZ | 2:F:239:THR:CB | 2.62 | 0.82 |
| 1:G:101:ASN:ND2 | 1:G:143:GLY:HA2 | 1.94 | 0.82 |
| 1:E:287:THR:O | 1:E:288:VAL:HG23 | 1.79 | 0.82 |
| 2:D:67:PHE:CE1 | 2:D:87:PHE:HE1 | 1.96 | 0.82 |
| 1:G:346:TRP:HB2 | 2:H:401:LYS:HG3 | 1.61 | 0.82 |
| 1:E:257:VAL:HG13 | 2:F:407:TRP:CG | 2.15 | 0.82 |
| 1:E:191:VAL:HG11 | 1:E:425:MET:HG3 | 1.60 | 0.82 |
| 2:H:102:ASN:CG | 2:H:407:TRP:HE1 | 1.83 | 0.82 |
| 1:A:88:ARG:NH1 | 1:E:283:TYR:HE1 | 1.71 | 0.81 |
| 1:E:101:ASN:ND2 | 1:E:143:GLY:HA2 | 1.94 | 0.81 |
| 1:E:147:SER:HB2 | 1:E:190:SER:HB3 | 1.60 | 0.81 |
| 1:A:147:SER:HB2 | 1:A:190:SER:HB3 | 1.60 | 0.81 |
| 1:C:101:ASN:ND2 | 1:C:143:GLY:HA2 | 1.94 | 0.81 |
| 1:A:101:ASN:ND2 | 1:A:143:GLY:HA2 | 1.94 | 0.81 |
| 1:C:20:PHE:CZ | 1:C:24:ILE:HD12 | 2.15 | 0.81 |
| 1:C:147:SER:HB2 | 1:C:190:SER:HB3 | 1.60 | 0.81 |
| 2:F:52:PHE:CZ | 2:F:239:THR:HG21 | 2.15 | 0.81 |
| 1:G:191:VAL:HG11 | 1:G:425:MET:HG3 | 1.60 | 0.81 |
| 2:H:52:PHE:CZ | 2:H:239:THR:HG21 | 2.15 | 0.81 |
| 2:B:67:PHE:CE1 | 2:B:87:PHE:HE1 | 1.96 | 0.81 |
| 2:B:23:LEU:HD23 | 2:B:236:SER:HB2 | 1.60 | 0.81 |
| 2:H:52:PHE:CZ | 2:H:239:THR:CG2 | 2.64 | 0.81 |
| 2:D:23:LEU:HD23 | 2:D:236:SER:HB2 | 1.61 | 0.81 |
| 2:D:52:PHE:CZ | 2:D:239:THR:CG2 | 2.64 | 0.81 |
| 2:F:313:MET:HB3 | 2:F:344:VAL:HG21 | 1.63 | 0.81 |
| 2:F:326:LYS:CG | 1:G:222:PRO:HG2 | 2.05 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:156:LYS:HA | 1:G:156:LYS:HE2 | 1.61 | 0.81 |
| 2:H:313:MET:HB3 | 2:H:344:VAL:HG21 | 1.63 | 0.81 |
| 2:F:23:LEU:HD23 | 2:F:236:SER:HB2 | 1.61 | 0.81 |
| 1:G:20:PHE:CZ | 1:G:24:ILE:HD12 | 2.15 | 0.81 |
| 1:G:352:LYS:HD3 | 2:H:181:VAL:HG21 | 1.61 | 0.81 |
| 2:H:267:PHE:N | 2:H:267:PHE:CD1 | 2.49 | 0.81 |
| 2:H:276:ILE:HG23 | 2:H:369:ALA:CB | 2.10 | 0.81 |
| 1:A:20:PHE:CZ | 1:A:24:ILE:HD12 | 2.15 | 0.81 |
| 1:E:20:PHE:CZ | 1:E:24:ILE:HD12 | 2.15 | 0.81 |
| 2:F:52:PHE:CZ | 2:F:239:THR:CG2 | 2.64 | 0.81 |
| 2:F:267:PHE:N | 2:F:267:PHE:CD1 | 2.49 | 0.81 |
| 2:F:276:ILE:HG23 | 2:F:369:ALA:CB | 2.10 | 0.81 |
| 2:B:6:SER:HB3 | 2:B:136:SER:OG | 1.81 | 0.81 |
| 2:F:6:SER:HB3 | 2:F:136:SER:OG | 1.81 | 0.81 |
| 1:G:2:ARG:NH2 | 2:H:98:ASP:CB | 2.44 | 0.81 |
| 1:G:147:SER:HB2 | 1:G:190:SER:HB3 | 1.60 | 0.81 |
| 2:H:6:SER:HB3 | 2:H:136:SER:OG | 1.81 | 0.81 |
| 2:H:23:LEU:HD23 | 2:H:236:SER:HB2 | 1.61 | 0.81 |
| 2:B:52:PHE:CZ | 2:B:239:THR:HB | 2.14 | 0.81 |
| 2:B:109:THR:CG2 | 2:B:110:ILE:N | 2.44 | 0.81 |
| 2:B:313:MET:HB3 | 2:B:344:VAL:HG21 | 1.63 | 0.81 |
| 1:C:156:LYS:HE2 | 1:C:156:LYS:HA | 1.61 | 0.81 |
| 2:F:220:GLU:C | 2:F:222:PRO:HD3 | 2.02 | 0.81 |
| 1:G:257:VAL:HG22 | 1:G:257:VAL:O | 1.78 | 0.81 |
| 2:H:109:THR:CG2 | 2:H:110:ILE:N | 2.44 | 0.81 |
| 2:H:220:GLU:C | 2:H:222:PRO:HD3 | 2.02 | 0.81 |
| 2:H:248:LEU:HD23 | 2:H:353:VAL:O | 1.80 | 0.81 |
| 2:B:184:PRO:HG2 | 2:B:398:MET:HE1 | 1.63 | 0.80 |
| 2:D:248:LEU:HD23 | 2:D:353:VAL:O | 1.80 | 0.80 |
| 1:E:156:LYS:HE2 | 1:E:156:LYS:HA | 1.61 | 0.80 |
| 2:F:7:ILE:HG22 | 2:F:66:VAL:HG22 | 1.63 | 0.80 |
| 2:F:109:THR:CG2 | 2:F:110:ILE:N | 2.44 | 0.80 |
| 2:H:7:ILE:HG22 | 2:H:66:VAL:HG22 | 1.63 | 0.80 |
| 2:H:132:LEU:HD23 | 2:H:132:LEU:H | 1.46 | 0.80 |
| 2:B:248:LEU:HD23 | 2:B:353:VAL:O | 1.80 | 0.80 |
| 2:B:267:PHE:N | 2:B:267:PHE:CD1 | 2.49 | 0.80 |
| 2:D:52:PHE:CZ | 2:D:239:THR:HG21 | 2.15 | 0.80 |
| 2:D:267:PHE:N | 2:D:267:PHE:CD1 | 2.49 | 0.80 |
| 2:B:52:PHE:HZ | 2:B:239:THR:CG2 | 1.94 | 0.80 |
| 2:D:6:SER:HB3 | 2:D:136:SER:OG | 1.81 | 0.80 |
| 2:F:248:LEU:HD23 | 2:F:353:VAL:O | 1.80 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:234:THR:CG2 | 1:A:270:PRO:HB2 | 2.11 | 0.80 |
| 2:B:7:ILE:HG22 | 2:B:66:VAL:HG22 | 1.63 | 0.80 |
| 2:D:109:THR:CG2 | 2:D:110:ILE:N | 2.44 | 0.80 |
| 2:D:313:MET:HB3 | 2:D:344:VAL:HG21 | 1.63 | 0.80 |
| 1:A:413:MET:HG3 | 1:A:414:ASP:H | 1.47 | 0.80 |
| 2:F:132:LEU:HD23 | 2:F:132:LEU:H | 1.46 | 0.80 |
| 2:F:241:SER:O | 2:F:244:PHE:HB3 | 1.82 | 0.80 |
| 2:B:70:LEU:CD1 | 2:B:145:THR:HG23 | 2.12 | 0.80 |
| 2:D:56:THR:O | 2:D:58:ALA:CB | 2.30 | 0.80 |
| 2:H:241:SER:O | 2:H:244:PHE:HB3 | 1.82 | 0.80 |
| 1:E:234:THR:CG2 | 1:E:270:PRO:HB2 | 2.11 | 0.80 |
| 1:E:413:MET:HG3 | 1:E:414:ASP:H | 1.47 | 0.80 |
| 1:G:413:MET:HG3 | 1:G:414:ASP:H | 1.47 | 0.80 |
| 2:D:70:LEU:CD1 | 2:D:145:THR:HG23 | 2.12 | 0.80 |
| 2:D:184:PRO:HG2 | 2:D:398:MET:HE1 | 1.62 | 0.80 |
| 2:D:276:ILE:HG23 | 2:D:369:ALA:CB | 2.10 | 0.80 |
| 1:G:236:SER:O | 1:G:240:THR:CG2 | 2.29 | 0.80 |
| 2:B:276:ILE:HG23 | 2:B:369:ALA:CB | 2.10 | 0.80 |
| 1:G:254:LYS:HE3 | 1:G:352:LYS:NZ | 1.97 | 0.80 |
| 2:B:67:PHE:HE1 | 2:B:87:PHE:CD1 | 2.00 | 0.79 |
| 2:B:220:GLU:C | 2:B:222:PRO:HD3 | 2.02 | 0.79 |
| 2:B:241:SER:O | 2:B:244:PHE:HB3 | 1.82 | 0.79 |
| 1:C:413:MET:HG3 | 1:C:414:ASP:H | 1.47 | 0.79 |
| 1:A:156:LYS:HE2 | 1:A:156:LYS:HA | 1.61 | 0.79 |
| 1:C:54:ASN:HD21 | 1:C:64:ARG:HD3 | 1.46 | 0.79 |
| 1:C:329:ASP:HB3 | 2:D:177:VAL:HG12 | 1.61 | 0.79 |
| 1:A:236:SER:O | 1:A:240:THR:CG2 | 2.29 | 0.79 |
| 2:D:7:ILE:HG22 | 2:D:66:VAL:HG22 | 1.63 | 0.79 |
| 1:E:54:ASN:HD21 | 1:E:64:ARG:HD3 | 1.46 | 0.79 |
| 2:F:67:PHE:HE1 | 2:F:87:PHE:CD1 | 1.99 | 0.79 |
| 2:D:67:PHE:HE1 | 2:D:87:PHE:CD1 | 2.00 | 0.79 |
| 1:E:236:SER:O | 1:E:240:THR:CG2 | 2.29 | 0.79 |
| 2:F:234:ILE:O | 2:F:234:ILE:HD13 | 1.81 | 0.79 |
| 2:H:234:ILE:O | 2:H:234:ILE:HD13 | 1.81 | 0.79 |
| 1:A:54:ASN:HD21 | 1:A:64:ARG:HD3 | 1.46 | 0.79 |
| 1:A:68:VAL:HG12 | 1:A:149:MET:SD | 2.22 | 0.79 |
| 1:C:236:SER:O | 1:C:240:THR:CG2 | 2.29 | 0.79 |
| 1:G:54:ASN:HD21 | 1:G:64:ARG:HD3 | 1.46 | 0.79 |
| 2:H:67:PHE:HE1 | 2:H:87:PHE:CD1 | 1.99 | 0.79 |
| 1:C:68:VAL:HG12 | 1:C:149:MET:SD | 2.22 | 0.79 |
| 1:C:264:ARG:HB2 | 1:C:266:HIS:HD2 | 1.45 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:265:LEU:HD12 | 1:C:265:LEU:O | 1.83 | 0.79 |
| 2:D:220:GLU:C | 2:D:222:PRO:HD3 | 2.02 | 0.79 |
| 2:D:234:ILE:HD13 | 2:D:234:ILE:O | 1.81 | 0.79 |
| 2:D:11:GLN:HE21 | 2:D:74:VAL:HG22 | 1.47 | 0.79 |
| 2:D:241:SER:O | 2:D:244:PHE:HB3 | 1.82 | 0.79 |
| 2:H:11:GLN:HE21 | 2:H:74:VAL:HG22 | 1.47 | 0.79 |
| 2:D:132:LEU:HD23 | 2:D:132:LEU:H | 1.46 | 0.79 |
| 2:F:11:GLN:HE21 | 2:F:74:VAL:HG22 | 1.47 | 0.79 |
| 2:H:70:LEU:CD1 | 2:H:145:THR:HG23 | 2.12 | 0.79 |
| 1:A:265:LEU:O | 1:A:265:LEU:HD12 | 1.83 | 0.79 |
| 2:B:243:ARG:HH21 | 2:B:252:LEU:H | 0.79 | 0.79 |
| 1:E:264:ARG:HB2 | 1:E:266:HIS:HD2 | 1.45 | 0.79 |
| 2:F:70:LEU:CD1 | 2:F:145:THR:HG23 | 2.12 | 0.79 |
| 1:G:264:ARG:HB2 | 1:G:266:HIS:HD2 | 1.45 | 0.79 |
| 1:A:264:ARG:HB2 | 1:A:266:HIS:HD2 | 1.45 | 0.79 |
| 2:B:56:THR:O | 2:B:58:ALA:CB | 2.30 | 0.79 |
| 1:E:68:VAL:HG12 | 1:E:149:MET:SD | 2.22 | 0.79 |
| 2:H:102:ASN:CG | 2:H:407:TRP:NE1 | 2.36 | 0.79 |
| 2:H:217:LEU:CD1 | 2:H:277:SER:HA | 2.13 | 0.78 |
| 2:H:296:PHE:CZ | 2:H:335:ILE:HG21 | 2.18 | 0.78 |
| 2:B:234:ILE:O | 2:B:234:ILE:HD13 | 1.81 | 0.78 |
| 2:D:217:LEU:CD1 | 2:D:277:SER:HA | 2.13 | 0.78 |
| 2:F:217:LEU:CD1 | 2:F:277:SER:HA | 2.13 | 0.78 |
| 2:F:243:ARG:HH21 | 2:F:252:LEU:H | 0.79 | 0.78 |
| 2:F:296:PHE:CZ | 2:F:335:ILE:HG21 | 2.18 | 0.78 |
| 1:G:68:VAL:HG12 | 1:G:149:MET:SD | 2.22 | 0.78 |
| 2:H:199:ASP:HB3 | 2:H:256:GLN:NE2 | 1.99 | 0.78 |
| 2:B:3:GLU:HG2 | 2:B:51:THR:HA | 0.80 | 0.78 |
| 1:C:257:VAL:HA | 2:D:407:TRP:CE2 | 2.18 | 0.78 |
| 1:G:352:LYS:CB | 2:H:181:VAL:HG21 | 2.13 | 0.78 |
| 2:H:3:GLU:HG2 | 2:H:51:THR:HA | 0.80 | 0.78 |
| 1:A:205:ASP:OD1 | 1:A:304:ALA:HB2 | 1.84 | 0.78 |
| 2:B:132:LEU:HD23 | 2:B:132:LEU:H | 1.46 | 0.78 |
| 2:B:199:ASP:HB3 | 2:B:256:GLN:NE2 | 1.99 | 0.78 |
| 1:C:259:MET:HA | 1:C:314:THR:HG21 | 1.65 | 0.78 |
| 2:D:243:ARG:HH21 | 2:D:252:LEU:H | 0.79 | 0.78 |
| 2:F:3:GLU:HG2 | 2:F:51:THR:HA | 0.80 | 0.78 |
| 2:F:199:ASP:HB3 | 2:F:256:GLN:NE2 | 1.99 | 0.78 |
| 2:F:346:TRP:HZ3 | 1:G:404:PHE:CZ | 2.01 | 0.78 |
| 1:G:205:ASP:OD1 | 1:G:304:ALA:HB2 | 1.84 | 0.78 |
| 2:H:102:ASN:ND2 | 2:H:407:TRP:CD1 | 2.51 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:243:ARG:HH21 | 2:H:252:LEU:H | 0.79 | 0.78 |
| 2:B:11:GLN:HE21 | 2:B:74:VAL:HG22 | 1.47 | 0.78 |
| 2:B:52:PHE:CZ | 2:B:239:THR:CB | 2.67 | 0.78 |
| 2:B:217:LEU:CD1 | 2:B:277:SER:HA | 2.13 | 0.78 |
| 1:C:205:ASP:OD1 | 1:C:304:ALA:HB2 | 1.84 | 0.78 |
| 2:D:199:ASP:HB3 | 2:D:256:GLN:NE2 | 1.98 | 0.78 |
| 2:D:276:ILE:O | 2:D:369:ALA:HB2 | 1.84 | 0.78 |
| 1:E:205:ASP:OD1 | 1:E:304:ALA:HB2 | 1.84 | 0.78 |
| 2:F:276:ILE:O | 2:F:369:ALA:HB2 | 1.83 | 0.78 |
| 2:H:30:ILE:HG12 | 2:H:36:MET:CB | 2.09 | 0.78 |
| 2:B:204:VAL:HG13 | 2:B:209:ILE:HD11 | 1.66 | 0.78 |
| 1:C:346:TRP:CB | 2:D:401:LYS:HD2 | 2.13 | 0.78 |
| 2:D:3:GLU:HG2 | 2:D:51:THR:HA | 0.80 | 0.78 |
| 2:H:204:VAL:HG13 | 2:H:209:ILE:HD11 | 1.65 | 0.78 |
| 2:H:276:ILE:O | 2:H:369:ALA:HB2 | 1.84 | 0.78 |
| 2:D:55:GLU:O | 2:D:57:GLY:N | 2.17 | 0.78 |
| 2:F:67:PHE:HD1 | 2:F:92:LEU:HD23 | 1.49 | 0.78 |
| 2:B:5:ILE:CG1 | 2:B:64:ARG:CZ | 2.56 | 0.78 |
| 1:C:325:MET:HG2 | 2:D:224:TYR:CE1 | 2.18 | 0.78 |
| 2:D:231:ILE:HA | 2:D:234:ILE:HG22 | 1.66 | 0.78 |
| 2:F:231:ILE:HA | 2:F:234:ILE:HG22 | 1.66 | 0.78 |
| 2:H:67:PHE:HD1 | 2:H:92:LEU:HD23 | 1.49 | 0.78 |
| 2:H:231:ILE:HA | 2:H:234:ILE:HG22 | 1.66 | 0.78 |
| 2:B:231:ILE:HA | 2:B:234:ILE:HG22 | 1.66 | 0.78 |
| 2:D:296:PHE:CD2 | 2:D:341:ILE:HD11 | 2.03 | 0.78 |
| 2:F:204:VAL:HG13 | 2:F:209:ILE:HD11 | 1.66 | 0.78 |
| 1:A:259:MET:HA | 1:A:314:THR:HG21 | 1.65 | 0.78 |
| 1:A:396:THR:HG23 | 1:A:422:GLU:OE2 | 1.83 | 0.78 |
| 2:B:172:TYR:C | 2:B:172:TYR:HD1 | 1.87 | 0.77 |
| 2:D:296:PHE:CZ | 2:D:335:ILE:HG21 | 2.18 | 0.77 |
| 1:E:35:SER:HB3 | 1:E:59:ASN:HA | 1.65 | 0.77 |
| 2:F:30:ILE:HG12 | 2:F:36:MET:CB | 2.09 | 0.77 |
| 2:B:223:THR:HB | 2:B:225:THR:HG22 | 1.67 | 0.77 |
| 2:B:348:PRO:HD2 | 1:C:398:MET:HE1 | 1.66 | 0.77 |
| 2:D:155:GLU:HA | 2:D:197:HIS:ND1 | 1.99 | 0.77 |
| 1:E:265:LEU:HD12 | 1:E:265:LEU:O | 1.83 | 0.77 |
| 1:E:332:MET:HE3 | 1:E:351:VAL:HG11 | 1.66 | 0.77 |
| 2:B:52:PHE:CZ | 2:B:239:THR:CG2 | 2.66 | 0.77 |
| 2:B:276:ILE:O | 2:B:369:ALA:HB2 | 1.84 | 0.77 |
| 2:B:296:PHE:CZ | 2:B:335:ILE:HG21 | 2.18 | 0.77 |
| 2:D:223:THR:HB | 2:D:225:THR:HG22 | 1.67 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:259:MET:HA | 1:E:314:THR:HG21 | 1.65 | 0.77 |
| 1:G:35:SER:HB3 | 1:G:59:ASN:HA | 1.65 | 0.77 |
| 2:B:110:ILE:HG23 | 2:B:111:GLY:N | 1.99 | 0.77 |
| 2:D:172:TYR:HD1 | 2:D:172:TYR:C | 1.87 | 0.77 |
| 2:D:204:VAL:HG13 | 2:D:209:ILE:HD11 | 1.66 | 0.77 |
| 2:D:67:PHE:HD1 | 2:D:92:LEU:HD23 | 1.49 | 0.77 |
| 2:F:5:ILE:HG23 | 2:F:135:PHE:HB3 | 1.66 | 0.77 |
| 2:F:425:MET:HE2 | 2:F:428:LEU:HD23 | 1.64 | 0.77 |
| 2:H:110:ILE:HG23 | 2:H:111:GLY:N | 1.99 | 0.77 |
| 2:H:155:GLU:HA | 2:H:197:HIS:ND1 | 1.99 | 0.77 |
| 2:F:110:ILE:HG23 | 2:F:111:GLY:N | 1.99 | 0.77 |
| 2:F:155:GLU:HA | 2:F:197:HIS:ND1 | 1.99 | 0.77 |
| 2:F:172:TYR:HD1 | 2:F:172:TYR:C | 1.87 | 0.77 |
| 2:H:425:MET:HE2 | 2:H:428:LEU:HD23 | 1.65 | 0.77 |
| 2:B:155:GLU:HA | 2:B:197:HIS:ND1 | 1.99 | 0.77 |
| 1:E:396:THR:HG23 | 1:E:422:GLU:OE2 | 1.83 | 0.77 |
| 2:F:223:THR:HB | 2:F:225:THR:HG22 | 1.67 | 0.77 |
| 1:G:259:MET:HA | 1:G:314:THR:HG21 | 1.65 | 0.77 |
| 1:G:265:LEU:HD12 | 1:G:265:LEU:O | 1.83 | 0.77 |
| 1:G:396:THR:HG23 | 1:G:422:GLU:OE2 | 1.83 | 0.77 |
| 2:F:261:PRO:CA | 1:G:404:PHE:HD2 | 1.82 | 0.77 |
| 2:H:5:ILE:HG23 | 2:H:135:PHE:HB3 | 1.66 | 0.77 |
| 2:H:172:TYR:C | 2:H:172:TYR:HD1 | 1.87 | 0.77 |
| 2:H:223:THR:HB | 2:H:225:THR:HG22 | 1.67 | 0.77 |
| 2:H:234:ILE:HG21 | 2:H:302:MET:HE3 | 1.66 | 0.77 |
| 1:C:396:THR:HG23 | 1:C:422:GLU:OE2 | 1.83 | 0.77 |
| 2:D:110:ILE:HG23 | 2:D:111:GLY:N | 1.99 | 0.77 |
| 2:F:298:PRO:HB3 | 2:F:307:PRO:CD | 2.15 | 0.77 |
| 2:H:298:PRO:HB3 | 2:H:307:PRO:CD | 2.15 | 0.77 |
| 2:B:67:PHE:HD1 | 2:B:92:LEU:HD23 | 1.49 | 0.77 |
| 1:C:35:SER:HB3 | 1:C:59:ASN:HA | 1.65 | 0.77 |
| 2:D:62:VAL:HG21 | 2:D:88:HIS:HE1 | 1.48 | 0.77 |
| 1:E:192:HIS:ND1 | 1:E:424:ASN:OD1 | 2.18 | 0.77 |
| 1:A:35:SER:HB3 | 1:A:59:ASN:HA | 1.65 | 0.76 |
| 1:C:247:GLN:HB3 | 2:D:224:TYR:HD1 | 1.50 | 0.76 |
| 2:F:63:PRO:HD3 | 2:F:86:LEU:O | 1.85 | 0.76 |
| 2:H:63:PRO:HD3 | 2:H:86:LEU:O | 1.85 | 0.76 |
| 2:F:324:VAL:HG11 | 1:G:221:THR:C | 2.05 | 0.76 |
| 1:A:192:HIS:ND1 | 1:A:424:ASN:OD1 | 2.18 | 0.76 |
| 2:F:70:LEU:CD1 | 2:F:145:THR:CG2 | 2.64 | 0.76 |
| 2:F:225:THR:O | 2:F:229:ARG:HG3 | 1.86 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:344:VAL:HG11 | 2:F:346:TRP:CE2 | 2.21 | 0.76 |
| 2:H:70:LEU:CD1 | 2:H:145:THR:CG2 | 2.64 | 0.76 |
| 2:B:70:LEU:CD1 | 2:B:145:THR:CG2 | 2.64 | 0.76 |
| 2:F:62:VAL:HG21 | 2:F:88:HIS:HE1 | 1.48 | 0.76 |
| 1:G:192:HIS:ND1 | 1:G:424:ASN:OD1 | 2.18 | 0.76 |
| 2:H:225:THR:O | 2:H:229:ARG:HG3 | 1.86 | 0.76 |
| 2:D:362:VAL:HG13 | 2:D:368:LEU:HD12 | 1.68 | 0.76 |
| 2:H:344:VAL:HG11 | 2:H:346:TRP:CE2 | 2.21 | 0.76 |
| 2:B:298:PRO:HB3 | 2:B:307:PRO:CD | 2.15 | 0.76 |
| 2:D:63:PRO:HD3 | 2:D:86:LEU:O | 1.85 | 0.76 |
| 2:H:163:LYS:O | 2:H:164:LYS:HG2 | 1.86 | 0.76 |
| 1:C:192:HIS:ND1 | 1:C:424:ASN:OD1 | 2.18 | 0.76 |
| 2:F:163:LYS:O | 2:F:164:LYS:HG2 | 1.86 | 0.76 |
| 2:F:331:ALA:O | 2:F:335:ILE:HG12 | 1.86 | 0.76 |
| 1:C:198:THR:O | 1:C:265:LEU:HD22 | 1.85 | 0.76 |
| 2:D:5:ILE:HG23 | 2:D:135:PHE:HB3 | 1.66 | 0.76 |
| 2:F:362:VAL:HG13 | 2:F:368:LEU:HD12 | 1.68 | 0.76 |
| 1:G:198:THR:O | 1:G:265:LEU:HD22 | 1.85 | 0.76 |
| 2:B:296:PHE:CD2 | 2:B:341:ILE:HD11 | 2.03 | 0.76 |
| 1:E:259:MET:HG2 | 1:E:314:THR:HG21 | 1.67 | 0.76 |
| 2:H:331:ALA:O | 2:H:335:ILE:HG12 | 1.86 | 0.76 |
| 2:D:163:LYS:O | 2:D:164:LYS:HG2 | 1.86 | 0.75 |
| 2:D:298:PRO:HB3 | 2:D:307:PRO:CD | 2.15 | 0.75 |
| 2:H:7:ILE:HD12 | 2:H:153:LEU:HD21 | 1.68 | 0.75 |
| 2:B:344:VAL:HG11 | 2:B:346:TRP:CE2 | 2.21 | 0.75 |
| 2:D:11:GLN:HG3 | 2:D:74:VAL:CG1 | 2.15 | 0.75 |
| 2:D:221:ARG:HD3 | 2:D:221:ARG:O | 1.85 | 0.75 |
| 1:E:19:LYS:HG3 | 1:E:228:ASN:CB | 2.17 | 0.75 |
| 2:F:7:ILE:HD12 | 2:F:153:LEU:HD21 | 1.68 | 0.75 |
| 2:H:62:VAL:HG21 | 2:H:88:HIS:HE1 | 1.48 | 0.75 |
| 1:A:198:THR:O | 1:A:265:LEU:HD22 | 1.85 | 0.75 |
| 2:B:30:ILE:HD13 | 2:B:61:HIS:CG | 2.20 | 0.75 |
| 2:D:70:LEU:CD1 | 2:D:145:THR:CG2 | 2.64 | 0.75 |
| 2:D:172:TYR:OH | 2:D:387:ALA:HB1 | 1.87 | 0.75 |
| 1:E:198:THR:O | 1:E:265:LEU:HD22 | 1.85 | 0.75 |
| 1:G:19:LYS:HG3 | 1:G:228:ASN:CB | 2.17 | 0.75 |
| 2:H:362:VAL:HG13 | 2:H:368:LEU:HD12 | 1.68 | 0.75 |
| 2:B:221:ARG:O | 2:B:221:ARG:HD3 | 1.85 | 0.75 |
| 2:B:362:VAL:HG13 | 2:B:368:LEU:HD12 | 1.68 | 0.75 |
| 2:D:7:ILE:HD12 | 2:D:153:LEU:HD21 | 1.68 | 0.75 |
| 2:D:331:ALA:O | 2:D:335:ILE:HG12 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:11:GLN:HG3 | 2:B:74:VAL:CG1 | 2.15 | 0.75 |
| 2:B:225:THR:O | 2:B:229:ARG:HG3 | 1.86 | 0.75 |
| 1:C:168:THR:HB | 1:C:201:THR:HG23 | 1.68 | 0.75 |
| 2:D:225:THR:O | 2:D:229:ARG:HG3 | 1.86 | 0.75 |
| 2:F:172:TYR:OH | 2:F:387:ALA:HB1 | 1.87 | 0.75 |
| 2:H:172:TYR:OH | 2:H:387:ALA:HB1 | 1.87 | 0.75 |
| 1:A:6:HIS:HE1 | 1:A:8:GLN:HG2 | 1.52 | 0.75 |
| 2:D:344:VAL:HG11 | 2:D:346:TRP:CE2 | 2.21 | 0.75 |
| 1:G:176:LYS:HE3 | 1:G:207:GLU:HG3 | 1.68 | 0.75 |
| 1:G:259:MET:HG2 | 1:G:314:THR:HG21 | 1.67 | 0.75 |
| 2:B:172:TYR:OH | 2:B:387:ALA:HB1 | 1.87 | 0.75 |
| 2:B:331:ALA:O | 2:B:335:ILE:HG12 | 1.86 | 0.75 |
| 1:C:19:LYS:HG3 | 1:C:228:ASN:CB | 2.17 | 0.75 |
| 1:A:19:LYS:HG3 | 1:A:228:ASN:CB | 2.17 | 0.75 |
| 1:A:168:THR:HB | 1:A:201:THR:HG23 | 1.68 | 0.75 |
| 1:A:217:LEU:C | 1:A:219:LEU:H | 1.91 | 0.75 |
| 2:D:167:LEU:HG | 2:D:200:CYS:HB3 | 1.69 | 0.75 |
| 2:B:425:MET:HE2 | 2:B:428:LEU:HD23 | 1.67 | 0.75 |
| 1:C:217:LEU:C | 1:C:219:LEU:H | 1.91 | 0.75 |
| 2:F:257:THR:CG2 | 1:G:101:ASN:HB3 | 2.16 | 0.75 |
| 2:F:317:LEU:HB3 | 2:F:319:TYR:HE1 | 1.52 | 0.75 |
| 1:A:103:TRP:CZ3 | 1:A:108:TYR:HE1 | 2.05 | 0.74 |
| 1:A:259:MET:HG2 | 1:A:314:THR:HG21 | 1.67 | 0.74 |
| 2:B:163:LYS:O | 2:B:164:LYS:HG2 | 1.86 | 0.74 |
| 2:B:167:LEU:HG | 2:B:200:CYS:HB3 | 1.69 | 0.74 |
| 2:D:317:LEU:HB3 | 2:D:319:TYR:HE1 | 1.52 | 0.74 |
| 1:E:250:ALA:HA | 1:E:254:LYS:HE2 | 1.68 | 0.74 |
| 1:G:2:ARG:NH2 | 2:H:98:ASP:CA | 2.49 | 0.74 |
| 1:A:176:LYS:HE3 | 1:A:207:GLU:HG3 | 1.68 | 0.74 |
| 2:B:317:LEU:HB3 | 2:B:319:TYR:HE1 | 1.52 | 0.74 |
| 2:B:349:THR:CB | 1:C:178:SER:HB2 | 2.17 | 0.74 |
| 2:D:205:ASP:CB | 2:D:303:VAL:HA | 2.17 | 0.74 |
| 2:F:221:ARG:O | 2:F:221:ARG:HD3 | 1.85 | 0.74 |
| 1:G:103:TRP:CZ3 | 1:G:108:TYR:HE1 | 2.05 | 0.74 |
| 2:H:70:LEU:HD11 | 2:H:145:THR:HG23 | 1.70 | 0.74 |
| 1:C:6:HIS:HE1 | 1:C:8:GLN:HG2 | 1.52 | 0.74 |
| 1:C:250:ALA:HA | 1:C:254:LYS:HE2 | 1.68 | 0.74 |
| 1:E:176:LYS:HE3 | 1:E:207:GLU:HG3 | 1.68 | 0.74 |
| 2:F:70:LEU:HD11 | 2:F:145:THR:HG23 | 1.70 | 0.74 |
| 2:F:329:ASN:OD1 | 1:G:210:TYR:HE1 | 1.70 | 0.74 |
| 2:B:7:ILE:HD12 | 2:B:153:LEU:HD21 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:103:TRP:CZ3 | 1:C:108:TYR:HE1 | 2.05 | 0.74 |
| 1:E:168:THR:HB | 1:E:201:THR:HG23 | 1.68 | 0.74 |
| 2:H:317:LEU:HB3 | 2:H:319:TYR:HE1 | 1.52 | 0.74 |
| 1:C:176:LYS:HE3 | 1:C:207:GLU:HG3 | 1.68 | 0.74 |
| 2:D:425:MET:HE2 | 2:D:428:LEU:HD23 | 1.68 | 0.74 |
| 1:E:103:TRP:CZ3 | 1:E:108:TYR:HE1 | 2.05 | 0.74 |
| 1:G:234:THR:CG2 | 1:G:270:PRO:HB2 | 2.11 | 0.74 |
| 2:H:167:LEU:HG | 2:H:200:CYS:HB3 | 1.69 | 0.74 |
| 2:H:221:ARG:O | 2:H:221:ARG:HD3 | 1.85 | 0.74 |
| 1:C:259:MET:HG2 | 1:C:314:THR:HG21 | 1.67 | 0.74 |
| 2:F:167:LEU:HG | 2:F:200:CYS:HB3 | 1.69 | 0.74 |
| 2:F:205:ASP:CB | 2:F:303:VAL:HA | 2.17 | 0.74 |
| 1:G:168:THR:HB | 1:G:201:THR:HG23 | 1.68 | 0.74 |
| 2:H:4:CYS:SG | 2:H:252:LEU:HD11 | 2.27 | 0.74 |
| 2:H:264:ARG:C | 2:H:266:HIS:H | 1.91 | 0.74 |
| 2:B:56:THR:O | 2:F:284:GLU:HB3 | 1.87 | 0.74 |
| 2:B:104:ALA:CB | 2:B:413:MET:HG3 | 2.18 | 0.74 |
| 2:F:264:ARG:C | 2:F:266:HIS:H | 1.91 | 0.74 |
| 1:G:6:HIS:HE1 | 1:G:8:GLN:HG2 | 1.52 | 0.74 |
| 2:H:104:ALA:CB | 2:H:413:MET:HG3 | 2.18 | 0.74 |
| 2:B:205:ASP:CB | 2:B:303:VAL:HA | 2.17 | 0.74 |
| 2:B:264:ARG:C | 2:B:266:HIS:H | 1.91 | 0.74 |
| 1:C:254:LYS:HZ3 | 2:D:101:ASN:HD21 | 1.34 | 0.74 |
| 1:C:257:VAL:HG13 | 2:D:407:TRP:CD1 | 2.22 | 0.74 |
| 2:D:264:ARG:C | 2:D:266:HIS:H | 1.91 | 0.74 |
| 1:E:6:HIS:HE1 | 1:E:8:GLN:HG2 | 1.52 | 0.74 |
| 2:F:234:ILE:HG21 | 2:F:302:MET:HE3 | 1.70 | 0.74 |
| 1:G:8:GLN:CD | 1:G:67:LEU:HD22 | 2.08 | 0.74 |
| 2:D:4:CYS:SG | 2:D:252:LEU:HD11 | 2.27 | 0.74 |
| 2:D:56:THR:CB | 2:H:284:GLU:HG3 | 2.16 | 0.74 |
| 2:F:4:CYS:SG | 2:F:252:LEU:HD11 | 2.27 | 0.74 |
| 2:F:104:ALA:CB | 2:F:413:MET:HG3 | 2.18 | 0.74 |
| 2:H:205:ASP:CB | 2:H:303:VAL:HA | 2.17 | 0.74 |
| 1:A:250:ALA:HA | 1:A:254:LYS:HE2 | 1.68 | 0.74 |
| 2:B:4:CYS:SG | 2:B:252:LEU:HD11 | 2.27 | 0.74 |
| 2:D:70:LEU:HD11 | 2:D:145:THR:HG23 | 1.70 | 0.74 |
| 2:D:104:ALA:CB | 2:D:413:MET:HG3 | 2.18 | 0.74 |
| 1:E:8:GLN:CD | 1:E:67:LEU:HD22 | 2.08 | 0.74 |
| 2:B:62:VAL:CG1 | 2:B:63:PRO:CD | 2.50 | 0.73 |
| 1:A:209:LEU:HG | 1:A:230:LEU:HD22 | 1.69 | 0.73 |
| 1:E:274:PRO:HG2 | 1:E:371:LEU:HD21 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:103:TYR:CD2 | 2:D:189:LEU:HD13 | 2.24 | 0.73 |
| 2:D:172:TYR:C | 2:D:172:TYR:CD1 | 2.61 | 0.73 |
| 2:H:102:ASN:CB | 2:H:407:TRP:CD1 | 2.71 | 0.73 |
| 1:A:8:GLN:CD | 1:A:67:LEU:HD22 | 2.08 | 0.73 |
| 1:A:274:PRO:HG2 | 1:A:371:LEU:HD21 | 1.70 | 0.73 |
| 2:B:242:LEU:HG | 2:B:250:VAL:O | 1.88 | 0.73 |
| 1:E:217:LEU:O | 1:E:219:LEU:N | 2.22 | 0.73 |
| 2:F:172:TYR:C | 2:F:172:TYR:CD1 | 2.61 | 0.73 |
| 1:G:217:LEU:O | 1:G:219:LEU:N | 2.22 | 0.73 |
| 2:H:11:GLN:HG3 | 2:H:74:VAL:CG1 | 2.15 | 0.73 |
| 2:H:172:TYR:C | 2:H:172:TYR:CD1 | 2.61 | 0.73 |
| 2:B:70:LEU:HD11 | 2:B:145:THR:HG23 | 1.70 | 0.73 |
| 2:B:172:TYR:C | 2:B:172:TYR:CD1 | 2.61 | 0.73 |
| 1:C:8:GLN:CD | 1:C:67:LEU:HD22 | 2.07 | 0.73 |
| 2:F:103:TYR:CD2 | 2:F:189:LEU:HD13 | 2.24 | 0.73 |
| 1:G:257:VAL:HG23 | 2:H:407:TRP:HB2 | 0.77 | 0.73 |
| 2:D:242:LEU:HG | 2:D:250:VAL:O | 1.88 | 0.73 |
| 2:F:62:VAL:HG11 | 2:F:88:HIS:ND1 | 2.04 | 0.73 |
| 2:H:103:TYR:CD2 | 2:H:189:LEU:HD13 | 2.24 | 0.73 |
| 2:B:103:TYR:CD2 | 2:B:189:LEU:HD13 | 2.24 | 0.73 |
| 2:D:306:ASP:O | 2:D:308:ARG:N | 2.20 | 0.73 |
| 1:G:2:ARG:NH1 | 2:H:98:ASP:HB3 | 2.04 | 0.73 |
| 2:H:242:LEU:HG | 2:H:250:VAL:O | 1.88 | 0.73 |
| 1:A:76:ASP:HA | 1:A:79:ARG:HG2 | 1.71 | 0.73 |
| 1:A:242:LEU:HD13 | 1:A:250:ALA:C | 2.08 | 0.73 |
| 1:E:76:ASP:HA | 1:E:79:ARG:HG2 | 1.71 | 0.73 |
| 2:F:242:LEU:HG | 2:F:250:VAL:O | 1.88 | 0.73 |
| 1:G:258:ASN:C | 2:H:404:PHE:HE2 | 1.90 | 0.73 |
| 2:B:234:ILE:HG21 | 2:B:302:MET:HE3 | 1.71 | 0.73 |
| 1:C:257:VAL:HA | 2:D:407:TRP:NE1 | 2.04 | 0.73 |
| 1:G:258:ASN:CA | 2:H:404:PHE:CE2 | 2.71 | 0.73 |
| 1:G:274:PRO:HG2 | 1:G:371:LEU:HD21 | 1.70 | 0.73 |
| 2:H:62:VAL:HG11 | 2:H:88:HIS:ND1 | 2.04 | 0.73 |
| 2:B:104:ALA:HB2 | 2:B:413:MET:HG3 | 1.71 | 0.73 |
| 1:C:209:LEU:HG | 1:C:230:LEU:HD22 | 1.69 | 0.73 |
| 1:C:242:LEU:HD13 | 1:C:250:ALA:C | 2.08 | 0.73 |
| 2:D:217:LEU:CD1 | 2:D:277:SER:CB | 2.54 | 0.73 |
| 2:D:234:ILE:HG21 | 2:D:302:MET:HE3 | 1.70 | 0.73 |
| 1:E:209:LEU:HG | 1:E:230:LEU:HD22 | 1.69 | 0.73 |
| 2:F:11:GLN:HG3 | 2:F:74:VAL:CG1 | 2.15 | 0.73 |
| 1:G:76:ASP:HA | 1:G:79:ARG:HG2 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:356:CYS:SG | 1:G:357:ASP:N | 2.62 | 0.73 |
| 2:H:104:ALA:HB2 | 2:H:413:MET:HG3 | 1.71 | 0.73 |
| 1:A:217:LEU:O | 1:A:219:LEU:N | 2.22 | 0.72 |
| 1:C:217:LEU:O | 1:C:219:LEU:N | 2.22 | 0.72 |
| 1:C:274:PRO:HG2 | 1:C:371:LEU:HD21 | 1.70 | 0.72 |
| 1:A:356:CYS:SG | 1:A:357:ASP:N | 2.62 | 0.72 |
| 1:C:88:ARG:CG | 1:G:283:TYR:OH | 2.36 | 0.72 |
| 2:D:105:ARG:O | 2:D:110:ILE:HG22 | 1.89 | 0.72 |
| 1:E:356:CYS:SG | 1:E:357:ASP:N | 2.62 | 0.72 |
| 2:F:112:LYS:O | 2:F:115:ILE:HG22 | 1.89 | 0.72 |
| 2:F:324:VAL:HG11 | 1:G:221:THR:HA | 1.70 | 0.72 |
| 2:H:112:LYS:O | 2:H:115:ILE:HG22 | 1.89 | 0.72 |
| 2:B:105:ARG:O | 2:B:110:ILE:HG22 | 1.89 | 0.72 |
| 1:C:76:ASP:HA | 1:C:79:ARG:HG2 | 1.71 | 0.72 |
| 1:E:191:VAL:CG1 | 1:E:425:MET:HG3 | 2.19 | 0.72 |
| 2:F:337:THR:CG2 | 3:I:99:GLN:OE1 | 2.37 | 0.72 |
| 1:G:209:LEU:HG | 1:G:230:LEU:HD22 | 1.69 | 0.72 |
| 1:A:299:LYS:HD3 | 1:A:299:LYS:N | 2.04 | 0.72 |
| 1:C:70:LEU:HG | 1:C:145:THR:CG2 | 2.20 | 0.72 |
| 1:C:234:THR:CG2 | 1:C:270:PRO:HB2 | 2.11 | 0.72 |
| 2:D:296:PHE:CE2 | 2:D:341:ILE:HD12 | 2.20 | 0.72 |
| 2:F:30:ILE:HD13 | 2:F:61:HIS:CD2 | 2.24 | 0.72 |
| 2:F:104:ALA:HB2 | 2:F:413:MET:HG3 | 1.71 | 0.72 |
| 1:G:111:GLY:O | 1:G:115:VAL:HG23 | 1.89 | 0.72 |
| 1:A:191:VAL:CG1 | 1:A:425:MET:HG3 | 2.19 | 0.72 |
| 1:A:325:MET:HA | 1:A:325:MET:HE3 | 1.70 | 0.72 |
| 1:G:191:VAL:CG1 | 1:G:425:MET:HG3 | 2.19 | 0.72 |
| 1:G:242:LEU:HD13 | 1:G:250:ALA:C | 2.08 | 0.72 |
| 1:A:70:LEU:HG | 1:A:145:THR:CG2 | 2.20 | 0.72 |
| 1:C:299:LYS:HD3 | 1:C:299:LYS:N | 2.04 | 0.72 |
| 2:D:242:LEU:HD21 | 2:D:250:VAL:HB | 1.71 | 0.72 |
| 2:F:263:PRO:HD3 | 1:G:406:HIS:CG | 2.24 | 0.72 |
| 2:B:7:ILE:CG1 | 2:B:137:VAL:HG22 | 2.20 | 0.72 |
| 2:B:166:LYS:HE3 | 2:B:199:ASP:OD1 | 1.90 | 0.72 |
| 2:B:306:ASP:O | 2:B:308:ARG:N | 2.20 | 0.72 |
| 1:C:191:VAL:CG1 | 1:C:425:MET:HG3 | 2.19 | 0.72 |
| 1:E:70:LEU:HG | 1:E:145:THR:CG2 | 2.20 | 0.72 |
| 1:E:243:ARG:NH2 | 1:E:252:LEU:HG | 2.05 | 0.72 |
| 2:F:346:TRP:CZ3 | 1:G:404:PHE:CZ | 2.76 | 0.72 |
| 2:H:306:ASP:O | 2:H:308:ARG:N | 2.20 | 0.72 |
| 1:C:356:CYS:SG | 1:C:357:ASP:N | 2.62 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:7:ILE:CG1 | 2:D:137:VAL:HG22 | 2.20 | 0.72 |
| 2:D:104:ALA:HB2 | 2:D:413:MET:HG3 | 1.71 | 0.72 |
| 2:F:7:ILE:CG1 | 2:F:137:VAL:HG22 | 2.20 | 0.72 |
| 2:F:166:LYS:HE3 | 2:F:199:ASP:OD1 | 1.89 | 0.72 |
| 1:G:217:LEU:C | 1:G:219:LEU:H | 1.91 | 0.72 |
| 1:G:243:ARG:NH2 | 1:G:252:LEU:HG | 2.05 | 0.72 |
| 1:G:258:ASN:O | 2:H:404:PHE:CE2 | 2.35 | 0.72 |
| 2:D:7:ILE:HD11 | 2:D:137:VAL:HG22 | 1.71 | 0.72 |
| 2:F:261:PRO:HA | 1:G:404:PHE:CE2 | 2.15 | 0.72 |
| 2:F:306:ASP:O | 2:F:308:ARG:N | 2.20 | 0.72 |
| 2:H:7:ILE:CG1 | 2:H:137:VAL:HG22 | 2.20 | 0.72 |
| 2:D:62:VAL:HG11 | 2:D:88:HIS:ND1 | 2.05 | 0.72 |
| 1:E:111:GLY:O | 1:E:115:VAL:HG23 | 1.89 | 0.72 |
| 1:G:70:LEU:HG | 1:G:145:THR:CG2 | 2.20 | 0.72 |
| 2:H:166:LYS:HE3 | 2:H:199:ASP:OD1 | 1.90 | 0.72 |
| 2:H:296:PHE:CE2 | 2:H:341:ILE:HD12 | 2.20 | 0.72 |
| 3:I:55:VAL:HG21 | 3:I:57:PHE:CE1 | 2.25 | 0.72 |
| 3:I:57:PHE:CE2 | 3:I:87:LEU:HD11 | 2.25 | 0.72 |
| 2:B:296:PHE:CE2 | 2:B:341:ILE:HD12 | 2.20 | 0.71 |
| 2:F:7:ILE:HD11 | 2:F:137:VAL:HG22 | 1.71 | 0.71 |
| 1:A:111:GLY:O | 1:A:115:VAL:HG23 | 1.89 | 0.71 |
| 1:C:111:GLY:O | 1:C:115:VAL:HG23 | 1.89 | 0.71 |
| 2:D:166:LYS:HE3 | 2:D:199:ASP:OD1 | 1.90 | 0.71 |
| 1:G:48:ARG:HG2 | 1:G:243:ARG:O | 1.90 | 0.71 |
| 1:A:201:THR:OG1 | 1:A:265:LEU:HD11 | 1.90 | 0.71 |
| 1:C:201:THR:OG1 | 1:C:265:LEU:HD11 | 1.90 | 0.71 |
| 1:E:217:LEU:C | 1:E:219:LEU:H | 1.91 | 0.71 |
| 1:E:242:LEU:HD13 | 1:E:250:ALA:C | 2.08 | 0.71 |
| 1:G:325:MET:HA | 1:G:325:MET:HE3 | 1.71 | 0.71 |
| 2:H:11:GLN:HE21 | 2:H:74:VAL:CG2 | 2.03 | 0.71 |
| 2:B:112:LYS:O | 2:B:115:ILE:HG22 | 1.89 | 0.71 |
| 2:B:242:LEU:HD21 | 2:B:250:VAL:HB | 1.71 | 0.71 |
| 2:D:112:LYS:O | 2:D:115:ILE:HG22 | 1.89 | 0.71 |
| 2:F:105:ARG:O | 2:F:110:ILE:HG22 | 1.89 | 0.71 |
| 2:H:105:ARG:O | 2:H:110:ILE:HG22 | 1.89 | 0.71 |
| 1:A:291:LEU:O | 1:A:295:MET:HG3 | 1.91 | 0.71 |
| 1:C:431:GLU:OE1 | 1:C:432:TYR:HA | 1.91 | 0.71 |
| 1:E:48:ARG:HG2 | 1:E:243:ARG:O | 1.90 | 0.71 |
| 2:H:7:ILE:HD11 | 2:H:137:VAL:HG22 | 1.71 | 0.71 |
| 1:A:431:GLU:OE1 | 1:A:432:TYR:HA | 1.91 | 0.71 |
| 2:B:7:ILE:HD11 | 2:B:137:VAL:HG22 | 1.71 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:88:ARG:HG3 | 1:G:283:TYR:OH | 1.90 | 0.71 |
| 1:E:10:GLY:O | 1:E:14:ASN:HB2 | 1.90 | 0.71 |
| 1:E:431:GLU:OE1 | 1:E:432:TYR:HA | 1.91 | 0.71 |
| 2:F:11:GLN:HE21 | 2:F:74:VAL:CG2 | 2.03 | 0.71 |
| 2:F:326:LYS:HB3 | 1:G:222:PRO:HD2 | 1.72 | 0.71 |
| 1:G:291:LEU:O | 1:G:295:MET:HG3 | 1.91 | 0.71 |
| 1:A:56:ALA:HB1 | 1:E:283:TYR:CE2 | 2.25 | 0.71 |
| 2:B:11:GLN:HE21 | 2:B:74:VAL:CG2 | 2.03 | 0.71 |
| 1:C:8:GLN:NE2 | 1:C:17:GLY:HA3 | 2.06 | 0.71 |
| 1:C:291:LEU:O | 1:C:295:MET:HG3 | 1.91 | 0.71 |
| 2:D:11:GLN:HE21 | 2:D:74:VAL:CG2 | 2.03 | 0.71 |
| 1:E:291:LEU:O | 1:E:295:MET:HG3 | 1.91 | 0.71 |
| 2:F:259:LEU:HD11 | 2:F:378:LEU:CD1 | 2.20 | 0.71 |
| 1:G:431:GLU:OE1 | 1:G:432:TYR:HA | 1.91 | 0.71 |
| 1:A:8:GLN:NE2 | 1:A:17:GLY:HA3 | 2.06 | 0.71 |
| 1:C:245:PRO:HA | 2:D:73:THR:CG2 | 2.21 | 0.71 |
| 1:E:237:GLY:O | 1:E:241:CYS:HB3 | 1.90 | 0.71 |
| 2:F:242:LEU:HD21 | 2:F:250:VAL:HB | 1.71 | 0.71 |
| 1:G:10:GLY:O | 1:G:14:ASN:HB2 | 1.90 | 0.71 |
| 1:G:258:ASN:HA | 2:H:404:PHE:HD2 | 1.52 | 0.71 |
| 2:H:242:LEU:HD21 | 2:H:250:VAL:HB | 1.71 | 0.71 |
| 2:H:259:LEU:HD11 | 2:H:378:LEU:CD1 | 2.20 | 0.71 |
| 2:B:259:LEU:HD11 | 2:B:378:LEU:CD1 | 2.20 | 0.71 |
| 2:D:259:LEU:HD11 | 2:D:378:LEU:CD1 | 2.20 | 0.71 |
| 2:F:12:ALA:HB3 | 2:F:140:SER:OG | 1.91 | 0.71 |
| 2:F:217:LEU:CD1 | 2:F:277:SER:CB | 2.54 | 0.71 |
| 2:F:296:PHE:CE2 | 2:F:341:ILE:HD12 | 2.20 | 0.71 |
| 2:F:317:LEU:HD12 | 2:F:351:PHE:HD2 | 1.56 | 0.71 |
| 2:H:12:ALA:HB3 | 2:H:140:SER:OG | 1.91 | 0.71 |
| 2:H:317:LEU:HD12 | 2:H:351:PHE:HD2 | 1.56 | 0.71 |
| 1:A:10:GLY:O | 1:A:14:ASN:HB2 | 1.90 | 0.71 |
| 1:A:175:PRO:HD2 | 1:A:207:GLU:OE2 | 1.91 | 0.71 |
| 1:C:237:GLY:O | 1:C:241:CYS:HB3 | 1.90 | 0.71 |
| 2:D:56:THR:C | 2:H:284:GLU:HB3 | 2.11 | 0.71 |
| 1:G:175:PRO:HD2 | 1:G:207:GLU:OE2 | 1.91 | 0.71 |
| 1:A:48:ARG:HG2 | 1:A:243:ARG:O | 1.90 | 0.70 |
| 1:A:243:ARG:NH2 | 1:A:252:LEU:HG | 2.05 | 0.70 |
| 2:B:343:PHE:CZ | 2:B:351:PHE:HE1 | 2.08 | 0.70 |
| 2:F:148:GLY:O | 2:F:151:SER:HB2 | 1.90 | 0.70 |
| 1:C:48:ARG:HG2 | 1:C:243:ARG:O | 1.90 | 0.70 |
| 1:E:175:PRO:HD2 | 1:E:207:GLU:OE2 | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:148:GLY:O | 2:H:151:SER:HB2 | 1.91 | 0.70 |
| 2:H:217:LEU:CD1 | 2:H:277:SER:CB | 2.54 | 0.70 |
| 2:B:312:TYR:O | 2:B:344:VAL:HG23 | 1.90 | 0.70 |
| 2:D:30:ILE:HD13 | 2:D:61:HIS:CD2 | 2.27 | 0.70 |
| 2:D:312:TYR:O | 2:D:344:VAL:HG23 | 1.90 | 0.70 |
| 1:A:237:GLY:O | 1:A:241:CYS:HB3 | 1.90 | 0.70 |
| 2:B:5:ILE:CD1 | 2:B:64:ARG:NH1 | 2.38 | 0.70 |
| 2:D:148:GLY:O | 2:D:151:SER:HB2 | 1.91 | 0.70 |
| 2:D:343:PHE:CZ | 2:D:351:PHE:HE1 | 2.08 | 0.70 |
| 1:G:237:GLY:O | 1:G:241:CYS:HB3 | 1.90 | 0.70 |
| 1:G:352:LYS:CB | 2:H:181:VAL:CG2 | 2.69 | 0.70 |
| 2:H:67:PHE:CD1 | 2:H:92:LEU:HD23 | 2.26 | 0.70 |
| 3:I:107:ILE:HD13 | 3:I:124:SER:HB3 | 1.73 | 0.70 |
| 1:C:325:MET:HE3 | 1:C:325:MET:HA | 1.71 | 0.70 |
| 1:E:8:GLN:NE2 | 1:E:17:GLY:HA3 | 2.06 | 0.70 |
| 1:E:201:THR:OG1 | 1:E:265:LEU:HD11 | 1.90 | 0.70 |
| 2:F:312:TYR:O | 2:F:344:VAL:HG23 | 1.90 | 0.70 |
| 1:G:8:GLN:NE2 | 1:G:17:GLY:HA3 | 2.06 | 0.70 |
| 1:C:175:PRO:HD2 | 1:C:207:GLU:OE2 | 1.91 | 0.70 |
| 1:C:243:ARG:NH2 | 1:C:252:LEU:HG | 2.05 | 0.70 |
| 2:F:51:THR:O | 2:F:52:PHE:CD1 | 2.44 | 0.70 |
| 2:F:67:PHE:CD1 | 2:F:92:LEU:HD23 | 2.26 | 0.70 |
| 1:G:179:ASP:HB2 | 4:G:600:GDP:C3' | 2.21 | 0.70 |
| 1:G:234:THR:O | 1:G:238:VAL:HG23 | 1.92 | 0.70 |
| 2:H:51:THR:O | 2:H:52:PHE:CD1 | 2.44 | 0.70 |
| 2:H:312:TYR:O | 2:H:344:VAL:HG23 | 1.90 | 0.70 |
| 2:B:199:ASP:HB3 | 2:B:256:GLN:HE21 | 1.57 | 0.70 |
| 2:D:317:LEU:HD12 | 2:D:351:PHE:HD2 | 1.55 | 0.70 |
| 1:E:234:THR:O | 1:E:238:VAL:HG23 | 1.92 | 0.70 |
| 1:G:306:ASP:OD2 | 3:I:95:ILE:HD13 | 1.91 | 0.70 |
| 1:C:10:GLY:O | 1:C:14:ASN:HB2 | 1.90 | 0.70 |
| 2:D:12:ALA:HB3 | 2:D:140:SER:OG | 1.91 | 0.70 |
| 2:D:67:PHE:CD1 | 2:D:92:LEU:HD23 | 2.26 | 0.70 |
| 2:D:51:THR:O | 2:D:52:PHE:CD1 | 2.45 | 0.70 |
| 2:F:343:PHE:CZ | 2:F:351:PHE:HE1 | 2.08 | 0.70 |
| 2:H:381:THR:C | 2:H:383:ALA:H | 1.95 | 0.70 |
| 1:A:234:THR:O | 1:A:238:VAL:HG23 | 1.92 | 0.70 |
| 2:B:67:PHE:CD1 | 2:B:92:LEU:HD23 | 2.26 | 0.70 |
| 2:B:217:LEU:CD1 | 2:B:277:SER:CB | 2.55 | 0.70 |
| 2:B:371:VAL:HG12 | 2:B:372:GLN:H | 1.57 | 0.70 |
| 2:D:199:ASP:HB3 | 2:D:256:GLN:HE21 | 1.57 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:371:VAL:HG12 | 2:D:372:GLN:H | 1.57 | 0.70 |
| 2:F:237:SER:CB | 2:F:376:CYS:SG | 2.80 | 0.70 |
| 2:H:237:SER:CB | 2:H:376:CYS:SG | 2.80 | 0.70 |
| 2:B:5:ILE:HG22 | 2:B:6:SER:N | 2.07 | 0.69 |
| 2:B:12:ALA:HB3 | 2:B:140:SER:OG | 1.91 | 0.69 |
| 2:B:148:GLY:O | 2:B:151:SER:HB2 | 1.91 | 0.69 |
| 2:D:237:SER:CB | 2:D:376:CYS:SG | 2.80 | 0.69 |
| 1:G:201:THR:OG1 | 1:G:265:LEU:HD11 | 1.90 | 0.69 |
| 2:B:317:LEU:HD12 | 2:B:351:PHE:HD2 | 1.55 | 0.69 |
| 1:C:255:LEU:O | 1:C:259:MET:HG3 | 1.91 | 0.69 |
| 2:D:244:PHE:HD2 | 2:D:245:ASP:N | 1.89 | 0.69 |
| 1:G:255:LEU:O | 1:G:259:MET:HG3 | 1.91 | 0.69 |
| 1:A:255:LEU:O | 1:A:259:MET:HG3 | 1.91 | 0.69 |
| 1:C:70:LEU:HG | 1:C:145:THR:HG23 | 1.74 | 0.69 |
| 1:E:180:THR:HG22 | 1:E:181:VAL:N | 2.07 | 0.69 |
| 2:F:349:THR:CG2 | 1:G:178:SER:O | 2.40 | 0.69 |
| 2:F:381:THR:C | 2:F:383:ALA:H | 1.95 | 0.69 |
| 2:B:243:ARG:NH2 | 2:B:252:LEU:N | 2.29 | 0.69 |
| 2:F:244:PHE:HD2 | 2:F:245:ASP:N | 1.89 | 0.69 |
| 1:A:70:LEU:HG | 1:A:145:THR:HG23 | 1.74 | 0.69 |
| 2:H:244:PHE:HD2 | 2:H:245:ASP:N | 1.89 | 0.69 |
| 1:A:180:THR:HG22 | 1:A:181:VAL:N | 2.07 | 0.69 |
| 1:A:260:VAL:HG23 | 2:B:407:TRP:HE1 | 1.57 | 0.69 |
| 2:B:237:SER:CB | 2:B:376:CYS:SG | 2.80 | 0.69 |
| 1:C:24:ILE:HD11 | 1:C:52:TYR:CE1 | 2.28 | 0.69 |
| 1:C:234:THR:O | 1:C:238:VAL:HG23 | 1.92 | 0.69 |
| 2:D:56:THR:CA | 2:H:284:GLU:HG3 | 2.22 | 0.69 |
| 1:A:24:ILE:HD11 | 1:A:52:TYR:CE1 | 2.28 | 0.69 |
| 2:B:115:ILE:CD1 | 2:B:119:LEU:HG | 2.23 | 0.69 |
| 2:B:205:ASP:HB3 | 2:B:303:VAL:HA | 1.73 | 0.69 |
| 2:B:333:ALA:CA | 1:C:177:VAL:HG21 | 2.23 | 0.69 |
| 1:C:180:THR:HG22 | 1:C:181:VAL:N | 2.07 | 0.69 |
| 1:E:255:LEU:O | 1:E:259:MET:HG3 | 1.91 | 0.69 |
| 2:F:205:ASP:HB3 | 2:F:303:VAL:HA | 1.73 | 0.69 |
| 2:F:261:PRO:CG | 1:G:404:PHE:CE2 | 2.69 | 0.69 |
| 1:G:180:THR:HG22 | 1:G:181:VAL:N | 2.07 | 0.69 |
| 1:G:253:ARG:CG | 2:H:407:TRP:HH2 | 2.06 | 0.69 |
| 2:H:205:ASP:HB3 | 2:H:303:VAL:HA | 1.73 | 0.69 |
| 2:H:343:PHE:CZ | 2:H:351:PHE:HE1 | 2.08 | 0.69 |
| 2:H:343:PHE:HZ | 2:H:351:PHE:CE1 | 2.10 | 0.69 |
| 2:H:371:VAL:HG12 | 2:H:372:GLN:H | 1.57 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:359:PRO:HB2 | 1:A:360:PRO:HD2 | 1.74 | 0.69 |
| 2:B:244:PHE:HD2 | 2:B:245:ASP:N | 1.90 | 0.69 |
| 2:B:343:PHE:HZ | 2:B:351:PHE:CE1 | 2.10 | 0.69 |
| 2:D:205:ASP:HB3 | 2:D:303:VAL:HA | 1.73 | 0.69 |
| 1:E:24:ILE:HD11 | 1:E:52:TYR:CE1 | 2.28 | 0.69 |
| 1:E:257:VAL:O | 1:E:257:VAL:HG12 | 1.93 | 0.69 |
| 2:F:343:PHE:HZ | 2:F:351:PHE:CE1 | 2.10 | 0.69 |
| 2:H:276:ILE:O | 2:H:369:ALA:N | 2.25 | 0.69 |
| 2:D:115:ILE:CD1 | 2:D:119:LEU:HG | 2.23 | 0.69 |
| 1:E:70:LEU:HG | 1:E:145:THR:HG23 | 1.74 | 0.69 |
| 1:E:242:LEU:CD2 | 1:E:250:ALA:H | 2.06 | 0.68 |
| 2:F:115:ILE:CD1 | 2:F:119:LEU:HG | 2.23 | 0.68 |
| 2:F:276:ILE:O | 2:F:369:ALA:N | 2.25 | 0.68 |
| 2:F:371:VAL:HG12 | 2:F:372:GLN:H | 1.57 | 0.68 |
| 1:G:242:LEU:CD2 | 1:G:250:ALA:H | 2.07 | 0.68 |
| 1:A:242:LEU:CD2 | 1:A:250:ALA:H | 2.06 | 0.68 |
| 1:C:242:LEU:CD2 | 1:C:250:ALA:H | 2.06 | 0.68 |
| 1:E:251:ASP:O | 1:E:253:ARG:N | 2.26 | 0.68 |
| 1:E:325:MET:HA | 1:E:325:MET:HE3 | 1.75 | 0.68 |
| 1:G:24:ILE:HD11 | 1:G:52:TYR:CE1 | 2.28 | 0.68 |
| 2:B:141:PHE:O | 2:B:147:SER:HB3 | 1.94 | 0.68 |
| 2:D:343:PHE:HZ | 2:D:351:PHE:CE1 | 2.10 | 0.68 |
| 1:G:209:LEU:HD23 | 1:G:227:LEU:HB3 | 1.75 | 0.68 |
| 1:G:243:ARG:HH22 | 1:G:252:LEU:HG | 1.59 | 0.68 |
| 1:G:251:ASP:O | 1:G:253:ARG:N | 2.26 | 0.68 |
| 2:H:115:ILE:CD1 | 2:H:119:LEU:HG | 2.23 | 0.68 |
| 1:A:256:ALA:O | 1:A:260:VAL:HG22 | 1.94 | 0.68 |
| 2:B:349:THR:HB | 1:C:178:SER:HB2 | 1.75 | 0.68 |
| 2:B:381:THR:C | 2:B:383:ALA:H | 1.95 | 0.68 |
| 2:D:102:ASN:HB2 | 2:D:408:TYR:CE2 | 2.29 | 0.68 |
| 1:E:243:ARG:HH22 | 1:E:252:LEU:HG | 1.59 | 0.68 |
| 1:E:250:ALA:HB1 | 1:E:254:LYS:HB2 | 1.75 | 0.68 |
| 1:E:256:ALA:O | 1:E:260:VAL:HG22 | 1.94 | 0.68 |
| 2:F:217:LEU:HD12 | 2:F:277:SER:CA | 2.23 | 0.68 |
| 2:B:102:ASN:HB2 | 2:B:408:TYR:CE2 | 2.29 | 0.68 |
| 2:D:221:ARG:N | 2:D:222:PRO:HD3 | 2.09 | 0.68 |
| 1:E:209:LEU:HD23 | 1:E:227:LEU:HB3 | 1.75 | 0.68 |
| 1:G:70:LEU:HG | 1:G:145:THR:HG23 | 1.74 | 0.68 |
| 1:G:256:ALA:O | 1:G:260:VAL:HG22 | 1.94 | 0.68 |
| 2:H:141:PHE:O | 2:H:147:SER:HB3 | 1.94 | 0.68 |
| 2:H:217:LEU:HD12 | 2:H:277:SER:CA | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:250:ALA:HB1 | 1:A:254:LYS:HB2 | 1.75 | 0.68 |
| 2:D:141:PHE:O | 2:D:147:SER:HB3 | 1.94 | 0.68 |
| 1:A:257:VAL:O | 1:A:257:VAL:HG12 | 1.93 | 0.68 |
| 2:D:293:ASN:HD21 | 2:D:338:LYS:HZ1 | 1.41 | 0.68 |
| 2:D:381:THR:C | 2:D:383:ALA:H | 1.95 | 0.68 |
| 2:F:141:PHE:O | 2:F:147:SER:HB3 | 1.94 | 0.68 |
| 2:F:348:PRO:HD3 | 1:G:398:MET:HE3 | 1.75 | 0.68 |
| 1:G:2:ARG:NH2 | 2:H:98:ASP:HA | 2.09 | 0.68 |
| 1:G:325:MET:CE | 1:G:355:VAL:HG21 | 2.24 | 0.68 |
| 1:A:251:ASP:O | 1:A:253:ARG:N | 2.26 | 0.68 |
| 1:A:325:MET:CE | 1:A:355:VAL:HG21 | 2.24 | 0.68 |
| 1:E:44:LEU:HD12 | 1:E:49:ILE:HD13 | 1.76 | 0.68 |
| 1:E:325:MET:CE | 1:E:355:VAL:HG21 | 2.24 | 0.68 |
| 1:A:209:LEU:HD23 | 1:A:227:LEU:HB3 | 1.75 | 0.68 |
| 2:B:70:LEU:HD12 | 2:B:145:THR:CG2 | 2.24 | 0.68 |
| 1:C:256:ALA:O | 1:C:260:VAL:HG22 | 1.94 | 0.68 |
| 1:C:359:PRO:HB2 | 1:C:360:PRO:HD2 | 1.74 | 0.68 |
| 1:E:267:PHE:CD1 | 1:E:267:PHE:N | 2.62 | 0.68 |
| 1:E:359:PRO:HB2 | 1:E:360:PRO:HD2 | 1.74 | 0.68 |
| 2:F:261:PRO:HG3 | 1:G:404:PHE:CE2 | 2.23 | 0.68 |
| 2:F:284:GLU:O | 2:F:284:GLU:HG2 | 1.93 | 0.68 |
| 1:G:359:PRO:HB2 | 1:G:360:PRO:HD2 | 1.74 | 0.68 |
| 2:H:102:ASN:HB2 | 2:H:408:TYR:CE2 | 2.29 | 0.68 |
| 2:B:133:GLN:HG2 | 2:B:243:ARG:HH22 | 1.57 | 0.68 |
| 2:B:221:ARG:N | 2:B:222:PRO:HD3 | 2.09 | 0.68 |
| 1:C:209:LEU:HD23 | 1:C:227:LEU:HB3 | 1.75 | 0.68 |
| 1:C:257:VAL:O | 1:C:257:VAL:HG12 | 1.93 | 0.68 |
| 2:F:102:ASN:HB2 | 2:F:408:TYR:CE2 | 2.29 | 0.68 |
| 1:G:44:LEU:HD12 | 1:G:49:ILE:HD13 | 1.76 | 0.68 |
| 1:G:267:PHE:N | 1:G:267:PHE:CD1 | 2.62 | 0.68 |
| 2:H:70:LEU:HD12 | 2:H:145:THR:CG2 | 2.24 | 0.68 |
| 2:B:49:PHE:CE1 | 2:B:61:HIS:HE1 | 2.12 | 0.67 |
| 2:B:296:PHE:CE1 | 2:B:335:ILE:CG2 | 2.73 | 0.67 |
| 1:C:251:ASP:O | 1:C:253:ARG:N | 2.26 | 0.67 |
| 1:C:325:MET:CE | 1:C:355:VAL:HG21 | 2.24 | 0.67 |
| 2:D:56:THR:C | 2:H:284:GLU:HB2 | 2.14 | 0.67 |
| 2:D:70:LEU:HD12 | 2:D:145:THR:CG2 | 2.24 | 0.67 |
| 2:D:133:GLN:HG2 | 2:D:243:ARG:HH22 | 1.57 | 0.67 |
| 2:D:276:ILE:O | 2:D:369:ALA:N | 2.25 | 0.67 |
| 2:F:3:GLU:HG2 | 2:F:51:THR:C | 2.14 | 0.67 |
| 1:G:107:HIS:CD2 | 1:G:151:THR:CG2 | 2.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:284:GLU:HG2 | 2:H:284:GLU:O | 1.93 | 0.67 |
| 3:I:97:LEU:HD22 | 3:I:100:GLY:O | 1.94 | 0.67 |
| 1:A:267:PHE:N | 1:A:267:PHE:CD1 | 2.62 | 0.67 |
| 1:C:250:ALA:HB1 | 1:C:254:LYS:HB2 | 1.75 | 0.67 |
| 1:C:328:VAL:O | 1:C:332:MET:HG2 | 1.94 | 0.67 |
| 2:D:152:LEU:HA | 2:D:155:GLU:HB2 | 1.77 | 0.67 |
| 2:D:243:ARG:NH2 | 2:D:252:LEU:N | 2.29 | 0.67 |
| 2:F:70:LEU:HD12 | 2:F:145:THR:CG2 | 2.24 | 0.67 |
| 2:F:133:GLN:HG2 | 2:F:243:ARG:HH22 | 1.57 | 0.67 |
| 2:F:152:LEU:HA | 2:F:155:GLU:HB2 | 1.77 | 0.67 |
| 2:H:7:ILE:HD12 | 2:H:153:LEU:CD2 | 2.24 | 0.67 |
| 2:H:133:GLN:HG2 | 2:H:243:ARG:HH22 | 1.57 | 0.67 |
| 1:E:107:HIS:CD2 | 1:E:151:THR:CG2 | 2.77 | 0.67 |
| 2:F:251:ASP:O | 2:F:254:GLU:HB2 | 1.94 | 0.67 |
| 1:G:258:ASN:CA | 2:H:404:PHE:CD2 | 2.70 | 0.67 |
| 2:H:152:LEU:HA | 2:H:155:GLU:HB2 | 1.77 | 0.67 |
| 3:I:84:LEU:HD13 | 3:I:102:ARG:O | 1.93 | 0.67 |
| 1:A:4:ILE:HG21 | 1:A:136:GLN:HG2 | 1.76 | 0.67 |
| 2:B:276:ILE:O | 2:B:369:ALA:N | 2.25 | 0.67 |
| 2:F:7:ILE:HD12 | 2:F:153:LEU:CD2 | 2.24 | 0.67 |
| 2:H:221:ARG:N | 2:H:222:PRO:HD3 | 2.09 | 0.67 |
| 2:B:175:PRO:HG3 | 2:B:304:LYS:HG2 | 1.76 | 0.67 |
| 1:C:310:GLY:HA3 | 1:C:436:GLN:HE21 | 1.59 | 0.67 |
| 2:D:3:GLU:HG2 | 2:D:51:THR:C | 2.15 | 0.67 |
| 2:H:3:GLU:HG2 | 2:H:51:THR:C | 2.14 | 0.67 |
| 2:H:95:GLY:O | 2:H:97:GLU:N | 2.27 | 0.67 |
| 2:H:251:ASP:O | 2:H:254:GLU:HB2 | 1.94 | 0.67 |
| 3:I:97:LEU:HD13 | 3:I:100:GLY:O | 1.94 | 0.67 |
| 1:A:328:VAL:O | 1:A:332:MET:HG2 | 1.94 | 0.67 |
| 2:B:3:GLU:HG2 | 2:B:51:THR:C | 2.15 | 0.67 |
| 2:B:251:ASP:O | 2:B:254:GLU:HB2 | 1.94 | 0.67 |
| 2:B:348:PRO:HD2 | 1:C:398:MET:HE2 | 1.76 | 0.67 |
| 1:C:44:LEU:HD12 | 1:C:49:ILE:HD13 | 1.76 | 0.67 |
| 2:D:7:ILE:HD12 | 2:D:153:LEU:CD2 | 2.24 | 0.67 |
| 1:E:4:ILE:HG21 | 1:E:136:GLN:HG2 | 1.76 | 0.67 |
| 1:E:66:ILE:C | 1:E:67:LEU:HD23 | 2.15 | 0.67 |
| 2:F:221:ARG:N | 2:F:222:PRO:HD3 | 2.09 | 0.67 |
| 2:F:326:LYS:HB2 | 1:G:222:PRO:HG2 | 0.71 | 0.67 |
| 1:G:4:ILE:HG21 | 1:G:136:GLN:HG2 | 1.76 | 0.67 |
| 1:A:107:HIS:CD2 | 1:A:151:THR:CG2 | 2.77 | 0.67 |
| 1:A:230:LEU:HD23 | 1:A:231:VAL:N | 2.10 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:95:GLY:O | 2:F:97:GLU:N | 2.27 | 0.67 |
| 1:G:66:ILE:C | 1:G:67:LEU:HD23 | 2.15 | 0.67 |
| 1:G:328:VAL:O | 1:G:332:MET:HG2 | 1.95 | 0.67 |
| 1:A:66:ILE:C | 1:A:67:LEU:HD23 | 2.15 | 0.67 |
| 2:B:7:ILE:HD12 | 2:B:153:LEU:CD2 | 2.24 | 0.67 |
| 2:B:152:LEU:HA | 2:B:155:GLU:HB2 | 1.77 | 0.67 |
| 2:B:333:ALA:CA | 1:C:177:VAL:CG2 | 2.73 | 0.67 |
| 1:C:230:LEU:HD23 | 1:C:231:VAL:N | 2.10 | 0.67 |
| 1:E:328:VAL:O | 1:E:332:MET:HG2 | 1.95 | 0.67 |
| 2:H:199:ASP:HB3 | 2:H:256:GLN:HE21 | 1.57 | 0.67 |
| 1:A:44:LEU:HD12 | 1:A:49:ILE:HD13 | 1.76 | 0.67 |
| 1:A:310:GLY:HA3 | 1:A:436:GLN:HE21 | 1.59 | 0.67 |
| 1:C:4:ILE:HG21 | 1:C:136:GLN:HG2 | 1.76 | 0.67 |
| 2:D:251:ASP:O | 2:D:254:GLU:HB2 | 1.94 | 0.67 |
| 2:F:175:PRO:HG3 | 2:F:304:LYS:HG2 | 1.76 | 0.67 |
| 1:G:204:ILE:HD13 | 1:G:231:VAL:HG22 | 1.76 | 0.67 |
| 1:G:260:VAL:HG23 | 2:H:406:HIS:CE1 | 2.29 | 0.67 |
| 2:H:22:GLU:HG3 | 2:H:83:TYR:OH | 1.95 | 0.67 |
| 2:D:95:GLY:O | 2:D:97:GLU:N | 2.27 | 0.67 |
| 2:F:199:ASP:HB3 | 2:F:256:GLN:HE21 | 1.57 | 0.67 |
| 2:F:243:ARG:NH2 | 2:F:252:LEU:N | 2.29 | 0.67 |
| 2:B:95:GLY:O | 2:B:97:GLU:N | 2.27 | 0.66 |
| 2:B:348:PRO:CG | 1:C:398:MET:CE | 2.67 | 0.66 |
| 1:C:242:LEU:CD1 | 1:C:255:LEU:HD11 | 2.25 | 0.66 |
| 2:D:175:PRO:HG3 | 2:D:304:LYS:HG2 | 1.76 | 0.66 |
| 1:E:204:ILE:HD13 | 1:E:231:VAL:HG22 | 1.76 | 0.66 |
| 2:F:22:GLU:HG3 | 2:F:83:TYR:OH | 1.95 | 0.66 |
| 2:F:293:ASN:HD21 | 2:F:338:LYS:HZ1 | 1.43 | 0.66 |
| 2:H:172:TYR:HD1 | 2:H:173:PRO:N | 1.93 | 0.66 |
| 2:H:175:PRO:HG3 | 2:H:304:LYS:HG2 | 1.76 | 0.66 |
| 2:H:341:ILE:O | 2:H:341:ILE:HG12 | 1.95 | 0.66 |
| 1:C:107:HIS:CD2 | 1:C:151:THR:CG2 | 2.77 | 0.66 |
| 1:C:265:LEU:HD12 | 1:C:265:LEU:C | 2.16 | 0.66 |
| 2:F:341:ILE:O | 2:F:341:ILE:HG12 | 1.95 | 0.66 |
| 1:A:243:ARG:HH22 | 1:A:252:LEU:HG | 1.59 | 0.66 |
| 2:B:172:TYR:HD1 | 2:B:173:PRO:N | 1.93 | 0.66 |
| 1:C:204:ILE:HD13 | 1:C:231:VAL:HG22 | 1.76 | 0.66 |
| 2:D:22:GLU:HG3 | 2:D:83:TYR:OH | 1.95 | 0.66 |
| 1:E:230:LEU:HD23 | 1:E:231:VAL:N | 2.10 | 0.66 |
| 2:F:172:TYR:HD1 | 2:F:173:PRO:N | 1.93 | 0.66 |
| 1:A:242:LEU:CD1 | 1:A:255:LEU:HD11 | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:265:LEU:HD12 | 1:A:265:LEU:C | 2.16 | 0.66 |
| 2:B:67:PHE:CD1 | 2:B:92:LEU:CD2 | 2.79 | 0.66 |
| 2:B:100:ALA:CB | 2:B:105:ARG:HD3 | 2.26 | 0.66 |
| 2:D:172:TYR:HD1 | 2:D:173:PRO:N | 1.93 | 0.66 |
| 2:F:67:PHE:CD1 | 2:F:92:LEU:CD2 | 2.79 | 0.66 |
| 1:G:230:LEU:HD23 | 1:G:231:VAL:N | 2.10 | 0.66 |
| 1:G:265:LEU:HD12 | 1:G:265:LEU:C | 2.16 | 0.66 |
| 1:G:310:GLY:HA3 | 1:G:436:GLN:HE21 | 1.59 | 0.66 |
| 2:H:100:ALA:CB | 2:H:105:ARG:HD3 | 2.26 | 0.66 |
| 1:A:204:ILE:HD13 | 1:A:231:VAL:HG22 | 1.76 | 0.66 |
| 1:C:242:LEU:HD12 | 1:C:255:LEU:HD11 | 1.77 | 0.66 |
| 2:D:67:PHE:CD1 | 2:D:92:LEU:CD2 | 2.79 | 0.66 |
| 2:D:68:VAL:HG11 | 2:D:149:PHE:CZ | 2.30 | 0.66 |
| 1:E:310:GLY:HA3 | 1:E:436:GLN:HE21 | 1.59 | 0.66 |
| 2:F:100:ALA:CB | 2:F:105:ARG:HD3 | 2.26 | 0.66 |
| 1:G:242:LEU:CD1 | 1:G:255:LEU:HD11 | 2.25 | 0.66 |
| 1:G:352:LYS:CA | 2:H:181:VAL:CG2 | 2.73 | 0.66 |
| 1:G:413:MET:HG2 | 1:G:418:PHE:HE1 | 1.61 | 0.66 |
| 2:H:67:PHE:CD1 | 2:H:92:LEU:CD2 | 2.79 | 0.66 |
| 1:C:66:ILE:C | 1:C:67:LEU:HD23 | 2.15 | 0.66 |
| 1:E:413:MET:HG2 | 1:E:418:PHE:HE1 | 1.61 | 0.66 |
| 2:F:68:VAL:HG11 | 2:F:149:PHE:CZ | 2.30 | 0.66 |
| 2:H:68:VAL:HG11 | 2:H:149:PHE:CZ | 2.30 | 0.66 |
| 1:A:413:MET:HG2 | 1:A:418:PHE:HE1 | 1.61 | 0.66 |
| 2:B:313:MET:HB3 | 2:B:344:VAL:CG2 | 2.26 | 0.66 |
| 1:C:245:PRO:HA | 2:D:73:THR:HG21 | 1.77 | 0.66 |
| 1:E:242:LEU:CD1 | 1:E:255:LEU:HD11 | 2.25 | 0.66 |
| 2:H:313:MET:HB3 | 2:H:344:VAL:CG2 | 2.26 | 0.66 |
| 1:A:242:LEU:HD12 | 1:A:255:LEU:HD11 | 1.77 | 0.66 |
| 2:B:22:GLU:HG3 | 2:B:83:TYR:OH | 1.95 | 0.66 |
| 2:B:49:PHE:CE1 | 2:B:61:HIS:CE1 | 2.84 | 0.66 |
| 2:B:68:VAL:HG11 | 2:B:149:PHE:CZ | 2.30 | 0.66 |
| 1:C:172:VAL:HG11 | 1:C:387:LEU:CD2 | 2.22 | 0.66 |
| 2:D:100:ALA:CB | 2:D:105:ARG:HD3 | 2.26 | 0.66 |
| 2:D:313:MET:HB3 | 2:D:344:VAL:CG2 | 2.26 | 0.66 |
| 1:E:182:VAL:HG23 | 1:E:186:ASN:HD21 | 1.60 | 0.66 |
| 1:E:265:LEU:HD12 | 1:E:265:LEU:C | 2.16 | 0.66 |
| 2:F:30:ILE:CD1 | 2:F:61:HIS:CD2 | 2.78 | 0.66 |
| 2:F:313:MET:HB3 | 2:F:344:VAL:CG2 | 2.26 | 0.66 |
| 2:F:326:LYS:HE2 | 1:G:214:PHE:CB | 2.26 | 0.66 |
| 2:H:243:ARG:NH2 | 2:H:252:LEU:N | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:182:VAL:HG23 | 1:A:186:ASN:HD21 | 1.60 | 0.66 |
| 1:C:413:MET:HG2 | 1:C:418:PHE:HE1 | 1.61 | 0.66 |
| 1:G:299:LYS:HD3 | 1:G:299:LYS:N | 2.04 | 0.66 |
| 1:A:88:ARG:HD2 | 1:E:283:TYR:OH | 1.96 | 0.66 |
| 2:B:372:GLN:O | 2:B:373:ARG:HB3 | 1.96 | 0.66 |
| 1:C:182:VAL:HG23 | 1:C:186:ASN:HD21 | 1.60 | 0.66 |
| 1:C:243:ARG:HH22 | 1:C:252:LEU:HG | 1.59 | 0.66 |
| 1:C:267:PHE:N | 1:C:267:PHE:CD1 | 2.62 | 0.66 |
| 1:C:281:GLN:O | 1:C:283:TYR:HB2 | 1.96 | 0.66 |
| 1:E:281:GLN:O | 1:E:283:TYR:HB2 | 1.96 | 0.66 |
| 1:G:242:LEU:HD12 | 1:G:255:LEU:HD11 | 1.78 | 0.66 |
| 1:A:35:SER:HB3 | 1:A:59:ASN:CA | 2.26 | 0.65 |
| 1:A:281:GLN:O | 1:A:283:TYR:HB2 | 1.96 | 0.65 |
| 2:B:206:ASN:OD1 | 2:B:227:LEU:HD13 | 1.96 | 0.65 |
| 1:C:35:SER:HB3 | 1:C:59:ASN:CA | 2.26 | 0.65 |
| 1:C:103:TRP:HZ3 | 1:C:108:TYR:HE1 | 1.42 | 0.65 |
| 1:E:242:LEU:HD12 | 1:E:255:LEU:HD11 | 1.77 | 0.65 |
| 1:G:248:LEU:HD13 | 2:H:179:THR:HG21 | 1.76 | 0.65 |
| 1:A:66:ILE:CD1 | 1:A:122:VAL:HG12 | 2.26 | 0.65 |
| 2:B:63:PRO:CG | 2:B:87:PHE:HA | 2.26 | 0.65 |
| 2:B:296:PHE:CZ | 2:B:341:ILE:HD11 | 2.22 | 0.65 |
| 2:B:439:SER:CA | 1:C:401:ARG:NH2 | 2.59 | 0.65 |
| 1:C:66:ILE:CD1 | 1:C:122:VAL:HG12 | 2.26 | 0.65 |
| 2:B:317:LEU:HD12 | 2:B:351:PHE:CD2 | 2.32 | 0.65 |
| 1:C:352:LYS:NZ | 2:D:180:ALA:HA | 2.11 | 0.65 |
| 1:E:66:ILE:CD1 | 1:E:122:VAL:HG12 | 2.26 | 0.65 |
| 1:G:108:TYR:CD1 | 1:G:413:MET:HE1 | 2.32 | 0.65 |
| 1:G:182:VAL:HG23 | 1:G:186:ASN:HD21 | 1.60 | 0.65 |
| 2:H:102:ASN:HB3 | 2:H:407:TRP:CD1 | 2.31 | 0.65 |
| 1:A:103:TRP:HZ3 | 1:A:108:TYR:HE1 | 1.42 | 0.65 |
| 2:D:317:LEU:HD12 | 2:D:351:PHE:CD2 | 2.32 | 0.65 |
| 1:G:66:ILE:CD1 | 1:G:122:VAL:HG12 | 2.26 | 0.65 |
| 1:G:281:GLN:O | 1:G:283:TYR:HB2 | 1.96 | 0.65 |
| 2:H:317:LEU:HD12 | 2:H:351:PHE:CD2 | 2.32 | 0.65 |
| 2:D:217:LEU:HD11 | 2:D:367:ASP:O | 1.96 | 0.65 |
| 2:D:372:GLN:O | 2:D:373:ARG:HB3 | 1.96 | 0.65 |
| 1:E:108:TYR:CD1 | 1:E:413:MET:HE1 | 2.32 | 0.65 |
| 2:F:261:PRO:CB | 1:G:404:PHE:HE2 | 1.95 | 0.65 |
| 2:F:317:LEU:HD12 | 2:F:351:PHE:CD2 | 2.32 | 0.65 |
| 1:G:250:ALA:HB1 | 1:G:254:LYS:HB3 | 1.78 | 0.65 |
| 1:G:306:ASP:OD2 | 3:I:95:ILE:CD1 | 2.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:206:ASN:OD1 | 2:H:227:LEU:HD13 | 1.97 | 0.65 |
| 1:C:254:LYS:HZ2 | 2:D:101:ASN:CG | 1.99 | 0.65 |
| 2:D:206:ASN:OD1 | 2:D:227:LEU:HD13 | 1.97 | 0.65 |
| 2:F:206:ASN:OD1 | 2:F:227:LEU:HD13 | 1.96 | 0.65 |
| 2:D:341:ILE:HG12 | 2:D:341:ILE:O | 1.95 | 0.65 |
| 1:E:299:LYS:HD3 | 1:E:299:LYS:N | 2.04 | 0.65 |
| 1:E:431:GLU:O | 1:E:434:GLN:HG2 | 1.97 | 0.65 |
| 1:G:431:GLU:O | 1:G:434:GLN:HG2 | 1.97 | 0.65 |
| 2:B:271:THR:HG23 | 2:B:300:ASN:O | 1.97 | 0.65 |
| 2:B:293:ASN:OD1 | 2:B:338:LYS:NZ | 2.30 | 0.65 |
| 2:B:341:ILE:O | 2:B:341:ILE:HG12 | 1.95 | 0.65 |
| 2:D:3:GLU:HA | 2:D:51:THR:CB | 2.27 | 0.65 |
| 2:F:115:ILE:HG23 | 2:F:116:ASP:N | 2.12 | 0.65 |
| 2:F:296:PHE:CZ | 2:F:341:ILE:HD11 | 2.22 | 0.65 |
| 2:F:349:THR:HG23 | 1:G:178:SER:H | 1.58 | 0.65 |
| 1:C:282:GLN:O | 1:C:282:GLN:HG2 | 1.97 | 0.65 |
| 1:E:241:CYS:O | 1:E:244:PHE:HB2 | 1.97 | 0.65 |
| 2:H:115:ILE:HG23 | 2:H:116:ASP:N | 2.12 | 0.65 |
| 2:B:3:GLU:HA | 2:B:51:THR:CB | 2.27 | 0.65 |
| 2:B:217:LEU:HD11 | 2:B:367:ASP:O | 1.97 | 0.65 |
| 2:D:293:ASN:OD1 | 2:D:338:LYS:NZ | 2.30 | 0.65 |
| 2:F:217:LEU:HD11 | 2:F:367:ASP:O | 1.96 | 0.65 |
| 1:G:35:SER:HB3 | 1:G:59:ASN:CA | 2.26 | 0.65 |
| 1:G:241:CYS:O | 1:G:244:PHE:HB2 | 1.97 | 0.65 |
| 1:G:276:THR:HB | 1:G:281:GLN:CG | 2.25 | 0.65 |
| 2:H:296:PHE:CZ | 2:H:341:ILE:HD11 | 2.22 | 0.65 |
| 1:A:282:GLN:HG2 | 1:A:282:GLN:O | 1.97 | 0.64 |
| 2:D:271:THR:HG23 | 2:D:300:ASN:O | 1.97 | 0.64 |
| 2:D:305:CYS:SG | 2:D:384:ILE:HD13 | 2.37 | 0.64 |
| 1:E:35:SER:HB3 | 1:E:59:ASN:CA | 2.26 | 0.64 |
| 1:E:103:TRP:HZ3 | 1:E:108:TYR:HE1 | 1.42 | 0.64 |
| 1:E:282:GLN:O | 1:E:282:GLN:HG2 | 1.97 | 0.64 |
| 2:F:3:GLU:HA | 2:F:51:THR:CB | 2.27 | 0.64 |
| 2:F:349:THR:O | 1:G:181:VAL:HA | 1.96 | 0.64 |
| 1:G:158:ARG:NE | 1:G:197:ASN:O | 2.30 | 0.64 |
| 2:H:3:GLU:HA | 2:H:51:THR:CB | 2.27 | 0.64 |
| 2:H:217:LEU:HD11 | 2:H:367:ASP:O | 1.96 | 0.64 |
| 1:A:241:CYS:O | 1:A:244:PHE:HB2 | 1.97 | 0.64 |
| 1:A:431:GLU:O | 1:A:434:GLN:HG2 | 1.97 | 0.64 |
| 2:D:296:PHE:CZ | 2:D:341:ILE:HD11 | 2.22 | 0.64 |
| 1:G:70:LEU:N | 1:G:145:THR:HG21 | 2.11 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:282:GLN:HG2 | 1:G:282:GLN:O | 1.97 | 0.64 |
| 2:H:209:ILE:HG23 | 2:H:230:LEU:HD23 | 1.79 | 0.64 |
| 2:H:271:THR:HG23 | 2:H:300:ASN:O | 1.97 | 0.64 |
| 1:A:114:LEU:O | 1:A:118:VAL:HG23 | 1.97 | 0.64 |
| 1:A:276:THR:HB | 1:A:281:GLN:CG | 2.25 | 0.64 |
| 1:C:114:LEU:O | 1:C:118:VAL:HG23 | 1.97 | 0.64 |
| 1:C:241:CYS:O | 1:C:244:PHE:HB2 | 1.98 | 0.64 |
| 1:E:180:THR:CG2 | 1:E:181:VAL:N | 2.61 | 0.64 |
| 1:E:422:GLU:O | 1:E:426:ASN:HB2 | 1.97 | 0.64 |
| 1:A:66:ILE:HD13 | 1:A:122:VAL:HG12 | 1.79 | 0.64 |
| 1:A:158:ARG:NE | 1:A:197:ASN:O | 2.30 | 0.64 |
| 1:C:70:LEU:N | 1:C:145:THR:HG21 | 2.11 | 0.64 |
| 1:C:158:ARG:NE | 1:C:197:ASN:O | 2.30 | 0.64 |
| 2:F:271:THR:HG23 | 2:F:300:ASN:O | 1.97 | 0.64 |
| 2:F:305:CYS:SG | 2:F:384:ILE:HD13 | 2.37 | 0.64 |
| 2:F:372:GLN:O | 2:F:373:ARG:HB3 | 1.96 | 0.64 |
| 2:B:305:CYS:SG | 2:B:384:ILE:HD13 | 2.37 | 0.64 |
| 2:B:344:VAL:HG12 | 2:B:345:ASP:N | 2.12 | 0.64 |
| 1:C:66:ILE:HD13 | 1:C:122:VAL:HG12 | 1.79 | 0.64 |
| 1:C:276:THR:HB | 1:C:281:GLN:CG | 2.25 | 0.64 |
| 1:C:427:ASP:O | 1:C:430:SER:HB3 | 1.97 | 0.64 |
| 1:C:431:GLU:O | 1:C:434:GLN:HG2 | 1.97 | 0.64 |
| 1:E:276:THR:HB | 1:E:281:GLN:CG | 2.25 | 0.64 |
| 2:F:209:ILE:HG23 | 2:F:230:LEU:HD23 | 1.79 | 0.64 |
| 1:G:427:ASP:O | 1:G:430:SER:HB3 | 1.97 | 0.64 |
| 1:A:70:LEU:N | 1:A:145:THR:HG21 | 2.11 | 0.64 |
| 2:B:56:THR:CB | 2:F:284:GLU:CG | 2.76 | 0.64 |
| 2:B:63:PRO:HG3 | 2:B:87:PHE:HA | 1.79 | 0.64 |
| 1:E:158:ARG:NE | 1:E:197:ASN:O | 2.30 | 0.64 |
| 1:G:103:TRP:HZ3 | 1:G:108:TYR:HE1 | 1.42 | 0.64 |
| 1:G:180:THR:CG2 | 1:G:181:VAL:N | 2.61 | 0.64 |
| 2:H:305:CYS:SG | 2:H:384:ILE:HD13 | 2.37 | 0.64 |
| 1:C:192:HIS:O | 1:C:195:VAL:HG12 | 1.98 | 0.64 |
| 1:C:422:GLU:O | 1:C:426:ASN:HB2 | 1.97 | 0.64 |
| 2:H:372:GLN:O | 2:H:373:ARG:HB3 | 1.96 | 0.64 |
| 1:A:284:ARG:O | 1:A:286:LEU:N | 2.31 | 0.64 |
| 1:A:422:GLU:O | 1:A:426:ASN:HB2 | 1.97 | 0.64 |
| 2:D:115:ILE:HG23 | 2:D:116:ASP:N | 2.12 | 0.64 |
| 2:D:209:ILE:HG23 | 2:D:230:LEU:HD23 | 1.79 | 0.64 |
| 2:D:344:VAL:HG12 | 2:D:345:ASP:N | 2.12 | 0.64 |
| 1:E:70:LEU:N | 1:E:145:THR:HG21 | 2.11 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:284:ARG:O | 1:G:286:LEU:N | 2.31 | 0.64 |
| 1:G:422:GLU:O | 1:G:426:ASN:HB2 | 1.97 | 0.64 |
| 1:A:427:ASP:O | 1:A:430:SER:HB3 | 1.97 | 0.64 |
| 2:B:25:CYS:HB2 | 2:B:30:ILE:O | 1.98 | 0.64 |
| 2:B:234:ILE:HD13 | 2:B:234:ILE:C | 2.18 | 0.64 |
| 1:C:133:GLN:HG3 | 1:C:165:ILE:HD11 | 1.80 | 0.64 |
| 1:C:284:ARG:O | 1:C:286:LEU:N | 2.31 | 0.64 |
| 1:E:66:ILE:HD13 | 1:E:122:VAL:HG12 | 1.79 | 0.64 |
| 2:F:175:PRO:HG2 | 2:F:207:GLU:OE1 | 1.98 | 0.64 |
| 2:H:175:PRO:HG2 | 2:H:207:GLU:OE1 | 1.98 | 0.64 |
| 2:H:402:ARG:O | 2:H:403:ALA:C | 2.36 | 0.64 |
| 2:B:209:ILE:HG23 | 2:B:230:LEU:HD23 | 1.79 | 0.64 |
| 2:D:30:ILE:CD1 | 2:D:61:HIS:CD2 | 2.81 | 0.64 |
| 1:E:284:ARG:O | 1:E:286:LEU:N | 2.31 | 0.64 |
| 2:F:402:ARG:O | 2:F:403:ALA:C | 2.36 | 0.64 |
| 1:G:299:LYS:H | 1:G:299:LYS:CD | 2.07 | 0.64 |
| 1:A:133:GLN:HG3 | 1:A:165:ILE:HD11 | 1.80 | 0.63 |
| 1:A:192:HIS:O | 1:A:195:VAL:HG12 | 1.98 | 0.63 |
| 2:D:317:LEU:HB3 | 2:D:319:TYR:CE1 | 2.33 | 0.63 |
| 1:E:137:LEU:HD22 | 1:E:154:ILE:CG2 | 2.28 | 0.63 |
| 2:F:151:SER:O | 2:F:155:GLU:HB2 | 1.98 | 0.63 |
| 2:F:293:ASN:OD1 | 2:F:338:LYS:NZ | 2.30 | 0.63 |
| 1:G:105:LYS:O | 1:G:110:GLU:HB2 | 1.97 | 0.63 |
| 1:G:137:LEU:HD22 | 1:G:154:ILE:CG2 | 2.28 | 0.63 |
| 2:B:115:ILE:HG23 | 2:B:116:ASP:N | 2.12 | 0.63 |
| 1:E:63:PRO:HD2 | 1:E:86:ILE:HG12 | 1.80 | 0.63 |
| 1:E:427:ASP:O | 1:E:430:SER:HB3 | 1.97 | 0.63 |
| 2:F:284:GLU:OE1 | 2:F:284:GLU:N | 2.30 | 0.63 |
| 1:G:66:ILE:HD13 | 1:G:122:VAL:HG12 | 1.79 | 0.63 |
| 2:H:151:SER:O | 2:H:155:GLU:HB2 | 1.98 | 0.63 |
| 2:H:284:GLU:OE1 | 2:H:284:GLU:N | 2.30 | 0.63 |
| 1:A:63:PRO:HD2 | 1:A:86:ILE:HG12 | 1.80 | 0.63 |
| 1:A:107:HIS:HD2 | 1:A:151:THR:CG2 | 2.12 | 0.63 |
| 1:C:137:LEU:HD22 | 1:C:154:ILE:CG2 | 2.28 | 0.63 |
| 1:E:105:LYS:O | 1:E:110:GLU:HB2 | 1.97 | 0.63 |
| 2:H:7:ILE:HG22 | 2:H:66:VAL:CG2 | 2.28 | 0.63 |
| 1:A:137:LEU:HD22 | 1:A:154:ILE:CG2 | 2.28 | 0.63 |
| 2:B:386:GLU:O | 2:B:389:ALA:N | 2.31 | 0.63 |
| 2:D:25:CYS:HB2 | 2:D:30:ILE:O | 1.98 | 0.63 |
| 2:D:175:PRO:HG2 | 2:D:207:GLU:OE1 | 1.98 | 0.63 |
| 2:D:234:ILE:HD13 | 2:D:234:ILE:C | 2.18 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:386:GLU:O | 2:D:389:ALA:N | 2.31 | 0.63 |
| 1:E:299:LYS:H | 1:E:299:LYS:CD | 2.07 | 0.63 |
| 2:F:386:GLU:O | 2:F:389:ALA:N | 2.31 | 0.63 |
| 1:G:114:LEU:O | 1:G:118:VAL:HG23 | 1.97 | 0.63 |
| 1:G:133:GLN:HG3 | 1:G:165:ILE:HD11 | 1.80 | 0.63 |
| 1:G:318:VAL:HA | 1:G:354:ALA:HB3 | 1.81 | 0.63 |
| 1:A:180:THR:CG2 | 1:A:181:VAL:N | 2.61 | 0.63 |
| 1:A:318:VAL:HA | 1:A:354:ALA:HB3 | 1.81 | 0.63 |
| 2:B:175:PRO:HG2 | 2:B:207:GLU:OE1 | 1.98 | 0.63 |
| 1:C:107:HIS:HD2 | 1:C:151:THR:CG2 | 2.12 | 0.63 |
| 1:C:180:THR:CG2 | 1:C:181:VAL:N | 2.61 | 0.63 |
| 1:C:318:VAL:HA | 1:C:354:ALA:HB3 | 1.81 | 0.63 |
| 1:C:346:TRP:CD1 | 2:D:401:LYS:NZ | 2.65 | 0.63 |
| 2:F:7:ILE:HG22 | 2:F:66:VAL:CG2 | 2.28 | 0.63 |
| 2:F:234:ILE:HD13 | 2:F:234:ILE:C | 2.18 | 0.63 |
| 2:F:296:PHE:CE1 | 2:F:335:ILE:CG2 | 2.73 | 0.63 |
| 1:G:192:HIS:O | 1:G:195:VAL:HG12 | 1.98 | 0.63 |
| 1:G:352:LYS:CA | 2:H:181:VAL:HG22 | 2.24 | 0.63 |
| 2:H:234:ILE:HD13 | 2:H:234:ILE:C | 2.18 | 0.63 |
| 2:H:293:ASN:OD1 | 2:H:338:LYS:NZ | 2.30 | 0.63 |
| 2:H:296:PHE:CE1 | 2:H:335:ILE:CG2 | 2.73 | 0.63 |
| 2:H:386:GLU:O | 2:H:389:ALA:N | 2.31 | 0.63 |
| 1:C:105:LYS:O | 1:C:110:GLU:HB2 | 1.97 | 0.63 |
| 2:D:88:HIS:HB2 | 2:D:91:GLN:NE2 | 2.06 | 0.63 |
| 1:E:114:LEU:O | 1:E:118:VAL:HG23 | 1.97 | 0.63 |
| 1:E:192:HIS:O | 1:E:195:VAL:HG12 | 1.98 | 0.63 |
| 2:F:278:ALA:O | 2:F:279:GLU:CB | 2.43 | 0.63 |
| 1:G:63:PRO:HD2 | 1:G:86:ILE:HG12 | 1.80 | 0.63 |
| 2:H:88:HIS:HB2 | 2:H:91:GLN:NE2 | 2.06 | 0.63 |
| 2:B:151:SER:O | 2:B:155:GLU:HB2 | 1.98 | 0.63 |
| 2:B:152:LEU:HD12 | 2:B:153:LEU:N | 2.14 | 0.63 |
| 2:B:317:LEU:HB3 | 2:B:319:TYR:CE1 | 2.33 | 0.63 |
| 1:C:315:VAL:HG13 | 1:C:377:PHE:CE1 | 2.34 | 0.63 |
| 1:E:318:VAL:HA | 1:E:354:ALA:HB3 | 1.81 | 0.63 |
| 2:F:88:HIS:HB2 | 2:F:91:GLN:NE2 | 2.06 | 0.63 |
| 2:F:317:LEU:HB3 | 2:F:319:TYR:CE1 | 2.33 | 0.63 |
| 2:H:278:ALA:O | 2:H:279:GLU:CB | 2.43 | 0.63 |
| 2:H:317:LEU:HB3 | 2:H:319:TYR:CE1 | 2.33 | 0.63 |
| 2:H:344:VAL:HG12 | 2:H:345:ASP:N | 2.12 | 0.63 |
| 1:A:315:VAL:HG13 | 1:A:377:PHE:CE1 | 2.34 | 0.63 |
| 2:B:159:VAL:CG1 | 3:I:78:ARG:HG3 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:243:ARG:HH21 | 1:C:252:LEU:H | 1.45 | 0.63 |
| 1:C:247:GLN:HB3 | 2:D:224:TYR:CD1 | 2.31 | 0.63 |
| 2:D:7:ILE:HG22 | 2:D:66:VAL:CG2 | 2.28 | 0.63 |
| 2:D:102:ASN:OD1 | 2:D:105:ARG:HB3 | 1.99 | 0.63 |
| 1:E:172:VAL:HG11 | 1:E:387:LEU:CD2 | 2.22 | 0.63 |
| 1:E:299:LYS:O | 1:E:300:ASN:HB2 | 1.97 | 0.63 |
| 2:B:102:ASN:OD1 | 2:B:105:ARG:HB3 | 1.99 | 0.63 |
| 1:C:299:LYS:O | 1:C:300:ASN:HB2 | 1.97 | 0.63 |
| 2:D:7:ILE:CD1 | 2:D:137:VAL:HG22 | 2.29 | 0.63 |
| 1:E:133:GLN:HG3 | 1:E:165:ILE:HD11 | 1.80 | 0.63 |
| 2:F:344:VAL:HG12 | 2:F:345:ASP:N | 2.12 | 0.63 |
| 1:G:245:PRO:HB3 | 2:H:73:THR:CG2 | 2.29 | 0.63 |
| 1:G:258:ASN:OD1 | 2:H:181:VAL:HB | 1.99 | 0.63 |
| 1:A:105:LYS:O | 1:A:110:GLU:HB2 | 1.97 | 0.62 |
| 1:C:205:ASP:OD1 | 1:C:304:ALA:N | 2.32 | 0.62 |
| 1:G:107:HIS:HD2 | 1:G:151:THR:CG2 | 2.12 | 0.62 |
| 1:G:172:VAL:HG11 | 1:G:387:LEU:CD2 | 2.22 | 0.62 |
| 1:C:63:PRO:HD2 | 1:C:86:ILE:HG12 | 1.80 | 0.62 |
| 2:D:151:SER:O | 2:D:155:GLU:HB2 | 1.98 | 0.62 |
| 2:H:267:PHE:H | 2:H:267:PHE:HD1 | 1.47 | 0.62 |
| 1:A:108:TYR:CD1 | 1:A:413:MET:HE1 | 2.33 | 0.62 |
| 1:A:299:LYS:H | 1:A:299:LYS:CD | 2.07 | 0.62 |
| 2:B:7:ILE:CD1 | 2:B:137:VAL:HG22 | 2.29 | 0.62 |
| 2:B:166:LYS:H | 2:B:199:ASP:CG | 2.03 | 0.62 |
| 2:D:267:PHE:HD1 | 2:D:267:PHE:H | 1.47 | 0.62 |
| 2:F:152:LEU:HD12 | 2:F:153:LEU:N | 2.14 | 0.62 |
| 1:G:243:ARG:HH21 | 1:G:252:LEU:H | 1.45 | 0.62 |
| 1:G:250:ALA:HB1 | 1:G:254:LYS:CD | 2.17 | 0.62 |
| 2:H:152:LEU:HD12 | 2:H:153:LEU:N | 2.14 | 0.62 |
| 2:H:269:LEU:O | 2:H:378:LEU:HA | 1.99 | 0.62 |
| 1:A:243:ARG:HH21 | 1:A:252:LEU:H | 1.45 | 0.62 |
| 1:C:4:ILE:HA | 1:C:134:GLY:O | 1.99 | 0.62 |
| 2:D:152:LEU:HD12 | 2:D:153:LEU:N | 2.14 | 0.62 |
| 2:D:315:CYS:HB3 | 2:D:377:MET:CE | 2.29 | 0.62 |
| 2:F:115:ILE:HG13 | 2:F:152:LEU:HD13 | 1.81 | 0.62 |
| 2:F:273:ALA:HB3 | 2:F:274:PRO:HD3 | 1.81 | 0.62 |
| 2:F:315:CYS:HB3 | 2:F:377:MET:CE | 2.29 | 0.62 |
| 1:G:258:ASN:C | 2:H:404:PHE:CE2 | 2.72 | 0.62 |
| 1:G:299:LYS:O | 1:G:300:ASN:HB2 | 1.98 | 0.62 |
| 2:H:70:LEU:O | 2:H:95:GLY:O | 2.17 | 0.62 |
| 1:A:56:ALA:CB | 1:E:283:TYR:CD2 | 2.76 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:205:ASP:OD1 | 1:A:304:ALA:N | 2.32 | 0.62 |
| 1:A:253:ARG:O | 1:A:256:ALA:N | 2.33 | 0.62 |
| 2:B:205:ASP:HB2 | 2:B:303:VAL:HA | 1.82 | 0.62 |
| 2:D:166:LYS:H | 2:D:199:ASP:CG | 2.03 | 0.62 |
| 1:E:315:VAL:HG13 | 1:E:377:PHE:CE1 | 2.34 | 0.62 |
| 1:E:325:MET:HE2 | 1:E:355:VAL:HG21 | 1.80 | 0.62 |
| 2:F:62:VAL:CG1 | 2:F:91:GLN:HE22 | 2.13 | 0.62 |
| 2:F:102:ASN:OD1 | 2:F:105:ARG:HB3 | 1.99 | 0.62 |
| 2:F:166:LYS:H | 2:F:199:ASP:CG | 2.03 | 0.62 |
| 2:H:115:ILE:HG13 | 2:H:152:LEU:HD13 | 1.81 | 0.62 |
| 2:H:236:SER:O | 2:H:240:ALA:HB3 | 1.99 | 0.62 |
| 2:H:273:ALA:HB3 | 2:H:274:PRO:HD3 | 1.81 | 0.62 |
| 2:B:7:ILE:HG22 | 2:B:66:VAL:CG2 | 2.28 | 0.62 |
| 1:C:70:LEU:CG | 1:C:145:THR:HG23 | 2.30 | 0.62 |
| 1:C:253:ARG:O | 1:C:256:ALA:N | 2.33 | 0.62 |
| 2:D:115:ILE:HG13 | 2:D:152:LEU:HD13 | 1.81 | 0.62 |
| 2:D:205:ASP:HB2 | 2:D:303:VAL:HA | 1.82 | 0.62 |
| 2:D:236:SER:O | 2:D:240:ALA:HB3 | 1.99 | 0.62 |
| 1:E:243:ARG:HH21 | 1:E:252:LEU:H | 1.45 | 0.62 |
| 1:G:4:ILE:HG23 | 1:G:134:GLY:O | 2.00 | 0.62 |
| 2:H:62:VAL:CG1 | 2:H:91:GLN:HE22 | 2.13 | 0.62 |
| 2:H:166:LYS:H | 2:H:199:ASP:CG | 2.03 | 0.62 |
| 2:H:315:CYS:HB3 | 2:H:377:MET:CE | 2.29 | 0.62 |
| 1:A:211:ASP:OD1 | 1:A:212:ILE:N | 2.33 | 0.62 |
| 1:A:299:LYS:O | 1:A:300:ASN:HB2 | 1.98 | 0.62 |
| 2:B:267:PHE:H | 2:B:267:PHE:HD1 | 1.47 | 0.62 |
| 2:B:317:LEU:HD11 | 2:B:351:PHE:HE2 | 1.63 | 0.62 |
| 1:C:211:ASP:OD1 | 1:C:212:ILE:N | 2.33 | 0.62 |
| 1:C:254:LYS:NZ | 2:D:101:ASN:ND2 | 2.47 | 0.62 |
| 1:E:70:LEU:CG | 1:E:145:THR:HG23 | 2.30 | 0.62 |
| 1:E:107:HIS:HD2 | 1:E:151:THR:CG2 | 2.12 | 0.62 |
| 1:E:253:ARG:O | 1:E:256:ALA:N | 2.33 | 0.62 |
| 2:F:7:ILE:CD1 | 2:F:137:VAL:HG22 | 2.29 | 0.62 |
| 2:F:70:LEU:O | 2:F:95:GLY:O | 2.18 | 0.62 |
| 2:F:269:LEU:O | 2:F:378:LEU:HA | 1.99 | 0.62 |
| 1:G:205:ASP:OD1 | 1:G:304:ALA:N | 2.32 | 0.62 |
| 1:G:230:LEU:O | 1:G:233:ALA:HB3 | 2.00 | 0.62 |
| 1:G:315:VAL:HG13 | 1:G:377:PHE:CE1 | 2.34 | 0.62 |
| 2:H:102:ASN:OD1 | 2:H:105:ARG:HB3 | 1.99 | 0.62 |
| 1:A:115:VAL:HG21 | 1:A:152:LEU:CD2 | 2.30 | 0.62 |
| 2:B:115:ILE:HG13 | 2:B:152:LEU:HD13 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:118:VAL:HG11 | 2:B:149:PHE:HZ | 1.65 | 0.62 |
| 2:B:236:SER:O | 2:B:240:ALA:HB3 | 1.99 | 0.62 |
| 2:B:269:LEU:O | 2:B:378:LEU:HA | 1.99 | 0.62 |
| 2:B:315:CYS:HB3 | 2:B:377:MET:CE | 2.29 | 0.62 |
| 1:C:249:ASN:OD1 | 2:D:71:GLU:OE1 | 2.17 | 0.62 |
| 2:D:118:VAL:HG11 | 2:D:149:PHE:HZ | 1.65 | 0.62 |
| 1:E:4:ILE:HA | 1:E:134:GLY:O | 1.99 | 0.62 |
| 1:E:205:ASP:OD1 | 1:E:304:ALA:N | 2.32 | 0.62 |
| 2:F:326:LYS:CB | 1:G:222:PRO:CD | 2.77 | 0.62 |
| 2:H:7:ILE:CD1 | 2:H:137:VAL:HG22 | 2.29 | 0.62 |
| 1:C:93:VAL:CG1 | 1:C:118:VAL:HG22 | 2.19 | 0.62 |
| 2:D:402:ARG:O | 2:D:403:ALA:C | 2.36 | 0.62 |
| 1:E:4:ILE:HG23 | 1:E:134:GLY:O | 2.00 | 0.62 |
| 2:F:236:SER:O | 2:F:240:ALA:HB3 | 1.99 | 0.62 |
| 1:G:70:LEU:CG | 1:G:145:THR:HG23 | 2.30 | 0.62 |
| 1:G:115:VAL:HG21 | 1:G:152:LEU:CD2 | 2.30 | 0.62 |
| 1:A:4:ILE:HA | 1:A:134:GLY:O | 1.99 | 0.62 |
| 1:A:70:LEU:CG | 1:A:145:THR:HG23 | 2.30 | 0.62 |
| 2:B:62:VAL:HG11 | 2:B:88:HIS:ND1 | 2.15 | 0.62 |
| 2:B:159:VAL:HG13 | 3:I:78:ARG:HG2 | 1.81 | 0.62 |
| 2:B:296:PHE:CZ | 2:B:341:ILE:CD1 | 2.79 | 0.62 |
| 1:C:108:TYR:CD1 | 1:C:413:MET:HE1 | 2.34 | 0.62 |
| 1:C:115:VAL:HG21 | 1:C:152:LEU:CD2 | 2.30 | 0.62 |
| 2:D:317:LEU:HD11 | 2:D:351:PHE:HE2 | 1.63 | 0.62 |
| 1:E:115:VAL:HG21 | 1:E:152:LEU:CD2 | 2.30 | 0.62 |
| 1:E:230:LEU:O | 1:E:233:ALA:HB3 | 2.00 | 0.62 |
| 2:F:277:SER:HA | 2:F:367:ASP:O | 2.00 | 0.62 |
| 1:G:4:ILE:HA | 1:G:134:GLY:O | 1.99 | 0.62 |
| 1:G:248:LEU:CD2 | 2:H:179:THR:HG21 | 2.21 | 0.62 |
| 2:B:402:ARG:O | 2:B:403:ALA:C | 2.36 | 0.61 |
| 2:D:62:VAL:CG1 | 2:D:91:GLN:HE22 | 2.13 | 0.61 |
| 2:D:269:LEU:O | 2:D:378:LEU:HA | 1.99 | 0.61 |
| 2:D:277:SER:HA | 2:D:367:ASP:O | 2.00 | 0.61 |
| 2:D:70:LEU:O | 2:D:95:GLY:O | 2.17 | 0.61 |
| 2:F:205:ASP:HB2 | 2:F:303:VAL:HA | 1.82 | 0.61 |
| 2:F:296:PHE:CZ | 2:F:341:ILE:CD1 | 2.79 | 0.61 |
| 1:G:253:ARG:O | 1:G:256:ALA:N | 2.33 | 0.61 |
| 2:H:277:SER:HA | 2:H:367:ASP:O | 2.00 | 0.61 |
| 2:B:70:LEU:O | 2:B:95:GLY:O | 2.17 | 0.61 |
| 2:B:88:HIS:HB2 | 2:B:91:GLN:NE2 | 2.06 | 0.61 |
| 1:C:299:LYS:H | 1:C:299:LYS:CD | 2.07 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:23:LEU:HD22 | 2:D:232:GLY:O | 1.99 | 0.61 |
| 2:D:30:ILE:HG12 | 2:D:36:MET:CB | 2.12 | 0.61 |
| 2:F:23:LEU:HD22 | 2:F:232:GLY:O | 1.99 | 0.61 |
| 1:G:211:ASP:OD1 | 1:G:212:ILE:N | 2.33 | 0.61 |
| 2:H:205:ASP:HB2 | 2:H:303:VAL:HA | 1.82 | 0.61 |
| 1:A:4:ILE:HG23 | 1:A:134:GLY:O | 2.00 | 0.61 |
| 1:A:70:LEU:H | 1:A:145:THR:CG2 | 2.10 | 0.61 |
| 2:B:62:VAL:HG13 | 2:B:63:PRO:HD2 | 1.78 | 0.61 |
| 2:B:217:LEU:HD11 | 2:B:277:SER:HA | 1.83 | 0.61 |
| 2:B:277:SER:HA | 2:B:367:ASP:O | 2.00 | 0.61 |
| 1:C:70:LEU:H | 1:C:145:THR:CG2 | 2.10 | 0.61 |
| 1:C:324:SER:CB | 1:C:327:GLU:HG2 | 2.30 | 0.61 |
| 1:E:204:ILE:CD1 | 1:E:231:VAL:HG13 | 2.30 | 0.61 |
| 2:F:118:VAL:HG11 | 2:F:149:PHE:HZ | 1.65 | 0.61 |
| 2:F:168:GLU:OE1 | 2:F:198:SER:HB2 | 2.00 | 0.61 |
| 2:H:118:VAL:HG11 | 2:H:149:PHE:HZ | 1.65 | 0.61 |
| 1:A:93:VAL:CG1 | 1:A:118:VAL:HG22 | 2.19 | 0.61 |
| 2:B:5:ILE:HD11 | 2:B:64:ARG:HH22 | 1.65 | 0.61 |
| 2:B:23:LEU:HD22 | 2:B:232:GLY:O | 1.99 | 0.61 |
| 2:B:168:GLU:OE1 | 2:B:198:SER:HB2 | 2.00 | 0.61 |
| 2:B:273:ALA:HB3 | 2:B:274:PRO:HD3 | 1.81 | 0.61 |
| 1:C:114:LEU:HD23 | 1:C:149:MET:CE | 2.30 | 0.61 |
| 2:D:217:LEU:HD11 | 2:D:277:SER:HA | 1.82 | 0.61 |
| 1:E:324:SER:C | 1:E:326:LYS:H | 2.03 | 0.61 |
| 2:F:317:LEU:HD11 | 2:F:351:PHE:HE2 | 1.63 | 0.61 |
| 1:G:114:LEU:HD23 | 1:G:149:MET:CE | 2.30 | 0.61 |
| 2:H:23:LEU:HD22 | 2:H:232:GLY:O | 1.99 | 0.61 |
| 2:H:168:GLU:OE1 | 2:H:198:SER:HB2 | 2.01 | 0.61 |
| 1:A:88:ARG:HD3 | 1:E:283:TYR:CE1 | 2.34 | 0.61 |
| 2:B:30:ILE:CD1 | 2:B:61:HIS:CG | 2.82 | 0.61 |
| 2:D:119:LEU:CD2 | 2:D:122:ILE:HD11 | 2.28 | 0.61 |
| 1:G:204:ILE:CD1 | 1:G:231:VAL:HG13 | 2.30 | 0.61 |
| 1:A:230:LEU:O | 1:A:233:ALA:HB3 | 2.00 | 0.61 |
| 2:D:273:ALA:HB3 | 2:D:274:PRO:HD3 | 1.81 | 0.61 |
| 1:E:211:ASP:OD1 | 1:E:212:ILE:N | 2.33 | 0.61 |
| 2:H:296:PHE:CZ | 2:H:341:ILE:CD1 | 2.79 | 0.61 |
| 1:A:324:SER:CB | 1:A:327:GLU:HG2 | 2.30 | 0.61 |
| 2:B:169:PHE:CE1 | 2:B:235:VAL:HG22 | 2.36 | 0.61 |
| 2:B:229:ARG:NH1 | 2:B:363:VAL:HG21 | 2.16 | 0.61 |
| 2:B:348:PRO:HD3 | 1:C:398:MET:CE | 2.12 | 0.61 |
| 1:C:4:ILE:HG23 | 1:C:134:GLY:O | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:54:ASN:ND2 | 1:C:64:ARG:HD3 | 2.15 | 0.61 |
| 1:C:248:LEU:HD22 | 2:D:179:THR:CG2 | 2.27 | 0.61 |
| 2:D:168:GLU:OE1 | 2:D:198:SER:HB2 | 2.00 | 0.61 |
| 2:F:346:TRP:HZ3 | 1:G:404:PHE:HZ | 1.47 | 0.61 |
| 1:A:114:LEU:HD23 | 1:A:149:MET:CE | 2.30 | 0.61 |
| 2:B:345:ASP:C | 2:B:347:CYS:H | 2.04 | 0.61 |
| 1:C:324:SER:C | 1:C:326:LYS:H | 2.03 | 0.61 |
| 2:D:248:LEU:CD2 | 2:D:353:VAL:O | 2.49 | 0.61 |
| 2:D:296:PHE:CZ | 2:D:341:ILE:CD1 | 2.79 | 0.61 |
| 1:G:324:SER:C | 1:G:326:LYS:H | 2.03 | 0.61 |
| 2:H:317:LEU:HD11 | 2:H:351:PHE:HE2 | 1.63 | 0.61 |
| 2:B:293:ASN:HD21 | 2:B:338:LYS:HZ1 | 1.49 | 0.61 |
| 1:C:230:LEU:O | 1:C:233:ALA:HB3 | 2.00 | 0.61 |
| 2:D:229:ARG:NH1 | 2:D:363:VAL:HG21 | 2.16 | 0.61 |
| 2:F:119:LEU:CD2 | 2:F:122:ILE:HD11 | 2.28 | 0.61 |
| 2:F:191:THR:HG21 | 2:F:425:MET:SD | 2.41 | 0.61 |
| 1:G:93:VAL:CG1 | 1:G:118:VAL:HG22 | 2.19 | 0.61 |
| 1:G:245:PRO:HA | 2:H:73:THR:HG21 | 1.83 | 0.61 |
| 2:H:119:LEU:CD2 | 2:H:122:ILE:HD11 | 2.28 | 0.61 |
| 2:H:169:PHE:CE1 | 2:H:235:VAL:HG22 | 2.36 | 0.61 |
| 2:H:191:THR:HG21 | 2:H:425:MET:SD | 2.41 | 0.61 |
| 1:A:54:ASN:ND2 | 1:A:64:ARG:HD3 | 2.15 | 0.60 |
| 2:B:5:ILE:HD13 | 2:B:64:ARG:HH12 | 1.59 | 0.60 |
| 1:E:114:LEU:HD23 | 1:E:149:MET:CE | 2.30 | 0.60 |
| 2:F:87:PHE:CD2 | 2:F:87:PHE:N | 2.69 | 0.60 |
| 2:F:169:PHE:CE1 | 2:F:235:VAL:HG22 | 2.36 | 0.60 |
| 2:H:87:PHE:N | 2:H:87:PHE:CD2 | 2.69 | 0.60 |
| 2:H:102:ASN:CG | 2:H:407:TRP:CD1 | 2.75 | 0.60 |
| 2:H:315:CYS:HB3 | 2:H:377:MET:HE2 | 1.81 | 0.60 |
| 2:H:362:VAL:HG13 | 2:H:368:LEU:HB2 | 1.83 | 0.60 |
| 2:B:30:ILE:HG12 | 2:B:36:MET:CB | 2.12 | 0.60 |
| 2:D:169:PHE:CE1 | 2:D:235:VAL:HG22 | 2.36 | 0.60 |
| 1:E:93:VAL:CG1 | 1:E:118:VAL:HG22 | 2.19 | 0.60 |
| 2:F:267:PHE:HD1 | 2:F:267:PHE:H | 1.47 | 0.60 |
| 2:F:329:ASN:CB | 1:G:210:TYR:CZ | 2.81 | 0.60 |
| 3:I:63:ARG:HB3 | 3:I:136:VAL:HG11 | 1.83 | 0.60 |
| 1:A:204:ILE:HG21 | 1:A:231:VAL:HG22 | 1.84 | 0.60 |
| 2:B:88:HIS:CE1 | 2:F:284:GLU:OE2 | 2.54 | 0.60 |
| 2:B:119:LEU:CD2 | 2:B:122:ILE:HD11 | 2.28 | 0.60 |
| 2:B:191:THR:HG21 | 2:B:425:MET:SD | 2.41 | 0.60 |
| 1:C:115:VAL:HG21 | 1:C:152:LEU:HD23 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:273:ALA:HB3 | 1:C:274:PRO:CD | 2.29 | 0.60 |
| 1:C:285:ALA:HB1 | 1:C:290:GLU:HG2 | 1.82 | 0.60 |
| 1:A:172:VAL:HG11 | 1:A:387:LEU:CD2 | 2.22 | 0.60 |
| 1:A:273:ALA:HB3 | 1:A:274:PRO:CD | 2.29 | 0.60 |
| 1:C:204:ILE:CD1 | 1:C:231:VAL:HG13 | 2.30 | 0.60 |
| 2:D:345:ASP:C | 2:D:347:CYS:H | 2.04 | 0.60 |
| 1:E:204:ILE:HG21 | 1:E:231:VAL:HG22 | 1.84 | 0.60 |
| 2:F:345:ASP:C | 2:F:347:CYS:H | 2.04 | 0.60 |
| 1:A:115:VAL:HG21 | 1:A:152:LEU:HD23 | 1.84 | 0.60 |
| 1:A:204:ILE:CD1 | 1:A:231:VAL:HG13 | 2.30 | 0.60 |
| 1:A:324:SER:C | 1:A:326:LYS:H | 2.03 | 0.60 |
| 1:C:332:MET:HE3 | 1:C:351:VAL:HG11 | 1.82 | 0.60 |
| 2:D:191:THR:HG21 | 2:D:425:MET:SD | 2.41 | 0.60 |
| 2:F:362:VAL:HG13 | 2:F:368:LEU:HB2 | 1.83 | 0.60 |
| 1:A:49:ILE:O | 1:A:51:VAL:N | 2.35 | 0.60 |
| 1:A:325:MET:HE1 | 1:A:355:VAL:HG11 | 1.82 | 0.60 |
| 2:B:87:PHE:N | 2:B:87:PHE:CD2 | 2.69 | 0.60 |
| 2:B:311:LYS:HE3 | 2:B:342:GLN:CD | 2.22 | 0.60 |
| 2:D:362:VAL:HG13 | 2:D:368:LEU:HB2 | 1.83 | 0.60 |
| 2:F:63:PRO:CD | 2:F:87:PHE:HA | 2.32 | 0.60 |
| 2:H:345:ASP:C | 2:H:347:CYS:H | 2.04 | 0.60 |
| 1:C:141:LEU:N | 1:C:141:LEU:CD1 | 2.65 | 0.60 |
| 1:C:204:ILE:HG21 | 1:C:231:VAL:HG22 | 1.84 | 0.60 |
| 2:D:3:GLU:HG3 | 2:D:51:THR:HA | 1.75 | 0.60 |
| 2:D:57:GLY:HA3 | 2:D:58:ALA:HB2 | 0.66 | 0.60 |
| 2:D:87:PHE:CD2 | 2:D:87:PHE:N | 2.69 | 0.60 |
| 2:F:371:VAL:HG12 | 2:F:372:GLN:N | 2.17 | 0.60 |
| 1:G:2:ARG:HH21 | 2:H:98:ASP:HA | 1.64 | 0.60 |
| 1:G:49:ILE:O | 1:G:51:VAL:N | 2.35 | 0.60 |
| 1:G:204:ILE:HG21 | 1:G:231:VAL:HG22 | 1.84 | 0.60 |
| 1:G:332:MET:CE | 1:G:351:VAL:HG11 | 2.32 | 0.60 |
| 1:C:254:LYS:HZ3 | 2:D:101:ASN:ND2 | 2.00 | 0.60 |
| 2:D:344:VAL:HG11 | 2:D:346:TRP:NE1 | 2.16 | 0.60 |
| 1:E:115:VAL:HG21 | 1:E:152:LEU:HD23 | 1.84 | 0.60 |
| 1:E:273:ALA:HB3 | 1:E:274:PRO:CD | 2.29 | 0.60 |
| 2:H:63:PRO:CD | 2:H:87:PHE:HA | 2.32 | 0.60 |
| 2:H:229:ARG:NH1 | 2:H:363:VAL:HG21 | 2.16 | 0.60 |
| 2:H:371:VAL:HG12 | 2:H:372:GLN:N | 2.17 | 0.60 |
| 1:A:332:MET:CE | 1:A:351:VAL:HG11 | 2.32 | 0.60 |
| 2:B:362:VAL:HG13 | 2:B:368:LEU:HB2 | 1.83 | 0.60 |
| 1:C:49:ILE:O | 1:C:51:VAL:N | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:254:LYS:NZ | 2:D:101:ASN:HD21 | 1.98 | 0.60 |
| 2:F:229:ARG:NH1 | 2:F:363:VAL:HG21 | 2.16 | 0.60 |
| 2:F:344:VAL:HG11 | 2:F:346:TRP:NE1 | 2.16 | 0.60 |
| 1:G:115:VAL:HG21 | 1:G:152:LEU:HD23 | 1.84 | 0.60 |
| 2:H:311:LYS:HE3 | 2:H:342:GLN:CD | 2.22 | 0.60 |
| 1:A:141:LEU:N | 1:A:141:LEU:CD1 | 2.65 | 0.60 |
| 1:A:285:ALA:HB1 | 1:A:290:GLU:HG2 | 1.82 | 0.60 |
| 1:E:49:ILE:O | 1:E:51:VAL:N | 2.35 | 0.60 |
| 1:E:285:ALA:HB1 | 1:E:290:GLU:HG2 | 1.82 | 0.60 |
| 2:F:3:GLU:HG3 | 2:F:51:THR:HA | 1.74 | 0.60 |
| 2:F:217:LEU:HD11 | 2:F:277:SER:HA | 1.82 | 0.60 |
| 2:F:311:LYS:HE3 | 2:F:342:GLN:CD | 2.22 | 0.60 |
| 1:G:102:ASN:ND2 | 1:G:407:TRP:O | 2.35 | 0.60 |
| 1:G:408:TYR:CG | 1:G:418:PHE:HZ | 2.20 | 0.60 |
| 2:H:167:LEU:HA | 2:H:200:CYS:O | 2.01 | 0.60 |
| 2:H:248:LEU:CD2 | 2:H:353:VAL:O | 2.49 | 0.60 |
| 2:H:344:VAL:HG11 | 2:H:346:TRP:NE1 | 2.16 | 0.60 |
| 1:A:102:ASN:ND2 | 1:A:407:TRP:O | 2.35 | 0.59 |
| 1:C:102:ASN:ND2 | 1:C:407:TRP:O | 2.35 | 0.59 |
| 1:C:161:TYR:C | 1:C:163:ASP:H | 2.05 | 0.59 |
| 1:C:279:GLY:O | 1:C:282:GLN:HB3 | 2.01 | 0.59 |
| 1:E:102:ASN:ND2 | 1:E:407:TRP:O | 2.35 | 0.59 |
| 2:F:407:TRP:O | 2:F:411:GLU:HG2 | 2.02 | 0.59 |
| 1:G:279:GLY:O | 1:G:282:GLN:HB3 | 2.01 | 0.59 |
| 2:B:276:ILE:HD11 | 2:B:280:LYS:HD2 | 1.85 | 0.59 |
| 2:B:371:VAL:HG12 | 2:B:372:GLN:N | 2.17 | 0.59 |
| 2:B:435:VAL:O | 2:B:435:VAL:HG12 | 2.02 | 0.59 |
| 2:D:311:LYS:HE3 | 2:D:342:GLN:CD | 2.22 | 0.59 |
| 2:D:435:VAL:O | 2:D:435:VAL:HG12 | 2.02 | 0.59 |
| 1:E:324:SER:O | 1:E:328:VAL:HG23 | 2.02 | 0.59 |
| 1:G:285:ALA:HB1 | 1:G:290:GLU:HG2 | 1.82 | 0.59 |
| 1:G:324:SER:O | 1:G:328:VAL:HG23 | 2.01 | 0.59 |
| 2:H:407:TRP:O | 2:H:411:GLU:HG2 | 2.02 | 0.59 |
| 3:I:91:LEU:HD12 | 3:I:127:CYS:SG | 2.42 | 0.59 |
| 1:A:332:MET:HE3 | 1:A:351:VAL:HG11 | 1.83 | 0.59 |
| 2:B:57:GLY:HA3 | 2:B:58:ALA:HB2 | 0.66 | 0.59 |
| 1:C:30:ILE:HD13 | 1:C:53:TYR:CE2 | 2.38 | 0.59 |
| 1:C:128:SER:OG | 1:C:129:CYS:N | 2.34 | 0.59 |
| 2:D:63:PRO:CD | 2:D:87:PHE:HA | 2.32 | 0.59 |
| 1:E:161:TYR:C | 1:E:163:ASP:H | 2.05 | 0.59 |
| 1:E:408:TYR:CG | 1:E:418:PHE:HZ | 2.20 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:167:LEU:HA | 2:F:200:CYS:O | 2.01 | 0.59 |
| 1:A:30:ILE:HD13 | 1:A:53:TYR:CE2 | 2.38 | 0.59 |
| 2:B:344:VAL:HG11 | 2:B:346:TRP:NE1 | 2.16 | 0.59 |
| 1:C:332:MET:CE | 1:C:351:VAL:HG11 | 2.32 | 0.59 |
| 2:D:276:ILE:HD11 | 2:D:280:LYS:HD2 | 1.85 | 0.59 |
| 2:D:407:TRP:O | 2:D:411:GLU:HG2 | 2.02 | 0.59 |
| 2:D:413:MET:O | 2:D:414:GLU:HG3 | 2.02 | 0.59 |
| 1:E:30:ILE:HD13 | 1:E:53:TYR:CE2 | 2.38 | 0.59 |
| 1:E:172:VAL:CG1 | 1:E:387:LEU:HD21 | 2.24 | 0.59 |
| 2:F:248:LEU:CD2 | 2:F:353:VAL:O | 2.49 | 0.59 |
| 2:F:435:VAL:O | 2:F:435:VAL:HG12 | 2.02 | 0.59 |
| 1:G:30:ILE:HD13 | 1:G:53:TYR:CE2 | 2.38 | 0.59 |
| 1:G:70:LEU:H | 1:G:145:THR:CG2 | 2.10 | 0.59 |
| 2:H:217:LEU:HD11 | 2:H:277:SER:HA | 1.82 | 0.59 |
| 2:H:435:VAL:HG12 | 2:H:435:VAL:O | 2.02 | 0.59 |
| 2:D:371:VAL:HG12 | 2:D:372:GLN:N | 2.17 | 0.59 |
| 1:E:19:LYS:CG | 1:E:228:ASN:HB3 | 2.31 | 0.59 |
| 1:E:70:LEU:H | 1:E:145:THR:CG2 | 2.10 | 0.59 |
| 1:E:205:ASP:OD1 | 1:E:304:ALA:CB | 2.50 | 0.59 |
| 2:F:346:TRP:O | 1:G:398:MET:HE2 | 2.03 | 0.59 |
| 2:F:369:ALA:O | 2:F:370:LYS:HB3 | 2.03 | 0.59 |
| 1:G:172:VAL:CG1 | 1:G:387:LEU:HD21 | 2.24 | 0.59 |
| 1:G:273:ALA:HB3 | 1:G:274:PRO:CD | 2.29 | 0.59 |
| 3:I:72:VAL:HG13 | 3:I:83:LEU:HD13 | 1.84 | 0.59 |
| 1:A:205:ASP:OD1 | 1:A:304:ALA:CB | 2.50 | 0.59 |
| 2:B:369:ALA:O | 2:B:370:LYS:HB3 | 2.03 | 0.59 |
| 1:C:19:LYS:CG | 1:C:228:ASN:HB3 | 2.31 | 0.59 |
| 1:C:408:TYR:CG | 1:C:418:PHE:HZ | 2.20 | 0.59 |
| 2:D:296:PHE:CE1 | 2:D:335:ILE:CG2 | 2.73 | 0.59 |
| 2:D:369:ALA:O | 2:D:370:LYS:HB3 | 2.03 | 0.59 |
| 1:E:279:GLY:O | 1:E:282:GLN:HB3 | 2.01 | 0.59 |
| 1:G:161:TYR:C | 1:G:163:ASP:H | 2.05 | 0.59 |
| 2:H:369:ALA:O | 2:H:370:LYS:HB3 | 2.03 | 0.59 |
| 1:A:324:SER:O | 1:A:328:VAL:HG23 | 2.01 | 0.59 |
| 1:A:408:TYR:CG | 1:A:418:PHE:HZ | 2.20 | 0.59 |
| 1:C:205:ASP:OD1 | 1:C:304:ALA:CB | 2.50 | 0.59 |
| 1:C:324:SER:O | 1:C:328:VAL:HG23 | 2.01 | 0.59 |
| 1:G:19:LYS:CG | 1:G:228:ASN:HB3 | 2.31 | 0.59 |
| 1:G:254:LYS:HE3 | 1:G:352:LYS:CE | 2.27 | 0.59 |
| 2:H:115:ILE:O | 2:H:115:ILE:HD13 | 2.02 | 0.59 |
| 1:A:161:TYR:C | 1:A:163:ASP:H | 2.05 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:279:GLY:O | 1:A:282:GLN:HB3 | 2.01 | 0.59 |
| 2:D:115:ILE:O | 2:D:115:ILE:HD13 | 2.02 | 0.59 |
| 2:D:167:LEU:HA | 2:D:200:CYS:O | 2.01 | 0.59 |
| 2:F:115:ILE:O | 2:F:115:ILE:HD13 | 2.02 | 0.59 |
| 1:G:325:MET:HE2 | 1:G:355:VAL:HG21 | 1.85 | 0.59 |
| 2:H:276:ILE:HD11 | 2:H:280:LYS:HD2 | 1.85 | 0.59 |
| 1:A:128:SER:OG | 1:A:129:CYS:N | 2.34 | 0.59 |
| 2:B:167:LEU:HA | 2:B:200:CYS:O | 2.01 | 0.59 |
| 2:B:407:TRP:O | 2:B:411:GLU:HG2 | 2.02 | 0.59 |
| 2:F:276:ILE:HD11 | 2:F:280:LYS:HD2 | 1.85 | 0.59 |
| 2:F:413:MET:O | 2:F:414:GLU:HG3 | 2.02 | 0.59 |
| 1:G:324:SER:CB | 1:G:327:GLU:HG2 | 2.30 | 0.59 |
| 2:H:3:GLU:HG3 | 2:H:51:THR:HA | 1.75 | 0.59 |
| 2:H:413:MET:O | 2:H:414:GLU:HG3 | 2.02 | 0.59 |
| 2:B:381:THR:C | 2:B:383:ALA:N | 2.56 | 0.59 |
| 2:B:413:MET:O | 2:B:414:GLU:HG3 | 2.02 | 0.59 |
| 1:C:151:THR:OG1 | 1:C:193:GLN:HB3 | 2.03 | 0.59 |
| 2:D:119:LEU:O | 2:D:122:ILE:HG12 | 2.02 | 0.59 |
| 1:E:128:SER:OG | 1:E:129:CYS:N | 2.34 | 0.59 |
| 1:E:141:LEU:CD1 | 1:E:141:LEU:N | 2.65 | 0.59 |
| 3:I:113:ILE:HD12 | 3:I:118:GLU:HB3 | 1.85 | 0.59 |
| 1:A:19:LYS:CG | 1:A:228:ASN:HB3 | 2.31 | 0.58 |
| 2:B:3:GLU:HG3 | 2:B:51:THR:HA | 1.75 | 0.58 |
| 1:C:349:ASN:O | 2:D:181:VAL:HG13 | 2.03 | 0.58 |
| 2:D:6:SER:HA | 2:D:136:SER:O | 2.03 | 0.58 |
| 1:G:2:ARG:NH2 | 2:H:99:ALA:H | 2.00 | 0.58 |
| 1:G:68:VAL:CG1 | 1:G:149:MET:SD | 2.90 | 0.58 |
| 1:G:141:LEU:N | 1:G:141:LEU:CD1 | 2.65 | 0.58 |
| 1:G:205:ASP:OD1 | 1:G:304:ALA:CB | 2.50 | 0.58 |
| 1:G:332:MET:HE3 | 1:G:351:VAL:HG11 | 1.84 | 0.58 |
| 2:H:202:PHE:CE2 | 2:H:378:LEU:HD22 | 2.38 | 0.58 |
| 1:A:151:THR:OG1 | 1:A:193:GLN:HB3 | 2.03 | 0.58 |
| 1:A:307:PRO:HB3 | 1:A:312:TYR:OH | 2.04 | 0.58 |
| 1:C:68:VAL:CG1 | 1:C:149:MET:SD | 2.90 | 0.58 |
| 1:C:254:LYS:NZ | 2:D:101:ASN:OD1 | 2.26 | 0.58 |
| 2:D:381:THR:C | 2:D:383:ALA:N | 2.56 | 0.58 |
| 2:F:6:SER:HA | 2:F:136:SER:O | 2.03 | 0.58 |
| 2:F:202:PHE:CE2 | 2:F:378:LEU:HD22 | 2.38 | 0.58 |
| 1:G:349:ASN:C | 1:G:349:ASN:HD22 | 2.06 | 0.58 |
| 3:I:100:GLY:O | 3:I:101:VAL:HG23 | 2.02 | 0.58 |
| 1:A:70:LEU:C | 1:A:99:ALA:HB2 | 2.24 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:88:ARG:CZ | 1:E:283:TYR:HE1 | 2.16 | 0.58 |
| 1:A:89:PRO:HA | 1:A:92:PHE:CD1 | 2.38 | 0.58 |
| 1:A:349:ASN:C | 1:A:349:ASN:HD22 | 2.07 | 0.58 |
| 2:B:6:SER:HA | 2:B:136:SER:O | 2.03 | 0.58 |
| 2:B:119:LEU:O | 2:B:122:ILE:HG12 | 2.02 | 0.58 |
| 2:B:202:PHE:CE2 | 2:B:378:LEU:HD22 | 2.38 | 0.58 |
| 2:B:317:LEU:HD11 | 2:B:351:PHE:CE2 | 2.38 | 0.58 |
| 1:C:217:LEU:C | 1:C:219:LEU:N | 2.55 | 0.58 |
| 1:C:307:PRO:HB3 | 1:C:312:TYR:OH | 2.04 | 0.58 |
| 1:C:325:MET:HG2 | 2:D:224:TYR:CD1 | 2.37 | 0.58 |
| 2:D:317:LEU:HD11 | 2:D:351:PHE:CE2 | 2.38 | 0.58 |
| 1:E:89:PRO:HA | 1:E:92:PHE:CD1 | 2.38 | 0.58 |
| 1:E:324:SER:CB | 1:E:327:GLU:HG2 | 2.30 | 0.58 |
| 1:E:332:MET:CE | 1:E:351:VAL:HG11 | 2.32 | 0.58 |
| 1:E:349:ASN:C | 1:E:349:ASN:HD22 | 2.07 | 0.58 |
| 2:F:326:LYS:HB3 | 1:G:222:PRO:CD | 2.33 | 0.58 |
| 1:G:151:THR:OG1 | 1:G:193:GLN:HB3 | 2.03 | 0.58 |
| 2:B:5:ILE:HD11 | 2:B:64:ARG:HH12 | 1.59 | 0.58 |
| 2:B:115:ILE:HD13 | 2:B:115:ILE:O | 2.02 | 0.58 |
| 1:C:349:ASN:HD22 | 1:C:349:ASN:C | 2.07 | 0.58 |
| 2:D:202:PHE:CE2 | 2:D:378:LEU:HD22 | 2.38 | 0.58 |
| 2:F:2:ARG:N | 2:F:131:GLY:O | 2.36 | 0.58 |
| 2:F:119:LEU:O | 2:F:122:ILE:HG12 | 2.02 | 0.58 |
| 1:G:258:ASN:ND2 | 1:G:352:LYS:CE | 2.55 | 0.58 |
| 1:A:319:PHE:HA | 1:A:375:ALA:HA | 1.86 | 0.58 |
| 1:C:89:PRO:HA | 1:C:92:PHE:CD1 | 2.38 | 0.58 |
| 1:C:325:MET:HE2 | 1:C:355:VAL:HG21 | 1.83 | 0.58 |
| 2:D:264:ARG:HB2 | 2:D:266:HIS:HD2 | 1.67 | 0.58 |
| 1:E:198:THR:HG22 | 1:E:265:LEU:HD22 | 1.86 | 0.58 |
| 2:F:67:PHE:CZ | 2:F:87:PHE:CE1 | 2.92 | 0.58 |
| 1:G:70:LEU:C | 1:G:99:ALA:HB2 | 2.24 | 0.58 |
| 1:G:253:ARG:O | 1:G:257:VAL:N | 2.33 | 0.58 |
| 1:C:70:LEU:C | 1:C:99:ALA:HB2 | 2.24 | 0.58 |
| 1:C:319:PHE:HA | 1:C:375:ALA:HA | 1.86 | 0.58 |
| 2:D:5:ILE:HD12 | 2:D:64:ARG:HH12 | 1.69 | 0.58 |
| 1:E:68:VAL:CG1 | 1:E:149:MET:SD | 2.90 | 0.58 |
| 1:E:151:THR:OG1 | 1:E:193:GLN:HB3 | 2.03 | 0.58 |
| 1:G:128:SER:OG | 1:G:129:CYS:N | 2.34 | 0.58 |
| 1:G:273:ALA:CB | 1:G:274:PRO:HD3 | 2.30 | 0.58 |
| 2:H:2:ARG:N | 2:H:131:GLY:O | 2.36 | 0.58 |
| 2:H:6:SER:HA | 2:H:136:SER:O | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:67:PHE:CZ | 2:H:87:PHE:CE1 | 2.92 | 0.58 |
| 2:B:51:THR:O | 2:B:52:PHE:CD1 | 2.57 | 0.58 |
| 2:B:218:ASP:O | 2:B:219:ILE:HG23 | 2.04 | 0.58 |
| 2:D:2:ARG:N | 2:D:131:GLY:O | 2.36 | 0.58 |
| 2:D:67:PHE:CZ | 2:D:87:PHE:CE1 | 2.92 | 0.58 |
| 2:F:5:ILE:HD12 | 2:F:64:ARG:HH12 | 1.68 | 0.58 |
| 2:F:30:ILE:HD13 | 2:F:61:HIS:CG | 2.38 | 0.58 |
| 1:G:89:PRO:HA | 1:G:92:PHE:CD1 | 2.38 | 0.58 |
| 2:B:67:PHE:CZ | 2:B:87:PHE:CE1 | 2.92 | 0.58 |
| 1:C:183:GLU:HB3 | 1:C:184:PRO:CD | 2.33 | 0.58 |
| 2:H:5:ILE:HD12 | 2:H:64:ARG:HH12 | 1.69 | 0.58 |
| 2:H:119:LEU:O | 2:H:122:ILE:HG12 | 2.02 | 0.58 |
| 2:H:268:PRO:HA | 2:H:379:SER:O | 2.04 | 0.58 |
| 1:C:299:LYS:O | 1:C:300:ASN:CB | 2.51 | 0.58 |
| 2:D:110:ILE:CG2 | 2:D:111:GLY:H | 2.15 | 0.58 |
| 2:D:218:ASP:O | 2:D:219:ILE:HG23 | 2.04 | 0.58 |
| 1:E:70:LEU:C | 1:E:99:ALA:HB2 | 2.24 | 0.58 |
| 2:F:218:ASP:O | 2:F:219:ILE:HG23 | 2.04 | 0.58 |
| 2:F:268:PRO:HA | 2:F:379:SER:O | 2.04 | 0.58 |
| 1:G:198:THR:HG22 | 1:G:265:LEU:HD22 | 1.86 | 0.58 |
| 1:G:325:MET:HE1 | 1:G:355:VAL:HG11 | 1.85 | 0.58 |
| 2:H:218:ASP:O | 2:H:219:ILE:HG23 | 2.04 | 0.58 |
| 2:H:317:LEU:HD11 | 2:H:351:PHE:CE2 | 2.38 | 0.58 |
| 2:H:381:THR:C | 2:H:383:ALA:N | 2.56 | 0.58 |
| 1:A:68:VAL:CG1 | 1:A:149:MET:SD | 2.90 | 0.58 |
| 2:B:63:PRO:HG3 | 2:B:87:PHE:CB | 2.34 | 0.58 |
| 2:B:159:VAL:HG13 | 3:I:78:ARG:CG | 2.33 | 0.58 |
| 2:B:165:SER:HA | 2:B:199:ASP:OD2 | 2.04 | 0.58 |
| 2:B:260:VAL:HG22 | 1:C:407:TRP:HE1 | 1.68 | 0.58 |
| 2:D:268:PRO:HA | 2:D:379:SER:O | 2.04 | 0.58 |
| 1:E:274:PRO:CG | 1:E:371:LEU:HD21 | 2.34 | 0.58 |
| 1:E:307:PRO:HB3 | 1:E:312:TYR:OH | 2.04 | 0.58 |
| 2:F:317:LEU:HD11 | 2:F:351:PHE:CE2 | 2.38 | 0.58 |
| 2:F:381:THR:C | 2:F:383:ALA:N | 2.56 | 0.58 |
| 1:G:307:PRO:HB3 | 1:G:312:TYR:OH | 2.04 | 0.58 |
| 2:B:248:LEU:CD2 | 2:B:353:VAL:O | 2.49 | 0.57 |
| 1:C:422:GLU:O | 1:C:426:ASN:N | 2.37 | 0.57 |
| 1:E:54:ASN:ND2 | 1:E:64:ARG:HD3 | 2.15 | 0.57 |
| 1:E:253:ARG:O | 1:E:257:VAL:N | 2.33 | 0.57 |
| 1:G:274:PRO:CG | 1:G:371:LEU:HD21 | 2.34 | 0.57 |
| 1:A:5:VAL:CG2 | 1:A:135:PHE:HD2 | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:217:LEU:C | 1:A:219:LEU:N | 2.55 | 0.57 |
| 1:A:274:PRO:CG | 1:A:371:LEU:HD21 | 2.34 | 0.57 |
| 1:A:299:LYS:O | 1:A:300:ASN:CB | 2.51 | 0.57 |
| 2:B:345:ASP:O | 2:B:347:CYS:N | 2.37 | 0.57 |
| 1:C:274:PRO:CG | 1:C:371:LEU:HD21 | 2.34 | 0.57 |
| 1:C:301:MET:CE | 1:C:377:PHE:HE2 | 2.17 | 0.57 |
| 2:F:329:ASN:OD1 | 1:G:210:TYR:CE1 | 2.53 | 0.57 |
| 1:G:5:VAL:CG2 | 1:G:135:PHE:HD2 | 2.18 | 0.57 |
| 1:G:149:MET:O | 1:G:153:LEU:HD13 | 2.05 | 0.57 |
| 3:I:55:VAL:HG21 | 3:I:57:PHE:CZ | 2.39 | 0.57 |
| 1:A:183:GLU:HB3 | 1:A:184:PRO:CD | 2.33 | 0.57 |
| 1:A:198:THR:HG22 | 1:A:265:LEU:HD22 | 1.85 | 0.57 |
| 2:B:313:MET:O | 2:B:314:ALA:HB2 | 2.04 | 0.57 |
| 1:C:149:MET:O | 1:C:153:LEU:HD13 | 2.05 | 0.57 |
| 1:C:180:THR:CG2 | 1:C:181:VAL:H | 2.17 | 0.57 |
| 1:E:5:VAL:CG2 | 1:E:135:PHE:HD2 | 2.18 | 0.57 |
| 2:F:165:SER:HA | 2:F:199:ASP:OD2 | 2.04 | 0.57 |
| 2:F:166:LYS:HD2 | 2:F:197:HIS:O | 2.04 | 0.57 |
| 2:H:165:SER:HA | 2:H:199:ASP:OD2 | 2.04 | 0.57 |
| 2:H:345:ASP:O | 2:H:347:CYS:N | 2.37 | 0.57 |
| 1:A:301:MET:CE | 1:A:377:PHE:HE2 | 2.17 | 0.57 |
| 2:B:2:ARG:N | 2:B:131:GLY:O | 2.36 | 0.57 |
| 2:B:110:ILE:CG2 | 2:B:111:GLY:H | 2.15 | 0.57 |
| 1:C:5:VAL:CG2 | 1:C:135:PHE:HD2 | 2.18 | 0.57 |
| 1:C:6:HIS:HB3 | 1:C:65:ALA:HB2 | 1.87 | 0.57 |
| 2:D:165:SER:HA | 2:D:199:ASP:OD2 | 2.04 | 0.57 |
| 2:D:345:ASP:O | 2:D:347:CYS:N | 2.37 | 0.57 |
| 1:E:273:ALA:CB | 1:E:274:PRO:HD3 | 2.30 | 0.57 |
| 1:E:320:ARG:O | 1:E:359:PRO:HA | 2.04 | 0.57 |
| 1:A:180:THR:CG2 | 1:A:181:VAL:H | 2.17 | 0.57 |
| 1:A:320:ARG:O | 1:A:359:PRO:HA | 2.04 | 0.57 |
| 2:B:216:ASN:O | 2:B:217:LEU:HB2 | 2.05 | 0.57 |
| 1:E:149:MET:O | 1:E:153:LEU:HD13 | 2.05 | 0.57 |
| 1:E:301:MET:CE | 1:E:377:PHE:HE2 | 2.17 | 0.57 |
| 2:F:345:ASP:O | 2:F:347:CYS:N | 2.37 | 0.57 |
| 1:G:301:MET:CE | 1:G:377:PHE:HE2 | 2.17 | 0.57 |
| 1:A:149:MET:O | 1:A:153:LEU:HD13 | 2.05 | 0.57 |
| 2:B:117:LEU:HD11 | 2:B:121:ARG:HH22 | 1.69 | 0.57 |
| 2:B:264:ARG:HB2 | 2:B:266:HIS:HD2 | 1.67 | 0.57 |
| 2:B:268:PRO:HA | 2:B:379:SER:O | 2.04 | 0.57 |
| 1:C:270:PRO:HA | 1:C:377:PHE:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:152:LEU:HA | 2:D:155:GLU:CB | 2.35 | 0.57 |
| 2:D:216:ASN:O | 2:D:217:LEU:HB2 | 2.05 | 0.57 |
| 1:E:6:HIS:HB3 | 1:E:65:ALA:HB2 | 1.87 | 0.57 |
| 1:G:6:HIS:HB3 | 1:G:65:ALA:HB2 | 1.87 | 0.57 |
| 1:G:299:LYS:O | 1:G:300:ASN:CB | 2.51 | 0.57 |
| 1:G:320:ARG:O | 1:G:359:PRO:HA | 2.04 | 0.57 |
| 1:A:6:HIS:HB3 | 1:A:65:ALA:HB2 | 1.87 | 0.57 |
| 1:A:70:LEU:CD1 | 1:A:145:THR:HG23 | 2.35 | 0.57 |
| 2:B:152:LEU:HA | 2:B:155:GLU:CB | 2.35 | 0.57 |
| 2:B:209:ILE:CG2 | 2:B:227:LEU:HD22 | 2.35 | 0.57 |
| 1:C:30:ILE:HA | 1:C:35:SER:O | 2.04 | 0.57 |
| 1:C:198:THR:HG22 | 1:C:265:LEU:HD22 | 1.86 | 0.57 |
| 1:C:319:PHE:CD2 | 1:C:375:ALA:HB2 | 2.40 | 0.57 |
| 2:D:313:MET:O | 2:D:314:ALA:HB2 | 2.04 | 0.57 |
| 2:D:436:GLY:C | 2:D:438:ASP:H | 2.08 | 0.57 |
| 1:E:70:LEU:CD1 | 1:E:145:THR:HG23 | 2.35 | 0.57 |
| 2:F:117:LEU:HD11 | 2:F:121:ARG:HH22 | 1.69 | 0.57 |
| 2:F:152:LEU:HA | 2:F:155:GLU:CB | 2.35 | 0.57 |
| 1:G:270:PRO:HA | 1:G:377:PHE:O | 2.04 | 0.57 |
| 1:G:319:PHE:HA | 1:G:375:ALA:HA | 1.86 | 0.57 |
| 2:H:152:LEU:HA | 2:H:155:GLU:CB | 2.35 | 0.57 |
| 2:H:166:LYS:HD2 | 2:H:197:HIS:O | 2.04 | 0.57 |
| 2:H:362:VAL:CG1 | 2:H:368:LEU:HB2 | 2.35 | 0.57 |
| 2:B:278:ALA:O | 2:B:279:GLU:CB | 2.43 | 0.57 |
| 2:B:349:THR:O | 1:C:181:VAL:HG13 | 2.05 | 0.57 |
| 2:B:436:GLY:C | 2:B:438:ASP:H | 2.08 | 0.57 |
| 2:D:63:PRO:HG2 | 2:D:87:PHE:HA | 1.86 | 0.57 |
| 2:D:117:LEU:HD11 | 2:D:121:ARG:HH22 | 1.69 | 0.57 |
| 2:D:209:ILE:CG2 | 2:D:227:LEU:HD22 | 2.35 | 0.57 |
| 1:E:14:ASN:OD1 | 1:E:75:MET:HG2 | 2.05 | 0.57 |
| 1:E:183:GLU:HB3 | 1:E:184:PRO:CD | 2.33 | 0.57 |
| 1:G:54:ASN:ND2 | 1:G:64:ARG:HD3 | 2.15 | 0.57 |
| 1:G:70:LEU:CD1 | 1:G:145:THR:HG23 | 2.35 | 0.57 |
| 2:H:209:ILE:CG2 | 2:H:227:LEU:HD22 | 2.35 | 0.57 |
| 1:A:319:PHE:CD2 | 1:A:375:ALA:HB2 | 2.40 | 0.57 |
| 1:C:70:LEU:CD1 | 1:C:145:THR:HG23 | 2.35 | 0.57 |
| 1:C:320:ARG:O | 1:C:359:PRO:HA | 2.04 | 0.57 |
| 2:D:139:HIS:CE1 | 2:D:170:SER:HB3 | 2.40 | 0.57 |
| 1:E:180:THR:CG2 | 1:E:181:VAL:H | 2.17 | 0.57 |
| 1:E:253:ARG:O | 1:E:254:LYS:C | 2.42 | 0.57 |
| 1:E:270:PRO:HA | 1:E:377:PHE:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:209:ILE:CG2 | 2:F:227:LEU:HD22 | 2.35 | 0.57 |
| 2:F:216:ASN:O | 2:F:217:LEU:HB2 | 2.05 | 0.57 |
| 2:F:276:ILE:CG2 | 2:F:369:ALA:HB2 | 2.26 | 0.57 |
| 2:F:329:ASN:HB3 | 1:G:210:TYR:CZ | 2.35 | 0.57 |
| 2:F:436:GLY:C | 2:F:438:ASP:H | 2.08 | 0.57 |
| 1:G:2:ARG:HH21 | 2:H:99:ALA:H | 1.50 | 0.57 |
| 2:H:293:ASN:HD21 | 2:H:338:LYS:HZ1 | 1.52 | 0.57 |
| 2:H:436:GLY:C | 2:H:438:ASP:H | 2.08 | 0.57 |
| 1:A:30:ILE:HA | 1:A:35:SER:O | 2.04 | 0.57 |
| 1:A:270:PRO:HA | 1:A:377:PHE:O | 2.04 | 0.57 |
| 2:B:139:HIS:CE1 | 2:B:170:SER:HB3 | 2.40 | 0.57 |
| 2:B:166:LYS:HD2 | 2:B:197:HIS:O | 2.04 | 0.57 |
| 2:D:210:TYR:CE2 | 2:D:227:LEU:HD11 | 2.40 | 0.57 |
| 1:E:283:TYR:C | 1:E:284:ARG:HG2 | 2.24 | 0.57 |
| 2:F:139:HIS:CE1 | 2:F:170:SER:HB3 | 2.40 | 0.57 |
| 2:F:175:PRO:HG3 | 2:F:304:LYS:CG | 2.35 | 0.57 |
| 2:F:362:VAL:CG1 | 2:F:368:LEU:HB2 | 2.35 | 0.57 |
| 1:G:257:VAL:O | 2:H:404:PHE:HD2 | 1.88 | 0.57 |
| 1:G:319:PHE:CD2 | 1:G:375:ALA:HB2 | 2.40 | 0.57 |
| 2:H:63:PRO:HG2 | 2:H:87:PHE:HA | 1.86 | 0.57 |
| 2:H:117:LEU:HD11 | 2:H:121:ARG:HH22 | 1.69 | 0.57 |
| 2:H:175:PRO:HG3 | 2:H:304:LYS:CG | 2.35 | 0.57 |
| 2:H:216:ASN:O | 2:H:217:LEU:HB2 | 2.05 | 0.57 |
| 1:A:50:ASN:O | 1:A:64:ARG:NH2 | 2.38 | 0.56 |
| 1:C:50:ASN:O | 1:C:64:ARG:NH2 | 2.38 | 0.56 |
| 1:C:248:LEU:CD2 | 2:D:179:THR:CG2 | 2.82 | 0.56 |
| 2:D:166:LYS:HD2 | 2:D:197:HIS:O | 2.04 | 0.56 |
| 1:E:50:ASN:O | 1:E:64:ARG:NH2 | 2.38 | 0.56 |
| 1:E:299:LYS:O | 1:E:300:ASN:CB | 2.51 | 0.56 |
| 1:E:319:PHE:HA | 1:E:375:ALA:HA | 1.86 | 0.56 |
| 1:G:4:ILE:HD13 | 1:G:136:GLN:NE2 | 2.18 | 0.56 |
| 1:G:180:THR:CG2 | 1:G:181:VAL:H | 2.17 | 0.56 |
| 1:G:253:ARG:O | 1:G:254:LYS:C | 2.42 | 0.56 |
| 2:H:102:ASN:ND2 | 2:H:407:TRP:NE1 | 2.52 | 0.56 |
| 2:B:210:TYR:CE2 | 2:B:227:LEU:HD11 | 2.40 | 0.56 |
| 2:B:362:VAL:CG1 | 2:B:368:LEU:HB2 | 2.35 | 0.56 |
| 2:D:362:VAL:CG1 | 2:D:368:LEU:HB2 | 2.35 | 0.56 |
| 1:E:319:PHE:CD2 | 1:E:375:ALA:HB2 | 2.40 | 0.56 |
| 2:F:63:PRO:HG2 | 2:F:87:PHE:HA | 1.86 | 0.56 |
| 1:G:183:GLU:HB3 | 1:G:184:PRO:CD | 2.33 | 0.56 |
| 1:G:245:PRO:HG3 | 2:H:73:THR:HG23 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:276:ILE:CG2 | 2:H:369:ALA:HB2 | 2.26 | 0.56 |
| 1:A:283:TYR:C | 1:A:284:ARG:HG2 | 2.24 | 0.56 |
| 2:B:242:LEU:C | 2:B:244:PHE:H | 2.09 | 0.56 |
| 2:B:362:VAL:HG11 | 2:B:368:LEU:O | 2.04 | 0.56 |
| 2:B:382:THR:O | 2:B:382:THR:HG22 | 2.05 | 0.56 |
| 2:D:276:ILE:O | 2:D:369:ALA:CB | 2.53 | 0.56 |
| 2:D:382:THR:O | 2:D:382:THR:HG22 | 2.05 | 0.56 |
| 2:D:409:VAL:C | 2:D:411:GLU:H | 2.09 | 0.56 |
| 2:F:210:TYR:CE2 | 2:F:227:LEU:HD11 | 2.40 | 0.56 |
| 2:F:242:LEU:C | 2:F:244:PHE:H | 2.09 | 0.56 |
| 2:F:362:VAL:HG11 | 2:F:368:LEU:O | 2.04 | 0.56 |
| 1:G:14:ASN:OD1 | 1:G:75:MET:HG2 | 2.05 | 0.56 |
| 1:G:30:ILE:HA | 1:G:35:SER:O | 2.04 | 0.56 |
| 1:G:50:ASN:O | 1:G:64:ARG:NH2 | 2.38 | 0.56 |
| 2:H:139:HIS:CE1 | 2:H:170:SER:HB3 | 2.40 | 0.56 |
| 2:H:210:TYR:CE2 | 2:H:227:LEU:HD11 | 2.40 | 0.56 |
| 2:H:242:LEU:C | 2:H:244:PHE:H | 2.09 | 0.56 |
| 2:H:409:VAL:C | 2:H:411:GLU:H | 2.09 | 0.56 |
| 1:A:216:THR:O | 1:A:217:LEU:HD12 | 2.05 | 0.56 |
| 1:C:223:THR:HG22 | 1:C:224:TYR:N | 2.21 | 0.56 |
| 1:E:4:ILE:HD13 | 1:E:136:GLN:NE2 | 2.18 | 0.56 |
| 1:E:223:THR:HG22 | 1:E:224:TYR:N | 2.21 | 0.56 |
| 2:F:382:THR:HG22 | 2:F:382:THR:O | 2.06 | 0.56 |
| 2:F:409:VAL:C | 2:F:411:GLU:H | 2.09 | 0.56 |
| 1:G:223:THR:HG22 | 1:G:224:TYR:N | 2.21 | 0.56 |
| 1:G:283:TYR:C | 1:G:284:ARG:HG2 | 2.24 | 0.56 |
| 2:H:313:MET:O | 2:H:314:ALA:HB2 | 2.04 | 0.56 |
| 2:H:362:VAL:HG11 | 2:H:368:LEU:O | 2.04 | 0.56 |
| 2:H:382:THR:O | 2:H:382:THR:HG22 | 2.06 | 0.56 |
| 1:A:325:MET:HE2 | 1:A:355:VAL:HG21 | 1.86 | 0.56 |
| 1:C:132:LEU:CD2 | 1:C:164:ARG:HG3 | 2.32 | 0.56 |
| 1:C:250:ALA:CA | 1:C:254:LYS:HE2 | 2.35 | 0.56 |
| 2:D:362:VAL:HG11 | 2:D:368:LEU:O | 2.04 | 0.56 |
| 1:E:312:TYR:O | 1:E:344:VAL:HB | 2.05 | 0.56 |
| 1:A:223:THR:HG22 | 1:A:224:TYR:N | 2.21 | 0.56 |
| 1:A:311:ARG:HG2 | 1:A:311:ARG:HH11 | 1.71 | 0.56 |
| 2:B:56:THR:CB | 2:F:284:GLU:HG3 | 2.35 | 0.56 |
| 1:C:216:THR:O | 1:C:217:LEU:HD12 | 2.05 | 0.56 |
| 1:C:311:ARG:HG2 | 1:C:311:ARG:HH11 | 1.71 | 0.56 |
| 1:E:30:ILE:HA | 1:E:35:SER:O | 2.05 | 0.56 |
| 2:F:313:MET:O | 2:F:314:ALA:HB2 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:312:TYR:O | 1:G:344:VAL:HB | 2.05 | 0.56 |
| 1:A:132:LEU:CD2 | 1:A:164:ARG:HG3 | 2.32 | 0.56 |
| 1:A:151:THR:OG1 | 1:A:193:GLN:CB | 2.54 | 0.56 |
| 2:B:19:ALA:CB | 2:B:228:ASN:HB3 | 2.35 | 0.56 |
| 2:B:409:VAL:C | 2:B:411:GLU:H | 2.09 | 0.56 |
| 1:C:19:LYS:O | 1:C:23:VAL:HG23 | 2.06 | 0.56 |
| 1:C:312:TYR:O | 1:C:344:VAL:HB | 2.05 | 0.56 |
| 2:D:242:LEU:C | 2:D:244:PHE:H | 2.09 | 0.56 |
| 1:E:311:ARG:HD2 | 1:E:344:VAL:H | 1.71 | 0.56 |
| 1:G:424:ASN:C | 1:G:424:ASN:HD22 | 2.09 | 0.56 |
| 1:A:297:ASP:OD1 | 1:A:298:ALA:N | 2.39 | 0.56 |
| 2:B:56:THR:CB | 2:F:284:GLU:CD | 2.74 | 0.56 |
| 2:B:277:SER:O | 2:B:280:LYS:HB2 | 2.06 | 0.56 |
| 1:C:151:THR:OG1 | 1:C:193:GLN:CB | 2.54 | 0.56 |
| 1:C:283:TYR:C | 1:C:284:ARG:HG2 | 2.24 | 0.56 |
| 2:D:175:PRO:HG3 | 2:D:304:LYS:CG | 2.35 | 0.56 |
| 2:D:253:THR:O | 2:D:256:GLN:HG2 | 2.06 | 0.56 |
| 1:E:19:LYS:O | 1:E:23:VAL:HG23 | 2.06 | 0.56 |
| 1:E:311:ARG:HG2 | 1:E:311:ARG:HH11 | 1.71 | 0.56 |
| 1:E:424:ASN:HD22 | 1:E:424:ASN:C | 2.09 | 0.56 |
| 2:F:331:ALA:O | 2:F:334:THR:HG22 | 2.05 | 0.56 |
| 1:G:139:HIS:HE1 | 1:G:168:THR:HG23 | 1.71 | 0.56 |
| 1:A:139:HIS:HE1 | 1:A:168:THR:HG23 | 1.71 | 0.56 |
| 1:A:250:ALA:CA | 1:A:254:LYS:HE2 | 2.35 | 0.56 |
| 1:A:324:SER:C | 1:A:326:LYS:N | 2.59 | 0.56 |
| 1:C:14:ASN:OD1 | 1:C:75:MET:HG2 | 2.05 | 0.56 |
| 1:C:165:ILE:HD13 | 1:C:165:ILE:H | 1.71 | 0.56 |
| 1:E:139:HIS:HE1 | 1:E:168:THR:HG23 | 1.71 | 0.56 |
| 1:E:204:ILE:HG21 | 1:E:231:VAL:CG2 | 2.36 | 0.56 |
| 2:F:253:THR:O | 2:F:256:GLN:HG2 | 2.06 | 0.56 |
| 1:G:19:LYS:O | 1:G:23:VAL:HG23 | 2.06 | 0.56 |
| 1:G:216:THR:O | 1:G:217:LEU:HD12 | 2.05 | 0.56 |
| 1:G:311:ARG:HG2 | 1:G:311:ARG:HH11 | 1.71 | 0.56 |
| 1:G:311:ARG:HD2 | 1:G:344:VAL:H | 1.71 | 0.56 |
| 2:H:16:ILE:HD12 | 2:H:171:ILE:HD11 | 1.87 | 0.56 |
| 2:H:276:ILE:O | 2:H:369:ALA:CB | 2.53 | 0.56 |
| 1:A:19:LYS:O | 1:A:23:VAL:HG23 | 2.06 | 0.56 |
| 1:A:311:ARG:HD2 | 1:A:344:VAL:H | 1.71 | 0.56 |
| 2:B:175:PRO:HG3 | 2:B:304:LYS:CG | 2.35 | 0.56 |
| 2:B:276:ILE:O | 2:B:369:ALA:CB | 2.53 | 0.56 |
| 2:B:329:ASN:HB3 | 1:C:210:TYR:HE1 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:408:TYR:CD1 | 2:B:418:PHE:HZ | 2.24 | 0.56 |
| 1:C:139:HIS:HE1 | 1:C:168:THR:HG23 | 1.71 | 0.56 |
| 1:C:272:PHE:HB3 | 1:C:275:LEU:HD22 | 1.88 | 0.56 |
| 2:D:19:ALA:CB | 2:D:228:ASN:HB3 | 2.35 | 0.56 |
| 2:D:388:TRP:HA | 2:D:388:TRP:CE3 | 2.41 | 0.56 |
| 1:E:182:VAL:HG23 | 1:E:186:ASN:ND2 | 2.20 | 0.56 |
| 1:G:191:VAL:HA | 1:G:194:LEU:HD12 | 1.88 | 0.56 |
| 1:G:352:LYS:HD2 | 2:H:181:VAL:CG2 | 2.11 | 0.56 |
| 1:A:182:VAL:HG23 | 1:A:186:ASN:ND2 | 2.20 | 0.55 |
| 1:C:182:VAL:HG23 | 1:C:186:ASN:ND2 | 2.20 | 0.55 |
| 1:C:297:ASP:OD1 | 1:C:298:ALA:N | 2.39 | 0.55 |
| 1:C:311:ARG:HD2 | 1:C:344:VAL:H | 1.71 | 0.55 |
| 1:C:424:ASN:HD22 | 1:C:424:ASN:C | 2.09 | 0.55 |
| 2:F:5:ILE:HG22 | 2:F:135:PHE:CD2 | 2.40 | 0.55 |
| 2:F:276:ILE:O | 2:F:369:ALA:CB | 2.52 | 0.55 |
| 1:G:2:ARG:NH2 | 2:H:99:ALA:N | 2.54 | 0.55 |
| 1:G:151:THR:OG1 | 1:G:193:GLN:CB | 2.54 | 0.55 |
| 1:G:204:ILE:HG21 | 1:G:231:VAL:CG2 | 2.36 | 0.55 |
| 2:H:253:THR:O | 2:H:256:GLN:HG2 | 2.06 | 0.55 |
| 2:H:277:SER:O | 2:H:280:LYS:HB2 | 2.06 | 0.55 |
| 2:H:331:ALA:O | 2:H:334:THR:HG22 | 2.05 | 0.55 |
| 1:A:190:SER:O | 1:A:194:LEU:HG | 2.06 | 0.55 |
| 1:A:204:ILE:HG21 | 1:A:231:VAL:CG2 | 2.36 | 0.55 |
| 1:A:312:TYR:O | 1:A:344:VAL:HB | 2.05 | 0.55 |
| 2:B:388:TRP:HA | 2:B:388:TRP:CE3 | 2.41 | 0.55 |
| 1:C:31:ASP:O | 1:C:32:PRO:C | 2.44 | 0.55 |
| 1:C:253:ARG:O | 1:C:254:LYS:C | 2.42 | 0.55 |
| 1:C:324:SER:C | 1:C:326:LYS:N | 2.59 | 0.55 |
| 1:E:191:VAL:HA | 1:E:194:LEU:HD12 | 1.88 | 0.55 |
| 1:G:182:VAL:HG23 | 1:G:186:ASN:ND2 | 2.20 | 0.55 |
| 2:H:19:ALA:CB | 2:H:228:ASN:HB3 | 2.35 | 0.55 |
| 2:H:30:ILE:HG23 | 2:H:34:GLY:O | 2.07 | 0.55 |
| 1:A:14:ASN:OD1 | 1:A:75:MET:HG2 | 2.05 | 0.55 |
| 1:A:272:PHE:HB3 | 1:A:275:LEU:HD22 | 1.88 | 0.55 |
| 1:C:191:VAL:HA | 1:C:194:LEU:HD12 | 1.88 | 0.55 |
| 2:D:278:ALA:O | 2:D:279:GLU:CB | 2.43 | 0.55 |
| 1:E:216:THR:O | 1:E:217:LEU:HD12 | 2.05 | 0.55 |
| 2:F:16:ILE:HD12 | 2:F:171:ILE:HD11 | 1.88 | 0.55 |
| 2:F:260:VAL:CG2 | 1:G:407:TRP:HE1 | 2.20 | 0.55 |
| 2:F:277:SER:O | 2:F:280:LYS:HB2 | 2.06 | 0.55 |
| 2:H:5:ILE:HG22 | 2:H:135:PHE:CD2 | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:150:THR:O | 2:H:153:LEU:N | 2.40 | 0.55 |
| 2:H:264:ARG:HB2 | 2:H:266:HIS:HD2 | 1.67 | 0.55 |
| 3:I:113:ILE:HG23 | 3:I:118:GLU:HB2 | 1.88 | 0.55 |
| 1:A:165:ILE:H | 1:A:165:ILE:HD13 | 1.71 | 0.55 |
| 2:B:209:ILE:HG22 | 2:B:227:LEU:HD22 | 1.88 | 0.55 |
| 2:B:253:THR:O | 2:B:256:GLN:HG2 | 2.06 | 0.55 |
| 2:B:276:ILE:CG2 | 2:B:369:ALA:HB2 | 2.26 | 0.55 |
| 2:B:331:ALA:O | 2:B:334:THR:HG22 | 2.05 | 0.55 |
| 2:B:346:TRP:HB3 | 1:C:401:ARG:CG | 2.36 | 0.55 |
| 1:C:310:GLY:CA | 1:C:436:GLN:HE21 | 2.19 | 0.55 |
| 2:D:5:ILE:HG22 | 2:D:135:PHE:CD2 | 2.40 | 0.55 |
| 2:D:331:ALA:O | 2:D:334:THR:HG22 | 2.05 | 0.55 |
| 1:E:132:LEU:CD2 | 1:E:164:ARG:HG3 | 2.32 | 0.55 |
| 2:F:30:ILE:HG23 | 2:F:34:GLY:O | 2.07 | 0.55 |
| 2:F:150:THR:O | 2:F:153:LEU:N | 2.40 | 0.55 |
| 1:G:119:LEU:O | 1:G:123:ARG:HG3 | 2.06 | 0.55 |
| 1:G:239:THR:HG22 | 1:G:240:THR:N | 2.22 | 0.55 |
| 2:B:150:THR:O | 2:B:153:LEU:N | 2.40 | 0.55 |
| 2:B:260:VAL:HG22 | 1:C:407:TRP:NE1 | 2.22 | 0.55 |
| 1:C:204:ILE:HG21 | 1:C:231:VAL:CG2 | 2.36 | 0.55 |
| 2:D:150:THR:O | 2:D:153:LEU:N | 2.40 | 0.55 |
| 2:D:277:SER:O | 2:D:280:LYS:HB2 | 2.06 | 0.55 |
| 2:H:209:ILE:HG22 | 2:H:227:LEU:HD22 | 1.88 | 0.55 |
| 1:A:191:VAL:HA | 1:A:194:LEU:HD12 | 1.88 | 0.55 |
| 1:A:310:GLY:CA | 1:A:436:GLN:HE21 | 2.19 | 0.55 |
| 2:D:209:ILE:HG22 | 2:D:227:LEU:HD22 | 1.88 | 0.55 |
| 1:E:151:THR:OG1 | 1:E:193:GLN:CB | 2.54 | 0.55 |
| 1:E:239:THR:HG22 | 1:E:240:THR:N | 2.22 | 0.55 |
| 1:E:272:PHE:HB3 | 1:E:275:LEU:HD22 | 1.88 | 0.55 |
| 1:E:310:GLY:CA | 1:E:436:GLN:HE21 | 2.19 | 0.55 |
| 2:F:19:ALA:CB | 2:F:228:ASN:HB3 | 2.35 | 0.55 |
| 2:F:349:THR:HG21 | 1:G:178:SER:O | 2.05 | 0.55 |
| 1:A:67:LEU:HD23 | 1:A:67:LEU:N | 2.22 | 0.55 |
| 1:A:210:TYR:HD2 | 1:A:227:LEU:HD21 | 1.71 | 0.55 |
| 2:B:5:ILE:CG2 | 2:B:6:SER:N | 2.70 | 0.55 |
| 1:C:190:SER:O | 1:C:194:LEU:HG | 2.06 | 0.55 |
| 2:F:6:SER:O | 2:F:65:ALA:HB1 | 2.07 | 0.55 |
| 2:F:209:ILE:HG22 | 2:F:227:LEU:HD22 | 1.88 | 0.55 |
| 2:F:264:ARG:HB2 | 2:F:266:HIS:HD2 | 1.67 | 0.55 |
| 1:G:107:HIS:HD2 | 1:G:151:THR:HG22 | 1.72 | 0.55 |
| 1:G:310:GLY:CA | 1:G:436:GLN:HE21 | 2.19 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:253:ARG:O | 1:A:254:LYS:C | 2.42 | 0.55 |
| 1:A:424:ASN:C | 1:A:424:ASN:HD22 | 2.09 | 0.55 |
| 2:D:6:SER:O | 2:D:65:ALA:HB1 | 2.07 | 0.55 |
| 2:D:30:ILE:HD13 | 2:D:61:HIS:CG | 2.41 | 0.55 |
| 1:E:119:LEU:O | 1:E:123:ARG:HG3 | 2.06 | 0.55 |
| 1:E:190:SER:O | 1:E:194:LEU:HG | 2.06 | 0.55 |
| 2:F:231:ILE:HA | 2:F:234:ILE:CG2 | 2.36 | 0.55 |
| 2:F:388:TRP:CE3 | 2:F:388:TRP:HA | 2.41 | 0.55 |
| 1:G:190:SER:O | 1:G:194:LEU:HG | 2.06 | 0.55 |
| 1:A:239:THR:HG22 | 1:A:240:THR:N | 2.22 | 0.55 |
| 1:C:67:LEU:HD23 | 1:C:67:LEU:N | 2.22 | 0.55 |
| 2:D:408:TYR:CD1 | 2:D:418:PHE:HZ | 2.24 | 0.55 |
| 1:E:67:LEU:HD23 | 1:E:67:LEU:N | 2.22 | 0.55 |
| 1:G:5:VAL:HG22 | 1:G:135:PHE:CD2 | 2.42 | 0.55 |
| 1:A:5:VAL:HG22 | 1:A:135:PHE:CD2 | 2.42 | 0.55 |
| 1:A:31:ASP:O | 1:A:32:PRO:C | 2.44 | 0.55 |
| 1:A:119:LEU:O | 1:A:123:ARG:HG3 | 2.06 | 0.55 |
| 1:A:172:VAL:CG1 | 1:A:387:LEU:HD21 | 2.24 | 0.55 |
| 2:B:6:SER:O | 2:B:65:ALA:HB1 | 2.07 | 0.55 |
| 2:B:288:VAL:HG22 | 2:B:373:ARG:NH1 | 2.22 | 0.55 |
| 1:C:5:VAL:HG22 | 1:C:135:PHE:CD2 | 2.42 | 0.55 |
| 1:E:5:VAL:HG22 | 1:E:135:PHE:CD2 | 2.42 | 0.55 |
| 1:E:107:HIS:HD2 | 1:E:151:THR:HG22 | 1.72 | 0.55 |
| 1:E:210:TYR:HD2 | 1:E:227:LEU:HD21 | 1.71 | 0.55 |
| 2:F:30:ILE:O | 2:F:30:ILE:HG22 | 2.07 | 0.55 |
| 2:F:408:TYR:CD1 | 2:F:418:PHE:HZ | 2.24 | 0.55 |
| 1:G:67:LEU:HD23 | 1:G:67:LEU:N | 2.22 | 0.55 |
| 1:G:166:MET:HB3 | 1:G:198:THR:OG1 | 2.06 | 0.55 |
| 1:G:210:TYR:HD2 | 1:G:227:LEU:HD21 | 1.71 | 0.55 |
| 1:G:342:TYR:HD2 | 3:I:64:TYR:HH | 1.47 | 0.55 |
| 2:H:6:SER:O | 2:H:65:ALA:HB1 | 2.07 | 0.55 |
| 2:H:231:ILE:HA | 2:H:234:ILE:CG2 | 2.36 | 0.55 |
| 2:H:388:TRP:HA | 2:H:388:TRP:CE3 | 2.41 | 0.55 |
| 2:H:408:TYR:CD1 | 2:H:418:PHE:HZ | 2.24 | 0.55 |
| 2:B:24:TYR:OH | 2:B:239:THR:OG1 | 2.24 | 0.54 |
| 2:B:30:ILE:HG23 | 2:B:34:GLY:O | 2.07 | 0.54 |
| 2:B:231:ILE:HA | 2:B:234:ILE:CG2 | 2.36 | 0.54 |
| 1:C:204:ILE:HD13 | 1:C:231:VAL:HG13 | 1.89 | 0.54 |
| 1:C:210:TYR:HD2 | 1:C:227:LEU:HD21 | 1.71 | 0.54 |
| 2:D:231:ILE:HA | 2:D:234:ILE:CG2 | 2.36 | 0.54 |
| 2:D:288:VAL:HG22 | 2:D:373:ARG:NH1 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:339:ARG:C | 2:D:341:ILE:H | 2.11 | 0.54 |
| 1:E:166:MET:HB3 | 1:E:198:THR:OG1 | 2.06 | 0.54 |
| 1:G:165:ILE:H | 1:G:165:ILE:HD13 | 1.71 | 0.54 |
| 1:G:272:PHE:HB3 | 1:G:275:LEU:HD22 | 1.88 | 0.54 |
| 2:B:346:TRP:HB3 | 1:C:401:ARG:HG3 | 1.89 | 0.54 |
| 2:B:381:THR:OG1 | 2:B:383:ALA:HB3 | 2.07 | 0.54 |
| 1:C:4:ILE:HD13 | 1:C:136:GLN:NE2 | 2.18 | 0.54 |
| 1:C:119:LEU:O | 1:C:123:ARG:HG3 | 2.06 | 0.54 |
| 1:C:239:THR:HG22 | 1:C:240:THR:N | 2.22 | 0.54 |
| 2:D:110:ILE:O | 2:D:112:LYS:N | 2.41 | 0.54 |
| 1:G:132:LEU:CD2 | 1:G:164:ARG:HG3 | 2.32 | 0.54 |
| 3:I:55:VAL:CG2 | 3:I:57:PHE:CE1 | 2.90 | 0.54 |
| 1:A:204:ILE:HD13 | 1:A:231:VAL:HG13 | 1.89 | 0.54 |
| 2:B:56:THR:O | 2:F:284:GLU:CB | 2.53 | 0.54 |
| 1:C:239:THR:O | 1:C:241:CYS:N | 2.41 | 0.54 |
| 2:D:381:THR:OG1 | 2:D:383:ALA:HB3 | 2.07 | 0.54 |
| 1:E:250:ALA:CA | 1:E:254:LYS:HE2 | 2.36 | 0.54 |
| 2:F:64:ARG:HG3 | 2:F:64:ARG:O | 2.06 | 0.54 |
| 2:F:248:LEU:HB3 | 2:F:355:ILE:H | 1.73 | 0.54 |
| 2:F:258:ASN:OD1 | 1:G:180:THR:HG23 | 2.06 | 0.54 |
| 2:F:288:VAL:HG22 | 2:F:373:ARG:NH1 | 2.22 | 0.54 |
| 2:F:324:VAL:CG1 | 1:G:221:THR:C | 2.74 | 0.54 |
| 2:F:339:ARG:C | 2:F:341:ILE:H | 2.11 | 0.54 |
| 2:H:248:LEU:HB3 | 2:H:355:ILE:H | 1.73 | 0.54 |
| 2:H:288:VAL:HG22 | 2:H:373:ARG:NH1 | 2.23 | 0.54 |
| 1:A:166:MET:HB3 | 1:A:198:THR:OG1 | 2.06 | 0.54 |
| 2:B:16:ILE:HD12 | 2:B:171:ILE:HD11 | 1.87 | 0.54 |
| 1:C:427:ASP:OD1 | 1:C:428:LEU:N | 2.41 | 0.54 |
| 2:D:16:ILE:HD12 | 2:D:171:ILE:HD11 | 1.87 | 0.54 |
| 2:D:64:ARG:HG3 | 2:D:64:ARG:O | 2.07 | 0.54 |
| 1:E:44:LEU:O | 1:E:49:ILE:HG12 | 2.07 | 0.54 |
| 1:E:165:ILE:HD13 | 1:E:165:ILE:H | 1.71 | 0.54 |
| 1:E:239:THR:O | 1:E:241:CYS:N | 2.40 | 0.54 |
| 1:E:297:ASP:OD1 | 1:E:298:ALA:N | 2.39 | 0.54 |
| 1:E:325:MET:O | 1:E:329:ASP:HB2 | 2.07 | 0.54 |
| 2:F:261:PRO:CB | 1:G:404:PHE:CD2 | 2.78 | 0.54 |
| 2:F:381:THR:OG1 | 2:F:383:ALA:HB3 | 2.07 | 0.54 |
| 1:G:239:THR:O | 1:G:241:CYS:N | 2.41 | 0.54 |
| 2:H:64:ARG:HG3 | 2:H:64:ARG:O | 2.07 | 0.54 |
| 2:H:102:ASN:CB | 2:H:407:TRP:NE1 | 2.71 | 0.54 |
| 3:I:113:ILE:HG13 | 3:I:125:TYR:CE1 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:239:THR:O | 1:A:241:CYS:N | 2.41 | 0.54 |
| 2:B:17:GLY:O | 2:B:21:TRP:HB2 | 2.08 | 0.54 |
| 2:B:110:ILE:O | 2:B:112:LYS:N | 2.41 | 0.54 |
| 2:D:17:GLY:O | 2:D:21:TRP:HB2 | 2.08 | 0.54 |
| 2:D:118:VAL:HG21 | 2:D:149:PHE:CZ | 2.42 | 0.54 |
| 1:E:249:ASN:OD1 | 2:F:71:GLU:OE1 | 2.25 | 0.54 |
| 1:E:259:MET:CA | 1:E:314:THR:HG21 | 2.35 | 0.54 |
| 2:F:23:LEU:HD23 | 2:F:236:SER:CB | 2.37 | 0.54 |
| 2:F:118:VAL:HG21 | 2:F:149:PHE:CZ | 2.42 | 0.54 |
| 2:F:163:LYS:O | 2:F:163:LYS:HG2 | 2.08 | 0.54 |
| 1:G:68:VAL:HG12 | 1:G:149:MET:CE | 2.38 | 0.54 |
| 1:G:259:MET:CA | 1:G:314:THR:HG21 | 2.35 | 0.54 |
| 2:H:9:VAL:CG1 | 2:H:139:HIS:HB3 | 2.38 | 0.54 |
| 2:H:30:ILE:HG22 | 2:H:30:ILE:O | 2.07 | 0.54 |
| 2:H:339:ARG:C | 2:H:341:ILE:H | 2.11 | 0.54 |
| 1:A:331:GLN:O | 1:A:335:VAL:HG23 | 2.08 | 0.54 |
| 2:B:64:ARG:HG3 | 2:B:64:ARG:O | 2.07 | 0.54 |
| 2:B:110:ILE:CG2 | 2:B:111:GLY:N | 2.71 | 0.54 |
| 1:C:2:ARG:NH2 | 2:D:98:ASP:HA | 2.22 | 0.54 |
| 1:C:166:MET:HB3 | 1:C:198:THR:OG1 | 2.06 | 0.54 |
| 1:C:253:ARG:O | 1:C:257:VAL:N | 2.33 | 0.54 |
| 1:C:323:MET:HG3 | 1:C:328:VAL:HG21 | 1.90 | 0.54 |
| 1:C:325:MET:O | 1:C:329:ASP:HB2 | 2.07 | 0.54 |
| 2:D:5:ILE:HG23 | 2:D:135:PHE:CB | 2.38 | 0.54 |
| 1:E:213:CYS:SG | 1:E:219:LEU:HD23 | 2.48 | 0.54 |
| 1:E:257:VAL:HA | 2:F:407:TRP:CE2 | 2.42 | 0.54 |
| 1:G:297:ASP:OD1 | 1:G:298:ALA:N | 2.39 | 0.54 |
| 2:H:23:LEU:HD23 | 2:H:236:SER:CB | 2.37 | 0.54 |
| 2:H:115:ILE:HD13 | 2:H:115:ILE:C | 2.28 | 0.54 |
| 2:H:163:LYS:O | 2:H:163:LYS:HG2 | 2.08 | 0.54 |
| 2:H:381:THR:OG1 | 2:H:383:ALA:HB3 | 2.07 | 0.54 |
| 1:A:133:GLN:HE21 | 1:A:252:LEU:HB2 | 1.73 | 0.54 |
| 1:A:343:PHE:O | 1:A:344:VAL:O | 2.26 | 0.54 |
| 1:A:427:ASP:OD1 | 1:A:428:LEU:N | 2.41 | 0.54 |
| 1:C:343:PHE:O | 1:C:344:VAL:O | 2.26 | 0.54 |
| 2:D:62:VAL:CG1 | 2:D:88:HIS:ND1 | 2.71 | 0.54 |
| 2:F:9:VAL:CG1 | 2:F:139:HIS:HB3 | 2.38 | 0.54 |
| 2:F:17:GLY:O | 2:F:21:TRP:HB2 | 2.08 | 0.54 |
| 1:G:31:ASP:O | 1:G:32:PRO:C | 2.44 | 0.54 |
| 1:G:44:LEU:O | 1:G:49:ILE:HG12 | 2.07 | 0.54 |
| 1:G:323:MET:HG3 | 1:G:328:VAL:HG21 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:324:SER:C | 1:G:326:LYS:N | 2.59 | 0.54 |
| 1:G:343:PHE:O | 1:G:344:VAL:O | 2.26 | 0.54 |
| 2:H:98:ASP:O | 2:H:110:ILE:HD13 | 2.08 | 0.54 |
| 1:A:323:MET:HG3 | 1:A:328:VAL:HG21 | 1.90 | 0.54 |
| 1:A:325:MET:O | 1:A:329:ASP:HB2 | 2.07 | 0.54 |
| 2:B:98:ASP:O | 2:B:110:ILE:HD13 | 2.08 | 0.54 |
| 2:B:115:ILE:HD13 | 2:B:115:ILE:C | 2.28 | 0.54 |
| 2:B:339:ARG:C | 2:B:341:ILE:H | 2.11 | 0.54 |
| 2:D:9:VAL:CG1 | 2:D:139:HIS:HB3 | 2.38 | 0.54 |
| 2:D:30:ILE:HG23 | 2:D:34:GLY:O | 2.08 | 0.54 |
| 2:D:115:ILE:HD13 | 2:D:115:ILE:C | 2.28 | 0.54 |
| 2:D:315:CYS:HB3 | 2:D:377:MET:HE2 | 1.89 | 0.54 |
| 1:E:31:ASP:O | 1:E:32:PRO:C | 2.44 | 0.54 |
| 1:E:343:PHE:O | 1:E:344:VAL:O | 2.26 | 0.54 |
| 2:F:115:ILE:HD13 | 2:F:115:ILE:C | 2.28 | 0.54 |
| 2:F:182:VAL:O | 2:F:184:PRO:N | 2.41 | 0.54 |
| 2:F:257:THR:HG21 | 1:G:101:ASN:CB | 2.32 | 0.54 |
| 1:G:213:CYS:SG | 1:G:219:LEU:HD23 | 2.48 | 0.54 |
| 1:G:322:ARG:HH11 | 1:G:322:ARG:HG3 | 1.73 | 0.54 |
| 2:H:98:ASP:CB | 2:H:105:ARG:HH21 | 2.14 | 0.54 |
| 2:H:118:VAL:HG21 | 2:H:149:PHE:CZ | 2.42 | 0.54 |
| 2:H:182:VAL:O | 2:H:184:PRO:N | 2.41 | 0.54 |
| 1:A:44:LEU:O | 1:A:49:ILE:HG12 | 2.07 | 0.54 |
| 1:A:213:CYS:SG | 1:A:219:LEU:HD23 | 2.48 | 0.54 |
| 1:A:229:HIS:C | 1:A:229:HIS:ND1 | 2.62 | 0.54 |
| 1:A:253:ARG:O | 1:A:257:VAL:N | 2.33 | 0.54 |
| 2:B:118:VAL:HG21 | 2:B:149:PHE:CZ | 2.42 | 0.54 |
| 2:B:439:SER:O | 1:C:401:ARG:NH2 | 2.33 | 0.54 |
| 1:C:2:ARG:HH22 | 2:D:99:ALA:H | 1.54 | 0.54 |
| 1:C:31:ASP:HB3 | 1:C:32:PRO:HD2 | 1.89 | 0.54 |
| 2:D:24:TYR:OH | 2:D:239:THR:OG1 | 2.24 | 0.54 |
| 2:D:264:ARG:C | 2:D:266:HIS:N | 2.60 | 0.54 |
| 1:E:322:ARG:HH11 | 1:E:322:ARG:HG3 | 1.73 | 0.54 |
| 2:F:98:ASP:O | 2:F:110:ILE:HD13 | 2.08 | 0.54 |
| 2:F:215:ARG:C | 2:F:216:ASN:HD22 | 2.12 | 0.54 |
| 2:H:5:ILE:HG23 | 2:H:135:PHE:CB | 2.38 | 0.54 |
| 2:H:17:GLY:O | 2:H:21:TRP:HB2 | 2.08 | 0.54 |
| 1:A:4:ILE:HD13 | 1:A:136:GLN:NE2 | 2.18 | 0.54 |
| 2:B:9:VAL:CG1 | 2:B:139:HIS:HB3 | 2.38 | 0.54 |
| 1:C:68:VAL:HG12 | 1:C:149:MET:CE | 2.38 | 0.54 |
| 1:C:133:GLN:HE21 | 1:C:252:LEU:HB2 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:194:LEU:C | 1:C:196:GLU:H | 2.11 | 0.54 |
| 1:C:331:GLN:O | 1:C:335:VAL:HG23 | 2.08 | 0.54 |
| 2:D:98:ASP:O | 2:D:110:ILE:HD13 | 2.08 | 0.54 |
| 2:D:173:PRO:HB2 | 2:D:391:LEU:CD1 | 2.38 | 0.54 |
| 2:D:215:ARG:C | 2:D:216:ASN:HD22 | 2.12 | 0.54 |
| 1:E:4:ILE:CG2 | 1:E:136:GLN:HG2 | 2.38 | 0.54 |
| 2:F:110:ILE:O | 2:F:112:LYS:N | 2.41 | 0.54 |
| 1:G:194:LEU:C | 1:G:196:GLU:H | 2.11 | 0.54 |
| 2:H:110:ILE:O | 2:H:112:LYS:N | 2.41 | 0.54 |
| 2:H:215:ARG:C | 2:H:216:ASN:HD22 | 2.12 | 0.54 |
| 2:B:61:HIS:C | 2:B:62:VAL:HG23 | 2.28 | 0.53 |
| 2:B:163:LYS:O | 2:B:163:LYS:HG2 | 2.08 | 0.53 |
| 1:C:213:CYS:SG | 1:C:219:LEU:HD23 | 2.48 | 0.53 |
| 1:C:259:MET:CA | 1:C:314:THR:HG21 | 2.35 | 0.53 |
| 1:C:325:MET:CE | 1:C:355:VAL:HG11 | 2.38 | 0.53 |
| 1:C:431:GLU:O | 1:C:434:GLN:CG | 2.56 | 0.53 |
| 1:E:323:MET:HG3 | 1:E:328:VAL:HG21 | 1.90 | 0.53 |
| 2:F:5:ILE:HG23 | 2:F:135:PHE:CB | 2.38 | 0.53 |
| 1:G:4:ILE:CG2 | 1:G:136:GLN:HG2 | 2.38 | 0.53 |
| 1:G:204:ILE:HD13 | 1:G:231:VAL:HG13 | 1.89 | 0.53 |
| 1:C:229:HIS:ND1 | 1:C:229:HIS:C | 2.62 | 0.53 |
| 2:D:5:ILE:O | 2:D:135:PHE:HA | 2.09 | 0.53 |
| 2:D:276:ILE:CG2 | 2:D:369:ALA:HB2 | 2.27 | 0.53 |
| 1:E:5:VAL:HG23 | 1:E:5:VAL:O | 2.09 | 0.53 |
| 1:E:194:LEU:C | 1:E:196:GLU:H | 2.11 | 0.53 |
| 1:E:324:SER:C | 1:E:326:LYS:N | 2.59 | 0.53 |
| 1:E:325:MET:CE | 1:E:355:VAL:HG11 | 2.38 | 0.53 |
| 1:E:431:GLU:O | 1:E:434:GLN:CG | 2.56 | 0.53 |
| 1:G:31:ASP:HB3 | 1:G:32:PRO:HD2 | 1.89 | 0.53 |
| 2:H:5:ILE:O | 2:H:135:PHE:HA | 2.08 | 0.53 |
| 1:A:107:HIS:HD2 | 1:A:151:THR:HG22 | 1.72 | 0.53 |
| 1:A:194:LEU:C | 1:A:196:GLU:H | 2.11 | 0.53 |
| 2:B:159:VAL:CG1 | 3:I:78:ARG:CG | 2.86 | 0.53 |
| 1:C:44:LEU:O | 1:C:49:ILE:HG12 | 2.07 | 0.53 |
| 1:C:147:SER:O | 1:C:151:THR:CB | 2.51 | 0.53 |
| 2:D:163:LYS:O | 2:D:163:LYS:HG2 | 2.08 | 0.53 |
| 1:E:31:ASP:HB3 | 1:E:32:PRO:HD2 | 1.89 | 0.53 |
| 1:E:229:HIS:C | 1:E:229:HIS:ND1 | 2.62 | 0.53 |
| 2:F:5:ILE:O | 2:F:135:PHE:HA | 2.08 | 0.53 |
| 2:F:98:ASP:CB | 2:F:105:ARG:HH21 | 2.14 | 0.53 |
| 2:F:173:PRO:HB2 | 2:F:391:LEU:CD1 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:332:ILE:CG2 | 1:G:177:VAL:HG11 | 2.38 | 0.53 |
| 2:F:408:TYR:O | 2:F:411:GLU:N | 2.39 | 0.53 |
| 1:G:325:MET:CE | 1:G:355:VAL:HG11 | 2.38 | 0.53 |
| 1:G:431:GLU:O | 1:G:434:GLN:CG | 2.56 | 0.53 |
| 2:H:101:ASN:ND2 | 5:H:500:GTP:O3G | 2.42 | 0.53 |
| 1:A:68:VAL:HG12 | 1:A:149:MET:CE | 2.38 | 0.53 |
| 1:A:259:MET:CG | 1:A:314:THR:HG21 | 2.37 | 0.53 |
| 2:B:173:PRO:HB2 | 2:B:391:LEU:CD1 | 2.39 | 0.53 |
| 1:C:172:VAL:CG1 | 1:C:387:LEU:HD21 | 2.24 | 0.53 |
| 2:D:98:ASP:CB | 2:D:105:ARG:HH21 | 2.14 | 0.53 |
| 2:D:150:THR:O | 2:D:151:SER:C | 2.47 | 0.53 |
| 1:E:204:ILE:HD13 | 1:E:231:VAL:HG13 | 1.89 | 0.53 |
| 2:F:101:ASN:ND2 | 5:F:500:GTP:O3G | 2.42 | 0.53 |
| 2:F:121:ARG:O | 2:F:125:LEU:HB2 | 2.08 | 0.53 |
| 1:G:229:HIS:C | 1:G:229:HIS:ND1 | 2.62 | 0.53 |
| 1:G:427:ASP:OD1 | 1:G:428:LEU:N | 2.41 | 0.53 |
| 2:H:173:PRO:HB2 | 2:H:391:LEU:CD1 | 2.38 | 0.53 |
| 2:B:88:HIS:HE1 | 2:F:284:GLU:OE2 | 1.92 | 0.53 |
| 2:B:215:ARG:C | 2:B:216:ASN:HD22 | 2.12 | 0.53 |
| 2:B:349:THR:HG21 | 1:C:178:SER:CB | 2.38 | 0.53 |
| 2:B:408:TYR:O | 2:B:411:GLU:N | 2.39 | 0.53 |
| 1:E:331:GLN:O | 1:E:335:VAL:HG23 | 2.08 | 0.53 |
| 1:G:5:VAL:HG23 | 1:G:5:VAL:O | 2.09 | 0.53 |
| 2:H:67:PHE:CZ | 2:H:87:PHE:HE1 | 2.27 | 0.53 |
| 2:H:121:ARG:O | 2:H:125:LEU:HB2 | 2.08 | 0.53 |
| 2:H:408:TYR:O | 2:H:411:GLU:N | 2.39 | 0.53 |
| 1:A:31:ASP:HB3 | 1:A:32:PRO:HD2 | 1.89 | 0.53 |
| 1:A:226:ASP:O | 1:A:227:LEU:C | 2.46 | 0.53 |
| 2:B:5:ILE:O | 2:B:135:PHE:HA | 2.09 | 0.53 |
| 2:B:150:THR:O | 2:B:151:SER:C | 2.47 | 0.53 |
| 2:B:182:VAL:O | 2:B:184:PRO:N | 2.41 | 0.53 |
| 2:B:231:ILE:CA | 2:B:234:ILE:HG22 | 2.38 | 0.53 |
| 1:C:4:ILE:CG2 | 1:C:136:GLN:HG2 | 2.38 | 0.53 |
| 1:C:36:TYR:CZ | 1:C:38:GLY:HA3 | 2.43 | 0.53 |
| 1:C:259:MET:CG | 1:C:314:THR:HG21 | 2.36 | 0.53 |
| 1:E:20:PHE:CE2 | 1:E:24:ILE:HD12 | 2.43 | 0.53 |
| 1:E:168:THR:CB | 1:E:201:THR:HG23 | 2.38 | 0.53 |
| 1:E:226:ASP:O | 1:E:227:LEU:C | 2.46 | 0.53 |
| 2:F:67:PHE:CZ | 2:F:87:PHE:HE1 | 2.27 | 0.53 |
| 1:G:8:GLN:OE1 | 1:G:14:ASN:ND2 | 2.42 | 0.53 |
| 1:G:331:GLN:O | 1:G:335:VAL:HG23 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:322:ARG:HG3 | 1:A:322:ARG:HH11 | 1.73 | 0.53 |
| 2:B:121:ARG:O | 2:B:125:LEU:HB2 | 2.08 | 0.53 |
| 1:C:107:HIS:HD2 | 1:C:151:THR:HG22 | 1.72 | 0.53 |
| 1:C:259:MET:HG2 | 1:C:314:THR:CG2 | 2.38 | 0.53 |
| 2:D:101:ASN:ND2 | 5:D:500:GTP:O3G | 2.42 | 0.53 |
| 2:D:231:ILE:CA | 2:D:234:ILE:HG22 | 2.38 | 0.53 |
| 1:E:8:GLN:OE1 | 1:E:14:ASN:ND2 | 2.42 | 0.53 |
| 1:E:427:ASP:OD1 | 1:E:428:LEU:N | 2.41 | 0.53 |
| 2:F:231:ILE:CA | 2:F:234:ILE:HG22 | 2.38 | 0.53 |
| 2:F:243:ARG:CZ | 2:F:252:LEU:HG | 2.39 | 0.53 |
| 1:G:27:GLU:HG2 | 1:G:27:GLU:O | 2.08 | 0.53 |
| 1:A:259:MET:HG2 | 1:A:314:THR:CG2 | 2.38 | 0.53 |
| 1:A:259:MET:CA | 1:A:314:THR:HG21 | 2.35 | 0.53 |
| 1:A:431:GLU:O | 1:A:434:GLN:CG | 2.56 | 0.53 |
| 2:B:30:ILE:HD12 | 2:B:61:HIS:ND1 | 2.22 | 0.53 |
| 2:B:315:CYS:HB3 | 2:B:377:MET:HE2 | 1.89 | 0.53 |
| 1:C:21:TRP:CZ2 | 1:C:65:ALA:HB2 | 2.44 | 0.53 |
| 1:C:210:TYR:CD2 | 1:C:227:LEU:HD21 | 2.44 | 0.53 |
| 2:D:121:ARG:O | 2:D:125:LEU:HB2 | 2.08 | 0.53 |
| 1:E:21:TRP:CZ2 | 1:E:65:ALA:HB2 | 2.44 | 0.53 |
| 1:E:36:TYR:CZ | 1:E:38:GLY:HA3 | 2.43 | 0.53 |
| 2:F:196:GLU:C | 2:F:197:HIS:CD2 | 2.82 | 0.53 |
| 1:G:226:ASP:O | 1:G:227:LEU:C | 2.46 | 0.53 |
| 2:H:150:THR:O | 2:H:151:SER:C | 2.47 | 0.53 |
| 2:H:231:ILE:CA | 2:H:234:ILE:HG22 | 2.38 | 0.53 |
| 1:A:70:LEU:HD12 | 1:A:145:THR:HG23 | 1.91 | 0.53 |
| 2:B:101:ASN:ND2 | 5:B:500:GTP:O3G | 2.42 | 0.53 |
| 2:B:122:ILE:CD1 | 2:B:157:LEU:HD21 | 2.35 | 0.53 |
| 2:D:196:GLU:C | 2:D:197:HIS:CD2 | 2.82 | 0.53 |
| 1:E:198:THR:HG22 | 1:E:265:LEU:CD2 | 2.39 | 0.53 |
| 1:G:20:PHE:CE2 | 1:G:24:ILE:HD12 | 2.42 | 0.53 |
| 1:G:424:ASN:C | 1:G:424:ASN:ND2 | 2.61 | 0.53 |
| 2:H:102:ASN:HB3 | 2:H:407:TRP:NE1 | 2.24 | 0.53 |
| 2:H:196:GLU:C | 2:H:197:HIS:CD2 | 2.82 | 0.53 |
| 2:H:243:ARG:CZ | 2:H:252:LEU:HG | 2.39 | 0.53 |
| 1:A:168:THR:CB | 1:A:201:THR:HG23 | 2.38 | 0.53 |
| 1:A:179:ASP:HB2 | 4:A:600:GDP:H3' | 1.90 | 0.53 |
| 1:A:325:MET:CE | 1:A:355:VAL:HG11 | 2.38 | 0.53 |
| 1:A:424:ASN:C | 1:A:424:ASN:ND2 | 2.61 | 0.53 |
| 1:C:5:VAL:O | 1:C:5:VAL:HG23 | 2.09 | 0.53 |
| 1:C:264:ARG:HA | 1:C:264:ARG:HE | 1.75 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:424:ASN:C | 1:C:424:ASN:ND2 | 2.61 | 0.53 |
| 1:E:27:GLU:O | 1:E:27:GLU:HG2 | 2.08 | 0.53 |
| 1:E:68:VAL:HG12 | 1:E:149:MET:CE | 2.38 | 0.53 |
| 1:E:212:ILE:O | 1:E:216:THR:HB | 2.09 | 0.53 |
| 2:F:11:GLN:NE2 | 2:F:74:VAL:HG22 | 2.22 | 0.53 |
| 1:G:21:TRP:CZ2 | 1:G:65:ALA:HB2 | 2.44 | 0.53 |
| 1:G:36:TYR:CZ | 1:G:38:GLY:HA3 | 2.43 | 0.53 |
| 1:G:133:GLN:HE21 | 1:G:252:LEU:HB2 | 1.73 | 0.53 |
| 1:G:168:THR:CB | 1:G:201:THR:HG23 | 2.38 | 0.53 |
| 1:G:212:ILE:O | 1:G:216:THR:HB | 2.09 | 0.53 |
| 1:G:425:MET:O | 1:G:428:LEU:HB3 | 2.09 | 0.53 |
| 1:G:431:GLU:OE1 | 1:G:432:TYR:CA | 2.57 | 0.53 |
| 1:A:4:ILE:CG2 | 1:A:136:GLN:HG2 | 2.38 | 0.52 |
| 1:A:5:VAL:HG23 | 1:A:5:VAL:O | 2.09 | 0.52 |
| 1:A:21:TRP:CZ2 | 1:A:65:ALA:HB2 | 2.44 | 0.52 |
| 1:A:36:TYR:CZ | 1:A:38:GLY:HA3 | 2.43 | 0.52 |
| 1:A:210:TYR:CD2 | 1:A:227:LEU:HD21 | 2.44 | 0.52 |
| 1:A:425:MET:O | 1:A:428:LEU:HB3 | 2.09 | 0.52 |
| 2:B:172:TYR:OH | 2:B:387:ALA:O | 2.24 | 0.52 |
| 2:B:196:GLU:C | 2:B:197:HIS:CD2 | 2.82 | 0.52 |
| 1:C:27:GLU:O | 1:C:27:GLU:HG2 | 2.08 | 0.52 |
| 1:C:425:MET:O | 1:C:428:LEU:HB3 | 2.09 | 0.52 |
| 2:D:67:PHE:CZ | 2:D:87:PHE:HE1 | 2.27 | 0.52 |
| 2:D:182:VAL:O | 2:D:184:PRO:N | 2.41 | 0.52 |
| 2:D:324:VAL:O | 2:D:327:ASP:HB2 | 2.08 | 0.52 |
| 1:E:425:MET:O | 1:E:428:LEU:HB3 | 2.09 | 0.52 |
| 1:E:431:GLU:OE1 | 1:E:432:TYR:CA | 2.57 | 0.52 |
| 2:F:206:ASN:OD1 | 2:F:227:LEU:CD1 | 2.58 | 0.52 |
| 2:F:326:LYS:HE2 | 1:G:214:PHE:HB3 | 1.91 | 0.52 |
| 2:F:332:ILE:HG22 | 1:G:177:VAL:HG21 | 1.89 | 0.52 |
| 2:F:348:PRO:HD3 | 1:G:398:MET:CE | 2.38 | 0.52 |
| 1:G:210:TYR:CD2 | 1:G:227:LEU:HD21 | 2.44 | 0.52 |
| 2:H:206:ASN:OD1 | 2:H:227:LEU:CD1 | 2.58 | 0.52 |
| 1:A:264:ARG:HA | 1:A:264:ARG:HE | 1.75 | 0.52 |
| 2:B:8:HIS:HB3 | 2:B:13:GLY:O | 2.10 | 0.52 |
| 2:B:67:PHE:CZ | 2:B:87:PHE:HE1 | 2.27 | 0.52 |
| 1:C:20:PHE:CE2 | 1:C:24:ILE:HD12 | 2.43 | 0.52 |
| 1:C:141:LEU:HA | 1:C:147:SER:HB3 | 1.91 | 0.52 |
| 1:C:168:THR:CB | 1:C:201:THR:HG23 | 2.38 | 0.52 |
| 1:C:322:ARG:HH11 | 1:C:322:ARG:HG3 | 1.73 | 0.52 |
| 2:D:8:HIS:HB3 | 2:D:13:GLY:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:151:SER:HB3 | 2:D:193:THR:CG2 | 2.34 | 0.52 |
| 2:D:173:PRO:HB2 | 2:D:391:LEU:HD11 | 1.92 | 0.52 |
| 2:D:248:LEU:HB3 | 2:D:355:ILE:H | 1.73 | 0.52 |
| 1:E:210:TYR:CD2 | 1:E:227:LEU:HD21 | 2.44 | 0.52 |
| 2:F:173:PRO:HB2 | 2:F:391:LEU:HD11 | 1.92 | 0.52 |
| 1:G:259:MET:HG2 | 1:G:314:THR:CG2 | 2.38 | 0.52 |
| 1:G:259:MET:CG | 1:G:314:THR:HG21 | 2.36 | 0.52 |
| 1:A:27:GLU:HG2 | 1:A:27:GLU:O | 2.08 | 0.52 |
| 1:A:149:MET:O | 1:A:149:MET:HG2 | 2.10 | 0.52 |
| 1:A:209:LEU:O | 1:A:210:TYR:C | 2.48 | 0.52 |
| 1:A:431:GLU:OE1 | 1:A:432:TYR:CA | 2.57 | 0.52 |
| 2:B:147:SER:CB | 2:B:190:THR:OG1 | 2.52 | 0.52 |
| 1:C:149:MET:O | 1:C:149:MET:HG2 | 2.10 | 0.52 |
| 1:C:176:LYS:CE | 1:C:207:GLU:HG3 | 2.39 | 0.52 |
| 1:C:209:LEU:O | 1:C:210:TYR:C | 2.48 | 0.52 |
| 1:C:320:ARG:HA | 1:C:356:CYS:HB3 | 1.92 | 0.52 |
| 1:E:133:GLN:HE21 | 1:E:252:LEU:HB2 | 1.73 | 0.52 |
| 1:E:179:ASP:HB2 | 4:E:600:GDP:H3' | 1.90 | 0.52 |
| 1:E:209:LEU:O | 1:E:210:TYR:C | 2.48 | 0.52 |
| 2:F:172:TYR:OH | 2:F:387:ALA:O | 2.24 | 0.52 |
| 1:G:198:THR:HG22 | 1:G:265:LEU:CD2 | 2.39 | 0.52 |
| 2:H:11:GLN:NE2 | 2:H:74:VAL:HG22 | 2.22 | 0.52 |
| 2:H:25:CYS:HB2 | 2:H:30:ILE:O | 2.10 | 0.52 |
| 2:H:173:PRO:HB2 | 2:H:391:LEU:HD11 | 1.92 | 0.52 |
| 3:I:100:GLY:O | 3:I:101:VAL:CG2 | 2.57 | 0.52 |
| 1:A:8:GLN:OE1 | 1:A:14:ASN:ND2 | 2.42 | 0.52 |
| 1:A:176:LYS:CE | 1:A:207:GLU:HG3 | 2.39 | 0.52 |
| 1:A:320:ARG:HA | 1:A:356:CYS:HB3 | 1.92 | 0.52 |
| 2:B:98:ASP:CB | 2:B:105:ARG:HH21 | 2.14 | 0.52 |
| 2:B:231:ILE:HD13 | 2:B:231:ILE:N | 2.25 | 0.52 |
| 1:C:226:ASP:O | 1:C:227:LEU:C | 2.46 | 0.52 |
| 2:D:172:TYR:OH | 2:D:387:ALA:O | 2.24 | 0.52 |
| 1:E:141:LEU:HA | 1:E:147:SER:HB3 | 1.91 | 0.52 |
| 1:E:226:ASP:O | 1:E:229:HIS:N | 2.42 | 0.52 |
| 2:F:4:CYS:HA | 2:F:134:GLY:O | 2.10 | 0.52 |
| 2:F:25:CYS:HB2 | 2:F:30:ILE:O | 2.10 | 0.52 |
| 1:G:103:TRP:CE2 | 1:G:189:LEU:HB3 | 2.45 | 0.52 |
| 1:G:141:LEU:HA | 1:G:147:SER:HB3 | 1.91 | 0.52 |
| 1:G:226:ASP:O | 1:G:229:HIS:N | 2.42 | 0.52 |
| 1:G:345:GLU:C | 1:G:347:ILE:H | 2.13 | 0.52 |
| 2:H:110:ILE:CG2 | 2:H:111:GLY:N | 2.71 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:20:PHE:CE2 | 1:A:24:ILE:HD12 | 2.43 | 0.52 |
| 1:A:103:TRP:CE2 | 1:A:189:LEU:HB3 | 2.45 | 0.52 |
| 1:A:141:LEU:HA | 1:A:147:SER:HB3 | 1.91 | 0.52 |
| 1:A:212:ILE:O | 1:A:216:THR:HB | 2.09 | 0.52 |
| 2:B:5:ILE:O | 2:B:136:SER:N | 2.40 | 0.52 |
| 2:B:173:PRO:HB2 | 2:B:391:LEU:HD11 | 1.92 | 0.52 |
| 2:B:248:LEU:HB3 | 2:B:355:ILE:H | 1.73 | 0.52 |
| 2:B:349:THR:O | 1:C:181:VAL:HA | 2.09 | 0.52 |
| 1:C:70:LEU:HD12 | 1:C:145:THR:HG23 | 1.91 | 0.52 |
| 1:C:103:TRP:CE2 | 1:C:189:LEU:HB3 | 2.45 | 0.52 |
| 1:E:345:GLU:C | 1:E:347:ILE:H | 2.13 | 0.52 |
| 1:E:424:ASN:C | 1:E:424:ASN:ND2 | 2.61 | 0.52 |
| 2:F:110:ILE:CG2 | 2:F:111:GLY:H | 2.15 | 0.52 |
| 2:H:4:CYS:HA | 2:H:134:GLY:O | 2.10 | 0.52 |
| 2:H:62:VAL:CG1 | 2:H:88:HIS:ND1 | 2.71 | 0.52 |
| 2:H:172:TYR:OH | 2:H:387:ALA:O | 2.24 | 0.52 |
| 1:A:226:ASP:O | 1:A:229:HIS:N | 2.42 | 0.52 |
| 2:B:324:VAL:O | 2:B:327:ASP:HB2 | 2.08 | 0.52 |
| 1:C:226:ASP:O | 1:C:229:HIS:N | 2.42 | 0.52 |
| 2:D:24:TYR:CE2 | 2:D:240:ALA:HB2 | 2.45 | 0.52 |
| 1:E:103:TRP:CE2 | 1:E:189:LEU:HB3 | 2.45 | 0.52 |
| 1:E:320:ARG:HA | 1:E:356:CYS:HB3 | 1.92 | 0.52 |
| 2:F:62:VAL:CG1 | 2:F:88:HIS:ND1 | 2.71 | 0.52 |
| 2:F:231:ILE:N | 2:F:231:ILE:HD13 | 2.25 | 0.52 |
| 2:F:345:ASP:OD2 | 2:F:439:SER:HB3 | 2.10 | 0.52 |
| 2:F:348:PRO:HG3 | 1:G:394:GLN:HB3 | 1.91 | 0.52 |
| 2:H:110:ILE:CG2 | 2:H:111:GLY:H | 2.15 | 0.52 |
| 2:H:345:ASP:OD2 | 2:H:439:SER:HB3 | 2.09 | 0.52 |
| 1:A:147:SER:O | 1:A:151:THR:CB | 2.51 | 0.52 |
| 2:B:243:ARG:CZ | 2:B:252:LEU:HG | 2.39 | 0.52 |
| 1:C:107:HIS:CD2 | 1:C:151:THR:HG22 | 2.45 | 0.52 |
| 1:C:345:GLU:C | 1:C:347:ILE:H | 2.13 | 0.52 |
| 2:D:231:ILE:HD13 | 2:D:231:ILE:N | 2.25 | 0.52 |
| 1:E:259:MET:HG2 | 1:E:314:THR:CG2 | 2.38 | 0.52 |
| 1:E:259:MET:CG | 1:E:314:THR:HG21 | 2.37 | 0.52 |
| 2:F:8:HIS:HB3 | 2:F:13:GLY:O | 2.10 | 0.52 |
| 1:G:70:LEU:HD12 | 1:G:145:THR:HG23 | 1.91 | 0.52 |
| 1:G:422:GLU:O | 1:G:426:ASN:N | 2.37 | 0.52 |
| 1:A:277:SER:OG | 1:A:281:GLN:HB2 | 2.10 | 0.52 |
| 1:A:345:GLU:C | 1:A:347:ILE:H | 2.13 | 0.52 |
| 2:B:4:CYS:HA | 2:B:134:GLY:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:345:ASP:OD2 | 2:B:439:SER:HB3 | 2.10 | 0.52 |
| 1:C:212:ILE:O | 1:C:216:THR:HB | 2.09 | 0.52 |
| 1:C:431:GLU:OE1 | 1:C:432:TYR:CA | 2.57 | 0.52 |
| 2:D:206:ASN:OD1 | 2:D:227:LEU:CD1 | 2.58 | 0.52 |
| 2:D:243:ARG:CZ | 2:D:252:LEU:HG | 2.39 | 0.52 |
| 2:D:345:ASP:OD2 | 2:D:439:SER:HB3 | 2.09 | 0.52 |
| 2:D:408:TYR:O | 2:D:411:GLU:N | 2.39 | 0.52 |
| 1:E:70:LEU:HD12 | 1:E:145:THR:HG23 | 1.91 | 0.52 |
| 1:E:147:SER:O | 1:E:151:THR:CB | 2.51 | 0.52 |
| 1:E:251:ASP:O | 1:E:252:LEU:C | 2.49 | 0.52 |
| 1:E:295:MET:SD | 1:E:375:ALA:O | 2.68 | 0.52 |
| 2:F:315:CYS:HB3 | 2:F:377:MET:HE2 | 1.90 | 0.52 |
| 1:G:209:LEU:O | 1:G:210:TYR:C | 2.48 | 0.52 |
| 1:G:320:ARG:HA | 1:G:356:CYS:HB3 | 1.92 | 0.52 |
| 2:H:231:ILE:HD13 | 2:H:231:ILE:N | 2.25 | 0.52 |
| 2:H:234:ILE:CG1 | 2:H:270:ALA:HB1 | 2.38 | 0.52 |
| 2:B:119:LEU:HD11 | 2:B:156:ARG:CD | 2.40 | 0.52 |
| 2:B:244:PHE:CD2 | 2:B:245:ASP:N | 2.76 | 0.52 |
| 2:B:333:ALA:N | 1:C:177:VAL:HG21 | 2.25 | 0.52 |
| 1:C:8:GLN:OE1 | 1:C:14:ASN:ND2 | 2.42 | 0.52 |
| 1:C:352:LYS:HZ3 | 2:D:180:ALA:HA | 1.75 | 0.52 |
| 2:D:4:CYS:HA | 2:D:134:GLY:O | 2.10 | 0.52 |
| 1:G:251:ASP:O | 1:G:252:LEU:C | 2.49 | 0.52 |
| 2:H:8:HIS:HB3 | 2:H:13:GLY:O | 2.10 | 0.52 |
| 2:H:239:THR:O | 2:H:240:ALA:C | 2.48 | 0.52 |
| 2:H:251:ASP:OD1 | 2:H:252:LEU:N | 2.43 | 0.52 |
| 1:A:198:THR:HG22 | 1:A:265:LEU:CD2 | 2.39 | 0.52 |
| 2:B:24:TYR:CE2 | 2:B:240:ALA:HB2 | 2.45 | 0.52 |
| 2:B:201:ALA:O | 2:B:267:PHE:HA | 2.10 | 0.52 |
| 2:B:239:THR:O | 2:B:240:ALA:C | 2.48 | 0.52 |
| 2:B:417:GLU:OE1 | 2:B:417:GLU:HA | 2.10 | 0.52 |
| 1:C:325:MET:HE1 | 1:C:355:VAL:HG11 | 1.91 | 0.52 |
| 2:D:201:ALA:O | 2:D:267:PHE:HA | 2.10 | 0.52 |
| 2:D:244:PHE:CD2 | 2:D:245:ASP:N | 2.76 | 0.52 |
| 1:E:149:MET:O | 1:E:149:MET:HG2 | 2.10 | 0.52 |
| 1:E:149:MET:O | 1:E:153:LEU:HD22 | 2.10 | 0.52 |
| 1:E:188:THR:HA | 1:E:425:MET:CE | 2.40 | 0.52 |
| 2:F:239:THR:O | 2:F:240:ALA:C | 2.48 | 0.52 |
| 2:F:350:GLY:HA2 | 1:G:181:VAL:HG22 | 1.90 | 0.52 |
| 1:G:200:GLU:N | 1:G:265:LEU:HD13 | 2.25 | 0.52 |
| 2:B:9:VAL:HG21 | 2:B:149:PHE:CD1 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:63:PRO:HG3 | 2:B:87:PHE:CA | 2.40 | 0.51 |
| 2:B:243:ARG:NH2 | 2:B:251:ASP:OD1 | 2.44 | 0.51 |
| 1:C:277:SER:OG | 1:C:281:GLN:HB2 | 2.10 | 0.51 |
| 1:C:295:MET:SD | 1:C:375:ALA:O | 2.68 | 0.51 |
| 2:D:147:SER:CB | 2:D:190:THR:OG1 | 2.52 | 0.51 |
| 1:E:200:GLU:N | 1:E:265:LEU:HD13 | 2.25 | 0.51 |
| 2:F:24:TYR:CE2 | 2:F:240:ALA:HB2 | 2.45 | 0.51 |
| 2:F:63:PRO:CG | 2:F:87:PHE:HA | 2.40 | 0.51 |
| 2:F:147:SER:CB | 2:F:190:THR:OG1 | 2.52 | 0.51 |
| 2:F:251:ASP:OD1 | 2:F:252:LEU:N | 2.43 | 0.51 |
| 1:G:147:SER:O | 1:G:151:THR:CB | 2.51 | 0.51 |
| 1:G:188:THR:HA | 1:G:425:MET:CE | 2.40 | 0.51 |
| 1:G:260:VAL:HG23 | 1:G:260:VAL:O | 2.10 | 0.51 |
| 1:G:295:MET:SD | 1:G:375:ALA:O | 2.68 | 0.51 |
| 2:H:63:PRO:CG | 2:H:87:PHE:HA | 2.40 | 0.51 |
| 1:A:107:HIS:CD2 | 1:A:151:THR:HG22 | 2.45 | 0.51 |
| 1:A:188:THR:HA | 1:A:425:MET:CE | 2.40 | 0.51 |
| 1:A:295:MET:SD | 1:A:375:ALA:O | 2.68 | 0.51 |
| 2:B:206:ASN:OD1 | 2:B:227:LEU:CD1 | 2.57 | 0.51 |
| 1:C:198:THR:HG22 | 1:C:265:LEU:CD2 | 2.39 | 0.51 |
| 1:C:200:GLU:N | 1:C:265:LEU:HD13 | 2.25 | 0.51 |
| 1:C:254:LYS:NZ | 2:D:101:ASN:CG | 2.62 | 0.51 |
| 2:D:5:ILE:O | 2:D:136:SER:N | 2.40 | 0.51 |
| 2:D:9:VAL:HG21 | 2:D:149:PHE:CD1 | 2.46 | 0.51 |
| 2:D:239:THR:O | 2:D:240:ALA:C | 2.48 | 0.51 |
| 2:D:417:GLU:HA | 2:D:417:GLU:OE1 | 2.10 | 0.51 |
| 1:E:260:VAL:O | 1:E:260:VAL:HG23 | 2.10 | 0.51 |
| 1:E:264:ARG:HA | 1:E:264:ARG:HE | 1.75 | 0.51 |
| 1:E:422:GLU:O | 1:E:426:ASN:N | 2.37 | 0.51 |
| 2:F:150:THR:O | 2:F:151:SER:C | 2.47 | 0.51 |
| 2:F:234:ILE:CG1 | 2:F:270:ALA:HB1 | 2.38 | 0.51 |
| 2:F:324:VAL:O | 2:F:327:ASP:HB2 | 2.08 | 0.51 |
| 1:G:176:LYS:HG3 | 1:G:177:VAL:H | 1.76 | 0.51 |
| 2:H:24:TYR:CE2 | 2:H:240:ALA:HB2 | 2.45 | 0.51 |
| 2:H:147:SER:CB | 2:H:190:THR:OG1 | 2.52 | 0.51 |
| 2:H:324:VAL:O | 2:H:327:ASP:HB2 | 2.08 | 0.51 |
| 2:B:11:GLN:NE2 | 2:B:74:VAL:HG22 | 2.22 | 0.51 |
| 2:B:14:VAL:HG11 | 2:B:75:ILE:HD13 | 1.93 | 0.51 |
| 2:D:14:VAL:HG11 | 2:D:75:ILE:HD13 | 1.93 | 0.51 |
| 1:E:21:TRP:HZ2 | 1:E:65:ALA:HB2 | 1.76 | 0.51 |
| 1:G:149:MET:O | 1:G:153:LEU:HD22 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:264:ARG:HA | 1:G:264:ARG:HE | 1.75 | 0.51 |
| 2:H:191:THR:HG23 | 2:H:192:HIS:N | 2.25 | 0.51 |
| 1:A:200:GLU:N | 1:A:265:LEU:HD13 | 2.25 | 0.51 |
| 1:A:260:VAL:HG23 | 1:A:260:VAL:O | 2.10 | 0.51 |
| 2:B:191:THR:HG23 | 2:B:192:HIS:N | 2.25 | 0.51 |
| 1:C:5:VAL:CG2 | 1:C:135:PHE:CD2 | 2.94 | 0.51 |
| 1:C:260:VAL:HG23 | 1:C:260:VAL:O | 2.10 | 0.51 |
| 2:D:243:ARG:NH2 | 2:D:251:ASP:OD1 | 2.44 | 0.51 |
| 1:E:257:VAL:HA | 2:F:407:TRP:NE1 | 2.24 | 0.51 |
| 2:F:119:LEU:HD11 | 2:F:156:ARG:CD | 2.40 | 0.51 |
| 2:F:191:THR:HG23 | 2:F:192:HIS:N | 2.25 | 0.51 |
| 1:G:21:TRP:HZ2 | 1:G:65:ALA:HB2 | 1.76 | 0.51 |
| 1:G:149:MET:O | 1:G:149:MET:HG2 | 2.10 | 0.51 |
| 1:G:257:VAL:CB | 2:H:407:TRP:CE3 | 2.65 | 0.51 |
| 1:A:149:MET:O | 1:A:153:LEU:HD22 | 2.10 | 0.51 |
| 1:A:251:ASP:O | 1:A:252:LEU:C | 2.49 | 0.51 |
| 1:C:188:THR:HA | 1:C:425:MET:CE | 2.40 | 0.51 |
| 2:D:119:LEU:HD11 | 2:D:156:ARG:CD | 2.40 | 0.51 |
| 1:E:277:SER:OG | 1:E:281:GLN:HB2 | 2.10 | 0.51 |
| 1:G:5:VAL:CG2 | 1:G:135:PHE:CD2 | 2.94 | 0.51 |
| 2:H:14:VAL:HG11 | 2:H:75:ILE:HD13 | 1.93 | 0.51 |
| 2:H:119:LEU:HD11 | 2:H:156:ARG:CD | 2.40 | 0.51 |
| 2:H:201:ALA:O | 2:H:267:PHE:HA | 2.10 | 0.51 |
| 1:A:5:VAL:CG2 | 1:A:135:PHE:CD2 | 2.94 | 0.51 |
| 1:A:240:THR:HG23 | 1:A:241:CYS:H | 1.76 | 0.51 |
| 1:A:314:THR:CG2 | 1:A:315:VAL:N | 2.73 | 0.51 |
| 2:B:87:PHE:H | 2:B:87:PHE:HD2 | 1.59 | 0.51 |
| 1:C:251:ASP:O | 1:C:252:LEU:C | 2.49 | 0.51 |
| 2:D:63:PRO:CG | 2:D:87:PHE:HA | 2.40 | 0.51 |
| 2:D:191:THR:HG23 | 2:D:192:HIS:N | 2.25 | 0.51 |
| 2:D:251:ASP:OD1 | 2:D:252:LEU:N | 2.43 | 0.51 |
| 2:D:338:LYS:O | 2:D:340:THR:N | 2.34 | 0.51 |
| 2:D:402:ARG:O | 2:D:403:ALA:O | 2.29 | 0.51 |
| 2:F:14:VAL:HG11 | 2:F:75:ILE:HD13 | 1.93 | 0.51 |
| 2:F:201:ALA:O | 2:F:267:PHE:HA | 2.10 | 0.51 |
| 1:G:107:HIS:CD2 | 1:G:151:THR:HG22 | 2.45 | 0.51 |
| 1:G:277:SER:OG | 1:G:281:GLN:HB2 | 2.10 | 0.51 |
| 2:H:9:VAL:HG21 | 2:H:149:PHE:CD1 | 2.46 | 0.51 |
| 3:I:84:LEU:CD2 | 3:I:101:VAL:HG12 | 2.41 | 0.51 |
| 2:B:251:ASP:OD1 | 2:B:252:LEU:N | 2.43 | 0.51 |
| 1:E:107:HIS:CD2 | 1:E:151:THR:HG22 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:240:THR:HG23 | 1:E:241:CYS:H | 1.76 | 0.51 |
| 2:F:9:VAL:HG21 | 2:F:149:PHE:CD1 | 2.46 | 0.51 |
| 2:F:263:PRO:HD3 | 1:G:406:HIS:CE1 | 2.45 | 0.51 |
| 1:G:314:THR:CG2 | 1:G:315:VAL:N | 2.73 | 0.51 |
| 2:H:243:ARG:NH2 | 2:H:251:ASP:OD1 | 2.44 | 0.51 |
| 3:I:84:LEU:HD22 | 3:I:101:VAL:HG12 | 1.92 | 0.51 |
| 2:B:171:ILE:O | 2:B:171:ILE:HG22 | 2.10 | 0.51 |
| 1:C:240:THR:HG23 | 1:C:241:CYS:H | 1.76 | 0.51 |
| 2:D:11:GLN:NE2 | 2:D:74:VAL:HG22 | 2.22 | 0.51 |
| 2:D:87:PHE:H | 2:D:87:PHE:HD2 | 1.59 | 0.51 |
| 2:D:238:ILE:O | 2:D:242:LEU:HB2 | 2.11 | 0.51 |
| 1:E:113:GLU:HG3 | 1:E:114:LEU:N | 2.26 | 0.51 |
| 2:F:87:PHE:H | 2:F:87:PHE:HD2 | 1.59 | 0.51 |
| 2:F:243:ARG:NH2 | 2:F:251:ASP:OD1 | 2.44 | 0.51 |
| 2:F:260:VAL:HG22 | 1:G:407:TRP:HE1 | 1.76 | 0.51 |
| 2:F:305:CYS:O | 2:F:306:ASP:C | 2.49 | 0.51 |
| 2:F:338:LYS:O | 2:F:340:THR:N | 2.34 | 0.51 |
| 1:G:240:THR:HG23 | 1:G:241:CYS:H | 1.76 | 0.51 |
| 2:H:305:CYS:O | 2:H:306:ASP:C | 2.49 | 0.51 |
| 2:H:362:VAL:HG13 | 2:H:368:LEU:CD1 | 2.38 | 0.51 |
| 2:B:362:VAL:HG13 | 2:B:368:LEU:CD1 | 2.38 | 0.51 |
| 1:C:314:THR:CG2 | 1:C:315:VAL:N | 2.73 | 0.51 |
| 2:D:132:LEU:CD2 | 2:D:164:LYS:HE3 | 2.41 | 0.51 |
| 1:E:5:VAL:CG2 | 1:E:135:PHE:CD2 | 2.94 | 0.51 |
| 2:F:133:GLN:CB | 2:F:243:ARG:HH12 | 2.24 | 0.51 |
| 2:F:238:ILE:O | 2:F:242:LEU:HB2 | 2.11 | 0.51 |
| 2:F:332:ILE:HG21 | 1:G:177:VAL:HG11 | 1.91 | 0.51 |
| 1:G:113:GLU:HG3 | 1:G:114:LEU:N | 2.26 | 0.51 |
| 1:G:342:TYR:CD2 | 3:I:64:TYR:OH | 2.63 | 0.51 |
| 2:H:87:PHE:H | 2:H:87:PHE:HD2 | 1.59 | 0.51 |
| 2:H:171:ILE:HG22 | 2:H:171:ILE:O | 2.10 | 0.51 |
| 2:H:238:ILE:O | 2:H:242:LEU:HB2 | 2.11 | 0.51 |
| 1:A:422:GLU:O | 1:A:426:ASN:N | 2.37 | 0.51 |
| 2:B:402:ARG:O | 2:B:403:ALA:O | 2.29 | 0.51 |
| 1:E:49:ILE:HG13 | 1:E:50:ASN:H | 1.76 | 0.51 |
| 1:E:314:THR:CG2 | 1:E:315:VAL:N | 2.73 | 0.51 |
| 2:F:133:GLN:HB3 | 2:F:243:ARG:HH12 | 1.76 | 0.51 |
| 2:F:196:GLU:O | 2:F:197:HIS:CD2 | 2.64 | 0.51 |
| 2:F:315:CYS:HB3 | 2:F:377:MET:HE1 | 1.93 | 0.51 |
| 2:F:362:VAL:HG13 | 2:F:368:LEU:CD1 | 2.38 | 0.51 |
| 1:G:265:LEU:O | 1:G:266:HIS:O | 2.29 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:323:MET:HG3 | 1:G:328:VAL:CG2 | 2.41 | 0.51 |
| 1:G:348:PRO:HD3 | 2:H:397:LEU:HB3 | 1.92 | 0.51 |
| 2:H:132:LEU:CD2 | 2:H:164:LYS:HE3 | 2.41 | 0.51 |
| 2:H:133:GLN:HB3 | 2:H:243:ARG:HH12 | 1.76 | 0.51 |
| 2:H:151:SER:HB3 | 2:H:193:THR:CG2 | 2.34 | 0.51 |
| 1:A:265:LEU:O | 1:A:266:HIS:O | 2.29 | 0.50 |
| 2:B:119:LEU:HA | 2:B:122:ILE:HG12 | 1.93 | 0.50 |
| 2:B:348:PRO:CD | 1:C:398:MET:HE2 | 2.30 | 0.50 |
| 1:C:149:MET:O | 1:C:153:LEU:HD22 | 2.10 | 0.50 |
| 2:D:305:CYS:O | 2:D:306:ASP:C | 2.49 | 0.50 |
| 1:E:49:ILE:O | 1:E:50:ASN:C | 2.48 | 0.50 |
| 1:E:323:MET:HG3 | 1:E:328:VAL:CG2 | 2.41 | 0.50 |
| 2:F:132:LEU:CD2 | 2:F:164:LYS:HE3 | 2.41 | 0.50 |
| 2:F:140:SER:O | 2:F:142:GLY:N | 2.44 | 0.50 |
| 2:F:171:ILE:HG22 | 2:F:171:ILE:O | 2.10 | 0.50 |
| 2:H:102:ASN:CB | 2:H:407:TRP:HD1 | 2.23 | 0.50 |
| 2:H:133:GLN:CB | 2:H:243:ARG:HH12 | 2.24 | 0.50 |
| 2:H:140:SER:O | 2:H:142:GLY:N | 2.44 | 0.50 |
| 2:H:196:GLU:O | 2:H:197:HIS:CD2 | 2.64 | 0.50 |
| 2:H:338:LYS:O | 2:H:340:THR:N | 2.34 | 0.50 |
| 1:A:49:ILE:O | 1:A:50:ASN:C | 2.48 | 0.50 |
| 2:B:70:LEU:CD1 | 2:B:145:THR:CB | 2.89 | 0.50 |
| 2:B:132:LEU:CD2 | 2:B:164:LYS:HE3 | 2.42 | 0.50 |
| 2:D:133:GLN:CB | 2:D:243:ARG:HH12 | 2.24 | 0.50 |
| 2:D:133:GLN:HB3 | 2:D:243:ARG:HH12 | 1.76 | 0.50 |
| 2:D:244:PHE:CD2 | 2:D:244:PHE:C | 2.84 | 0.50 |
| 1:E:369:ARG:HD2 | 1:E:369:ARG:C | 2.32 | 0.50 |
| 1:E:383:ALA:C | 1:E:385:GLN:H | 2.15 | 0.50 |
| 2:F:119:LEU:HA | 2:F:122:ILE:HG12 | 1.93 | 0.50 |
| 2:F:151:SER:HB3 | 2:F:193:THR:CG2 | 2.34 | 0.50 |
| 1:G:24:ILE:HG22 | 1:G:25:SER:N | 2.26 | 0.50 |
| 2:H:70:LEU:CD1 | 2:H:145:THR:CB | 2.89 | 0.50 |
| 1:A:383:ALA:C | 1:A:385:GLN:H | 2.15 | 0.50 |
| 2:B:133:GLN:CB | 2:B:243:ARG:HH12 | 2.24 | 0.50 |
| 2:B:144:GLY:H | 5:B:500:GTP:PG | 2.33 | 0.50 |
| 2:B:196:GLU:O | 2:B:197:HIS:CD2 | 2.64 | 0.50 |
| 1:C:298:ALA:O | 1:C:299:LYS:C | 2.50 | 0.50 |
| 2:D:119:LEU:HA | 2:D:122:ILE:HG12 | 1.93 | 0.50 |
| 2:D:362:VAL:HG13 | 2:D:368:LEU:CD1 | 2.38 | 0.50 |
| 1:E:24:ILE:HG22 | 1:E:25:SER:N | 2.27 | 0.50 |
| 1:E:265:LEU:O | 1:E:266:HIS:O | 2.29 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:49:ILE:O | 1:G:50:ASN:C | 2.48 | 0.50 |
| 1:G:383:ALA:C | 1:G:385:GLN:H | 2.15 | 0.50 |
| 2:H:119:LEU:HA | 2:H:122:ILE:HG12 | 1.93 | 0.50 |
| 1:A:265:LEU:HD12 | 1:A:266:HIS:O | 2.12 | 0.50 |
| 2:B:238:ILE:O | 2:B:242:LEU:HB2 | 2.11 | 0.50 |
| 1:C:49:ILE:O | 1:C:50:ASN:C | 2.48 | 0.50 |
| 2:D:171:ILE:O | 2:D:171:ILE:HG22 | 2.10 | 0.50 |
| 2:D:310:GLY:HA3 | 2:D:383:ALA:N | 2.26 | 0.50 |
| 2:F:70:LEU:CD1 | 2:F:145:THR:CB | 2.89 | 0.50 |
| 1:G:49:ILE:HG13 | 1:G:50:ASN:H | 1.76 | 0.50 |
| 1:G:254:LYS:HE3 | 1:G:352:LYS:HZ2 | 1.74 | 0.50 |
| 1:G:257:VAL:CG2 | 1:G:257:VAL:O | 2.50 | 0.50 |
| 2:H:417:GLU:OE1 | 2:H:417:GLU:HA | 2.10 | 0.50 |
| 3:I:80:PHE:HE1 | 3:I:119:LEU:HD21 | 1.76 | 0.50 |
| 1:A:387:LEU:HD23 | 1:A:388:PHE:CD2 | 2.47 | 0.50 |
| 2:B:133:GLN:HB3 | 2:B:243:ARG:HH12 | 1.76 | 0.50 |
| 1:C:265:LEU:HD12 | 1:C:266:HIS:O | 2.12 | 0.50 |
| 2:D:11:GLN:O | 2:D:14:VAL:HB | 2.12 | 0.50 |
| 2:D:16:ILE:HG23 | 2:D:17:GLY:N | 2.26 | 0.50 |
| 2:D:70:LEU:CD1 | 2:D:145:THR:CB | 2.89 | 0.50 |
| 1:E:3:GLU:HA | 1:E:51:VAL:HA | 1.93 | 0.50 |
| 1:E:188:THR:HA | 1:E:425:MET:HE3 | 1.92 | 0.50 |
| 2:F:417:GLU:OE1 | 2:F:417:GLU:HA | 2.10 | 0.50 |
| 1:G:257:VAL:O | 2:H:404:PHE:CD2 | 2.64 | 0.50 |
| 1:G:280:SER:O | 1:G:282:GLN:N | 2.45 | 0.50 |
| 1:G:333:LEU:O | 1:G:336:GLN:N | 2.45 | 0.50 |
| 1:G:369:ARG:HD2 | 1:G:369:ARG:C | 2.32 | 0.50 |
| 2:H:16:ILE:HG23 | 2:H:17:GLY:N | 2.26 | 0.50 |
| 1:A:262:PHE:O | 1:A:264:ARG:N | 2.45 | 0.50 |
| 1:A:323:MET:HG3 | 1:A:328:VAL:CG2 | 2.41 | 0.50 |
| 2:B:11:GLN:O | 2:B:14:VAL:HB | 2.12 | 0.50 |
| 2:B:63:PRO:HD3 | 2:B:86:LEU:O | 2.11 | 0.50 |
| 1:C:113:GLU:HG3 | 1:C:114:LEU:N | 2.26 | 0.50 |
| 1:C:323:MET:HG3 | 1:C:328:VAL:CG2 | 2.41 | 0.50 |
| 1:C:387:LEU:HD23 | 1:C:388:PHE:CD2 | 2.47 | 0.50 |
| 2:D:234:ILE:HB | 2:D:302:MET:HE1 | 1.94 | 0.50 |
| 1:E:333:LEU:O | 1:E:336:GLN:N | 2.45 | 0.50 |
| 1:E:345:GLU:O | 1:E:347:ILE:N | 2.45 | 0.50 |
| 2:F:16:ILE:HG23 | 2:F:17:GLY:N | 2.26 | 0.50 |
| 1:G:253:ARG:CD | 2:H:407:TRP:HH2 | 2.24 | 0.50 |
| 1:G:269:MET:HB3 | 1:G:303:ALA:HB2 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:344:VAL:HG12 | 2:H:345:ASP:H | 1.74 | 0.50 |
| 1:A:24:ILE:HG22 | 1:A:25:SER:N | 2.27 | 0.50 |
| 1:A:298:ALA:O | 1:A:299:LYS:C | 2.50 | 0.50 |
| 1:A:369:ARG:HD2 | 1:A:369:ARG:C | 2.32 | 0.50 |
| 2:B:140:SER:O | 2:B:142:GLY:N | 2.44 | 0.50 |
| 2:B:234:ILE:HB | 2:B:302:MET:HE1 | 1.94 | 0.50 |
| 2:B:305:CYS:O | 2:B:306:ASP:C | 2.49 | 0.50 |
| 1:C:265:LEU:O | 1:C:266:HIS:O | 2.29 | 0.50 |
| 1:C:273:ALA:CB | 1:C:274:PRO:HD3 | 2.30 | 0.50 |
| 1:C:336:GLN:HE22 | 1:C:349:ASN:ND2 | 2.10 | 0.50 |
| 2:D:5:ILE:HG12 | 2:D:6:SER:N | 2.26 | 0.50 |
| 1:E:4:ILE:HG22 | 1:E:5:VAL:N | 2.27 | 0.50 |
| 1:E:168:THR:O | 1:E:201:THR:HA | 2.12 | 0.50 |
| 1:E:245:PRO:HA | 2:F:73:THR:CG2 | 2.42 | 0.50 |
| 1:E:262:PHE:O | 1:E:264:ARG:N | 2.45 | 0.50 |
| 1:E:269:MET:HB3 | 1:E:303:ALA:HB2 | 1.94 | 0.50 |
| 1:E:280:SER:O | 1:E:282:GLN:N | 2.45 | 0.50 |
| 2:F:12:ALA:CB | 2:F:140:SER:OG | 2.60 | 0.50 |
| 1:G:3:GLU:HA | 1:G:51:VAL:HA | 1.93 | 0.50 |
| 1:G:4:ILE:HG22 | 1:G:5:VAL:N | 2.27 | 0.50 |
| 1:G:262:PHE:O | 1:G:264:ARG:N | 2.45 | 0.50 |
| 2:H:12:ALA:CB | 2:H:140:SER:OG | 2.59 | 0.50 |
| 1:A:4:ILE:HD12 | 1:A:239:THR:CG2 | 2.42 | 0.50 |
| 1:A:173:PRO:HB3 | 1:A:183:GLU:CG | 2.42 | 0.50 |
| 1:A:431:GLU:HA | 1:A:434:GLN:CG | 2.42 | 0.50 |
| 2:B:261:PRO:HB2 | 2:B:262:TYR:CD1 | 2.46 | 0.50 |
| 2:B:310:GLY:HA3 | 2:B:383:ALA:N | 2.26 | 0.50 |
| 1:C:345:GLU:O | 1:C:347:ILE:N | 2.45 | 0.50 |
| 1:C:369:ARG:HD2 | 1:C:369:ARG:C | 2.32 | 0.50 |
| 1:E:173:PRO:HB3 | 1:E:183:GLU:CG | 2.42 | 0.50 |
| 1:E:336:GLN:HE22 | 1:E:349:ASN:ND2 | 2.10 | 0.50 |
| 2:F:344:VAL:HG12 | 2:F:345:ASP:H | 1.74 | 0.50 |
| 1:G:345:GLU:O | 1:G:347:ILE:N | 2.45 | 0.50 |
| 1:G:387:LEU:HD23 | 1:G:388:PHE:CD2 | 2.47 | 0.50 |
| 2:H:244:PHE:C | 2:H:244:PHE:CD2 | 2.83 | 0.50 |
| 2:H:261:PRO:HB2 | 2:H:262:TYR:CD1 | 2.46 | 0.50 |
| 2:H:310:GLY:HA3 | 2:H:383:ALA:N | 2.26 | 0.50 |
| 1:A:49:ILE:HG13 | 1:A:50:ASN:H | 1.76 | 0.50 |
| 1:A:333:LEU:O | 1:A:336:GLN:N | 2.45 | 0.50 |
| 1:A:336:GLN:HE22 | 1:A:349:ASN:ND2 | 2.10 | 0.50 |
| 1:A:345:GLU:O | 1:A:347:ILE:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:149:PHE:HE1 | 2:B:153:LEU:HD22 | 1.77 | 0.50 |
| 1:C:4:ILE:HD12 | 1:C:239:THR:CG2 | 2.42 | 0.50 |
| 1:C:262:PHE:O | 1:C:264:ARG:N | 2.45 | 0.50 |
| 1:C:269:MET:HB3 | 1:C:303:ALA:HB2 | 1.94 | 0.50 |
| 1:C:431:GLU:HA | 1:C:434:GLN:CG | 2.42 | 0.50 |
| 2:D:62:VAL:CG2 | 2:D:88:HIS:CE1 | 2.87 | 0.50 |
| 2:D:140:SER:O | 2:D:142:GLY:N | 2.44 | 0.50 |
| 2:D:196:GLU:O | 2:D:197:HIS:CD2 | 2.64 | 0.50 |
| 1:E:387:LEU:HD23 | 1:E:388:PHE:CD2 | 2.47 | 0.50 |
| 2:F:261:PRO:HB2 | 2:F:262:TYR:CD1 | 2.46 | 0.50 |
| 1:G:4:ILE:HD12 | 1:G:239:THR:CG2 | 2.42 | 0.50 |
| 1:A:88:ARG:NE | 1:E:283:TYR:HE1 | 2.09 | 0.49 |
| 1:A:133:GLN:NE2 | 1:A:252:LEU:HB2 | 2.27 | 0.49 |
| 1:A:273:ALA:CB | 1:A:274:PRO:HD3 | 2.30 | 0.49 |
| 1:A:296:PHE:CZ | 1:A:315:VAL:HG11 | 2.46 | 0.49 |
| 2:B:12:ALA:CB | 2:B:140:SER:OG | 2.59 | 0.49 |
| 1:C:4:ILE:HG22 | 1:C:5:VAL:N | 2.27 | 0.49 |
| 1:C:49:ILE:HG13 | 1:C:50:ASN:H | 1.76 | 0.49 |
| 2:D:115:ILE:CG2 | 2:D:116:ASP:N | 2.75 | 0.49 |
| 2:D:227:LEU:O | 2:D:231:ILE:HG12 | 2.12 | 0.49 |
| 1:E:4:ILE:HD12 | 1:E:239:THR:CG2 | 2.42 | 0.49 |
| 1:E:298:ALA:O | 1:E:299:LYS:C | 2.50 | 0.49 |
| 2:F:244:PHE:C | 2:F:244:PHE:CD2 | 2.83 | 0.49 |
| 1:G:133:GLN:NE2 | 1:G:252:LEU:HB2 | 2.27 | 0.49 |
| 1:G:173:PRO:HB3 | 1:G:183:GLU:CG | 2.42 | 0.49 |
| 1:G:245:PRO:CB | 2:H:73:THR:CG2 | 2.89 | 0.49 |
| 1:G:298:ALA:O | 1:G:299:LYS:C | 2.50 | 0.49 |
| 2:H:2:ARG:NH1 | 2:H:47:ASP:CB | 2.75 | 0.49 |
| 1:A:4:ILE:HG22 | 1:A:5:VAL:N | 2.27 | 0.49 |
| 1:A:168:THR:O | 1:A:201:THR:HA | 2.12 | 0.49 |
| 1:A:280:SER:O | 1:A:282:GLN:N | 2.45 | 0.49 |
| 2:B:115:ILE:CG2 | 2:B:116:ASP:N | 2.75 | 0.49 |
| 1:C:24:ILE:HG22 | 1:C:25:SER:N | 2.27 | 0.49 |
| 1:C:173:PRO:HB3 | 1:C:183:GLU:CG | 2.42 | 0.49 |
| 1:C:296:PHE:CZ | 1:C:315:VAL:HG11 | 2.46 | 0.49 |
| 1:C:301:MET:HE1 | 1:C:377:PHE:HE2 | 1.77 | 0.49 |
| 1:C:383:ALA:C | 1:C:385:GLN:H | 2.15 | 0.49 |
| 2:D:62:VAL:O | 2:D:63:PRO:O | 2.30 | 0.49 |
| 2:D:414:GLU:OE1 | 2:D:414:GLU:N | 2.46 | 0.49 |
| 1:E:431:GLU:HA | 1:E:434:GLN:CG | 2.42 | 0.49 |
| 2:F:2:ARG:NH1 | 2:F:47:ASP:CB | 2.75 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:5:ILE:HG12 | 2:F:6:SER:N | 2.26 | 0.49 |
| 2:F:149:PHE:HE1 | 2:F:153:LEU:HD22 | 1.77 | 0.49 |
| 2:F:263:PRO:HD3 | 1:G:406:HIS:NE2 | 2.27 | 0.49 |
| 2:F:402:ARG:O | 2:F:403:ALA:O | 2.29 | 0.49 |
| 1:G:168:THR:O | 1:G:201:THR:HA | 2.12 | 0.49 |
| 1:G:336:GLN:HE22 | 1:G:349:ASN:ND2 | 2.10 | 0.49 |
| 2:H:402:ARG:O | 2:H:403:ALA:O | 2.29 | 0.49 |
| 1:A:113:GLU:HG3 | 1:A:114:LEU:N | 2.26 | 0.49 |
| 2:B:414:GLU:OE1 | 2:B:414:GLU:N | 2.46 | 0.49 |
| 1:C:133:GLN:NE2 | 1:C:252:LEU:HB2 | 2.28 | 0.49 |
| 1:C:168:THR:O | 1:C:201:THR:HA | 2.12 | 0.49 |
| 2:D:56:THR:HA | 2:H:284:GLU:HG3 | 1.92 | 0.49 |
| 2:D:261:PRO:HB2 | 2:D:262:TYR:CD1 | 2.46 | 0.49 |
| 2:D:293:ASN:HD21 | 2:D:338:LYS:NZ | 2.11 | 0.49 |
| 2:F:11:GLN:O | 2:F:14:VAL:HB | 2.12 | 0.49 |
| 2:F:293:ASN:HD21 | 2:F:338:LYS:NZ | 2.10 | 0.49 |
| 2:F:310:GLY:HA3 | 2:F:383:ALA:N | 2.26 | 0.49 |
| 1:G:352:LYS:CD | 2:H:181:VAL:HG21 | 2.26 | 0.49 |
| 1:G:431:GLU:HA | 1:G:434:GLN:CG | 2.42 | 0.49 |
| 2:H:11:GLN:O | 2:H:14:VAL:HB | 2.12 | 0.49 |
| 1:A:21:TRP:HZ2 | 1:A:65:ALA:HB2 | 1.76 | 0.49 |
| 2:B:5:ILE:CG1 | 2:B:64:ARG:NH2 | 2.75 | 0.49 |
| 2:B:244:PHE:CD2 | 2:B:244:PHE:C | 2.84 | 0.49 |
| 2:B:338:LYS:O | 2:B:340:THR:N | 2.34 | 0.49 |
| 1:C:280:SER:O | 1:C:282:GLN:N | 2.45 | 0.49 |
| 1:E:133:GLN:NE2 | 1:E:252:LEU:HB2 | 2.28 | 0.49 |
| 1:E:257:VAL:HG13 | 2:F:407:TRP:CD2 | 2.48 | 0.49 |
| 1:E:265:LEU:HD12 | 1:E:266:HIS:O | 2.12 | 0.49 |
| 1:G:258:ASN:HD21 | 1:G:352:LYS:HE2 | 1.69 | 0.49 |
| 1:G:265:LEU:HD12 | 1:G:266:HIS:O | 2.12 | 0.49 |
| 2:H:5:ILE:HG12 | 2:H:6:SER:N | 2.26 | 0.49 |
| 2:H:62:VAL:O | 2:H:63:PRO:O | 2.30 | 0.49 |
| 2:H:149:PHE:HE1 | 2:H:153:LEU:HD22 | 1.77 | 0.49 |
| 2:B:55:GLU:O | 2:B:56:THR:C | 2.50 | 0.49 |
| 2:B:293:ASN:HD21 | 2:B:338:LYS:NZ | 2.11 | 0.49 |
| 1:C:21:TRP:HZ2 | 1:C:65:ALA:HB2 | 1.76 | 0.49 |
| 2:D:12:ALA:CB | 2:D:140:SER:OG | 2.59 | 0.49 |
| 2:D:274:PRO:CB | 2:D:371:VAL:HG21 | 2.43 | 0.49 |
| 2:D:315:CYS:HB3 | 2:D:377:MET:HE1 | 1.94 | 0.49 |
| 1:E:173:PRO:HB3 | 1:E:183:GLU:HG2 | 1.93 | 0.49 |
| 2:F:105:ARG:HH11 | 2:F:105:ARG:HG3 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:192:HIS:CD2 | 2:F:424:ASP:OD2 | 2.66 | 0.49 |
| 2:F:297:GLU:HG3 | 2:F:299:ALA:N | 2.28 | 0.49 |
| 2:F:414:GLU:N | 2:F:414:GLU:OE1 | 2.46 | 0.49 |
| 1:G:137:LEU:HD22 | 1:G:154:ILE:HG21 | 1.94 | 0.49 |
| 2:H:105:ARG:HG3 | 2:H:105:ARG:HH11 | 1.78 | 0.49 |
| 2:H:293:ASN:HD21 | 2:H:338:LYS:NZ | 2.11 | 0.49 |
| 2:H:297:GLU:HG3 | 2:H:299:ALA:N | 2.28 | 0.49 |
| 1:A:269:MET:HB3 | 1:A:303:ALA:HB2 | 1.94 | 0.49 |
| 2:B:16:ILE:HG23 | 2:B:17:GLY:N | 2.26 | 0.49 |
| 2:B:115:ILE:O | 2:B:116:ASP:C | 2.51 | 0.49 |
| 2:B:118:VAL:HG21 | 2:B:149:PHE:CE2 | 2.48 | 0.49 |
| 2:B:192:HIS:CD2 | 2:B:424:ASP:OD2 | 2.66 | 0.49 |
| 2:B:230:LEU:O | 2:B:233:GLN:N | 2.35 | 0.49 |
| 1:C:333:LEU:O | 1:C:336:GLN:N | 2.45 | 0.49 |
| 2:D:149:PHE:HE1 | 2:D:153:LEU:HD22 | 1.77 | 0.49 |
| 2:D:192:HIS:CD2 | 2:D:424:ASP:OD2 | 2.66 | 0.49 |
| 2:D:392:ASP:O | 2:D:395:PHE:HB3 | 2.13 | 0.49 |
| 2:F:62:VAL:CG2 | 2:F:88:HIS:CE1 | 2.87 | 0.49 |
| 2:F:203:MET:SD | 2:F:267:PHE:HB3 | 2.53 | 0.49 |
| 1:G:296:PHE:CZ | 1:G:315:VAL:HG11 | 2.46 | 0.49 |
| 2:H:192:HIS:CD2 | 2:H:424:ASP:OD2 | 2.66 | 0.49 |
| 3:I:72:VAL:HG11 | 3:I:116:MET:SD | 2.52 | 0.49 |
| 1:A:3:GLU:HA | 1:A:51:VAL:HA | 1.93 | 0.49 |
| 1:A:8:GLN:HB3 | 1:A:14:ASN:HA | 1.94 | 0.49 |
| 2:B:188:ILE:O | 2:B:191:THR:HG22 | 2.13 | 0.49 |
| 2:B:227:LEU:O | 2:B:231:ILE:HG12 | 2.12 | 0.49 |
| 2:B:260:VAL:HG22 | 1:C:407:TRP:CZ2 | 2.48 | 0.49 |
| 2:B:274:PRO:CB | 2:B:371:VAL:HG21 | 2.43 | 0.49 |
| 2:B:392:ASP:O | 2:B:395:PHE:HB3 | 2.13 | 0.49 |
| 1:C:431:GLU:OE1 | 1:C:432:TYR:N | 2.46 | 0.49 |
| 2:D:2:ARG:NH1 | 2:D:47:ASP:CB | 2.75 | 0.49 |
| 2:D:115:ILE:O | 2:D:116:ASP:C | 2.51 | 0.49 |
| 2:D:158:SER:OG | 2:D:197:HIS:HB3 | 2.13 | 0.49 |
| 2:D:230:LEU:O | 2:D:233:GLN:N | 2.35 | 0.49 |
| 1:E:103:TRP:HZ3 | 1:E:108:TYR:CE1 | 2.27 | 0.49 |
| 2:F:62:VAL:O | 2:F:63:PRO:O | 2.30 | 0.49 |
| 2:H:70:LEU:HD12 | 2:H:70:LEU:N | 2.28 | 0.49 |
| 2:H:203:MET:SD | 2:H:267:PHE:HB3 | 2.53 | 0.49 |
| 2:H:414:GLU:OE1 | 2:H:414:GLU:N | 2.46 | 0.49 |
| 1:A:69:ASP:HA | 1:A:145:THR:HG21 | 1.95 | 0.49 |
| 2:B:158:SER:OG | 2:B:197:HIS:HB3 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:184:PRO:HG2 | 2:B:398:MET:CE | 2.40 | 0.49 |
| 2:B:297:GLU:HG3 | 2:B:299:ALA:N | 2.28 | 0.49 |
| 2:B:315:CYS:HB3 | 2:B:377:MET:HE1 | 1.94 | 0.49 |
| 1:C:8:GLN:HB3 | 1:C:14:ASN:HA | 1.94 | 0.49 |
| 2:D:23:LEU:HD23 | 2:D:236:SER:CB | 2.37 | 0.49 |
| 2:D:70:LEU:HD12 | 2:D:70:LEU:N | 2.28 | 0.49 |
| 2:D:115:ILE:HD11 | 2:D:119:LEU:HG | 1.92 | 0.49 |
| 2:D:118:VAL:HG21 | 2:D:149:PHE:CE2 | 2.48 | 0.49 |
| 2:D:297:GLU:HG3 | 2:D:299:ALA:N | 2.28 | 0.49 |
| 2:D:344:VAL:HG12 | 2:D:345:ASP:H | 1.74 | 0.49 |
| 1:E:175:PRO:CD | 1:E:207:GLU:OE1 | 2.61 | 0.49 |
| 1:E:199:ASP:O | 1:E:200:GLU:HG3 | 2.13 | 0.49 |
| 2:F:70:LEU:HD12 | 2:F:70:LEU:N | 2.28 | 0.49 |
| 2:F:118:VAL:HG21 | 2:F:149:PHE:CE2 | 2.48 | 0.49 |
| 1:G:175:PRO:CD | 1:G:207:GLU:OE1 | 2.61 | 0.49 |
| 1:G:199:ASP:O | 1:G:200:GLU:HG3 | 2.13 | 0.49 |
| 1:G:431:GLU:OE1 | 1:G:432:TYR:N | 2.46 | 0.49 |
| 3:I:113:ILE:HG21 | 3:I:119:LEU:HD21 | 1.95 | 0.49 |
| 1:A:431:GLU:OE1 | 1:A:432:TYR:N | 2.46 | 0.49 |
| 2:D:203:MET:SD | 2:D:267:PHE:HB3 | 2.53 | 0.49 |
| 1:E:137:LEU:HD22 | 1:E:154:ILE:HG21 | 1.95 | 0.49 |
| 1:E:211:ASP:OD1 | 1:E:212:ILE:HG13 | 2.13 | 0.49 |
| 1:E:296:PHE:CZ | 1:E:315:VAL:HG11 | 2.46 | 0.49 |
| 2:F:151:SER:OG | 2:F:193:THR:HG21 | 2.13 | 0.49 |
| 1:G:211:ASP:OD1 | 1:G:212:ILE:HG13 | 2.13 | 0.49 |
| 2:H:115:ILE:HD11 | 2:H:119:LEU:HG | 1.92 | 0.49 |
| 2:H:118:VAL:HG21 | 2:H:149:PHE:CE2 | 2.48 | 0.49 |
| 2:H:328:VAL:C | 2:H:330:ALA:H | 2.16 | 0.49 |
| 1:A:191:VAL:HG13 | 1:A:192:HIS:N | 2.28 | 0.49 |
| 1:A:260:VAL:HG23 | 2:B:407:TRP:NE1 | 2.25 | 0.49 |
| 2:B:2:ARG:NH1 | 2:B:47:ASP:CB | 2.76 | 0.49 |
| 2:B:105:ARG:HH11 | 2:B:105:ARG:HG3 | 1.78 | 0.49 |
| 2:B:203:MET:SD | 2:B:267:PHE:HB3 | 2.53 | 0.49 |
| 1:C:3:GLU:HA | 1:C:51:VAL:HA | 1.93 | 0.49 |
| 1:E:431:GLU:OE1 | 1:E:432:TYR:N | 2.46 | 0.49 |
| 2:F:115:ILE:HD11 | 2:F:119:LEU:HG | 1.93 | 0.49 |
| 2:F:155:GLU:OE1 | 2:F:197:HIS:HE1 | 1.96 | 0.49 |
| 2:F:158:SER:OG | 2:F:197:HIS:HB3 | 2.13 | 0.49 |
| 1:G:8:GLN:HB3 | 1:G:14:ASN:HA | 1.94 | 0.49 |
| 1:G:102:ASN:HB3 | 1:G:105:LYS:HB2 | 1.95 | 0.49 |
| 1:G:173:PRO:HB3 | 1:G:183:GLU:HG2 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:179:ASP:CB | 4:G:600:GDP:H3' | 2.36 | 0.49 |
| 2:H:115:ILE:CG2 | 2:H:116:ASP:N | 2.75 | 0.49 |
| 2:B:70:LEU:HD12 | 2:B:70:LEU:N | 2.28 | 0.48 |
| 2:B:115:ILE:HD11 | 2:B:119:LEU:HG | 1.92 | 0.48 |
| 2:B:344:VAL:HG12 | 2:B:345:ASP:H | 1.75 | 0.48 |
| 1:C:142:GLY:HA3 | 1:C:183:GLU:OE2 | 2.13 | 0.48 |
| 1:C:173:PRO:HB3 | 1:C:183:GLU:HG2 | 1.93 | 0.48 |
| 1:C:175:PRO:CD | 1:C:207:GLU:OE1 | 2.61 | 0.48 |
| 1:C:191:VAL:HG13 | 1:C:192:HIS:N | 2.28 | 0.48 |
| 2:D:50:ASN:ND2 | 2:D:53:PHE:O | 2.46 | 0.48 |
| 2:D:151:SER:OG | 2:D:193:THR:HG21 | 2.13 | 0.48 |
| 2:D:188:ILE:O | 2:D:191:THR:HG22 | 2.13 | 0.48 |
| 1:E:69:ASP:HA | 1:E:145:THR:HG21 | 1.95 | 0.48 |
| 2:F:115:ILE:O | 2:F:116:ASP:C | 2.51 | 0.48 |
| 2:F:188:ILE:O | 2:F:191:THR:HG22 | 2.13 | 0.48 |
| 1:G:191:VAL:HG13 | 1:G:192:HIS:N | 2.28 | 0.48 |
| 2:H:151:SER:OG | 2:H:193:THR:HG21 | 2.13 | 0.48 |
| 2:H:155:GLU:OE1 | 2:H:197:HIS:HE1 | 1.96 | 0.48 |
| 2:H:158:SER:OG | 2:H:197:HIS:HB3 | 2.13 | 0.48 |
| 1:A:137:LEU:HD22 | 1:A:154:ILE:HG21 | 1.95 | 0.48 |
| 1:A:142:GLY:HA3 | 1:A:183:GLU:OE2 | 2.13 | 0.48 |
| 1:A:154:ILE:HG22 | 1:A:166:MET:CE | 2.44 | 0.48 |
| 2:B:96:LYS:O | 2:B:97:GLU:O | 2.31 | 0.48 |
| 2:B:231:ILE:O | 2:B:235:VAL:HG23 | 2.12 | 0.48 |
| 1:C:281:GLN:C | 1:C:283:TYR:N | 2.67 | 0.48 |
| 2:D:155:GLU:OE1 | 2:D:197:HIS:HE1 | 1.96 | 0.48 |
| 2:D:231:ILE:O | 2:D:235:VAL:HG23 | 2.12 | 0.48 |
| 1:E:176:LYS:HG3 | 1:E:177:VAL:H | 1.78 | 0.48 |
| 1:E:257:VAL:HG13 | 2:F:407:TRP:CD1 | 2.48 | 0.48 |
| 2:F:50:ASN:ND2 | 2:F:53:PHE:O | 2.46 | 0.48 |
| 2:F:104:ALA:CB | 2:F:408:TYR:HD2 | 2.26 | 0.48 |
| 1:G:103:TRP:HZ3 | 1:G:108:TYR:CE1 | 2.27 | 0.48 |
| 2:H:50:ASN:ND2 | 2:H:53:PHE:O | 2.46 | 0.48 |
| 2:H:96:LYS:O | 2:H:97:GLU:O | 2.31 | 0.48 |
| 2:H:115:ILE:O | 2:H:116:ASP:C | 2.51 | 0.48 |
| 2:H:188:ILE:O | 2:H:191:THR:HG22 | 2.13 | 0.48 |
| 2:H:274:PRO:CB | 2:H:371:VAL:HG21 | 2.43 | 0.48 |
| 1:A:173:PRO:HB3 | 1:A:183:GLU:HG2 | 1.93 | 0.48 |
| 1:A:413:MET:HG3 | 1:A:414:ASP:N | 2.22 | 0.48 |
| 1:C:69:ASP:HA | 1:C:145:THR:HG21 | 1.95 | 0.48 |
| 1:C:103:TRP:HZ3 | 1:C:108:TYR:CE1 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:154:ILE:HG22 | 1:C:166:MET:CE | 2.44 | 0.48 |
| 1:E:8:GLN:HB3 | 1:E:14:ASN:HA | 1.94 | 0.48 |
| 1:E:20:PHE:CG | 1:E:235:MET:SD | 3.07 | 0.48 |
| 1:E:191:VAL:HG13 | 1:E:192:HIS:N | 2.28 | 0.48 |
| 2:F:24:TYR:OH | 2:F:239:THR:OG1 | 2.24 | 0.48 |
| 2:F:115:ILE:CG2 | 2:F:116:ASP:N | 2.75 | 0.48 |
| 2:F:242:LEU:C | 2:F:244:PHE:N | 2.66 | 0.48 |
| 2:F:274:PRO:CB | 2:F:371:VAL:HG21 | 2.43 | 0.48 |
| 1:G:176:LYS:CE | 1:G:207:GLU:HG3 | 2.39 | 0.48 |
| 2:H:231:ILE:O | 2:H:235:VAL:HG23 | 2.12 | 0.48 |
| 3:I:55:VAL:HG12 | 3:I:123:GLU:HB2 | 1.94 | 0.48 |
| 2:B:151:SER:OG | 2:B:193:THR:HG21 | 2.13 | 0.48 |
| 1:C:2:ARG:NH1 | 1:C:251:ASP:OD2 | 2.46 | 0.48 |
| 1:C:137:LEU:HD22 | 1:C:154:ILE:HG21 | 1.94 | 0.48 |
| 1:C:308:ARG:HG3 | 1:C:342:TYR:OH | 2.13 | 0.48 |
| 2:D:9:VAL:HG11 | 2:D:150:THR:OG1 | 2.13 | 0.48 |
| 1:E:264:ARG:HA | 1:E:264:ARG:NE | 2.29 | 0.48 |
| 2:F:5:ILE:O | 2:F:136:SER:N | 2.40 | 0.48 |
| 2:F:96:LYS:O | 2:F:97:GLU:O | 2.31 | 0.48 |
| 2:F:230:LEU:O | 2:F:233:GLN:N | 2.35 | 0.48 |
| 2:F:231:ILE:O | 2:F:235:VAL:HG23 | 2.12 | 0.48 |
| 2:F:234:ILE:HB | 2:F:302:MET:HE1 | 1.95 | 0.48 |
| 2:F:260:VAL:HG21 | 1:G:407:TRP:HZ2 | 1.77 | 0.48 |
| 1:G:69:ASP:HA | 1:G:145:THR:HG21 | 1.95 | 0.48 |
| 1:G:248:LEU:CD1 | 2:H:179:THR:HG21 | 2.41 | 0.48 |
| 1:G:264:ARG:HA | 1:G:264:ARG:NE | 2.29 | 0.48 |
| 2:H:24:TYR:OH | 2:H:239:THR:OG1 | 2.24 | 0.48 |
| 2:H:104:ALA:CB | 2:H:408:TYR:HD2 | 2.26 | 0.48 |
| 2:H:392:ASP:O | 2:H:395:PHE:HB3 | 2.13 | 0.48 |
| 2:B:155:GLU:OE1 | 2:B:197:HIS:HE1 | 1.96 | 0.48 |
| 2:B:242:LEU:C | 2:B:244:PHE:N | 2.66 | 0.48 |
| 1:C:102:ASN:HB3 | 1:C:105:LYS:HB2 | 1.95 | 0.48 |
| 1:C:179:ASP:HB3 | 4:C:600:GDP:H3' | 1.95 | 0.48 |
| 1:C:237:GLY:O | 1:C:241:CYS:CB | 2.61 | 0.48 |
| 2:D:96:LYS:O | 2:D:97:GLU:O | 2.31 | 0.48 |
| 2:D:99:ALA:O | 2:D:100:ALA:HB3 | 2.14 | 0.48 |
| 2:D:104:ALA:CB | 2:D:408:TYR:HD2 | 2.26 | 0.48 |
| 2:D:384:ILE:HG22 | 2:D:388:TRP:CD1 | 2.49 | 0.48 |
| 1:E:49:ILE:HG13 | 1:E:50:ASN:N | 2.28 | 0.48 |
| 1:E:102:ASN:HB3 | 1:E:105:LYS:HB2 | 1.95 | 0.48 |
| 1:E:142:GLY:HA3 | 1:E:183:GLU:OE2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:154:ILE:HG22 | 1:E:166:MET:CE | 2.44 | 0.48 |
| 1:G:49:ILE:HG13 | 1:G:50:ASN:N | 2.28 | 0.48 |
| 1:G:154:ILE:HG22 | 1:G:166:MET:CE | 2.44 | 0.48 |
| 2:H:62:VAL:CG2 | 2:H:88:HIS:CE1 | 2.87 | 0.48 |
| 1:A:2:ARG:NH1 | 1:A:251:ASP:OD2 | 2.46 | 0.48 |
| 1:A:102:ASN:HB3 | 1:A:105:LYS:HB2 | 1.95 | 0.48 |
| 1:A:188:THR:HA | 1:A:425:MET:HE3 | 1.95 | 0.48 |
| 1:A:199:ASP:O | 1:A:200:GLU:HG3 | 2.13 | 0.48 |
| 1:A:211:ASP:OD1 | 1:A:212:ILE:HG13 | 2.13 | 0.48 |
| 1:A:237:GLY:O | 1:A:241:CYS:CB | 2.61 | 0.48 |
| 1:A:263:PRO:O | 1:A:264:ARG:C | 2.52 | 0.48 |
| 1:A:281:GLN:C | 1:A:283:TYR:N | 2.67 | 0.48 |
| 2:B:104:ALA:CB | 2:B:408:TYR:HD2 | 2.26 | 0.48 |
| 1:C:115:VAL:CG2 | 1:C:152:LEU:HD23 | 2.44 | 0.48 |
| 1:C:346:TRP:HB3 | 2:D:401:LYS:NZ | 2.28 | 0.48 |
| 2:D:88:HIS:O | 2:D:89:PRO:C | 2.52 | 0.48 |
| 1:E:263:PRO:O | 1:E:264:ARG:C | 2.52 | 0.48 |
| 2:F:227:LEU:O | 2:F:231:ILE:HG12 | 2.12 | 0.48 |
| 1:G:209:LEU:CD2 | 1:G:227:LEU:HD13 | 2.44 | 0.48 |
| 2:H:227:LEU:O | 2:H:231:ILE:HG12 | 2.12 | 0.48 |
| 2:H:242:LEU:C | 2:H:244:PHE:N | 2.66 | 0.48 |
| 1:A:20:PHE:CG | 1:A:235:MET:SD | 3.07 | 0.48 |
| 1:A:103:TRP:HZ3 | 1:A:108:TYR:CE1 | 2.27 | 0.48 |
| 1:A:175:PRO:CD | 1:A:207:GLU:OE1 | 2.61 | 0.48 |
| 2:B:50:ASN:ND2 | 2:B:53:PHE:O | 2.46 | 0.48 |
| 2:B:62:VAL:HG12 | 2:B:63:PRO:N | 2.25 | 0.48 |
| 2:B:99:ALA:O | 2:B:100:ALA:HB3 | 2.14 | 0.48 |
| 2:B:386:GLU:O | 2:B:388:TRP:N | 2.47 | 0.48 |
| 1:C:156:LYS:HA | 1:C:156:LYS:CE | 2.38 | 0.48 |
| 1:C:263:PRO:O | 1:C:264:ARG:C | 2.52 | 0.48 |
| 2:D:105:ARG:HH11 | 2:D:105:ARG:HG3 | 1.78 | 0.48 |
| 2:D:163:LYS:C | 2:D:164:LYS:HG2 | 2.33 | 0.48 |
| 1:E:209:LEU:O | 1:E:213:CYS:N | 2.47 | 0.48 |
| 2:F:392:ASP:O | 2:F:395:PHE:HB3 | 2.13 | 0.48 |
| 1:G:20:PHE:CG | 1:G:235:MET:SD | 3.07 | 0.48 |
| 1:G:142:GLY:HA3 | 1:G:183:GLU:OE2 | 2.13 | 0.48 |
| 1:G:281:GLN:C | 1:G:283:TYR:N | 2.67 | 0.48 |
| 1:G:399:PHE:O | 1:G:400:ARG:C | 2.52 | 0.48 |
| 2:H:62:VAL:HG12 | 2:H:91:GLN:HE22 | 1.77 | 0.48 |
| 2:H:99:ALA:O | 2:H:100:ALA:HB3 | 2.13 | 0.48 |
| 2:H:230:LEU:O | 2:H:233:GLN:N | 2.35 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:115:VAL:CG2 | 1:A:152:LEU:HD23 | 2.44 | 0.48 |
| 1:A:308:ARG:HG3 | 1:A:342:TYR:OH | 2.13 | 0.48 |
| 2:B:67:PHE:CE1 | 2:B:87:PHE:CD1 | 2.89 | 0.48 |
| 2:B:253:THR:O | 2:B:254:GLU:C | 2.52 | 0.48 |
| 1:C:211:ASP:OD1 | 1:C:212:ILE:HG13 | 2.13 | 0.48 |
| 2:D:386:GLU:O | 2:D:388:TRP:N | 2.47 | 0.48 |
| 1:E:413:MET:HG3 | 1:E:414:ASP:N | 2.22 | 0.48 |
| 2:F:155:GLU:HG2 | 2:F:197:HIS:CE1 | 2.49 | 0.48 |
| 2:F:261:PRO:HB3 | 1:G:404:PHE:CD2 | 2.40 | 0.48 |
| 2:F:386:GLU:O | 2:F:388:TRP:N | 2.47 | 0.48 |
| 1:G:209:LEU:O | 1:G:213:CYS:N | 2.47 | 0.48 |
| 1:G:253:ARG:HB3 | 2:H:407:TRP:CZ3 | 2.34 | 0.48 |
| 1:G:287:THR:O | 1:G:288:VAL:CG2 | 2.58 | 0.48 |
| 1:G:413:MET:HG3 | 1:G:414:ASP:N | 2.22 | 0.48 |
| 2:H:155:GLU:HG2 | 2:H:197:HIS:CE1 | 2.49 | 0.48 |
| 3:I:113:ILE:HG21 | 3:I:119:LEU:CD2 | 2.44 | 0.48 |
| 2:B:6:SER:OG | 2:B:65:ALA:HB2 | 2.14 | 0.48 |
| 2:B:23:LEU:HD23 | 2:B:236:SER:CB | 2.37 | 0.48 |
| 2:B:384:ILE:HG22 | 2:B:388:TRP:CD1 | 2.49 | 0.48 |
| 1:C:199:ASP:O | 1:C:200:GLU:HG3 | 2.13 | 0.48 |
| 1:C:209:LEU:CD2 | 1:C:227:LEU:HD13 | 2.44 | 0.48 |
| 2:D:6:SER:OG | 2:D:65:ALA:HB2 | 2.14 | 0.48 |
| 1:E:2:ARG:NH1 | 1:E:251:ASP:OD2 | 2.46 | 0.48 |
| 1:E:296:PHE:HZ | 1:E:315:VAL:HG11 | 1.78 | 0.48 |
| 2:F:99:ALA:O | 2:F:100:ALA:HB3 | 2.13 | 0.48 |
| 2:F:107:HIS:CE1 | 2:F:152:LEU:HB3 | 2.49 | 0.48 |
| 2:F:261:PRO:HB3 | 1:G:404:PHE:CZ | 2.45 | 0.48 |
| 1:G:226:ASP:O | 1:G:229:HIS:HB3 | 2.14 | 0.48 |
| 2:H:386:GLU:O | 2:H:388:TRP:N | 2.47 | 0.48 |
| 2:B:5:ILE:HG22 | 2:B:6:SER:H | 1.78 | 0.48 |
| 2:B:9:VAL:HG11 | 2:B:150:THR:OG1 | 2.13 | 0.48 |
| 2:B:88:HIS:O | 2:B:89:PRO:C | 2.52 | 0.48 |
| 1:C:20:PHE:CG | 1:C:235:MET:SD | 3.07 | 0.48 |
| 1:C:49:ILE:HG13 | 1:C:50:ASN:N | 2.28 | 0.48 |
| 1:C:242:LEU:HD22 | 1:C:250:ALA:N | 2.19 | 0.48 |
| 2:D:70:LEU:HD12 | 2:D:145:THR:HG21 | 1.95 | 0.48 |
| 2:D:242:LEU:C | 2:D:244:PHE:N | 2.66 | 0.48 |
| 1:E:176:LYS:CE | 1:E:207:GLU:HG3 | 2.39 | 0.48 |
| 1:E:226:ASP:O | 1:E:229:HIS:HB3 | 2.14 | 0.48 |
| 1:E:399:PHE:O | 1:E:400:ARG:C | 2.52 | 0.48 |
| 2:F:9:VAL:HG11 | 2:F:150:THR:OG1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:70:LEU:HD12 | 2:F:145:THR:HG21 | 1.95 | 0.48 |
| 2:F:88:HIS:O | 2:F:89:PRO:C | 2.52 | 0.48 |
| 2:F:163:LYS:C | 2:F:164:LYS:HG2 | 2.33 | 0.48 |
| 2:F:191:THR:CG2 | 2:F:192:HIS:N | 2.76 | 0.48 |
| 1:G:296:PHE:HZ | 1:G:315:VAL:HG11 | 1.78 | 0.48 |
| 1:G:308:ARG:HG3 | 1:G:342:TYR:OH | 2.13 | 0.48 |
| 2:H:5:ILE:O | 2:H:136:SER:N | 2.40 | 0.48 |
| 2:H:147:SER:O | 2:H:190:THR:HG23 | 2.14 | 0.48 |
| 1:A:209:LEU:CD2 | 1:A:227:LEU:HD13 | 2.44 | 0.47 |
| 2:D:52:PHE:O | 2:D:64:ARG:HB3 | 2.14 | 0.47 |
| 2:D:115:ILE:HG23 | 2:D:116:ASP:H | 1.79 | 0.47 |
| 2:D:147:SER:O | 2:D:190:THR:HG23 | 2.14 | 0.47 |
| 1:E:209:LEU:CD2 | 1:E:227:LEU:HD13 | 2.44 | 0.47 |
| 1:E:308:ARG:HG3 | 1:E:342:TYR:OH | 2.13 | 0.47 |
| 2:F:147:SER:O | 2:F:190:THR:HG23 | 2.14 | 0.47 |
| 1:G:2:ARG:NH1 | 1:G:251:ASP:OD2 | 2.46 | 0.47 |
| 2:H:88:HIS:O | 2:H:89:PRO:C | 2.52 | 0.47 |
| 2:H:107:HIS:CE1 | 2:H:152:LEU:HB3 | 2.49 | 0.47 |
| 1:A:49:ILE:HG13 | 1:A:50:ASN:N | 2.28 | 0.47 |
| 2:B:260:VAL:O | 2:B:260:VAL:CG2 | 2.62 | 0.47 |
| 2:D:335:ILE:O | 2:D:337:THR:N | 2.47 | 0.47 |
| 1:G:115:VAL:CG2 | 1:G:152:LEU:HD23 | 2.44 | 0.47 |
| 2:H:9:VAL:HG11 | 2:H:150:THR:OG1 | 2.13 | 0.47 |
| 2:H:97:GLU:HB2 | 2:H:110:ILE:HD11 | 1.96 | 0.47 |
| 2:H:122:ILE:CD1 | 2:H:157:LEU:HD21 | 2.35 | 0.47 |
| 2:H:163:LYS:C | 2:H:164:LYS:HG2 | 2.33 | 0.47 |
| 2:H:191:THR:CG2 | 2:H:192:HIS:N | 2.76 | 0.47 |
| 1:A:20:PHE:O | 1:A:24:ILE:HB | 2.14 | 0.47 |
| 1:A:387:LEU:O | 1:A:387:LEU:HG | 2.14 | 0.47 |
| 2:B:115:ILE:HG23 | 2:B:116:ASP:H | 1.79 | 0.47 |
| 2:B:145:THR:H | 5:B:500:GTP:PG | 2.37 | 0.47 |
| 2:B:204:VAL:CG1 | 2:B:209:ILE:HD11 | 2.42 | 0.47 |
| 1:C:399:PHE:O | 1:C:400:ARG:C | 2.52 | 0.47 |
| 2:D:191:THR:CG2 | 2:D:192:HIS:N | 2.76 | 0.47 |
| 2:D:253:THR:O | 2:D:254:GLU:C | 2.52 | 0.47 |
| 2:D:260:VAL:CG2 | 2:D:260:VAL:O | 2.63 | 0.47 |
| 1:E:70:LEU:O | 1:E:99:ALA:HB2 | 2.15 | 0.47 |
| 2:F:241:SER:HB3 | 2:F:320:ARG:NH2 | 2.29 | 0.47 |
| 2:F:335:ILE:O | 2:F:337:THR:N | 2.47 | 0.47 |
| 1:G:20:PHE:O | 1:G:24:ILE:HB | 2.14 | 0.47 |
| 2:H:70:LEU:HD12 | 2:H:145:THR:HG21 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:154:MET:HA | 2:H:157:LEU:HD12 | 1.96 | 0.47 |
| 2:H:335:ILE:O | 2:H:337:THR:N | 2.47 | 0.47 |
| 2:H:384:ILE:HG22 | 2:H:388:TRP:CD1 | 2.49 | 0.47 |
| 1:A:264:ARG:HA | 1:A:264:ARG:NE | 2.29 | 0.47 |
| 1:A:296:PHE:HZ | 1:A:315:VAL:HG11 | 1.78 | 0.47 |
| 2:B:107:HIS:CE1 | 2:B:152:LEU:HB3 | 2.49 | 0.47 |
| 2:B:117:LEU:HD12 | 2:B:121:ARG:HH12 | 1.80 | 0.47 |
| 2:B:147:SER:O | 2:B:190:THR:HG23 | 2.14 | 0.47 |
| 2:B:154:MET:HA | 2:B:157:LEU:HD12 | 1.97 | 0.47 |
| 2:B:163:LYS:C | 2:B:164:LYS:HG2 | 2.33 | 0.47 |
| 1:C:188:THR:HA | 1:C:425:MET:HE3 | 1.95 | 0.47 |
| 1:C:209:LEU:O | 1:C:213:CYS:N | 2.47 | 0.47 |
| 1:C:242:LEU:CD1 | 1:C:250:ALA:HB3 | 2.45 | 0.47 |
| 1:C:274:PRO:HG2 | 1:C:371:LEU:CD2 | 2.43 | 0.47 |
| 2:D:97:GLU:HB2 | 2:D:110:ILE:HD11 | 1.96 | 0.47 |
| 2:D:154:MET:HA | 2:D:157:LEU:HD12 | 1.96 | 0.47 |
| 2:D:155:GLU:HA | 2:D:197:HIS:CE1 | 2.49 | 0.47 |
| 2:D:317:LEU:CD1 | 2:D:351:PHE:CD2 | 2.97 | 0.47 |
| 2:D:339:ARG:C | 2:D:341:ILE:N | 2.68 | 0.47 |
| 2:D:388:TRP:HA | 2:D:388:TRP:HE3 | 1.79 | 0.47 |
| 1:E:185:TYR:HD2 | 1:E:395:PHE:CE1 | 2.33 | 0.47 |
| 1:E:243:ARG:HA | 1:E:243:ARG:HD3 | 1.62 | 0.47 |
| 1:E:287:THR:O | 1:E:288:VAL:CG2 | 2.58 | 0.47 |
| 2:F:6:SER:OG | 2:F:65:ALA:HB2 | 2.14 | 0.47 |
| 2:F:122:ILE:CD1 | 2:F:157:LEU:HD21 | 2.35 | 0.47 |
| 2:F:154:MET:HA | 2:F:157:LEU:HD12 | 1.97 | 0.47 |
| 2:F:260:VAL:CG2 | 2:F:260:VAL:O | 2.63 | 0.47 |
| 2:F:369:ALA:O | 2:F:370:LYS:CB | 2.62 | 0.47 |
| 1:G:70:LEU:O | 1:G:99:ALA:HB2 | 2.15 | 0.47 |
| 2:H:5:ILE:CG2 | 2:H:135:PHE:HB3 | 2.41 | 0.47 |
| 2:H:6:SER:OG | 2:H:65:ALA:HB2 | 2.14 | 0.47 |
| 2:H:241:SER:HB3 | 2:H:320:ARG:NH2 | 2.29 | 0.47 |
| 2:H:253:THR:O | 2:H:254:GLU:C | 2.52 | 0.47 |
| 1:A:185:TYR:HD2 | 1:A:395:PHE:CE1 | 2.33 | 0.47 |
| 1:A:274:PRO:HG2 | 1:A:371:LEU:CD2 | 2.43 | 0.47 |
| 2:B:175:PRO:HD2 | 2:B:207:GLU:HB3 | 1.96 | 0.47 |
| 2:B:185:TYR:OH | 2:B:399:TYR:HA | 2.15 | 0.47 |
| 1:C:20:PHE:O | 1:C:24:ILE:HB | 2.14 | 0.47 |
| 1:C:387:LEU:O | 1:C:387:LEU:HG | 2.14 | 0.47 |
| 2:D:107:HIS:CE1 | 2:D:152:LEU:HB3 | 2.49 | 0.47 |
| 2:D:117:LEU:HD12 | 2:D:121:ARG:HH12 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:407:TRP:O | 2:D:411:GLU:CG | 2.63 | 0.47 |
| 1:E:20:PHE:O | 1:E:24:ILE:HB | 2.14 | 0.47 |
| 1:E:307:PRO:HB3 | 1:E:312:TYR:CZ | 2.49 | 0.47 |
| 1:E:384:ILE:O | 1:E:384:ILE:HG23 | 2.14 | 0.47 |
| 2:F:97:GLU:HB2 | 2:F:110:ILE:HD11 | 1.96 | 0.47 |
| 2:F:117:LEU:HD12 | 2:F:121:ARG:HH12 | 1.80 | 0.47 |
| 2:F:175:PRO:HD2 | 2:F:207:GLU:HB3 | 1.97 | 0.47 |
| 2:F:384:ILE:HG22 | 2:F:388:TRP:CD1 | 2.49 | 0.47 |
| 1:G:175:PRO:O | 1:G:176:LYS:C | 2.52 | 0.47 |
| 1:G:260:VAL:HG23 | 2:H:406:HIS:HE1 | 1.79 | 0.47 |
| 2:H:317:LEU:CD1 | 2:H:351:PHE:CD2 | 2.97 | 0.47 |
| 2:H:369:ALA:O | 2:H:370:LYS:CB | 2.62 | 0.47 |
| 1:A:176:LYS:HG3 | 1:A:177:VAL:H | 1.78 | 0.47 |
| 1:A:242:LEU:HD22 | 1:A:250:ALA:N | 2.19 | 0.47 |
| 1:A:384:ILE:O | 1:A:384:ILE:HG23 | 2.14 | 0.47 |
| 2:B:407:TRP:O | 2:B:411:GLU:CG | 2.63 | 0.47 |
| 1:C:176:LYS:HG3 | 1:C:177:VAL:H | 1.78 | 0.47 |
| 1:C:296:PHE:HZ | 1:C:315:VAL:HG11 | 1.78 | 0.47 |
| 1:C:384:ILE:O | 1:C:384:ILE:HG23 | 2.14 | 0.47 |
| 2:D:57:GLY:N | 2:H:284:GLU:HB2 | 2.30 | 0.47 |
| 2:D:62:VAL:HG12 | 2:D:91:GLN:HE22 | 1.78 | 0.47 |
| 2:D:210:TYR:CE2 | 2:D:227:LEU:HD21 | 2.49 | 0.47 |
| 1:E:101:ASN:ND2 | 1:E:101:ASN:O | 2.48 | 0.47 |
| 1:E:175:PRO:O | 1:E:176:LYS:C | 2.52 | 0.47 |
| 1:E:387:LEU:O | 1:E:387:LEU:HG | 2.14 | 0.47 |
| 2:F:62:VAL:HG12 | 2:F:91:GLN:HE22 | 1.77 | 0.47 |
| 2:F:120:ASP:O | 2:F:124:LYS:HB2 | 2.15 | 0.47 |
| 2:F:210:TYR:CE2 | 2:F:227:LEU:HD21 | 2.49 | 0.47 |
| 2:F:317:LEU:CD1 | 2:F:351:PHE:CD2 | 2.97 | 0.47 |
| 1:G:101:ASN:ND2 | 1:G:101:ASN:O | 2.48 | 0.47 |
| 1:G:185:TYR:HD2 | 1:G:395:PHE:CE1 | 2.33 | 0.47 |
| 1:G:253:ARG:CG | 2:H:407:TRP:CH2 | 2.92 | 0.47 |
| 2:H:175:PRO:HD2 | 2:H:207:GLU:HB3 | 1.97 | 0.47 |
| 2:H:210:TYR:CE2 | 2:H:227:LEU:HD21 | 2.49 | 0.47 |
| 2:H:260:VAL:O | 2:H:260:VAL:CG2 | 2.63 | 0.47 |
| 2:H:339:ARG:C | 2:H:341:ILE:N | 2.68 | 0.47 |
| 1:A:82:PRO:HB2 | 1:A:83:PHE:H | 1.56 | 0.47 |
| 1:A:101:ASN:ND2 | 1:A:101:ASN:O | 2.48 | 0.47 |
| 1:A:168:THR:N | 1:A:200:GLU:O | 2.43 | 0.47 |
| 1:A:242:LEU:CD1 | 1:A:250:ALA:HB3 | 2.45 | 0.47 |
| 1:A:307:PRO:C | 1:A:309:HIS:H | 2.18 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:360:PRO:HG2 | 1:A:371:LEU:CB | 2.38 | 0.47 |
| 1:A:399:PHE:O | 1:A:400:ARG:C | 2.52 | 0.47 |
| 2:B:70:LEU:HD12 | 2:B:145:THR:HG21 | 1.95 | 0.47 |
| 2:B:97:GLU:HB2 | 2:B:110:ILE:HD11 | 1.96 | 0.47 |
| 2:B:155:GLU:HG2 | 2:B:197:HIS:CE1 | 2.49 | 0.47 |
| 2:B:191:THR:O | 2:B:195:LEU:HB2 | 2.15 | 0.47 |
| 2:B:328:VAL:O | 2:B:330:ALA:N | 2.38 | 0.47 |
| 2:B:335:ILE:O | 2:B:337:THR:N | 2.47 | 0.47 |
| 2:B:339:ARG:C | 2:B:341:ILE:N | 2.68 | 0.47 |
| 2:B:388:TRP:HA | 2:B:388:TRP:HE3 | 1.79 | 0.47 |
| 1:C:185:TYR:HD2 | 1:C:395:PHE:CE1 | 2.33 | 0.47 |
| 1:C:226:ASP:O | 1:C:229:HIS:HB3 | 2.14 | 0.47 |
| 1:C:264:ARG:HA | 1:C:264:ARG:NE | 2.29 | 0.47 |
| 2:D:9:VAL:HG21 | 2:D:149:PHE:HD1 | 1.80 | 0.47 |
| 2:D:120:ASP:O | 2:D:124:LYS:HB2 | 2.15 | 0.47 |
| 2:D:132:LEU:HD21 | 2:D:164:LYS:HE3 | 1.96 | 0.47 |
| 2:D:148:GLY:O | 2:D:151:SER:CB | 2.61 | 0.47 |
| 2:D:172:TYR:CD1 | 2:D:173:PRO:N | 2.80 | 0.47 |
| 1:E:242:LEU:HD11 | 1:E:250:ALA:HB3 | 1.97 | 0.47 |
| 2:F:5:ILE:CG2 | 2:F:135:PHE:HB3 | 2.41 | 0.47 |
| 2:F:9:VAL:HG21 | 2:F:149:PHE:HD1 | 1.80 | 0.47 |
| 2:F:115:ILE:HG23 | 2:F:116:ASP:H | 1.79 | 0.47 |
| 2:F:132:LEU:HD21 | 2:F:164:LYS:HE3 | 1.96 | 0.47 |
| 2:F:253:THR:O | 2:F:254:GLU:C | 2.52 | 0.47 |
| 2:F:256:GLN:O | 2:F:260:VAL:HG13 | 2.15 | 0.47 |
| 2:F:339:ARG:C | 2:F:341:ILE:N | 2.67 | 0.47 |
| 2:F:348:PRO:CD | 1:G:398:MET:CE | 2.92 | 0.47 |
| 2:F:407:TRP:O | 2:F:411:GLU:CG | 2.63 | 0.47 |
| 1:G:168:THR:N | 1:G:200:GLU:O | 2.43 | 0.47 |
| 1:G:242:LEU:CD1 | 1:G:250:ALA:HB3 | 2.45 | 0.47 |
| 1:G:242:LEU:HD11 | 1:G:250:ALA:HB3 | 1.97 | 0.47 |
| 1:G:274:PRO:HG2 | 1:G:371:LEU:CD2 | 2.43 | 0.47 |
| 1:G:387:LEU:O | 1:G:387:LEU:HG | 2.14 | 0.47 |
| 2:H:9:VAL:HG21 | 2:H:149:PHE:HD1 | 1.80 | 0.47 |
| 2:H:102:ASN:CB | 2:H:407:TRP:HE1 | 2.25 | 0.47 |
| 2:H:115:ILE:HG23 | 2:H:116:ASP:H | 1.79 | 0.47 |
| 2:H:117:LEU:HD12 | 2:H:121:ARG:HH12 | 1.80 | 0.47 |
| 2:H:120:ASP:O | 2:H:124:LYS:HB2 | 2.15 | 0.47 |
| 2:H:132:LEU:HD21 | 2:H:164:LYS:HE3 | 1.96 | 0.47 |
| 2:H:256:GLN:O | 2:H:260:VAL:HG13 | 2.15 | 0.47 |
| 2:H:407:TRP:O | 2:H:411:GLU:CG | 2.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:156:LYS:HA | 1:A:156:LYS:CE | 2.38 | 0.47 |
| 1:A:175:PRO:O | 1:A:176:LYS:C | 2.52 | 0.47 |
| 1:A:209:LEU:O | 1:A:213:CYS:N | 2.47 | 0.47 |
| 2:B:120:ASP:O | 2:B:124:LYS:HB2 | 2.15 | 0.47 |
| 2:B:191:THR:CG2 | 2:B:192:HIS:N | 2.76 | 0.47 |
| 2:B:210:TYR:CE2 | 2:B:227:LEU:HD21 | 2.49 | 0.47 |
| 2:B:369:ALA:O | 2:B:370:LYS:CB | 2.62 | 0.47 |
| 2:B:392:ASP:OD2 | 2:B:422:ARG:NE | 2.48 | 0.47 |
| 1:C:101:ASN:ND2 | 1:C:101:ASN:O | 2.47 | 0.47 |
| 1:C:198:THR:HG23 | 1:C:200:GLU:H | 1.79 | 0.47 |
| 2:D:155:GLU:HG2 | 2:D:197:HIS:CE1 | 2.49 | 0.47 |
| 2:D:185:TYR:OH | 2:D:399:TYR:HA | 2.15 | 0.47 |
| 2:D:241:SER:HB3 | 2:D:320:ARG:NH2 | 2.29 | 0.47 |
| 2:D:265:GLY:O | 2:D:266:HIS:O | 2.33 | 0.47 |
| 2:D:369:ALA:O | 2:D:370:LYS:CB | 2.62 | 0.47 |
| 2:D:434:GLU:C | 2:D:436:GLY:H | 2.18 | 0.47 |
| 1:E:24:ILE:CD1 | 1:E:52:TYR:CE1 | 2.97 | 0.47 |
| 2:F:262:TYR:HE2 | 1:G:403:ALA:O | 1.91 | 0.47 |
| 2:F:346:TRP:CZ3 | 1:G:404:PHE:HZ | 2.27 | 0.47 |
| 1:G:301:MET:HE1 | 1:G:377:PHE:HE2 | 1.80 | 0.47 |
| 2:H:148:GLY:O | 2:H:151:SER:CB | 2.61 | 0.47 |
| 1:A:226:ASP:O | 1:A:229:HIS:HB3 | 2.14 | 0.47 |
| 1:A:242:LEU:HD11 | 1:A:250:ALA:HB3 | 1.97 | 0.47 |
| 2:B:243:ARG:NH2 | 2:B:252:LEU:CB | 2.78 | 0.47 |
| 1:C:175:PRO:O | 1:C:176:LYS:C | 2.52 | 0.47 |
| 1:C:257:VAL:CG1 | 2:D:407:TRP:CG | 2.76 | 0.47 |
| 1:C:287:THR:N | 1:C:290:GLU:OE1 | 2.48 | 0.47 |
| 1:C:307:PRO:HB3 | 1:C:312:TYR:CZ | 2.49 | 0.47 |
| 2:D:5:ILE:CG2 | 2:D:135:PHE:HB3 | 2.41 | 0.47 |
| 2:D:175:PRO:HD2 | 2:D:207:GLU:HB3 | 1.96 | 0.47 |
| 2:D:204:VAL:CG1 | 2:D:209:ILE:HD11 | 2.42 | 0.47 |
| 2:D:256:GLN:HA | 2:D:260:VAL:HG13 | 1.97 | 0.47 |
| 2:D:392:ASP:OD2 | 2:D:422:ARG:NE | 2.48 | 0.47 |
| 2:D:436:GLY:O | 2:D:438:ASP:N | 2.48 | 0.47 |
| 1:E:103:TRP:CE3 | 1:E:189:LEU:HD13 | 2.50 | 0.47 |
| 1:E:198:THR:HG23 | 1:E:200:GLU:H | 1.79 | 0.47 |
| 1:E:237:GLY:HA3 | 1:E:376:THR:OG1 | 2.15 | 0.47 |
| 1:E:297:ASP:OD2 | 1:E:299:LYS:HE2 | 2.14 | 0.47 |
| 2:F:148:GLY:O | 2:F:151:SER:CB | 2.61 | 0.47 |
| 1:G:103:TRP:CE3 | 1:G:189:LEU:HD13 | 2.50 | 0.47 |
| 1:G:243:ARG:HA | 1:G:243:ARG:HD3 | 1.62 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:307:PRO:HB3 | 1:G:312:TYR:CZ | 2.49 | 0.47 |
| 1:A:103:TRP:CE3 | 1:A:189:LEU:HD13 | 2.50 | 0.47 |
| 2:B:241:SER:HB3 | 2:B:320:ARG:NH2 | 2.29 | 0.47 |
| 2:B:381:THR:O | 2:B:383:ALA:N | 2.48 | 0.47 |
| 2:B:436:GLY:O | 2:B:438:ASP:N | 2.48 | 0.47 |
| 1:C:175:PRO:HD2 | 1:C:207:GLU:CD | 2.35 | 0.47 |
| 1:C:307:PRO:C | 1:C:309:HIS:H | 2.18 | 0.47 |
| 2:D:55:GLU:O | 2:D:56:THR:C | 2.52 | 0.47 |
| 2:D:67:PHE:CE1 | 2:D:87:PHE:CD1 | 2.89 | 0.47 |
| 2:D:191:THR:O | 2:D:195:LEU:HB2 | 2.15 | 0.47 |
| 2:D:381:THR:O | 2:D:383:ALA:N | 2.48 | 0.47 |
| 2:D:404:PHE:CD1 | 2:D:404:PHE:N | 2.83 | 0.47 |
| 1:E:307:PRO:C | 1:E:309:HIS:H | 2.18 | 0.47 |
| 2:F:191:THR:O | 2:F:195:LEU:HB2 | 2.15 | 0.47 |
| 2:F:204:VAL:HG21 | 2:F:231:ILE:HG23 | 1.97 | 0.47 |
| 2:F:265:GLY:O | 2:F:266:HIS:O | 2.33 | 0.47 |
| 1:G:24:ILE:CD1 | 1:G:52:TYR:CE1 | 2.97 | 0.47 |
| 1:G:188:THR:HA | 1:G:425:MET:HE3 | 1.95 | 0.47 |
| 1:G:384:ILE:O | 1:G:384:ILE:HG23 | 2.14 | 0.47 |
| 2:H:204:VAL:HG21 | 2:H:231:ILE:HG23 | 1.97 | 0.47 |
| 2:H:436:GLY:O | 2:H:438:ASP:N | 2.48 | 0.47 |
| 3:I:59:ARG:HG2 | 3:I:59:ARG:O | 2.14 | 0.47 |
| 1:A:287:THR:N | 1:A:290:GLU:OE1 | 2.48 | 0.46 |
| 1:A:297:ASP:OD2 | 1:A:299:LYS:HE2 | 2.14 | 0.46 |
| 2:B:9:VAL:HG21 | 2:B:149:PHE:HD1 | 1.80 | 0.46 |
| 2:B:132:LEU:HD21 | 2:B:164:LYS:HE3 | 1.96 | 0.46 |
| 2:B:256:GLN:HA | 2:B:260:VAL:HG13 | 1.97 | 0.46 |
| 2:B:353:VAL:HB | 1:C:179:ASP:OD1 | 2.15 | 0.46 |
| 2:D:19:ALA:HB2 | 2:D:228:ASN:HB3 | 1.96 | 0.46 |
| 2:D:145:THR:O | 2:D:149:PHE:HB3 | 2.15 | 0.46 |
| 1:E:35:SER:CB | 1:E:59:ASN:HA | 2.42 | 0.46 |
| 1:E:82:PRO:HB2 | 1:E:83:PHE:H | 1.56 | 0.46 |
| 1:E:242:LEU:CD1 | 1:E:250:ALA:HB3 | 2.45 | 0.46 |
| 2:F:114:ILE:O | 2:F:118:VAL:HG23 | 2.16 | 0.46 |
| 2:F:243:ARG:NH2 | 2:F:252:LEU:CB | 2.78 | 0.46 |
| 2:F:244:PHE:CD2 | 2:F:245:ASP:N | 2.76 | 0.46 |
| 2:F:324:VAL:HG12 | 2:F:326:LYS:H | 1.81 | 0.46 |
| 2:F:436:GLY:O | 2:F:438:ASP:N | 2.48 | 0.46 |
| 1:G:237:GLY:HA3 | 1:G:376:THR:OG1 | 2.15 | 0.46 |
| 1:G:254:LYS:CE | 1:G:352:LYS:NZ | 2.71 | 0.46 |
| 1:G:297:ASP:OD2 | 1:G:299:LYS:HE2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:360:PRO:HG2 | 1:G:371:LEU:CB | 2.38 | 0.46 |
| 2:H:114:ILE:O | 2:H:118:VAL:HG23 | 2.16 | 0.46 |
| 2:H:191:THR:O | 2:H:195:LEU:HB2 | 2.15 | 0.46 |
| 2:H:243:ARG:NH2 | 2:H:252:LEU:CB | 2.78 | 0.46 |
| 2:H:328:VAL:O | 2:H:330:ALA:N | 2.38 | 0.46 |
| 1:A:260:VAL:HG21 | 2:B:407:TRP:HZ2 | 1.80 | 0.46 |
| 1:C:103:TRP:CE3 | 1:C:189:LEU:HD13 | 2.50 | 0.46 |
| 1:C:168:THR:N | 1:C:200:GLU:O | 2.43 | 0.46 |
| 1:C:431:GLU:HA | 1:C:434:GLN:HG3 | 1.97 | 0.46 |
| 2:D:243:ARG:NH2 | 2:D:252:LEU:CB | 2.78 | 0.46 |
| 1:E:224:TYR:O | 1:E:225:GLY:C | 2.53 | 0.46 |
| 1:E:242:LEU:HD22 | 1:E:250:ALA:N | 2.19 | 0.46 |
| 2:F:256:GLN:HA | 2:F:260:VAL:HG13 | 1.97 | 0.46 |
| 1:G:179:ASP:OD2 | 4:G:600:GDP:O2' | 2.15 | 0.46 |
| 1:G:198:THR:HG23 | 1:G:200:GLU:H | 1.79 | 0.46 |
| 1:G:224:TYR:O | 1:G:225:GLY:C | 2.53 | 0.46 |
| 1:G:307:PRO:C | 1:G:309:HIS:H | 2.18 | 0.46 |
| 2:H:22:GLU:O | 2:H:23:LEU:C | 2.54 | 0.46 |
| 2:H:265:GLY:O | 2:H:266:HIS:O | 2.33 | 0.46 |
| 2:H:324:VAL:HG12 | 2:H:326:LYS:H | 1.81 | 0.46 |
| 1:A:198:THR:HG23 | 1:A:200:GLU:H | 1.79 | 0.46 |
| 1:A:301:MET:HE1 | 1:A:377:PHE:HE2 | 1.80 | 0.46 |
| 1:A:307:PRO:HB3 | 1:A:312:TYR:CZ | 2.49 | 0.46 |
| 2:B:56:THR:C | 2:F:284:GLU:CB | 2.83 | 0.46 |
| 2:B:148:GLY:O | 2:B:151:SER:CB | 2.61 | 0.46 |
| 2:B:210:TYR:CZ | 2:B:227:LEU:HD11 | 2.51 | 0.46 |
| 2:B:265:GLY:O | 2:B:266:HIS:O | 2.33 | 0.46 |
| 2:B:324:VAL:HG12 | 2:B:326:LYS:H | 1.81 | 0.46 |
| 1:C:242:LEU:HD11 | 1:C:250:ALA:HB3 | 1.97 | 0.46 |
| 1:C:360:PRO:HG2 | 1:C:371:LEU:CB | 2.38 | 0.46 |
| 2:D:22:GLU:O | 2:D:23:LEU:C | 2.54 | 0.46 |
| 2:D:210:TYR:CZ | 2:D:227:LEU:HD11 | 2.51 | 0.46 |
| 2:D:255:PHE:O | 2:D:256:GLN:C | 2.53 | 0.46 |
| 2:D:324:VAL:HG12 | 2:D:326:LYS:H | 1.81 | 0.46 |
| 1:E:115:VAL:CG2 | 1:E:152:LEU:HD23 | 2.44 | 0.46 |
| 1:E:156:LYS:HA | 1:E:156:LYS:CE | 2.38 | 0.46 |
| 1:E:274:PRO:HG2 | 1:E:371:LEU:CD2 | 2.43 | 0.46 |
| 1:E:324:SER:OG | 1:E:326:LYS:HB3 | 2.16 | 0.46 |
| 2:F:22:GLU:O | 2:F:23:LEU:C | 2.54 | 0.46 |
| 2:F:63:PRO:HG2 | 2:F:87:PHE:CG | 2.51 | 0.46 |
| 2:F:243:ARG:NH2 | 2:F:252:LEU:HB2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:117:LEU:HD11 | 2:H:121:ARG:NH2 | 2.30 | 0.46 |
| 2:H:243:ARG:NH2 | 2:H:252:LEU:HB2 | 2.30 | 0.46 |
| 2:H:244:PHE:CD2 | 2:H:245:ASP:N | 2.76 | 0.46 |
| 1:A:70:LEU:O | 1:A:99:ALA:HB2 | 2.15 | 0.46 |
| 2:B:19:ALA:HB2 | 2:B:228:ASN:HB3 | 1.96 | 0.46 |
| 2:B:204:VAL:HG21 | 2:B:231:ILE:HG23 | 1.97 | 0.46 |
| 2:B:328:VAL:C | 2:B:330:ALA:H | 2.16 | 0.46 |
| 2:D:166:LYS:CE | 2:D:199:ASP:OD1 | 2.62 | 0.46 |
| 1:E:113:GLU:CG | 1:E:114:LEU:N | 2.79 | 0.46 |
| 2:F:117:LEU:HD11 | 2:F:121:ARG:NH2 | 2.30 | 0.46 |
| 2:F:145:THR:O | 2:F:149:PHE:HB3 | 2.15 | 0.46 |
| 2:H:3:GLU:CD | 2:H:50:ASN:O | 2.54 | 0.46 |
| 2:H:256:GLN:HA | 2:H:260:VAL:HG13 | 1.97 | 0.46 |
| 3:I:54:LYS:O | 3:I:122:GLY:N | 2.49 | 0.46 |
| 3:I:72:VAL:HG11 | 3:I:83:LEU:HD22 | 1.98 | 0.46 |
| 1:A:154:ILE:HD12 | 1:A:155:SER:N | 2.31 | 0.46 |
| 1:A:224:TYR:O | 1:A:225:GLY:C | 2.53 | 0.46 |
| 2:B:63:PRO:HG3 | 2:B:87:PHE:CG | 2.50 | 0.46 |
| 2:B:255:PHE:O | 2:B:256:GLN:C | 2.53 | 0.46 |
| 2:B:317:LEU:CD1 | 2:B:351:PHE:CD2 | 2.97 | 0.46 |
| 2:B:434:GLU:C | 2:B:436:GLY:H | 2.18 | 0.46 |
| 1:C:70:LEU:O | 1:C:99:ALA:HB2 | 2.15 | 0.46 |
| 1:C:134:GLY:HA3 | 1:C:165:ILE:HG12 | 1.97 | 0.46 |
| 1:C:154:ILE:HD12 | 1:C:155:SER:N | 2.31 | 0.46 |
| 1:E:168:THR:N | 1:E:200:GLU:O | 2.43 | 0.46 |
| 1:E:250:ALA:HB1 | 1:E:254:LYS:CB | 2.44 | 0.46 |
| 2:F:3:GLU:CD | 2:F:50:ASN:O | 2.54 | 0.46 |
| 2:F:185:TYR:OH | 2:F:399:TYR:HA | 2.15 | 0.46 |
| 2:F:349:THR:HG22 | 1:G:178:SER:O | 2.13 | 0.46 |
| 1:G:324:SER:OG | 1:G:326:LYS:HB3 | 2.15 | 0.46 |
| 1:G:431:GLU:HA | 1:G:434:GLN:HG3 | 1.98 | 0.46 |
| 2:H:392:ASP:OD2 | 2:H:422:ARG:NE | 2.48 | 0.46 |
| 1:A:175:PRO:HD2 | 1:A:207:GLU:CD | 2.36 | 0.46 |
| 2:B:22:GLU:O | 2:B:23:LEU:C | 2.54 | 0.46 |
| 2:B:23:LEU:CD2 | 2:B:232:GLY:O | 2.64 | 0.46 |
| 2:B:62:VAL:HA | 2:B:86:LEU:O | 2.15 | 0.46 |
| 2:B:348:PRO:HD3 | 1:C:398:MET:HB3 | 1.97 | 0.46 |
| 2:D:204:VAL:HG21 | 2:D:231:ILE:HG23 | 1.97 | 0.46 |
| 2:D:345:ASP:C | 2:D:347:CYS:N | 2.68 | 0.46 |
| 2:F:67:PHE:CE1 | 2:F:87:PHE:CD1 | 2.89 | 0.46 |
| 2:F:316:CYS:HB3 | 2:F:378:LEU:HD12 | 1.94 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:328:VAL:O | 2:F:330:ALA:N | 2.38 | 0.46 |
| 1:G:113:GLU:CG | 1:G:114:LEU:N | 2.79 | 0.46 |
| 1:G:156:LYS:HA | 1:G:156:LYS:CE | 2.38 | 0.46 |
| 1:G:196:GLU:O | 1:G:197:ASN:OD1 | 2.34 | 0.46 |
| 1:G:208:ALA:O | 1:G:212:ILE:HG13 | 2.16 | 0.46 |
| 1:G:245:PRO:CB | 2:H:73:THR:HG21 | 2.45 | 0.46 |
| 1:G:245:PRO:CA | 2:H:73:THR:HG21 | 2.44 | 0.46 |
| 1:G:287:THR:N | 1:G:290:GLU:OE1 | 2.48 | 0.46 |
| 1:G:342:TYR:HD2 | 3:I:64:TYR:OH | 1.99 | 0.46 |
| 2:H:11:GLN:O | 2:H:15:GLN:HG3 | 2.15 | 0.46 |
| 2:H:63:PRO:HG2 | 2:H:87:PHE:CG | 2.51 | 0.46 |
| 2:H:185:TYR:OH | 2:H:399:TYR:HA | 2.15 | 0.46 |
| 2:H:210:TYR:CZ | 2:H:227:LEU:HD11 | 2.51 | 0.46 |
| 2:H:316:CYS:HB3 | 2:H:378:LEU:HD12 | 1.95 | 0.46 |
| 1:A:196:GLU:O | 1:A:197:ASN:OD1 | 2.34 | 0.46 |
| 1:A:237:GLY:HA3 | 1:A:376:THR:OG1 | 2.15 | 0.46 |
| 1:A:245:PRO:HA | 2:B:73:THR:CG2 | 2.46 | 0.46 |
| 1:A:431:GLU:HA | 1:A:434:GLN:HG3 | 1.97 | 0.46 |
| 2:B:114:ILE:O | 2:B:118:VAL:HG23 | 2.15 | 0.46 |
| 2:B:166:LYS:CE | 2:B:199:ASP:OD1 | 2.62 | 0.46 |
| 1:C:196:GLU:O | 1:C:197:ASN:OD1 | 2.34 | 0.46 |
| 1:C:224:TYR:O | 1:C:225:GLY:C | 2.53 | 0.46 |
| 1:C:237:GLY:HA3 | 1:C:376:THR:OG1 | 2.15 | 0.46 |
| 2:D:63:PRO:HG2 | 2:D:87:PHE:CG | 2.51 | 0.46 |
| 2:D:328:VAL:O | 2:D:330:ALA:N | 2.38 | 0.46 |
| 1:E:208:ALA:O | 1:E:212:ILE:HG13 | 2.16 | 0.46 |
| 1:E:360:PRO:HG2 | 1:E:371:LEU:CB | 2.38 | 0.46 |
| 2:F:11:GLN:O | 2:F:15:GLN:HG3 | 2.15 | 0.46 |
| 2:F:210:TYR:CZ | 2:F:227:LEU:HD11 | 2.51 | 0.46 |
| 2:F:210:TYR:CD2 | 2:F:227:LEU:HD21 | 2.51 | 0.46 |
| 2:F:392:ASP:OD2 | 2:F:422:ARG:NE | 2.48 | 0.46 |
| 1:G:102:ASN:ND2 | 1:G:104:ALA:HB3 | 2.31 | 0.46 |
| 2:H:145:THR:O | 2:H:149:PHE:HB3 | 2.15 | 0.46 |
| 2:H:210:TYR:CD2 | 2:H:227:LEU:HD21 | 2.51 | 0.46 |
| 2:H:434:GLU:C | 2:H:436:GLY:H | 2.18 | 0.46 |
| 1:A:113:GLU:CG | 1:A:114:LEU:N | 2.79 | 0.46 |
| 2:B:5:ILE:HD11 | 2:B:64:ARG:NH2 | 2.31 | 0.46 |
| 2:B:104:ALA:HB1 | 2:B:413:MET:HG3 | 1.96 | 0.46 |
| 2:B:145:THR:O | 2:B:149:PHE:HB3 | 2.15 | 0.46 |
| 2:B:308:ARG:O | 2:B:309:HIS:HB3 | 2.16 | 0.46 |
| 1:C:297:ASP:OD2 | 1:C:299:LYS:HE2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:114:ILE:O | 2:D:118:VAL:HG23 | 2.16 | 0.46 |
| 2:D:226:ASN:O | 2:D:229:ARG:N | 2.48 | 0.46 |
| 2:D:328:VAL:C | 2:D:330:ALA:H | 2.16 | 0.46 |
| 2:F:63:PRO:HD2 | 2:F:87:PHE:HA | 1.97 | 0.46 |
| 2:F:226:ASN:O | 2:F:229:ARG:N | 2.48 | 0.46 |
| 2:F:328:VAL:C | 2:F:330:ALA:H | 2.16 | 0.46 |
| 2:F:381:THR:O | 2:F:383:ALA:N | 2.49 | 0.46 |
| 2:F:388:TRP:HA | 2:F:388:TRP:HE3 | 1.79 | 0.46 |
| 1:G:35:SER:CB | 1:G:59:ASN:HA | 2.42 | 0.46 |
| 2:H:19:ALA:HB2 | 2:H:228:ASN:HB3 | 1.96 | 0.46 |
| 2:H:119:LEU:HD11 | 2:H:156:ARG:HD2 | 1.97 | 0.46 |
| 2:H:345:ASP:C | 2:H:347:CYS:N | 2.68 | 0.46 |
| 1:A:11:GLN:O | 1:A:14:ASN:HB3 | 2.16 | 0.46 |
| 1:A:134:GLY:HA3 | 1:A:165:ILE:HG12 | 1.97 | 0.46 |
| 2:B:3:GLU:CD | 2:B:50:ASN:O | 2.54 | 0.46 |
| 1:C:11:GLN:O | 1:C:14:ASN:HB3 | 2.16 | 0.46 |
| 2:D:23:LEU:CD2 | 2:D:232:GLY:O | 2.64 | 0.46 |
| 2:D:104:ALA:HB1 | 2:D:413:MET:HG3 | 1.95 | 0.46 |
| 1:E:196:GLU:O | 1:E:197:ASN:OD1 | 2.34 | 0.46 |
| 1:E:287:THR:N | 1:E:290:GLU:OE1 | 2.48 | 0.46 |
| 1:E:323:MET:CE | 1:E:328:VAL:HG22 | 2.46 | 0.46 |
| 1:E:431:GLU:HA | 1:E:434:GLN:HG3 | 1.98 | 0.46 |
| 2:F:434:GLU:C | 2:F:436:GLY:H | 2.18 | 0.46 |
| 1:G:133:GLN:O | 1:G:165:ILE:CD1 | 2.64 | 0.46 |
| 1:G:154:ILE:HD12 | 1:G:155:SER:N | 2.31 | 0.46 |
| 1:G:250:ALA:HB1 | 1:G:254:LYS:CB | 2.44 | 0.46 |
| 2:H:63:PRO:HD2 | 2:H:87:PHE:HA | 1.98 | 0.46 |
| 1:A:133:GLN:O | 1:A:165:ILE:CD1 | 2.64 | 0.46 |
| 1:A:242:LEU:C | 1:A:244:PHE:H | 2.20 | 0.46 |
| 1:A:310:GLY:HA3 | 1:A:436:GLN:NE2 | 2.29 | 0.46 |
| 2:B:119:LEU:HD11 | 2:B:156:ARG:HD2 | 1.97 | 0.46 |
| 2:B:210:TYR:CD2 | 2:B:227:LEU:HD21 | 2.51 | 0.46 |
| 2:B:256:GLN:O | 2:B:260:VAL:HG13 | 2.15 | 0.46 |
| 2:B:345:ASP:C | 2:B:347:CYS:N | 2.68 | 0.46 |
| 1:C:72:PRO:O | 1:C:74:THR:N | 2.50 | 0.46 |
| 1:C:137:LEU:HD22 | 1:C:154:ILE:HG23 | 1.97 | 0.46 |
| 1:C:310:GLY:HA3 | 1:C:436:GLN:NE2 | 2.29 | 0.46 |
| 1:C:408:TYR:O | 1:C:411:GLU:HB2 | 2.15 | 0.46 |
| 2:D:148:GLY:O | 2:D:149:PHE:C | 2.55 | 0.46 |
| 2:D:308:ARG:O | 2:D:309:HIS:HB3 | 2.16 | 0.46 |
| 1:E:11:GLN:O | 1:E:14:ASN:HB3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:133:GLN:O | 1:E:165:ILE:CD1 | 2.64 | 0.46 |
| 1:E:154:ILE:HD12 | 1:E:155:SER:N | 2.31 | 0.46 |
| 1:E:175:PRO:HG2 | 1:E:207:GLU:OE1 | 2.16 | 0.46 |
| 1:E:360:PRO:O | 1:E:369:ARG:C | 2.54 | 0.46 |
| 2:F:119:LEU:HD11 | 2:F:156:ARG:HD2 | 1.97 | 0.46 |
| 1:G:245:PRO:HB3 | 2:H:73:THR:HG22 | 1.98 | 0.46 |
| 1:G:245:PRO:HB3 | 2:H:73:THR:HG21 | 1.97 | 0.46 |
| 1:G:248:LEU:HD21 | 2:H:179:THR:HG22 | 1.92 | 0.46 |
| 1:G:257:VAL:CG2 | 2:H:407:TRP:HB3 | 2.28 | 0.46 |
| 1:G:323:MET:CE | 1:G:328:VAL:HG22 | 2.46 | 0.46 |
| 2:H:23:LEU:CD2 | 2:H:232:GLY:O | 2.64 | 0.46 |
| 2:H:52:PHE:O | 2:H:64:ARG:HB3 | 2.16 | 0.46 |
| 2:H:381:THR:O | 2:H:383:ALA:N | 2.49 | 0.46 |
| 2:H:388:TRP:HA | 2:H:388:TRP:HE3 | 1.79 | 0.46 |
| 1:A:72:PRO:O | 1:A:74:THR:N | 2.50 | 0.45 |
| 1:A:94:PHE:CD2 | 1:A:94:PHE:N | 2.84 | 0.45 |
| 1:A:175:PRO:HG2 | 1:A:207:GLU:OE1 | 2.17 | 0.45 |
| 1:A:208:ALA:O | 1:A:212:ILE:HG13 | 2.16 | 0.45 |
| 1:A:360:PRO:O | 1:A:369:ARG:C | 2.54 | 0.45 |
| 2:B:5:ILE:CG2 | 2:B:6:SER:H | 2.29 | 0.45 |
| 2:B:148:GLY:O | 2:B:149:PHE:C | 2.55 | 0.45 |
| 2:B:384:ILE:HG22 | 2:B:384:ILE:O | 2.15 | 0.45 |
| 1:C:6:HIS:HB3 | 1:C:21:TRP:HZ2 | 1.81 | 0.45 |
| 1:C:175:PRO:HG2 | 1:C:207:GLU:OE1 | 2.17 | 0.45 |
| 2:D:210:TYR:CD2 | 2:D:227:LEU:HD21 | 2.51 | 0.45 |
| 1:E:72:PRO:O | 1:E:74:THR:N | 2.49 | 0.45 |
| 1:E:102:ASN:ND2 | 1:E:104:ALA:HB3 | 2.31 | 0.45 |
| 1:E:134:GLY:HA3 | 1:E:165:ILE:HG12 | 1.97 | 0.45 |
| 1:E:242:LEU:C | 1:E:244:PHE:H | 2.19 | 0.45 |
| 2:F:148:GLY:O | 2:F:149:PHE:C | 2.55 | 0.45 |
| 2:F:203:MET:SD | 2:F:267:PHE:CB | 3.04 | 0.45 |
| 1:G:175:PRO:HG2 | 1:G:207:GLU:OE1 | 2.17 | 0.45 |
| 1:G:242:LEU:C | 1:G:244:PHE:H | 2.19 | 0.45 |
| 1:G:257:VAL:O | 2:H:404:PHE:HB3 | 2.15 | 0.45 |
| 1:G:408:TYR:O | 1:G:411:GLU:HB2 | 2.15 | 0.45 |
| 2:H:104:ALA:HB1 | 2:H:413:MET:HG3 | 1.95 | 0.45 |
| 2:H:148:GLY:O | 2:H:149:PHE:C | 2.55 | 0.45 |
| 2:H:203:MET:SD | 2:H:267:PHE:CB | 3.04 | 0.45 |
| 2:H:226:ASN:O | 2:H:229:ARG:N | 2.48 | 0.45 |
| 2:B:117:LEU:HD11 | 2:B:121:ARG:NH2 | 2.31 | 0.45 |
| 2:B:155:GLU:HA | 2:B:197:HIS:CE1 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:226:ASN:O | 2:B:229:ARG:N | 2.48 | 0.45 |
| 1:C:209:LEU:HD23 | 1:C:227:LEU:HD13 | 1.98 | 0.45 |
| 1:C:242:LEU:C | 1:C:244:PHE:H | 2.20 | 0.45 |
| 2:D:95:GLY:C | 2:D:97:GLU:N | 2.69 | 0.45 |
| 2:D:117:LEU:HD11 | 2:D:121:ARG:NH2 | 2.30 | 0.45 |
| 1:E:94:PHE:CD2 | 1:E:94:PHE:N | 2.84 | 0.45 |
| 1:E:409:THR:HA | 1:E:413:MET:HB3 | 1.99 | 0.45 |
| 2:F:23:LEU:CD2 | 2:F:232:GLY:O | 2.64 | 0.45 |
| 2:F:255:PHE:O | 2:F:256:GLN:C | 2.53 | 0.45 |
| 2:F:345:ASP:C | 2:F:347:CYS:N | 2.68 | 0.45 |
| 1:G:11:GLN:O | 1:G:14:ASN:HB3 | 2.16 | 0.45 |
| 1:G:175:PRO:HD2 | 1:G:207:GLU:CD | 2.35 | 0.45 |
| 1:G:360:PRO:O | 1:G:369:ARG:C | 2.54 | 0.45 |
| 1:G:409:THR:HA | 1:G:413:MET:HB3 | 1.99 | 0.45 |
| 1:A:137:LEU:HD22 | 1:A:154:ILE:HG23 | 1.97 | 0.45 |
| 1:A:408:TYR:O | 1:A:411:GLU:HB2 | 2.15 | 0.45 |
| 2:B:203:MET:SD | 2:B:267:PHE:CB | 3.04 | 0.45 |
| 2:B:346:TRP:HZ2 | 2:B:435:VAL:HG12 | 1.81 | 0.45 |
| 1:C:133:GLN:O | 1:C:165:ILE:CD1 | 2.64 | 0.45 |
| 1:C:313:LEU:O | 1:C:347:ILE:HD12 | 2.16 | 0.45 |
| 2:D:11:GLN:O | 2:D:15:GLN:HG3 | 2.15 | 0.45 |
| 2:D:384:ILE:HG22 | 2:D:384:ILE:O | 2.15 | 0.45 |
| 2:D:396:ASP:O | 2:D:397:LEU:C | 2.53 | 0.45 |
| 1:E:67:LEU:HD12 | 1:E:92:PHE:CD2 | 2.51 | 0.45 |
| 1:E:210:TYR:CE2 | 1:E:227:LEU:HD11 | 2.52 | 0.45 |
| 1:E:281:GLN:C | 1:E:283:TYR:N | 2.67 | 0.45 |
| 2:F:19:ALA:HB2 | 2:F:228:ASN:HB3 | 1.96 | 0.45 |
| 2:F:104:ALA:HB1 | 2:F:413:MET:HG3 | 1.95 | 0.45 |
| 2:F:413:MET:C | 2:F:414:GLU:HG3 | 2.36 | 0.45 |
| 1:G:82:PRO:HB2 | 1:G:83:PHE:H | 1.55 | 0.45 |
| 1:G:313:LEU:O | 1:G:347:ILE:HD12 | 2.16 | 0.45 |
| 1:A:67:LEU:HD12 | 1:A:92:PHE:CD2 | 2.51 | 0.45 |
| 1:A:135:PHE:N | 1:A:135:PHE:CD1 | 2.85 | 0.45 |
| 1:A:250:ALA:HB1 | 1:A:254:LYS:CB | 2.43 | 0.45 |
| 2:B:11:GLN:O | 2:B:15:GLN:HG3 | 2.15 | 0.45 |
| 2:B:392:ASP:OD2 | 2:B:422:ARG:CZ | 2.65 | 0.45 |
| 1:C:67:LEU:HD12 | 1:C:92:PHE:CD2 | 2.51 | 0.45 |
| 1:C:113:GLU:CG | 1:C:114:LEU:N | 2.79 | 0.45 |
| 1:C:135:PHE:CD1 | 1:C:135:PHE:N | 2.84 | 0.45 |
| 2:D:7:ILE:HG13 | 2:D:137:VAL:HG22 | 1.97 | 0.45 |
| 2:D:256:GLN:O | 2:D:260:VAL:HG13 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:423:GLU:O | 2:D:426:ALA:HB3 | 2.16 | 0.45 |
| 1:E:288:VAL:N | 1:E:289:PRO:CD | 2.79 | 0.45 |
| 1:E:408:TYR:O | 1:E:411:GLU:HB2 | 2.15 | 0.45 |
| 2:F:268:PRO:CA | 2:F:379:SER:O | 2.65 | 0.45 |
| 2:F:346:TRP:HZ2 | 2:F:435:VAL:HG12 | 1.81 | 0.45 |
| 1:G:72:PRO:O | 1:G:74:THR:N | 2.50 | 0.45 |
| 1:G:94:PHE:N | 1:G:94:PHE:CD2 | 2.84 | 0.45 |
| 1:G:257:VAL:HG11 | 2:H:407:TRP:CE2 | 2.52 | 0.45 |
| 1:A:24:ILE:CD1 | 1:A:52:TYR:CE1 | 2.97 | 0.45 |
| 2:B:317:LEU:CD1 | 2:B:351:PHE:CE2 | 2.99 | 0.45 |
| 2:B:396:ASP:O | 2:B:397:LEU:C | 2.53 | 0.45 |
| 2:B:408:TYR:CG | 2:B:418:PHE:HZ | 2.34 | 0.45 |
| 1:C:24:ILE:CD1 | 1:C:52:TYR:CE1 | 2.97 | 0.45 |
| 1:C:35:SER:CB | 1:C:59:ASN:HA | 2.42 | 0.45 |
| 1:C:94:PHE:CD2 | 1:C:94:PHE:N | 2.84 | 0.45 |
| 1:C:208:ALA:O | 1:C:212:ILE:HG13 | 2.16 | 0.45 |
| 2:D:243:ARG:NH2 | 2:D:252:LEU:HB2 | 2.30 | 0.45 |
| 1:E:175:PRO:HD2 | 1:E:207:GLU:CD | 2.36 | 0.45 |
| 1:E:288:VAL:C | 1:E:290:GLU:N | 2.70 | 0.45 |
| 1:E:324:SER:O | 1:E:326:LYS:N | 2.50 | 0.45 |
| 2:F:155:GLU:HA | 2:F:197:HIS:CE1 | 2.49 | 0.45 |
| 2:F:212:ILE:HD11 | 2:F:302:MET:H | 1.82 | 0.45 |
| 2:F:317:LEU:CD1 | 2:F:351:PHE:CE2 | 2.99 | 0.45 |
| 1:G:209:LEU:HD23 | 1:G:227:LEU:HD13 | 1.98 | 0.45 |
| 1:G:273:ALA:CB | 1:G:274:PRO:CD | 2.93 | 0.45 |
| 1:G:324:SER:O | 1:G:326:LYS:N | 2.50 | 0.45 |
| 1:G:409:THR:O | 1:G:412:GLY:N | 2.48 | 0.45 |
| 2:H:144:GLY:H | 5:H:500:GTP:PG | 2.40 | 0.45 |
| 2:H:212:ILE:HD11 | 2:H:302:MET:H | 1.82 | 0.45 |
| 2:H:255:PHE:O | 2:H:256:GLN:C | 2.53 | 0.45 |
| 2:H:346:TRP:HZ2 | 2:H:435:VAL:HG12 | 1.81 | 0.45 |
| 2:H:413:MET:C | 2:H:414:GLU:HG3 | 2.37 | 0.45 |
| 1:A:288:VAL:N | 1:A:289:PRO:CD | 2.80 | 0.45 |
| 1:A:313:LEU:O | 1:A:347:ILE:HD12 | 2.16 | 0.45 |
| 2:B:316:CYS:HB3 | 2:B:378:LEU:HD12 | 1.95 | 0.45 |
| 2:B:334:THR:CG2 | 2:B:335:ILE:N | 2.79 | 0.45 |
| 2:B:423:GLU:O | 2:B:426:ALA:HB3 | 2.16 | 0.45 |
| 1:C:360:PRO:O | 1:C:369:ARG:C | 2.54 | 0.45 |
| 1:C:413:MET:HG3 | 1:C:414:ASP:N | 2.22 | 0.45 |
| 2:D:3:GLU:CD | 2:D:50:ASN:O | 2.54 | 0.45 |
| 2:D:144:GLY:H | 5:D:500:GTP:PG | 2.39 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:303:VAL:O | 2:D:303:VAL:CG1 | 2.64 | 0.45 |
| 2:D:316:CYS:HB3 | 2:D:378:LEU:HD12 | 1.95 | 0.45 |
| 2:D:317:LEU:CD1 | 2:D:351:PHE:CE2 | 2.99 | 0.45 |
| 2:D:334:THR:CG2 | 2:D:335:ILE:N | 2.79 | 0.45 |
| 2:D:413:MET:C | 2:D:414:GLU:HG3 | 2.36 | 0.45 |
| 1:E:209:LEU:HD23 | 1:E:227:LEU:HD13 | 1.98 | 0.45 |
| 2:F:95:GLY:C | 2:F:97:GLU:N | 2.69 | 0.45 |
| 2:F:115:ILE:CG1 | 2:F:152:LEU:HD13 | 2.46 | 0.45 |
| 2:F:144:GLY:H | 5:F:500:GTP:PG | 2.40 | 0.45 |
| 1:G:210:TYR:CE2 | 1:G:227:LEU:HD11 | 2.52 | 0.45 |
| 1:G:242:LEU:HD22 | 1:G:250:ALA:N | 2.19 | 0.45 |
| 1:G:288:VAL:N | 1:G:289:PRO:CD | 2.79 | 0.45 |
| 2:H:62:VAL:CG1 | 2:H:91:GLN:NE2 | 2.80 | 0.45 |
| 2:H:155:GLU:HA | 2:H:197:HIS:CE1 | 2.49 | 0.45 |
| 2:H:268:PRO:CA | 2:H:379:SER:O | 2.65 | 0.45 |
| 2:H:317:LEU:CD1 | 2:H:351:PHE:CE2 | 2.99 | 0.45 |
| 3:I:80:PHE:CE1 | 3:I:119:LEU:HD21 | 2.52 | 0.45 |
| 1:A:4:ILE:HD12 | 1:A:239:THR:HG21 | 1.98 | 0.45 |
| 1:A:209:LEU:HD23 | 1:A:227:LEU:HD13 | 1.98 | 0.45 |
| 1:A:210:TYR:CE2 | 1:A:227:LEU:HD11 | 2.52 | 0.45 |
| 1:A:312:TYR:HA | 1:A:381:SER:HA | 1.99 | 0.45 |
| 1:A:324:SER:OG | 1:A:326:LYS:HB3 | 2.15 | 0.45 |
| 2:B:10:GLY:O | 2:B:11:GLN:C | 2.53 | 0.45 |
| 2:B:95:GLY:C | 2:B:97:GLU:N | 2.69 | 0.45 |
| 2:B:204:VAL:O | 2:B:204:VAL:HG12 | 2.17 | 0.45 |
| 2:B:253:THR:HG21 | 1:C:105:LYS:NZ | 2.32 | 0.45 |
| 1:C:210:TYR:CE2 | 1:C:227:LEU:HD11 | 2.51 | 0.45 |
| 1:C:324:SER:OG | 1:C:326:LYS:HB3 | 2.15 | 0.45 |
| 2:D:62:VAL:CG1 | 2:D:91:GLN:NE2 | 2.80 | 0.45 |
| 2:D:63:PRO:HD2 | 2:D:87:PHE:HA | 1.98 | 0.45 |
| 2:D:103:TYR:CD1 | 2:D:148:GLY:HA2 | 2.52 | 0.45 |
| 2:D:203:MET:SD | 2:D:267:PHE:CB | 3.04 | 0.45 |
| 1:E:106:GLY:O | 1:E:149:MET:HB2 | 2.17 | 0.45 |
| 1:E:135:PHE:N | 1:E:135:PHE:CD1 | 2.85 | 0.45 |
| 1:E:313:LEU:O | 1:E:347:ILE:HD12 | 2.16 | 0.45 |
| 2:F:52:PHE:O | 2:F:64:ARG:HB3 | 2.16 | 0.45 |
| 2:F:62:VAL:CG1 | 2:F:91:GLN:NE2 | 2.80 | 0.45 |
| 2:F:295:CYS:SG | 2:F:375:VAL:HG11 | 2.57 | 0.45 |
| 1:G:106:GLY:O | 1:G:149:MET:HB2 | 2.16 | 0.45 |
| 1:G:135:PHE:N | 1:G:135:PHE:CD1 | 2.85 | 0.45 |
| 1:G:263:PRO:O | 1:G:264:ARG:C | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:67:PHE:CE1 | 2:H:87:PHE:CD1 | 2.89 | 0.45 |
| 1:A:6:HIS:HB3 | 1:A:21:TRP:HZ2 | 1.81 | 0.45 |
| 1:A:8:GLN:CG | 1:A:67:LEU:HD22 | 2.47 | 0.45 |
| 1:A:35:SER:CB | 1:A:59:ASN:HA | 2.42 | 0.45 |
| 1:A:82:PRO:C | 1:A:84:GLY:H | 2.20 | 0.45 |
| 2:B:132:LEU:H | 2:B:132:LEU:CD2 | 2.23 | 0.45 |
| 1:C:8:GLN:CG | 1:C:67:LEU:HD22 | 2.47 | 0.45 |
| 1:C:102:ASN:ND2 | 1:C:104:ALA:HB3 | 2.31 | 0.45 |
| 1:C:194:LEU:O | 1:C:265:LEU:HD23 | 2.17 | 0.45 |
| 1:C:273:ALA:CB | 1:C:274:PRO:CD | 2.93 | 0.45 |
| 1:C:288:VAL:N | 1:C:289:PRO:CD | 2.80 | 0.45 |
| 1:C:324:SER:O | 1:C:326:LYS:N | 2.50 | 0.45 |
| 2:D:119:LEU:HD11 | 2:D:156:ARG:HD2 | 1.97 | 0.45 |
| 2:D:212:ILE:HD11 | 2:D:302:MET:H | 1.82 | 0.45 |
| 2:D:234:ILE:C | 2:D:234:ILE:CD1 | 2.85 | 0.45 |
| 1:E:194:LEU:O | 1:E:265:LEU:HD23 | 2.16 | 0.45 |
| 1:E:312:TYR:HA | 1:E:381:SER:HA | 1.99 | 0.45 |
| 2:F:182:VAL:O | 2:F:184:PRO:CD | 2.65 | 0.45 |
| 2:F:408:TYR:CG | 2:F:418:PHE:HZ | 2.34 | 0.45 |
| 1:G:67:LEU:HD12 | 1:G:92:PHE:CD2 | 2.51 | 0.45 |
| 1:G:254:LYS:HA | 1:G:257:VAL:HG12 | 1.99 | 0.45 |
| 2:H:103:TYR:CD1 | 2:H:148:GLY:HA2 | 2.52 | 0.45 |
| 2:H:295:CYS:SG | 2:H:375:VAL:HG11 | 2.57 | 0.45 |
| 1:A:102:ASN:ND2 | 1:A:104:ALA:HB3 | 2.31 | 0.45 |
| 1:A:102:ASN:OD1 | 1:A:408:TYR:CZ | 2.70 | 0.45 |
| 1:A:273:ALA:CB | 1:A:274:PRO:CD | 2.93 | 0.45 |
| 1:A:323:MET:CE | 1:A:328:VAL:HG22 | 2.46 | 0.45 |
| 2:B:63:PRO:CG | 2:B:91:GLN:CD | 2.71 | 0.45 |
| 2:B:103:TYR:CD1 | 2:B:148:GLY:HA2 | 2.52 | 0.45 |
| 2:B:218:ASP:C | 2:B:219:ILE:HG12 | 2.37 | 0.45 |
| 1:C:102:ASN:OD1 | 1:C:408:TYR:CZ | 2.70 | 0.45 |
| 1:C:409:THR:O | 1:C:412:GLY:N | 2.48 | 0.45 |
| 2:D:204:VAL:O | 2:D:204:VAL:HG12 | 2.17 | 0.45 |
| 2:D:274:PRO:HB2 | 2:D:371:VAL:HG21 | 1.98 | 0.45 |
| 2:D:346:TRP:HZ2 | 2:D:435:VAL:HG12 | 1.81 | 0.45 |
| 2:D:408:TYR:CG | 2:D:418:PHE:HZ | 2.34 | 0.45 |
| 1:E:115:VAL:HG21 | 1:E:152:LEU:HD21 | 1.98 | 0.45 |
| 2:F:274:PRO:HB2 | 2:F:371:VAL:HG21 | 1.98 | 0.45 |
| 2:F:334:THR:CG2 | 2:F:335:ILE:N | 2.79 | 0.45 |
| 1:G:6:HIS:HB3 | 1:G:21:TRP:HZ2 | 1.81 | 0.45 |
| 2:H:115:ILE:CG1 | 2:H:152:LEU:HD13 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:182:VAL:O | 2:H:184:PRO:CD | 2.65 | 0.45 |
| 2:H:308:ARG:O | 2:H:309:HIS:HB3 | 2.16 | 0.45 |
| 1:A:106:GLY:O | 1:A:149:MET:HB2 | 2.16 | 0.45 |
| 1:A:189:LEU:HD23 | 1:A:421:ALA:CB | 2.47 | 0.45 |
| 1:A:269:MET:HE1 | 1:A:381:SER:OG | 2.18 | 0.45 |
| 1:A:324:SER:O | 1:A:326:LYS:N | 2.50 | 0.45 |
| 1:A:409:THR:O | 1:A:412:GLY:N | 2.48 | 0.45 |
| 2:B:212:ILE:HD11 | 2:B:302:MET:H | 1.82 | 0.45 |
| 2:B:234:ILE:C | 2:B:234:ILE:CD1 | 2.86 | 0.45 |
| 2:B:243:ARG:NH2 | 2:B:252:LEU:HB2 | 2.30 | 0.45 |
| 2:B:276:ILE:CG2 | 2:B:369:ALA:CB | 2.91 | 0.45 |
| 2:B:295:CYS:SG | 2:B:375:VAL:HG11 | 2.57 | 0.45 |
| 2:B:303:VAL:O | 2:B:303:VAL:CG1 | 2.64 | 0.45 |
| 2:B:413:MET:C | 2:B:414:GLU:HG3 | 2.36 | 0.45 |
| 1:C:23:VAL:O | 1:C:25:SER:N | 2.50 | 0.45 |
| 1:C:312:TYR:HA | 1:C:381:SER:HA | 1.99 | 0.45 |
| 1:C:323:MET:CE | 1:C:328:VAL:HG22 | 2.46 | 0.45 |
| 2:D:218:ASP:C | 2:D:219:ILE:HG12 | 2.37 | 0.45 |
| 2:D:392:ASP:OD2 | 2:D:422:ARG:CZ | 2.65 | 0.45 |
| 1:E:23:VAL:O | 1:E:25:SER:N | 2.50 | 0.45 |
| 2:F:384:ILE:HG22 | 2:F:384:ILE:O | 2.15 | 0.45 |
| 1:G:8:GLN:CG | 1:G:67:LEU:HD22 | 2.47 | 0.45 |
| 1:G:115:VAL:HG21 | 1:G:152:LEU:HD21 | 1.98 | 0.45 |
| 1:G:134:GLY:HA3 | 1:G:165:ILE:HG12 | 1.97 | 0.45 |
| 1:G:312:TYR:HA | 1:G:381:SER:HA | 1.99 | 0.45 |
| 2:H:95:GLY:C | 2:H:97:GLU:N | 2.69 | 0.45 |
| 2:H:384:ILE:HG22 | 2:H:384:ILE:O | 2.15 | 0.45 |
| 2:H:408:TYR:CG | 2:H:418:PHE:HZ | 2.34 | 0.45 |
| 3:I:97:LEU:HB3 | 3:I:100:GLY:O | 2.16 | 0.45 |
| 1:A:194:LEU:O | 1:A:265:LEU:HD23 | 2.16 | 0.44 |
| 2:B:4:CYS:SG | 2:B:252:LEU:CD1 | 3.02 | 0.44 |
| 2:B:152:LEU:HD12 | 2:B:152:LEU:C | 2.38 | 0.44 |
| 2:B:402:ARG:O | 2:B:405:VAL:N | 2.49 | 0.44 |
| 2:B:404:PHE:CD1 | 2:B:404:PHE:N | 2.83 | 0.44 |
| 1:C:82:PRO:C | 1:C:84:GLY:H | 2.20 | 0.44 |
| 1:C:167:ASN:HA | 1:C:200:GLU:O | 2.17 | 0.44 |
| 1:C:189:LEU:HD23 | 1:C:421:ALA:CB | 2.47 | 0.44 |
| 2:D:152:LEU:HD12 | 2:D:152:LEU:C | 2.38 | 0.44 |
| 2:D:295:CYS:SG | 2:D:375:VAL:HG11 | 2.57 | 0.44 |
| 1:E:6:HIS:HB3 | 1:E:21:TRP:HZ2 | 1.81 | 0.44 |
| 1:E:52:TYR:HE1 | 1:E:240:THR:HB | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:137:LEU:HD22 | 1:E:154:ILE:HG23 | 1.97 | 0.44 |
| 1:E:409:THR:O | 1:E:412:GLY:N | 2.48 | 0.44 |
| 2:F:103:TYR:CD1 | 2:F:148:GLY:HA2 | 2.52 | 0.44 |
| 2:F:153:LEU:O | 2:F:157:LEU:HG | 2.18 | 0.44 |
| 2:F:231:ILE:HD13 | 2:F:231:ILE:H | 1.82 | 0.44 |
| 2:F:303:VAL:O | 2:F:303:VAL:CG1 | 2.65 | 0.44 |
| 2:F:344:VAL:CG1 | 2:F:345:ASP:N | 2.78 | 0.44 |
| 2:F:423:GLU:O | 2:F:426:ALA:HB3 | 2.16 | 0.44 |
| 1:G:52:TYR:HE1 | 1:G:240:THR:HB | 1.83 | 0.44 |
| 1:G:189:LEU:HD23 | 1:G:421:ALA:CB | 2.47 | 0.44 |
| 1:G:194:LEU:O | 1:G:265:LEU:HD23 | 2.16 | 0.44 |
| 1:G:217:LEU:C | 1:G:219:LEU:N | 2.55 | 0.44 |
| 2:H:153:LEU:O | 2:H:157:LEU:HG | 2.18 | 0.44 |
| 2:H:274:PRO:HB2 | 2:H:371:VAL:HG21 | 1.98 | 0.44 |
| 2:H:334:THR:CG2 | 2:H:335:ILE:N | 2.79 | 0.44 |
| 1:A:14:ASN:O | 1:A:17:GLY:N | 2.50 | 0.44 |
| 1:A:282:GLN:O | 1:A:282:GLN:CG | 2.65 | 0.44 |
| 2:B:344:VAL:CG1 | 2:B:345:ASP:N | 2.78 | 0.44 |
| 1:C:4:ILE:HD12 | 1:C:239:THR:HG21 | 1.99 | 0.44 |
| 1:C:194:LEU:C | 1:C:196:GLU:N | 2.70 | 0.44 |
| 1:C:257:VAL:CG1 | 2:D:407:TRP:CD1 | 2.98 | 0.44 |
| 1:C:269:MET:HE1 | 1:C:381:SER:OG | 2.18 | 0.44 |
| 2:D:271:THR:O | 2:D:376:CYS:HA | 2.17 | 0.44 |
| 1:E:8:GLN:CG | 1:E:67:LEU:HD22 | 2.47 | 0.44 |
| 1:E:167:ASN:HD21 | 1:E:252:LEU:HD22 | 1.82 | 0.44 |
| 1:E:242:LEU:HD22 | 1:E:250:ALA:O | 2.17 | 0.44 |
| 1:E:273:ALA:CB | 1:E:274:PRO:CD | 2.93 | 0.44 |
| 2:F:30:ILE:O | 2:F:31:GLN:O | 2.35 | 0.44 |
| 2:F:30:ILE:HD11 | 2:F:61:HIS:CD2 | 2.51 | 0.44 |
| 2:F:229:ARG:NH1 | 2:F:229:ARG:HG2 | 2.31 | 0.44 |
| 2:F:308:ARG:O | 2:F:309:HIS:HB3 | 2.17 | 0.44 |
| 2:F:396:ASP:O | 2:F:397:LEU:C | 2.53 | 0.44 |
| 1:G:4:ILE:HD12 | 1:G:239:THR:HG21 | 1.98 | 0.44 |
| 1:G:237:GLY:O | 1:G:241:CYS:CB | 2.61 | 0.44 |
| 2:H:204:VAL:O | 2:H:204:VAL:HG12 | 2.17 | 0.44 |
| 2:H:229:ARG:NH1 | 2:H:229:ARG:HG2 | 2.31 | 0.44 |
| 2:H:231:ILE:HD13 | 2:H:231:ILE:H | 1.82 | 0.44 |
| 2:H:234:ILE:C | 2:H:234:ILE:CD1 | 2.86 | 0.44 |
| 2:H:303:VAL:O | 2:H:303:VAL:CG1 | 2.65 | 0.44 |
| 2:H:392:ASP:OD2 | 2:H:422:ARG:CZ | 2.64 | 0.44 |
| 2:H:396:ASP:O | 2:H:397:LEU:C | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:11:GLN:O | 1:A:15:GLN:N | 2.41 | 0.44 |
| 1:A:288:VAL:N | 1:A:289:PRO:HD2 | 2.32 | 0.44 |
| 2:B:7:ILE:HG13 | 2:B:137:VAL:HG22 | 1.97 | 0.44 |
| 2:B:182:VAL:O | 2:B:184:PRO:CD | 2.65 | 0.44 |
| 1:C:282:GLN:O | 1:C:282:GLN:CG | 2.65 | 0.44 |
| 1:C:288:VAL:N | 1:C:289:PRO:HD2 | 2.32 | 0.44 |
| 1:C:346:TRP:CG | 2:D:401:LYS:NZ | 2.78 | 0.44 |
| 1:C:409:THR:HA | 1:C:413:MET:HB3 | 1.99 | 0.44 |
| 2:D:252:LEU:O | 2:D:253:THR:C | 2.56 | 0.44 |
| 1:E:82:PRO:C | 1:E:84:GLY:H | 2.20 | 0.44 |
| 1:E:102:ASN:OD1 | 1:E:408:TYR:CZ | 2.70 | 0.44 |
| 1:E:237:GLY:O | 1:E:241:CYS:CB | 2.61 | 0.44 |
| 1:E:257:VAL:O | 1:E:257:VAL:CG1 | 2.64 | 0.44 |
| 1:G:23:VAL:O | 1:G:25:SER:N | 2.50 | 0.44 |
| 1:G:82:PRO:C | 1:G:84:GLY:H | 2.20 | 0.44 |
| 1:G:102:ASN:OD1 | 1:G:408:TYR:CZ | 2.70 | 0.44 |
| 2:H:218:ASP:C | 2:H:219:ILE:HG12 | 2.37 | 0.44 |
| 2:H:271:THR:O | 2:H:376:CYS:HA | 2.17 | 0.44 |
| 2:H:344:VAL:CG1 | 2:H:345:ASP:N | 2.78 | 0.44 |
| 1:A:167:ASN:HA | 1:A:200:GLU:O | 2.17 | 0.44 |
| 2:B:271:THR:O | 2:B:376:CYS:HA | 2.17 | 0.44 |
| 1:C:14:ASN:O | 1:C:17:GLY:N | 2.50 | 0.44 |
| 1:C:250:ALA:HB1 | 1:C:254:LYS:CB | 2.44 | 0.44 |
| 2:D:8:HIS:HA | 2:D:138:PHE:HB2 | 1.99 | 0.44 |
| 2:F:204:VAL:O | 2:F:204:VAL:HG12 | 2.17 | 0.44 |
| 2:F:234:ILE:C | 2:F:234:ILE:CD1 | 2.86 | 0.44 |
| 2:F:262:TYR:CZ | 1:G:403:ALA:O | 2.70 | 0.44 |
| 2:F:272:TYR:CE2 | 2:F:274:PRO:HD2 | 2.53 | 0.44 |
| 2:F:392:ASP:OD2 | 2:F:422:ARG:CZ | 2.65 | 0.44 |
| 1:G:2:ARG:HD3 | 2:H:98:ASP:OD2 | 2.18 | 0.44 |
| 1:G:269:MET:HE1 | 1:G:381:SER:OG | 2.17 | 0.44 |
| 1:G:310:GLY:HA3 | 1:G:436:GLN:NE2 | 2.29 | 0.44 |
| 2:H:8:HIS:HA | 2:H:138:PHE:HB2 | 1.99 | 0.44 |
| 1:A:23:VAL:O | 1:A:25:SER:N | 2.50 | 0.44 |
| 1:A:52:TYR:HE1 | 1:A:240:THR:HB | 1.82 | 0.44 |
| 1:A:239:THR:O | 1:A:240:THR:C | 2.56 | 0.44 |
| 2:B:8:HIS:HA | 2:B:138:PHE:HB2 | 2.00 | 0.44 |
| 2:B:154:MET:CE | 2:B:166:LYS:HB3 | 2.48 | 0.44 |
| 2:B:252:LEU:O | 2:B:253:THR:C | 2.56 | 0.44 |
| 2:B:268:PRO:CA | 2:B:379:SER:O | 2.65 | 0.44 |
| 2:B:274:PRO:HB2 | 2:B:371:VAL:HG21 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:362:VAL:HG13 | 2:B:368:LEU:CG | 2.48 | 0.44 |
| 2:B:363:VAL:CG1 | 2:B:364:PRO:HD2 | 2.48 | 0.44 |
| 1:C:106:GLY:O | 1:C:149:MET:HB2 | 2.17 | 0.44 |
| 1:C:167:ASN:HD21 | 1:C:252:LEU:HD22 | 1.82 | 0.44 |
| 1:C:257:VAL:O | 1:C:257:VAL:CG1 | 2.64 | 0.44 |
| 2:D:11:GLN:NE2 | 2:D:74:VAL:CG2 | 2.76 | 0.44 |
| 2:D:182:VAL:O | 2:D:184:PRO:CD | 2.65 | 0.44 |
| 2:D:276:ILE:CG2 | 2:D:369:ALA:CB | 2.91 | 0.44 |
| 2:D:402:ARG:O | 2:D:405:VAL:N | 2.49 | 0.44 |
| 1:E:167:ASN:HA | 1:E:200:GLU:O | 2.17 | 0.44 |
| 1:E:189:LEU:HD23 | 1:E:421:ALA:CB | 2.47 | 0.44 |
| 1:E:217:LEU:C | 1:E:219:LEU:N | 2.55 | 0.44 |
| 1:E:310:GLY:HA3 | 1:E:436:GLN:NE2 | 2.29 | 0.44 |
| 2:F:8:HIS:HA | 2:F:138:PHE:HB2 | 2.00 | 0.44 |
| 2:F:23:LEU:O | 2:F:26:LEU:HB3 | 2.17 | 0.44 |
| 2:F:217:LEU:HD13 | 2:F:277:SER:N | 2.33 | 0.44 |
| 2:F:218:ASP:C | 2:F:219:ILE:HG12 | 2.37 | 0.44 |
| 1:G:137:LEU:HD22 | 1:G:154:ILE:HG23 | 1.98 | 0.44 |
| 1:G:167:ASN:HD21 | 1:G:252:LEU:HD22 | 1.82 | 0.44 |
| 1:G:242:LEU:HD22 | 1:G:250:ALA:O | 2.17 | 0.44 |
| 2:H:23:LEU:O | 2:H:26:LEU:HB3 | 2.17 | 0.44 |
| 2:H:30:ILE:O | 2:H:31:GLN:O | 2.35 | 0.44 |
| 2:H:272:TYR:CE2 | 2:H:274:PRO:HD2 | 2.53 | 0.44 |
| 2:H:343:PHE:CE1 | 2:H:351:PHE:HE1 | 2.36 | 0.44 |
| 2:H:423:GLU:O | 2:H:426:ALA:HB3 | 2.16 | 0.44 |
| 1:A:105:LYS:HG2 | 1:A:110:GLU:CG | 2.48 | 0.44 |
| 2:B:272:TYR:CE2 | 2:B:274:PRO:HD2 | 2.53 | 0.44 |
| 2:D:10:GLY:O | 2:D:11:GLN:C | 2.53 | 0.44 |
| 2:D:272:TYR:CE2 | 2:D:274:PRO:HD2 | 2.53 | 0.44 |
| 2:D:362:VAL:HG13 | 2:D:368:LEU:CG | 2.48 | 0.44 |
| 1:E:4:ILE:HD12 | 1:E:239:THR:HG21 | 1.98 | 0.44 |
| 1:E:147:SER:HB2 | 1:E:190:SER:CB | 2.41 | 0.44 |
| 2:F:343:PHE:CE1 | 2:F:351:PHE:HE1 | 2.36 | 0.44 |
| 2:F:402:ARG:O | 2:F:405:VAL:N | 2.49 | 0.44 |
| 1:G:204:ILE:HD13 | 1:G:231:VAL:CG2 | 2.45 | 0.44 |
| 2:H:121:ARG:HG2 | 2:H:121:ARG:HH11 | 1.83 | 0.44 |
| 2:H:217:LEU:HD13 | 2:H:277:SER:N | 2.33 | 0.44 |
| 2:H:363:VAL:CG1 | 2:H:364:PRO:HD2 | 2.48 | 0.44 |
| 2:H:402:ARG:O | 2:H:405:VAL:N | 2.49 | 0.44 |
| 3:I:77:PHE:HB2 | 3:I:116:MET:HE3 | 2.00 | 0.44 |
| 1:A:194:LEU:C | 1:A:196:GLU:N | 2.70 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:349:THR:O | 1:C:181:VAL:CG1 | 2.65 | 0.44 |
| 1:C:24:ILE:CG2 | 1:C:25:SER:N | 2.80 | 0.44 |
| 1:C:105:LYS:HG2 | 1:C:110:GLU:CG | 2.48 | 0.44 |
| 1:C:182:VAL:O | 1:C:183:GLU:C | 2.56 | 0.44 |
| 2:D:64:ARG:HD2 | 2:D:125:LEU:HD22 | 1.99 | 0.44 |
| 1:E:105:LYS:HG2 | 1:E:110:GLU:CG | 2.48 | 0.44 |
| 1:E:161:TYR:O | 1:E:163:ASP:N | 2.51 | 0.44 |
| 2:F:50:ASN:HD22 | 2:F:50:ASN:HA | 1.60 | 0.44 |
| 2:F:271:THR:O | 2:F:376:CYS:HA | 2.17 | 0.44 |
| 2:F:325:PRO:CD | 1:G:223:THR:HA | 2.30 | 0.44 |
| 1:G:105:LYS:HG2 | 1:G:110:GLU:CG | 2.48 | 0.44 |
| 1:G:161:TYR:O | 1:G:163:ASP:N | 2.51 | 0.44 |
| 3:I:60:ASN:HB2 | 3:I:126:VAL:CG1 | 2.48 | 0.44 |
| 3:I:77:PHE:CD2 | 3:I:83:LEU:HD13 | 2.52 | 0.44 |
| 1:A:115:VAL:HG21 | 1:A:152:LEU:HD21 | 1.98 | 0.44 |
| 1:A:242:LEU:HD23 | 1:A:242:LEU:HA | 1.76 | 0.44 |
| 1:A:287:THR:O | 1:A:288:VAL:CG2 | 2.58 | 0.44 |
| 2:B:12:ALA:HB2 | 5:B:500:GTP:C8 | 2.52 | 0.44 |
| 2:B:13:GLY:C | 2:B:16:ILE:HG22 | 2.38 | 0.44 |
| 2:B:23:LEU:O | 2:B:26:LEU:HB3 | 2.17 | 0.44 |
| 2:B:64:ARG:HD2 | 2:B:125:LEU:HD22 | 1.99 | 0.44 |
| 2:B:149:PHE:O | 2:B:150:THR:C | 2.56 | 0.44 |
| 1:C:52:TYR:HE1 | 1:C:240:THR:HB | 1.83 | 0.44 |
| 1:C:72:PRO:HG2 | 1:C:73:GLY:H | 1.83 | 0.44 |
| 1:C:115:VAL:HG21 | 1:C:152:LEU:HD21 | 1.99 | 0.44 |
| 1:C:239:THR:O | 1:C:240:THR:C | 2.56 | 0.44 |
| 1:C:346:TRP:CG | 2:D:401:LYS:HD2 | 2.52 | 0.44 |
| 2:D:363:VAL:CG1 | 2:D:364:PRO:HD2 | 2.48 | 0.44 |
| 2:D:390:ARG:HG3 | 2:D:390:ARG:HH11 | 1.83 | 0.44 |
| 1:E:67:LEU:HD12 | 1:E:92:PHE:CE2 | 2.52 | 0.44 |
| 1:E:288:VAL:N | 1:E:289:PRO:HD2 | 2.32 | 0.44 |
| 1:E:301:MET:O | 1:E:303:ALA:N | 2.51 | 0.44 |
| 1:E:301:MET:HE1 | 1:E:377:PHE:HE2 | 1.82 | 0.44 |
| 2:F:13:GLY:C | 2:F:16:ILE:HG22 | 2.38 | 0.44 |
| 2:F:121:ARG:NH1 | 2:F:121:ARG:HG2 | 2.33 | 0.44 |
| 2:F:152:LEU:HD12 | 2:F:152:LEU:C | 2.38 | 0.44 |
| 2:F:363:VAL:CG1 | 2:F:364:PRO:HD2 | 2.48 | 0.44 |
| 1:G:26:ASP:C | 1:G:28:HIS:H | 2.21 | 0.44 |
| 1:G:67:LEU:HD12 | 1:G:92:PHE:CE2 | 2.52 | 0.44 |
| 1:G:301:MET:O | 1:G:303:ALA:N | 2.51 | 0.44 |
| 2:H:13:GLY:C | 2:H:16:ILE:HG22 | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:121:ARG:HG2 | 2:H:121:ARG:NH1 | 2.33 | 0.44 |
| 2:H:263:PRO:O | 2:H:264:ARG:C | 2.56 | 0.44 |
| 2:H:362:VAL:HG13 | 2:H:368:LEU:CG | 2.48 | 0.44 |
| 3:I:46:LEU:N | 3:I:46:LEU:HD12 | 2.33 | 0.44 |
| 3:I:80:PHE:CZ | 3:I:104:ILE:HB | 2.53 | 0.44 |
| 3:I:102:ARG:HB3 | 3:I:103:TYR:CE1 | 2.52 | 0.44 |
| 1:A:257:VAL:O | 1:A:257:VAL:CG1 | 2.64 | 0.44 |
| 1:A:409:THR:HA | 1:A:413:MET:HB3 | 1.99 | 0.44 |
| 2:B:115:ILE:CG1 | 2:B:152:LEU:HD13 | 2.46 | 0.44 |
| 2:B:121:ARG:HG2 | 2:B:121:ARG:NH1 | 2.33 | 0.44 |
| 2:B:153:LEU:O | 2:B:157:LEU:HG | 2.18 | 0.44 |
| 2:B:175:PRO:CG | 2:B:304:LYS:HG2 | 2.47 | 0.44 |
| 2:B:390:ARG:HH11 | 2:B:390:ARG:HG3 | 1.83 | 0.44 |
| 2:D:13:GLY:C | 2:D:16:ILE:HG22 | 2.38 | 0.44 |
| 2:D:23:LEU:O | 2:D:26:LEU:HB3 | 2.17 | 0.44 |
| 2:D:50:ASN:HD22 | 2:D:50:ASN:HA | 1.61 | 0.44 |
| 2:D:153:LEU:O | 2:D:157:LEU:HG | 2.18 | 0.44 |
| 2:D:154:MET:CE | 2:D:166:LYS:HB3 | 2.48 | 0.44 |
| 2:D:175:PRO:CG | 2:D:304:LYS:HG2 | 2.47 | 0.44 |
| 1:E:7:ILE:N | 1:E:136:GLN:O | 2.51 | 0.44 |
| 1:E:161:TYR:CD1 | 1:E:161:TYR:N | 2.86 | 0.44 |
| 2:F:5:ILE:CG2 | 2:F:135:PHE:CB | 2.96 | 0.44 |
| 2:F:263:PRO:O | 2:F:264:ARG:C | 2.56 | 0.44 |
| 2:F:346:TRP:O | 1:G:398:MET:CE | 2.66 | 0.44 |
| 1:G:7:ILE:N | 1:G:136:GLN:O | 2.51 | 0.44 |
| 1:G:167:ASN:HA | 1:G:200:GLU:O | 2.17 | 0.44 |
| 1:G:288:VAL:N | 1:G:289:PRO:HD2 | 2.32 | 0.44 |
| 1:G:307:PRO:C | 1:G:309:HIS:N | 2.71 | 0.44 |
| 2:H:5:ILE:CG2 | 2:H:135:PHE:CB | 2.95 | 0.44 |
| 2:H:12:ALA:HB2 | 5:H:500:GTP:C8 | 2.52 | 0.44 |
| 2:H:152:LEU:HD12 | 2:H:152:LEU:C | 2.38 | 0.44 |
| 2:H:404:PHE:CD1 | 2:H:404:PHE:N | 2.83 | 0.44 |
| 1:A:72:PRO:HG2 | 1:A:73:GLY:H | 1.83 | 0.43 |
| 1:A:167:ASN:HD21 | 1:A:252:LEU:HD22 | 1.82 | 0.43 |
| 1:A:307:PRO:C | 1:A:309:HIS:N | 2.71 | 0.43 |
| 2:B:54:SER:O | 2:B:61:HIS:O | 2.35 | 0.43 |
| 2:B:436:GLY:C | 2:B:438:ASP:N | 2.72 | 0.43 |
| 1:C:141:LEU:N | 1:C:141:LEU:HD12 | 2.33 | 0.43 |
| 1:C:242:LEU:HD23 | 1:C:242:LEU:HA | 1.76 | 0.43 |
| 1:C:307:PRO:C | 1:C:309:HIS:N | 2.71 | 0.43 |
| 2:D:149:PHE:O | 2:D:150:THR:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:229:ARG:NH1 | 2:D:229:ARG:HG2 | 2.31 | 0.43 |
| 2:D:436:GLY:C | 2:D:438:ASP:N | 2.72 | 0.43 |
| 1:E:6:HIS:HB3 | 1:E:65:ALA:CB | 2.48 | 0.43 |
| 1:E:72:PRO:HG2 | 1:E:73:GLY:H | 1.83 | 0.43 |
| 1:E:168:THR:CG2 | 1:E:201:THR:HG23 | 2.48 | 0.43 |
| 1:E:243:ARG:HH21 | 1:E:252:LEU:N | 2.12 | 0.43 |
| 1:E:282:GLN:O | 1:E:282:GLN:CG | 2.65 | 0.43 |
| 2:F:7:ILE:HG13 | 2:F:137:VAL:HG22 | 1.97 | 0.43 |
| 2:F:362:VAL:HG13 | 2:F:368:LEU:CG | 2.48 | 0.43 |
| 1:G:6:HIS:HB3 | 1:G:65:ALA:CB | 2.48 | 0.43 |
| 2:H:7:ILE:HG13 | 2:H:137:VAL:HG22 | 1.98 | 0.43 |
| 2:H:10:GLY:O | 2:H:11:GLN:C | 2.53 | 0.43 |
| 2:H:50:ASN:HD22 | 2:H:50:ASN:HA | 1.61 | 0.43 |
| 2:H:304:LYS:HG3 | 2:H:304:LYS:O | 2.18 | 0.43 |
| 1:A:24:ILE:CG2 | 1:A:25:SER:N | 2.80 | 0.43 |
| 1:A:70:LEU:HB2 | 1:A:99:ALA:CB | 2.49 | 0.43 |
| 1:A:204:ILE:HD13 | 1:A:231:VAL:CG2 | 2.45 | 0.43 |
| 1:A:212:ILE:O | 1:A:212:ILE:HG22 | 2.18 | 0.43 |
| 1:A:239:THR:CG2 | 1:A:240:THR:N | 2.81 | 0.43 |
| 1:A:240:THR:HG23 | 1:A:241:CYS:N | 2.33 | 0.43 |
| 1:A:262:PHE:HA | 1:A:263:PRO:HD2 | 1.65 | 0.43 |
| 1:A:295:MET:SD | 1:A:375:ALA:HB3 | 2.58 | 0.43 |
| 2:B:296:PHE:HZ | 2:B:351:PHE:HZ | 1.66 | 0.43 |
| 1:C:70:LEU:HB2 | 1:C:99:ALA:CB | 2.49 | 0.43 |
| 1:C:295:MET:SD | 1:C:375:ALA:HB3 | 2.57 | 0.43 |
| 2:D:5:ILE:CG2 | 2:D:135:PHE:CB | 2.96 | 0.43 |
| 2:D:132:LEU:H | 2:D:132:LEU:CD2 | 2.23 | 0.43 |
| 2:D:196:GLU:C | 2:D:197:HIS:HD2 | 2.19 | 0.43 |
| 2:D:268:PRO:CA | 2:D:379:SER:O | 2.65 | 0.43 |
| 2:F:121:ARG:HG2 | 2:F:121:ARG:HH11 | 1.83 | 0.43 |
| 2:F:276:ILE:O | 2:F:369:ALA:CA | 2.66 | 0.43 |
| 2:F:292:THR:O | 2:F:295:CYS:HB2 | 2.18 | 0.43 |
| 2:F:304:LYS:HG3 | 2:F:304:LYS:O | 2.19 | 0.43 |
| 1:G:72:PRO:HG2 | 1:G:73:GLY:H | 1.83 | 0.43 |
| 2:H:175:PRO:CG | 2:H:304:LYS:HG2 | 2.47 | 0.43 |
| 2:H:276:ILE:O | 2:H:369:ALA:CA | 2.66 | 0.43 |
| 2:B:229:ARG:NH1 | 2:B:229:ARG:HG2 | 2.31 | 0.43 |
| 2:B:241:SER:C | 2:B:244:PHE:HB3 | 2.36 | 0.43 |
| 2:B:292:THR:O | 2:B:295:CYS:HB2 | 2.18 | 0.43 |
| 2:B:409:VAL:C | 2:B:411:GLU:N | 2.71 | 0.43 |
| 1:C:7:ILE:N | 1:C:136:GLN:O | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:67:LEU:HD12 | 1:C:92:PHE:CE2 | 2.52 | 0.43 |
| 1:C:248:LEU:HD21 | 2:D:179:THR:HG21 | 1.97 | 0.43 |
| 2:D:12:ALA:HB2 | 5:D:500:GTP:C8 | 2.53 | 0.43 |
| 2:D:199:ASP:OD2 | 2:D:256:GLN:NE2 | 2.46 | 0.43 |
| 2:D:209:ILE:CD1 | 2:D:231:ILE:HD11 | 2.47 | 0.43 |
| 1:E:70:LEU:HB2 | 1:E:99:ALA:CB | 2.49 | 0.43 |
| 1:E:194:LEU:C | 1:E:196:GLU:N | 2.70 | 0.43 |
| 1:E:204:ILE:HD13 | 1:E:231:VAL:CG2 | 2.45 | 0.43 |
| 1:E:307:PRO:C | 1:E:309:HIS:N | 2.71 | 0.43 |
| 2:F:5:ILE:CG1 | 2:F:6:SER:N | 2.82 | 0.43 |
| 2:F:12:ALA:HB2 | 5:F:500:GTP:C8 | 2.52 | 0.43 |
| 2:F:154:MET:CE | 2:F:166:LYS:HB3 | 2.48 | 0.43 |
| 1:G:194:LEU:C | 1:G:196:GLU:N | 2.70 | 0.43 |
| 1:G:282:GLN:O | 1:G:282:GLN:CG | 2.65 | 0.43 |
| 2:H:5:ILE:CG1 | 2:H:6:SER:N | 2.82 | 0.43 |
| 2:H:154:MET:CE | 2:H:166:LYS:HB3 | 2.48 | 0.43 |
| 2:H:196:GLU:C | 2:H:197:HIS:HD2 | 2.19 | 0.43 |
| 2:H:255:PHE:O | 2:H:259:LEU:N | 2.50 | 0.43 |
| 2:H:377:MET:HG3 | 2:H:377:MET:O | 2.18 | 0.43 |
| 1:A:67:LEU:HD12 | 1:A:92:PHE:CE2 | 2.52 | 0.43 |
| 1:A:161:TYR:CD1 | 1:A:161:TYR:N | 2.86 | 0.43 |
| 2:B:121:ARG:HG2 | 2:B:121:ARG:HH11 | 1.83 | 0.43 |
| 1:C:242:LEU:HD22 | 1:C:250:ALA:O | 2.17 | 0.43 |
| 1:C:287:THR:O | 1:C:288:VAL:CG2 | 2.58 | 0.43 |
| 2:D:121:ARG:NH1 | 2:D:121:ARG:HG2 | 2.33 | 0.43 |
| 2:D:217:LEU:HD13 | 2:D:277:SER:N | 2.32 | 0.43 |
| 2:D:409:VAL:C | 2:D:411:GLU:N | 2.71 | 0.43 |
| 2:D:425:MET:O | 2:D:428:LEU:N | 2.45 | 0.43 |
| 1:E:26:ASP:C | 1:E:28:HIS:H | 2.21 | 0.43 |
| 1:E:239:THR:O | 1:E:240:THR:C | 2.56 | 0.43 |
| 2:F:196:GLU:C | 2:F:197:HIS:HD2 | 2.19 | 0.43 |
| 2:F:252:LEU:O | 2:F:253:THR:C | 2.56 | 0.43 |
| 2:F:390:ARG:HH11 | 2:F:390:ARG:HG3 | 1.83 | 0.43 |
| 2:F:404:PHE:CD1 | 2:F:404:PHE:N | 2.83 | 0.43 |
| 1:G:24:ILE:CG2 | 1:G:25:SER:N | 2.80 | 0.43 |
| 1:G:70:LEU:HB2 | 1:G:99:ALA:CB | 2.49 | 0.43 |
| 1:G:161:TYR:CD1 | 1:G:161:TYR:N | 2.86 | 0.43 |
| 1:G:239:THR:O | 1:G:240:THR:C | 2.56 | 0.43 |
| 1:G:409:THR:C | 1:G:411:GLU:H | 2.22 | 0.43 |
| 2:H:4:CYS:SG | 2:H:252:LEU:CD1 | 3.02 | 0.43 |
| 2:H:292:THR:O | 2:H:295:CYS:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:7:ILE:N | 1:A:136:GLN:O | 2.51 | 0.43 |
| 1:A:243:ARG:HH21 | 1:A:252:LEU:N | 2.12 | 0.43 |
| 1:A:301:MET:O | 1:A:303:ALA:N | 2.51 | 0.43 |
| 1:A:399:PHE:O | 1:A:402:LYS:N | 2.29 | 0.43 |
| 1:C:161:TYR:O | 1:C:163:ASP:N | 2.51 | 0.43 |
| 1:C:204:ILE:HD13 | 1:C:231:VAL:CG2 | 2.45 | 0.43 |
| 1:C:240:THR:HG23 | 1:C:241:CYS:N | 2.33 | 0.43 |
| 2:D:115:ILE:CG1 | 2:D:152:LEU:HD13 | 2.46 | 0.43 |
| 2:D:231:ILE:HD13 | 2:D:231:ILE:H | 1.82 | 0.43 |
| 2:D:304:LYS:HG3 | 2:D:304:LYS:O | 2.18 | 0.43 |
| 1:E:212:ILE:O | 1:E:212:ILE:HG22 | 2.18 | 0.43 |
| 1:E:295:MET:SD | 1:E:375:ALA:HB3 | 2.57 | 0.43 |
| 2:F:10:GLY:O | 2:F:11:GLN:C | 2.54 | 0.43 |
| 2:F:175:PRO:CG | 2:F:304:LYS:HG2 | 2.47 | 0.43 |
| 2:F:209:ILE:CD1 | 2:F:231:ILE:HD11 | 2.47 | 0.43 |
| 2:F:296:PHE:HZ | 2:F:351:PHE:HZ | 1.66 | 0.43 |
| 2:F:310:GLY:HA3 | 2:F:383:ALA:CA | 2.48 | 0.43 |
| 1:G:168:THR:CG2 | 1:G:201:THR:HG23 | 2.48 | 0.43 |
| 1:G:295:MET:SD | 1:G:375:ALA:HB3 | 2.57 | 0.43 |
| 2:H:64:ARG:HD2 | 2:H:125:LEU:HD22 | 1.99 | 0.43 |
| 2:H:252:LEU:O | 2:H:253:THR:C | 2.56 | 0.43 |
| 2:H:296:PHE:HZ | 2:H:351:PHE:HZ | 1.66 | 0.43 |
| 2:H:390:ARG:HH11 | 2:H:390:ARG:HG3 | 1.83 | 0.43 |
| 2:H:409:VAL:C | 2:H:411:GLU:N | 2.71 | 0.43 |
| 1:A:141:LEU:N | 1:A:141:LEU:HD12 | 2.32 | 0.43 |
| 1:A:161:TYR:O | 1:A:163:ASP:N | 2.51 | 0.43 |
| 2:B:8:HIS:CD2 | 2:B:138:PHE:CD1 | 3.07 | 0.43 |
| 2:B:209:ILE:CD1 | 2:B:231:ILE:HD11 | 2.47 | 0.43 |
| 2:B:217:LEU:HD13 | 2:B:277:SER:N | 2.33 | 0.43 |
| 2:B:230:LEU:O | 2:B:231:ILE:C | 2.57 | 0.43 |
| 2:B:231:ILE:HD13 | 2:B:231:ILE:H | 1.82 | 0.43 |
| 2:B:234:ILE:CG1 | 2:B:270:ALA:HB1 | 2.37 | 0.43 |
| 2:B:304:LYS:HG3 | 2:B:304:LYS:O | 2.18 | 0.43 |
| 1:C:301:MET:O | 1:C:303:ALA:N | 2.51 | 0.43 |
| 1:C:359:PRO:CB | 1:C:360:PRO:HD2 | 2.45 | 0.43 |
| 2:D:122:ILE:CD1 | 2:D:157:LEU:HD21 | 2.35 | 0.43 |
| 2:D:343:PHE:HZ | 2:D:351:PHE:CZ | 2.36 | 0.43 |
| 1:E:182:VAL:O | 1:E:183:GLU:C | 2.56 | 0.43 |
| 2:F:11:GLN:NE2 | 2:F:74:VAL:CG2 | 2.76 | 0.43 |
| 2:F:64:ARG:HD2 | 2:F:125:LEU:HD22 | 1.99 | 0.43 |
| 2:F:255:PHE:O | 2:F:259:LEU:N | 2.50 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:264:ARG:C | 2:F:266:HIS:N | 2.60 | 0.43 |
| 2:F:377:MET:HG3 | 2:F:377:MET:O | 2.18 | 0.43 |
| 2:F:409:VAL:C | 2:F:411:GLU:N | 2.71 | 0.43 |
| 1:G:182:VAL:O | 1:G:183:GLU:C | 2.56 | 0.43 |
| 1:G:243:ARG:HH21 | 1:G:252:LEU:N | 2.13 | 0.43 |
| 2:H:310:GLY:HA3 | 2:H:383:ALA:CA | 2.49 | 0.43 |
| 1:A:26:ASP:C | 1:A:28:HIS:H | 2.21 | 0.43 |
| 1:A:242:LEU:HD22 | 1:A:250:ALA:O | 2.17 | 0.43 |
| 2:B:105:ARG:O | 2:B:110:ILE:CG2 | 2.64 | 0.43 |
| 2:B:397:LEU:HD23 | 2:B:397:LEU:HA | 1.81 | 0.43 |
| 1:C:161:TYR:CD1 | 1:C:161:TYR:N | 2.86 | 0.43 |
| 1:C:168:THR:CG2 | 1:C:201:THR:HG23 | 2.48 | 0.43 |
| 1:C:409:THR:C | 1:C:411:GLU:H | 2.22 | 0.43 |
| 2:D:241:SER:C | 2:D:244:PHE:HB3 | 2.36 | 0.43 |
| 2:D:296:PHE:HZ | 2:D:351:PHE:HZ | 1.66 | 0.43 |
| 1:E:11:GLN:O | 1:E:15:GLN:N | 2.41 | 0.43 |
| 1:G:11:GLN:O | 1:G:15:GLN:N | 2.41 | 0.43 |
| 1:G:212:ILE:O | 1:G:212:ILE:HG22 | 2.18 | 0.43 |
| 1:G:253:ARG:HD3 | 2:H:407:TRP:CH2 | 2.53 | 0.43 |
| 1:G:280:SER:OG | 1:G:281:GLN:N | 2.49 | 0.43 |
| 1:G:332:MET:HE2 | 1:G:351:VAL:HG11 | 2.01 | 0.43 |
| 2:H:166:LYS:CE | 2:H:199:ASP:OD1 | 2.62 | 0.43 |
| 2:H:384:ILE:C | 2:H:386:GLU:N | 2.72 | 0.43 |
| 1:A:6:HIS:HB3 | 1:A:65:ALA:CB | 2.49 | 0.43 |
| 1:A:168:THR:CG2 | 1:A:201:THR:HG23 | 2.48 | 0.43 |
| 1:A:192:HIS:NE2 | 1:A:420:GLU:HG2 | 2.34 | 0.43 |
| 1:A:249:ASN:OD1 | 2:B:71:GLU:OE1 | 2.36 | 0.43 |
| 2:B:5:ILE:HD11 | 2:B:64:ARG:NH1 | 2.27 | 0.43 |
| 2:B:104:ALA:HB3 | 2:B:408:TYR:HD2 | 1.84 | 0.43 |
| 2:B:196:GLU:C | 2:B:197:HIS:HD2 | 2.19 | 0.43 |
| 2:B:439:SER:HA | 1:C:401:ARG:NH2 | 2.32 | 0.43 |
| 1:C:153:LEU:HD13 | 1:C:153:LEU:N | 2.34 | 0.43 |
| 1:C:210:TYR:O | 1:C:214:PHE:N | 2.52 | 0.43 |
| 2:D:5:ILE:CG1 | 2:D:6:SER:N | 2.82 | 0.43 |
| 2:D:8:HIS:CD2 | 2:D:138:PHE:CD1 | 3.07 | 0.43 |
| 2:D:280:LYS:O | 2:D:282:TYR:N | 2.52 | 0.43 |
| 1:E:24:ILE:CG2 | 1:E:25:SER:N | 2.80 | 0.43 |
| 1:E:141:LEU:N | 1:E:141:LEU:HD12 | 2.33 | 0.43 |
| 1:E:431:GLU:O | 1:E:434:GLN:N | 2.48 | 0.43 |
| 2:F:8:HIS:CD2 | 2:F:138:PHE:CD1 | 3.07 | 0.43 |
| 2:F:104:ALA:HB3 | 2:F:408:TYR:HD2 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:166:LYS:CE | 2:F:199:ASP:OD1 | 2.62 | 0.43 |
| 2:F:238:ILE:O | 2:F:242:LEU:CB | 2.67 | 0.43 |
| 2:F:241:SER:C | 2:F:244:PHE:HB3 | 2.36 | 0.43 |
| 2:F:343:PHE:HZ | 2:F:351:PHE:CZ | 2.36 | 0.43 |
| 1:G:14:ASN:O | 1:G:17:GLY:N | 2.50 | 0.43 |
| 1:G:187:ALA:O | 1:G:188:THR:C | 2.57 | 0.43 |
| 2:H:8:HIS:CD2 | 2:H:138:PHE:CD1 | 3.07 | 0.43 |
| 2:H:209:ILE:CD1 | 2:H:231:ILE:HD11 | 2.47 | 0.43 |
| 1:A:288:VAL:C | 1:A:290:GLU:N | 2.70 | 0.43 |
| 2:B:56:THR:C | 2:F:284:GLU:HB2 | 2.40 | 0.43 |
| 2:B:296:PHE:CG | 2:B:341:ILE:HD12 | 2.53 | 0.43 |
| 2:B:343:PHE:CE1 | 2:B:351:PHE:HE1 | 2.36 | 0.43 |
| 1:C:6:HIS:HB3 | 1:C:65:ALA:CB | 2.48 | 0.43 |
| 1:C:114:LEU:HD23 | 1:C:149:MET:HE2 | 1.99 | 0.43 |
| 1:C:118:VAL:O | 1:C:122:VAL:HG13 | 2.19 | 0.43 |
| 2:D:4:CYS:SG | 2:D:252:LEU:CD1 | 3.02 | 0.43 |
| 2:D:104:ALA:HB3 | 2:D:408:TYR:HD2 | 1.84 | 0.43 |
| 2:D:292:THR:O | 2:D:295:CYS:HB2 | 2.18 | 0.43 |
| 2:D:343:PHE:CE1 | 2:D:351:PHE:HE1 | 2.36 | 0.43 |
| 2:D:428:LEU:HD12 | 2:D:428:LEU:HA | 1.78 | 0.43 |
| 1:E:68:VAL:HG11 | 1:E:153:LEU:HD21 | 2.00 | 0.43 |
| 1:E:114:LEU:HD23 | 1:E:149:MET:HE3 | 2.00 | 0.43 |
| 1:E:210:TYR:O | 1:E:214:PHE:N | 2.52 | 0.43 |
| 2:F:4:CYS:SG | 2:F:252:LEU:CD1 | 3.02 | 0.43 |
| 2:F:209:ILE:CD1 | 2:F:231:ILE:CD1 | 2.97 | 0.43 |
| 2:F:384:ILE:C | 2:F:386:GLU:N | 2.72 | 0.43 |
| 1:G:210:TYR:O | 1:G:214:PHE:N | 2.52 | 0.43 |
| 1:G:253:ARG:HD3 | 2:H:407:TRP:HH2 | 1.82 | 0.43 |
| 1:G:288:VAL:C | 1:G:290:GLU:N | 2.70 | 0.43 |
| 2:H:100:ALA:O | 2:H:102:ASN:N | 2.49 | 0.43 |
| 2:H:262:TYR:HB3 | 2:H:263:PRO:HD2 | 2.00 | 0.43 |
| 1:A:118:VAL:O | 1:A:122:VAL:HG13 | 2.19 | 0.43 |
| 1:A:210:TYR:O | 1:A:214:PHE:N | 2.52 | 0.43 |
| 2:B:49:PHE:HE1 | 2:B:61:HIS:CE1 | 2.34 | 0.43 |
| 2:B:209:ILE:CD1 | 2:B:231:ILE:CD1 | 2.97 | 0.43 |
| 2:B:377:MET:HG3 | 2:B:377:MET:O | 2.18 | 0.43 |
| 1:C:210:TYR:O | 1:C:211:ASP:C | 2.57 | 0.43 |
| 1:C:239:THR:CG2 | 1:C:240:THR:N | 2.80 | 0.43 |
| 1:C:243:ARG:HH21 | 1:C:252:LEU:N | 2.12 | 0.43 |
| 2:D:209:ILE:CD1 | 2:D:231:ILE:CD1 | 2.97 | 0.43 |
| 1:E:238:VAL:HB | 1:E:239:THR:H | 1.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:243:ARG:HD3 | 1:G:243:ARG:N | 2.26 | 0.43 |
| 2:H:104:ALA:HB3 | 2:H:408:TYR:HD2 | 1.84 | 0.43 |
| 2:H:204:VAL:CG1 | 2:H:209:ILE:HD11 | 2.42 | 0.43 |
| 2:H:238:ILE:O | 2:H:242:LEU:CB | 2.67 | 0.43 |
| 2:H:343:PHE:HZ | 2:H:351:PHE:CZ | 2.36 | 0.43 |
| 1:A:156:LYS:NZ | 1:A:159:GLU:OE1 | 2.47 | 0.42 |
| 1:A:280:SER:OG | 1:A:281:GLN:N | 2.49 | 0.42 |
| 2:B:16:ILE:CG2 | 2:B:17:GLY:N | 2.82 | 0.42 |
| 2:B:63:PRO:HG3 | 2:B:87:PHE:CD1 | 2.54 | 0.42 |
| 2:B:103:TYR:O | 2:B:104:ALA:C | 2.57 | 0.42 |
| 2:B:425:MET:O | 2:B:428:LEU:N | 2.45 | 0.42 |
| 1:C:383:ALA:C | 1:C:385:GLN:N | 2.72 | 0.42 |
| 2:D:115:ILE:CD1 | 2:D:115:ILE:C | 2.87 | 0.42 |
| 2:D:234:ILE:CG1 | 2:D:270:ALA:HB1 | 2.38 | 0.42 |
| 1:E:280:SER:OG | 1:E:281:GLN:N | 2.49 | 0.42 |
| 2:F:100:ALA:O | 2:F:102:ASN:N | 2.49 | 0.42 |
| 2:F:204:VAL:CG1 | 2:F:209:ILE:HD11 | 2.42 | 0.42 |
| 2:F:378:LEU:HD12 | 2:F:378:LEU:O | 2.19 | 0.42 |
| 1:G:359:PRO:CB | 1:G:360:PRO:HD2 | 2.45 | 0.42 |
| 2:H:11:GLN:NE2 | 2:H:74:VAL:CG2 | 2.76 | 0.42 |
| 2:H:70:LEU:HD13 | 2:H:145:THR:CB | 2.46 | 0.42 |
| 2:H:378:LEU:HD12 | 2:H:378:LEU:O | 2.19 | 0.42 |
| 1:A:153:LEU:HD13 | 1:A:153:LEU:N | 2.34 | 0.42 |
| 1:A:187:ALA:O | 1:A:188:THR:C | 2.57 | 0.42 |
| 1:A:409:THR:C | 1:A:411:GLU:H | 2.22 | 0.42 |
| 2:B:262:TYR:HB3 | 2:B:263:PRO:HD2 | 2.00 | 0.42 |
| 2:B:280:LYS:O | 2:B:282:TYR:N | 2.52 | 0.42 |
| 2:B:343:PHE:HZ | 2:B:351:PHE:CZ | 2.36 | 0.42 |
| 2:B:378:LEU:HD12 | 2:B:378:LEU:O | 2.19 | 0.42 |
| 2:D:16:ILE:CG2 | 2:D:17:GLY:N | 2.82 | 0.42 |
| 2:D:121:ARG:HG2 | 2:D:121:ARG:HH11 | 1.83 | 0.42 |
| 2:D:230:LEU:O | 2:D:231:ILE:C | 2.57 | 0.42 |
| 1:E:103:TRP:HB2 | 1:E:186:ASN:HA | 2.01 | 0.42 |
| 2:F:105:ARG:O | 2:F:110:ILE:CG2 | 2.64 | 0.42 |
| 2:F:262:TYR:HB3 | 2:F:263:PRO:HD2 | 2.01 | 0.42 |
| 1:G:210:TYR:O | 1:G:211:ASP:C | 2.57 | 0.42 |
| 2:H:115:ILE:CD1 | 2:H:115:ILE:C | 2.87 | 0.42 |
| 2:H:147:SER:HB2 | 2:H:186:ASN:O | 2.19 | 0.42 |
| 2:H:209:ILE:CD1 | 2:H:231:ILE:CD1 | 2.97 | 0.42 |
| 2:H:238:ILE:HD11 | 2:H:378:LEU:HD23 | 2.01 | 0.42 |
| 2:H:241:SER:C | 2:H:244:PHE:HB3 | 2.36 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:80:PHE:CE2 | 3:I:104:ILE:HB | 2.54 | 0.42 |
| 1:A:250:ALA:CB | 1:A:254:LYS:HE2 | 2.49 | 0.42 |
| 2:B:50:ASN:HD22 | 2:B:50:ASN:HA | 1.60 | 0.42 |
| 2:B:147:SER:HB2 | 2:B:186:ASN:O | 2.19 | 0.42 |
| 2:B:276:ILE:O | 2:B:369:ALA:CA | 2.66 | 0.42 |
| 2:B:363:VAL:HG13 | 2:B:364:PRO:HD2 | 2.02 | 0.42 |
| 1:C:192:HIS:NE2 | 1:C:420:GLU:HG2 | 2.34 | 0.42 |
| 2:D:103:TYR:O | 2:D:104:ALA:C | 2.57 | 0.42 |
| 2:D:276:ILE:O | 2:D:369:ALA:CA | 2.66 | 0.42 |
| 2:D:310:GLY:HA3 | 2:D:383:ALA:CA | 2.49 | 0.42 |
| 1:E:14:ASN:O | 1:E:17:GLY:N | 2.51 | 0.42 |
| 1:E:240:THR:HG23 | 1:E:241:CYS:N | 2.33 | 0.42 |
| 1:E:399:PHE:O | 1:E:402:LYS:N | 2.29 | 0.42 |
| 2:F:7:ILE:HD11 | 2:F:137:VAL:CG2 | 2.44 | 0.42 |
| 2:F:115:ILE:CD1 | 2:F:115:ILE:C | 2.87 | 0.42 |
| 2:F:238:ILE:HD11 | 2:F:378:LEU:HD23 | 2.01 | 0.42 |
| 2:F:280:LYS:O | 2:F:282:TYR:N | 2.52 | 0.42 |
| 1:G:68:VAL:HG11 | 1:G:153:LEU:HD21 | 2.00 | 0.42 |
| 1:G:114:LEU:HD23 | 1:G:149:MET:HE1 | 2.01 | 0.42 |
| 1:G:141:LEU:N | 1:G:141:LEU:HD12 | 2.33 | 0.42 |
| 1:G:254:LYS:HA | 1:G:257:VAL:CG1 | 2.49 | 0.42 |
| 1:G:348:PRO:HG3 | 2:H:397:LEU:HB2 | 2.01 | 0.42 |
| 1:G:399:PHE:O | 1:G:402:LYS:N | 2.29 | 0.42 |
| 1:G:431:GLU:O | 1:G:434:GLN:N | 2.48 | 0.42 |
| 2:H:105:ARG:O | 2:H:110:ILE:CG2 | 2.64 | 0.42 |
| 2:H:264:ARG:C | 2:H:266:HIS:N | 2.60 | 0.42 |
| 2:B:115:ILE:CG2 | 2:B:116:ASP:H | 2.32 | 0.42 |
| 2:B:260:VAL:HG22 | 1:C:407:TRP:CE2 | 2.54 | 0.42 |
| 2:B:263:PRO:O | 2:B:264:ARG:C | 2.56 | 0.42 |
| 1:C:250:ALA:CB | 1:C:254:LYS:HE2 | 2.49 | 0.42 |
| 1:C:288:VAL:C | 1:C:290:GLU:N | 2.70 | 0.42 |
| 2:D:147:SER:HB2 | 2:D:186:ASN:O | 2.19 | 0.42 |
| 2:D:262:TYR:HB3 | 2:D:263:PRO:HD2 | 2.00 | 0.42 |
| 2:D:378:LEU:HD12 | 2:D:378:LEU:O | 2.19 | 0.42 |
| 1:E:192:HIS:NE2 | 1:E:420:GLU:HG2 | 2.34 | 0.42 |
| 1:E:359:PRO:CB | 1:E:360:PRO:HD2 | 2.45 | 0.42 |
| 1:E:409:THR:C | 1:E:411:GLU:H | 2.22 | 0.42 |
| 2:F:70:LEU:HD13 | 2:F:145:THR:CB | 2.46 | 0.42 |
| 2:F:147:SER:HB2 | 2:F:186:ASN:O | 2.19 | 0.42 |
| 2:F:262:TYR:OH | 1:G:403:ALA:CA | 2.39 | 0.42 |
| 1:G:103:TRP:HB2 | 1:G:186:ASN:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:153:LEU:HD13 | 1:G:153:LEU:N | 2.34 | 0.42 |
| 2:H:280:LYS:O | 2:H:282:TYR:N | 2.52 | 0.42 |
| 3:I:65:PHE:CE2 | 3:I:67:GLY:CA | 3.02 | 0.42 |
| 3:I:105:TYR:HA | 3:I:112:LYS:HA | 2.00 | 0.42 |
| 1:A:68:VAL:HG11 | 1:A:153:LEU:HD21 | 2.00 | 0.42 |
| 1:A:359:PRO:CB | 1:A:360:PRO:HD2 | 2.45 | 0.42 |
| 2:B:329:ASN:HB3 | 1:C:210:TYR:CE1 | 2.52 | 0.42 |
| 1:C:26:ASP:C | 1:C:28:HIS:H | 2.21 | 0.42 |
| 1:C:106:GLY:O | 1:C:149:MET:CA | 2.68 | 0.42 |
| 1:C:187:ALA:O | 1:C:188:THR:C | 2.57 | 0.42 |
| 1:C:243:ARG:N | 1:C:243:ARG:HD3 | 2.26 | 0.42 |
| 2:D:263:PRO:O | 2:D:264:ARG:C | 2.56 | 0.42 |
| 1:E:175:PRO:O | 1:E:177:VAL:N | 2.53 | 0.42 |
| 1:E:250:ALA:CB | 1:E:254:LYS:HE2 | 2.50 | 0.42 |
| 1:E:269:MET:HE1 | 1:E:381:SER:OG | 2.19 | 0.42 |
| 1:E:273:ALA:HB1 | 1:E:291:LEU:HG | 2.01 | 0.42 |
| 1:G:12:CYS:C | 1:G:14:ASN:N | 2.71 | 0.42 |
| 1:G:192:HIS:NE2 | 1:G:420:GLU:HG2 | 2.34 | 0.42 |
| 1:G:253:ARG:O | 1:G:257:VAL:HG12 | 2.19 | 0.42 |
| 2:H:149:PHE:O | 2:H:150:THR:C | 2.56 | 0.42 |
| 3:I:107:ILE:HD11 | 3:I:139:THR:HG23 | 2.01 | 0.42 |
| 1:A:182:VAL:O | 1:A:183:GLU:C | 2.56 | 0.42 |
| 1:A:383:ALA:C | 1:A:385:GLN:N | 2.72 | 0.42 |
| 2:B:25:CYS:SG | 2:B:26:LEU:N | 2.92 | 0.42 |
| 2:B:115:ILE:CD1 | 2:B:115:ILE:C | 2.87 | 0.42 |
| 2:B:207:GLU:O | 2:B:210:TYR:N | 2.51 | 0.42 |
| 2:B:238:ILE:O | 2:B:242:LEU:CB | 2.67 | 0.42 |
| 1:C:2:ARG:NH1 | 1:C:251:ASP:CG | 2.73 | 0.42 |
| 1:C:102:ASN:ND2 | 1:C:408:TYR:HA | 2.20 | 0.42 |
| 1:C:409:THR:C | 1:C:411:GLU:N | 2.73 | 0.42 |
| 2:D:105:ARG:O | 2:D:110:ILE:CG2 | 2.64 | 0.42 |
| 2:D:238:ILE:O | 2:D:242:LEU:CB | 2.67 | 0.42 |
| 1:E:98:GLY:O | 1:E:100:GLY:N | 2.49 | 0.42 |
| 1:E:187:ALA:O | 1:E:188:THR:C | 2.57 | 0.42 |
| 1:E:242:LEU:HB3 | 1:E:250:ALA:O | 2.20 | 0.42 |
| 1:E:243:ARG:HD3 | 1:E:243:ARG:N | 2.26 | 0.42 |
| 2:F:16:ILE:CG2 | 2:F:17:GLY:N | 2.82 | 0.42 |
| 2:F:119:LEU:HD11 | 2:F:156:ARG:HD3 | 2.01 | 0.42 |
| 2:F:149:PHE:O | 2:F:150:THR:C | 2.56 | 0.42 |
| 2:F:296:PHE:CG | 2:F:341:ILE:HD12 | 2.53 | 0.42 |
| 2:H:7:ILE:HD11 | 2:H:137:VAL:CG2 | 2.44 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:296:PHE:CG | 2:H:341:ILE:HD12 | 2.53 | 0.42 |
| 1:A:102:ASN:ND2 | 1:A:408:TYR:HA | 2.20 | 0.42 |
| 1:A:103:TRP:HB2 | 1:A:186:ASN:HA | 2.01 | 0.42 |
| 1:C:147:SER:CB | 1:C:190:SER:HB3 | 2.42 | 0.42 |
| 1:C:154:ILE:HG22 | 1:C:166:MET:HE1 | 2.01 | 0.42 |
| 1:C:212:ILE:O | 1:C:212:ILE:HG22 | 2.18 | 0.42 |
| 1:C:307:PRO:O | 1:C:309:HIS:N | 2.53 | 0.42 |
| 2:D:293:ASN:ND2 | 2:D:338:LYS:HZ1 | 2.14 | 0.42 |
| 2:D:363:VAL:HG13 | 2:D:364:PRO:HD2 | 2.02 | 0.42 |
| 2:D:377:MET:HG3 | 2:D:377:MET:O | 2.18 | 0.42 |
| 1:E:261:PRO:HB2 | 1:E:262:PHE:CD1 | 2.54 | 0.42 |
| 2:F:115:ILE:CG2 | 2:F:116:ASP:H | 2.32 | 0.42 |
| 2:F:231:ILE:C | 2:F:233:GLN:N | 2.73 | 0.42 |
| 2:F:363:VAL:HG13 | 2:F:364:PRO:HD2 | 2.02 | 0.42 |
| 1:G:242:LEU:HB3 | 1:G:250:ALA:O | 2.20 | 0.42 |
| 1:G:273:ALA:HB1 | 1:G:291:LEU:HG | 2.02 | 0.42 |
| 2:H:16:ILE:CG2 | 2:H:17:GLY:N | 2.82 | 0.42 |
| 2:H:119:LEU:HD11 | 2:H:156:ARG:HD3 | 2.01 | 0.42 |
| 2:H:175:PRO:HG3 | 2:H:304:LYS:CB | 2.50 | 0.42 |
| 2:H:184:PRO:CG | 2:H:398:MET:HE1 | 2.37 | 0.42 |
| 2:H:231:ILE:C | 2:H:233:GLN:N | 2.73 | 0.42 |
| 2:H:363:VAL:HG13 | 2:H:364:PRO:HD2 | 2.02 | 0.42 |
| 3:I:102:ARG:HB3 | 3:I:103:TYR:CD1 | 2.54 | 0.42 |
| 1:A:2:ARG:NH1 | 1:A:251:ASP:CG | 2.73 | 0.42 |
| 1:A:106:GLY:O | 1:A:149:MET:CA | 2.68 | 0.42 |
| 1:A:185:TYR:HD2 | 1:A:185:TYR:HA | 1.76 | 0.42 |
| 1:A:230:LEU:HD21 | 1:A:302:MET:HE2 | 2.02 | 0.42 |
| 1:A:238:VAL:HB | 1:A:239:THR:H | 1.65 | 0.42 |
| 1:A:261:PRO:HB2 | 1:A:262:PHE:CD1 | 2.54 | 0.42 |
| 1:A:307:PRO:O | 1:A:309:HIS:N | 2.53 | 0.42 |
| 1:A:409:THR:C | 1:A:411:GLU:N | 2.73 | 0.42 |
| 1:A:427:ASP:OD1 | 1:A:427:ASP:C | 2.57 | 0.42 |
| 2:B:110:ILE:O | 2:B:111:GLY:C | 2.57 | 0.42 |
| 2:B:119:LEU:HD11 | 2:B:156:ARG:HD3 | 2.02 | 0.42 |
| 2:B:175:PRO:HG3 | 2:B:304:LYS:CB | 2.50 | 0.42 |
| 2:B:310:GLY:HA3 | 2:B:383:ALA:CA | 2.49 | 0.42 |
| 2:B:346:TRP:O | 1:C:398:MET:HB2 | 2.20 | 0.42 |
| 2:B:362:VAL:HG13 | 2:B:368:LEU:CB | 2.50 | 0.42 |
| 1:C:68:VAL:HG11 | 1:C:153:LEU:HD21 | 2.00 | 0.42 |
| 2:D:115:ILE:CG2 | 2:D:116:ASP:H | 2.32 | 0.42 |
| 2:D:119:LEU:HD11 | 2:D:156:ARG:HD3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:296:PHE:CG | 2:D:341:ILE:HD12 | 2.53 | 0.42 |
| 2:D:335:ILE:C | 2:D:337:THR:N | 2.73 | 0.42 |
| 1:E:2:ARG:NH1 | 1:E:251:ASP:CG | 2.73 | 0.42 |
| 1:E:138:THR:O | 1:E:139:HIS:HB3 | 2.19 | 0.42 |
| 1:E:307:PRO:O | 1:E:309:HIS:N | 2.53 | 0.42 |
| 2:F:110:ILE:O | 2:F:111:GLY:C | 2.57 | 0.42 |
| 2:F:175:PRO:HG3 | 2:F:304:LYS:CB | 2.50 | 0.42 |
| 2:F:335:ILE:C | 2:F:337:THR:N | 2.73 | 0.42 |
| 1:G:175:PRO:O | 1:G:177:VAL:N | 2.53 | 0.42 |
| 1:G:409:THR:C | 1:G:411:GLU:N | 2.73 | 0.42 |
| 1:G:427:ASP:OD1 | 1:G:427:ASP:C | 2.57 | 0.42 |
| 2:H:115:ILE:CG2 | 2:H:116:ASP:H | 2.32 | 0.42 |
| 2:H:335:ILE:C | 2:H:337:THR:N | 2.73 | 0.42 |
| 3:I:84:LEU:HD21 | 3:I:104:ILE:HG13 | 2.01 | 0.42 |
| 1:A:275:LEU:HD12 | 1:A:275:LEU:HA | 1.78 | 0.42 |
| 1:A:343:PHE:CD2 | 1:A:350:ASN:ND2 | 2.88 | 0.42 |
| 1:A:399:PHE:O | 1:A:401:ARG:N | 2.53 | 0.42 |
| 2:B:11:GLN:NE2 | 2:B:74:VAL:CG2 | 2.76 | 0.42 |
| 2:B:13:GLY:HA2 | 2:B:16:ILE:CG2 | 2.50 | 0.42 |
| 2:B:63:PRO:HG2 | 2:B:91:GLN:NE2 | 2.34 | 0.42 |
| 2:B:213:CYS:O | 2:B:219:ILE:HG13 | 2.20 | 0.42 |
| 2:B:264:ARG:C | 2:B:266:HIS:N | 2.60 | 0.42 |
| 2:B:335:ILE:C | 2:B:337:THR:N | 2.73 | 0.42 |
| 1:C:103:TRP:HB2 | 1:C:186:ASN:HA | 2.01 | 0.42 |
| 1:C:171:VAL:O | 1:C:171:VAL:HG12 | 2.20 | 0.42 |
| 1:C:273:ALA:HB1 | 1:C:291:LEU:HG | 2.01 | 0.42 |
| 2:D:207:GLU:O | 2:D:210:TYR:N | 2.51 | 0.42 |
| 2:D:213:CYS:O | 2:D:219:ILE:HG13 | 2.20 | 0.42 |
| 1:E:153:LEU:HD13 | 1:E:153:LEU:N | 2.34 | 0.42 |
| 1:E:399:PHE:O | 1:E:401:ARG:N | 2.53 | 0.42 |
| 1:E:409:THR:C | 1:E:411:GLU:N | 2.73 | 0.42 |
| 2:F:15:GLN:NE2 | 5:F:500:GTP:N7 | 2.67 | 0.42 |
| 1:G:240:THR:HG23 | 1:G:241:CYS:N | 2.34 | 0.42 |
| 1:G:261:PRO:HB2 | 1:G:262:PHE:CD1 | 2.54 | 0.42 |
| 1:G:307:PRO:O | 1:G:309:HIS:N | 2.53 | 0.42 |
| 2:H:213:CYS:O | 2:H:219:ILE:HG13 | 2.20 | 0.42 |
| 2:H:234:ILE:HB | 2:H:302:MET:HE1 | 2.02 | 0.42 |
| 1:A:199:ASP:C | 1:A:265:LEU:HD13 | 2.40 | 0.42 |
| 1:A:332:MET:HE2 | 1:A:351:VAL:HG11 | 2.02 | 0.42 |
| 2:B:238:ILE:HD11 | 2:B:378:LEU:HD23 | 2.01 | 0.42 |
| 2:B:255:PHE:O | 2:B:257:THR:N | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:230:LEU:HD21 | 1:C:302:MET:HE2 | 2.02 | 0.42 |
| 1:C:280:SER:OG | 1:C:281:GLN:N | 2.49 | 0.42 |
| 1:C:343:PHE:CD2 | 1:C:350:ASN:ND2 | 2.88 | 0.42 |
| 2:D:110:ILE:O | 2:D:111:GLY:C | 2.58 | 0.42 |
| 2:D:175:PRO:HG3 | 2:D:304:LYS:CB | 2.50 | 0.42 |
| 2:D:362:VAL:HG13 | 2:D:368:LEU:CB | 2.50 | 0.42 |
| 1:E:48:ARG:HG2 | 1:E:243:ARG:HB3 | 2.01 | 0.42 |
| 1:E:210:TYR:O | 1:E:211:ASP:C | 2.57 | 0.42 |
| 1:E:343:PHE:CD2 | 1:E:350:ASN:ND2 | 2.88 | 0.42 |
| 2:F:11:GLN:CG | 2:F:74:VAL:HG21 | 2.50 | 0.42 |
| 2:F:213:CYS:O | 2:F:219:ILE:HG13 | 2.20 | 0.42 |
| 2:F:230:LEU:O | 2:F:231:ILE:C | 2.57 | 0.42 |
| 1:G:2:ARG:NH1 | 1:G:251:ASP:CG | 2.73 | 0.42 |
| 1:G:306:ASP:HA | 1:G:307:PRO:HD3 | 1.92 | 0.42 |
| 2:H:255:PHE:O | 2:H:257:THR:N | 2.53 | 0.42 |
| 2:H:362:VAL:HG13 | 2:H:368:LEU:CB | 2.50 | 0.42 |
| 2:H:428:LEU:HD12 | 2:H:428:LEU:HA | 1.78 | 0.42 |
| 2:B:11:GLN:CG | 2:B:74:VAL:HG21 | 2.50 | 0.41 |
| 2:B:151:SER:HB3 | 2:B:193:THR:CG2 | 2.34 | 0.41 |
| 2:B:384:ILE:C | 2:B:386:GLU:N | 2.72 | 0.41 |
| 1:C:133:GLN:CG | 1:C:165:ILE:HD11 | 2.49 | 0.41 |
| 1:C:150:GLY:HA2 | 1:C:153:LEU:CD2 | 2.42 | 0.41 |
| 1:C:242:LEU:HB3 | 1:C:250:ALA:O | 2.20 | 0.41 |
| 1:C:306:ASP:HA | 1:C:307:PRO:HD3 | 1.91 | 0.41 |
| 1:C:399:PHE:O | 1:C:401:ARG:N | 2.53 | 0.41 |
| 1:C:417:GLU:O | 1:C:420:GLU:HB3 | 2.20 | 0.41 |
| 1:C:427:ASP:OD1 | 1:C:427:ASP:C | 2.57 | 0.41 |
| 2:D:11:GLN:CG | 2:D:74:VAL:HG21 | 2.50 | 0.41 |
| 2:D:15:GLN:NE2 | 5:D:500:GTP:N7 | 2.67 | 0.41 |
| 2:D:238:ILE:HD11 | 2:D:378:LEU:HD23 | 2.01 | 0.41 |
| 2:D:243:ARG:NH2 | 2:D:252:LEU:HG | 2.35 | 0.41 |
| 1:E:118:VAL:O | 1:E:122:VAL:HG13 | 2.19 | 0.41 |
| 1:E:262:PHE:HA | 1:E:263:PRO:HD2 | 1.65 | 0.41 |
| 1:E:325:MET:HA | 1:E:325:MET:CE | 2.49 | 0.41 |
| 2:F:71:GLU:HA | 2:F:72:PRO:HD3 | 1.88 | 0.41 |
| 2:F:132:LEU:H | 2:F:132:LEU:CD2 | 2.23 | 0.41 |
| 2:F:255:PHE:O | 2:F:257:THR:N | 2.53 | 0.41 |
| 2:F:347:CYS:SG | 1:G:181:VAL:HG13 | 2.60 | 0.41 |
| 2:F:362:VAL:HG13 | 2:F:368:LEU:CB | 2.50 | 0.41 |
| 1:G:399:PHE:O | 1:G:401:ARG:N | 2.53 | 0.41 |
| 2:H:11:GLN:CG | 2:H:74:VAL:HG21 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:15:GLN:NE2 | 5:H:500:GTP:N7 | 2.67 | 0.41 |
| 2:H:110:ILE:O | 2:H:111:GLY:C | 2.58 | 0.41 |
| 2:H:436:GLY:C | 2:H:438:ASP:N | 2.72 | 0.41 |
| 3:I:100:GLY:C | 3:I:101:VAL:HG23 | 2.39 | 0.41 |
| 1:A:25:SER:O | 1:A:28:HIS:N | 2.53 | 0.41 |
| 1:A:44:LEU:HD12 | 1:A:49:ILE:CD1 | 2.49 | 0.41 |
| 1:A:48:ARG:HG2 | 1:A:243:ARG:HB3 | 2.01 | 0.41 |
| 1:A:138:THR:O | 1:A:139:HIS:HB3 | 2.19 | 0.41 |
| 1:A:171:VAL:HG12 | 1:A:171:VAL:O | 2.20 | 0.41 |
| 1:A:273:ALA:HB1 | 1:A:291:LEU:HG | 2.01 | 0.41 |
| 1:A:417:GLU:O | 1:A:420:GLU:HB3 | 2.20 | 0.41 |
| 1:A:421:ALA:O | 1:A:422:GLU:C | 2.58 | 0.41 |
| 2:B:243:ARG:NH2 | 2:B:252:LEU:HG | 2.35 | 0.41 |
| 2:B:305:CYS:SG | 2:B:383:ALA:HB1 | 2.60 | 0.41 |
| 1:C:19:LYS:HG3 | 1:C:228:ASN:HB2 | 2.01 | 0.41 |
| 1:C:175:PRO:O | 1:C:177:VAL:N | 2.53 | 0.41 |
| 1:C:199:ASP:C | 1:C:265:LEU:HD13 | 2.41 | 0.41 |
| 2:D:30:ILE:HD11 | 2:D:61:HIS:CD2 | 2.54 | 0.41 |
| 2:D:305:CYS:SG | 2:D:383:ALA:HB1 | 2.60 | 0.41 |
| 2:D:384:ILE:C | 2:D:386:GLU:N | 2.72 | 0.41 |
| 1:E:171:VAL:O | 1:E:171:VAL:HG12 | 2.20 | 0.41 |
| 1:E:427:ASP:OD1 | 1:E:427:ASP:C | 2.57 | 0.41 |
| 2:F:13:GLY:HA2 | 2:F:16:ILE:CG2 | 2.50 | 0.41 |
| 2:F:243:ARG:NH2 | 2:F:252:LEU:HG | 2.35 | 0.41 |
| 1:G:2:ARG:HH21 | 2:H:99:ALA:N | 2.16 | 0.41 |
| 1:G:118:VAL:O | 1:G:122:VAL:HG13 | 2.19 | 0.41 |
| 1:G:138:THR:O | 1:G:139:HIS:HB3 | 2.20 | 0.41 |
| 1:G:383:ALA:C | 1:G:385:GLN:N | 2.72 | 0.41 |
| 2:H:95:GLY:C | 2:H:97:GLU:H | 2.23 | 0.41 |
| 2:H:103:TYR:O | 2:H:104:ALA:C | 2.57 | 0.41 |
| 2:H:132:LEU:H | 2:H:132:LEU:CD2 | 2.23 | 0.41 |
| 2:H:243:ARG:NH2 | 2:H:252:LEU:HG | 2.35 | 0.41 |
| 2:B:15:GLN:NE2 | 5:B:500:GTP:N7 | 2.67 | 0.41 |
| 1:C:118:VAL:O | 1:C:121:VAL:N | 2.54 | 0.41 |
| 1:C:352:LYS:HZ2 | 2:D:180:ALA:HA | 1.86 | 0.41 |
| 1:C:352:LYS:HG2 | 2:D:181:VAL:HG23 | 2.02 | 0.41 |
| 2:D:13:GLY:HA2 | 2:D:16:ILE:CG2 | 2.50 | 0.41 |
| 2:D:25:CYS:SG | 2:D:26:LEU:N | 2.92 | 0.41 |
| 2:D:255:PHE:O | 2:D:257:THR:N | 2.53 | 0.41 |
| 1:E:25:SER:O | 1:E:28:HIS:N | 2.53 | 0.41 |
| 1:E:199:ASP:C | 1:E:265:LEU:HD13 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:325:MET:HE2 | 1:E:355:VAL:CG2 | 2.48 | 0.41 |
| 1:E:383:ALA:C | 1:E:385:GLN:N | 2.72 | 0.41 |
| 2:F:95:GLY:C | 2:F:97:GLU:H | 2.23 | 0.41 |
| 2:F:103:TYR:O | 2:F:104:ALA:C | 2.57 | 0.41 |
| 2:F:184:PRO:HG2 | 2:F:398:MET:CE | 2.40 | 0.41 |
| 1:G:48:ARG:HG2 | 1:G:243:ARG:HB3 | 2.01 | 0.41 |
| 1:G:108:TYR:CE1 | 1:G:413:MET:HE1 | 2.56 | 0.41 |
| 1:G:171:VAL:O | 1:G:171:VAL:HG12 | 2.20 | 0.41 |
| 2:H:13:GLY:HA2 | 2:H:16:ILE:CG2 | 2.50 | 0.41 |
| 3:I:80:PHE:CZ | 3:I:104:ILE:HD12 | 2.56 | 0.41 |
| 1:A:118:VAL:O | 1:A:121:VAL:N | 2.54 | 0.41 |
| 1:A:150:GLY:HA2 | 1:A:153:LEU:CD2 | 2.42 | 0.41 |
| 1:A:175:PRO:O | 1:A:177:VAL:N | 2.53 | 0.41 |
| 2:B:224:TYR:HD2 | 2:B:224:TYR:HA | 1.73 | 0.41 |
| 2:B:242:LEU:HD11 | 2:B:250:VAL:HG23 | 2.02 | 0.41 |
| 2:B:332:ILE:CD1 | 2:B:353:VAL:HG22 | 2.51 | 0.41 |
| 1:C:72:PRO:O | 1:C:73:GLY:C | 2.58 | 0.41 |
| 1:C:261:PRO:HB2 | 1:C:262:PHE:CD1 | 2.54 | 0.41 |
| 2:D:56:THR:CB | 2:H:284:GLU:OE2 | 2.68 | 0.41 |
| 2:D:332:ILE:CD1 | 2:D:353:VAL:HG22 | 2.51 | 0.41 |
| 2:D:344:VAL:CG1 | 2:D:345:ASP:N | 2.78 | 0.41 |
| 1:E:12:CYS:C | 1:E:14:ASN:N | 2.71 | 0.41 |
| 1:E:108:TYR:CE1 | 1:E:413:MET:HE1 | 2.56 | 0.41 |
| 2:F:436:GLY:C | 2:F:438:ASP:N | 2.72 | 0.41 |
| 1:G:98:GLY:O | 1:G:100:GLY:N | 2.49 | 0.41 |
| 1:G:254:LYS:CA | 1:G:257:VAL:HG12 | 2.50 | 0.41 |
| 1:G:352:LYS:CG | 2:H:181:VAL:CG2 | 2.93 | 0.41 |
| 2:H:25:CYS:SG | 2:H:26:LEU:N | 2.92 | 0.41 |
| 2:H:242:LEU:HD11 | 2:H:250:VAL:HG23 | 2.02 | 0.41 |
| 2:H:251:ASP:CA | 2:H:254:GLU:HG3 | 2.48 | 0.41 |
| 2:H:318:LEU:HB2 | 2:H:376:CYS:SG | 2.61 | 0.41 |
| 1:A:119:LEU:O | 1:A:122:VAL:HG22 | 2.21 | 0.41 |
| 1:A:242:LEU:HB3 | 1:A:250:ALA:O | 2.20 | 0.41 |
| 1:C:399:PHE:O | 1:C:402:LYS:N | 2.29 | 0.41 |
| 2:D:242:LEU:HD11 | 2:D:250:VAL:HG23 | 2.02 | 0.41 |
| 2:D:401:LYS:C | 2:D:403:ALA:H | 2.24 | 0.41 |
| 1:E:182:VAL:O | 1:E:184:PRO:N | 2.54 | 0.41 |
| 2:F:25:CYS:SG | 2:F:26:LEU:N | 2.92 | 0.41 |
| 2:F:81:GLY:O | 2:F:82:THR:C | 2.59 | 0.41 |
| 2:F:226:ASN:O | 2:F:227:LEU:C | 2.59 | 0.41 |
| 2:F:297:GLU:HA | 2:F:298:PRO:HD2 | 1.87 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:305:CYS:SG | 2:F:383:ALA:HB1 | 2.60 | 0.41 |
| 2:F:318:LEU:HB2 | 2:F:376:CYS:SG | 2.61 | 0.41 |
| 1:G:118:VAL:O | 1:G:121:VAL:N | 2.54 | 0.41 |
| 1:G:199:ASP:C | 1:G:265:LEU:HD13 | 2.41 | 0.41 |
| 2:H:61:HIS:O | 2:H:62:VAL:C | 2.59 | 0.41 |
| 2:H:71:GLU:HA | 2:H:72:PRO:HD3 | 1.88 | 0.41 |
| 2:H:81:GLY:O | 2:H:82:THR:C | 2.59 | 0.41 |
| 1:A:72:PRO:O | 1:A:73:GLY:C | 2.58 | 0.41 |
| 1:A:105:LYS:HG2 | 1:A:110:GLU:HG3 | 2.03 | 0.41 |
| 2:B:81:GLY:O | 2:B:82:THR:C | 2.59 | 0.41 |
| 1:C:119:LEU:O | 1:C:122:VAL:HG22 | 2.21 | 0.41 |
| 1:C:138:THR:O | 1:C:139:HIS:HB3 | 2.20 | 0.41 |
| 1:C:168:THR:HB | 1:C:198:THR:HG21 | 2.03 | 0.41 |
| 1:C:421:ALA:O | 1:C:422:GLU:C | 2.58 | 0.41 |
| 2:D:130:THR:O | 2:D:131:GLY:C | 2.59 | 0.41 |
| 2:D:251:ASP:CA | 2:D:254:GLU:HG3 | 2.49 | 0.41 |
| 2:D:273:ALA:HB2 | 2:D:375:VAL:HB | 2.03 | 0.41 |
| 1:E:106:GLY:O | 1:E:149:MET:CA | 2.68 | 0.41 |
| 1:E:135:PHE:CD1 | 1:E:166:MET:SD | 3.14 | 0.41 |
| 1:E:168:THR:HB | 1:E:198:THR:HG21 | 2.03 | 0.41 |
| 1:E:202:TYR:CE2 | 1:E:268:PHE:HD1 | 2.38 | 0.41 |
| 2:F:251:ASP:CA | 2:F:254:GLU:HG3 | 2.49 | 0.41 |
| 2:F:273:ALA:HB2 | 2:F:375:VAL:HB | 2.03 | 0.41 |
| 2:F:332:ILE:CD1 | 2:F:353:VAL:HG22 | 2.51 | 0.41 |
| 2:F:428:LEU:HD12 | 2:F:428:LEU:HA | 1.79 | 0.41 |
| 1:G:106:GLY:O | 1:G:149:MET:CA | 2.68 | 0.41 |
| 1:G:343:PHE:CD2 | 1:G:350:ASN:ND2 | 2.88 | 0.41 |
| 2:H:226:ASN:O | 2:H:227:LEU:C | 2.59 | 0.41 |
| 2:H:305:CYS:SG | 2:H:383:ALA:HB1 | 2.60 | 0.41 |
| 2:H:315:CYS:HB3 | 2:H:377:MET:HE1 | 2.02 | 0.41 |
| 3:I:108:ASP:O | 3:I:133:PHE:CE2 | 2.74 | 0.41 |
| 1:A:19:LYS:HG3 | 1:A:228:ASN:HB2 | 2.01 | 0.41 |
| 1:A:168:THR:HB | 1:A:198:THR:HG21 | 2.03 | 0.41 |
| 2:B:34:GLY:O | 2:B:61:HIS:HB2 | 2.20 | 0.41 |
| 2:B:95:GLY:C | 2:B:97:GLU:H | 2.23 | 0.41 |
| 2:B:130:THR:O | 2:B:131:GLY:C | 2.59 | 0.41 |
| 2:B:166:LYS:HB2 | 2:B:199:ASP:OD1 | 2.20 | 0.41 |
| 2:B:292:THR:HG21 | 2:B:331:ALA:HB1 | 2.02 | 0.41 |
| 2:B:328:VAL:C | 2:B:330:ALA:N | 2.73 | 0.41 |
| 1:C:105:LYS:HG2 | 1:C:110:GLU:HG3 | 2.03 | 0.41 |
| 2:D:166:LYS:HB2 | 2:D:199:ASP:OD1 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:226:ASN:O | 2:D:227:LEU:C | 2.59 | 0.41 |
| 2:D:255:PHE:O | 2:D:259:LEU:N | 2.50 | 0.41 |
| 2:D:318:LEU:HB2 | 2:D:376:CYS:SG | 2.61 | 0.41 |
| 1:E:70:LEU:HB2 | 1:E:99:ALA:HB2 | 2.03 | 0.41 |
| 1:E:72:PRO:O | 1:E:73:GLY:C | 2.58 | 0.41 |
| 1:E:118:VAL:O | 1:E:121:VAL:N | 2.54 | 0.41 |
| 2:F:166:LYS:HB2 | 2:F:199:ASP:OD1 | 2.20 | 0.41 |
| 1:G:72:PRO:O | 1:G:73:GLY:C | 2.58 | 0.41 |
| 1:G:161:TYR:C | 1:G:163:ASP:N | 2.71 | 0.41 |
| 1:G:168:THR:HB | 1:G:198:THR:HG21 | 2.03 | 0.41 |
| 1:G:230:LEU:HD21 | 1:G:302:MET:HE2 | 2.02 | 0.41 |
| 1:G:333:LEU:HD11 | 1:G:337:ASN:HD21 | 1.85 | 0.41 |
| 1:G:417:GLU:O | 1:G:420:GLU:HB3 | 2.21 | 0.41 |
| 2:H:166:LYS:HB2 | 2:H:199:ASP:OD1 | 2.20 | 0.41 |
| 2:H:172:TYR:CD1 | 2:H:173:PRO:N | 2.80 | 0.41 |
| 2:H:230:LEU:O | 2:H:231:ILE:C | 2.57 | 0.41 |
| 2:H:287:SER:O | 2:H:291:ILE:HG12 | 2.21 | 0.41 |
| 2:H:332:ILE:CD1 | 2:H:353:VAL:HG22 | 2.51 | 0.41 |
| 1:A:133:GLN:CG | 1:A:165:ILE:HD11 | 2.49 | 0.41 |
| 2:B:7:ILE:HD11 | 2:B:137:VAL:CG2 | 2.44 | 0.41 |
| 2:B:273:ALA:HB2 | 2:B:375:VAL:HB | 2.03 | 0.41 |
| 1:C:44:LEU:HD12 | 1:C:49:ILE:CD1 | 2.49 | 0.41 |
| 1:C:48:ARG:HG2 | 1:C:243:ARG:HB3 | 2.01 | 0.41 |
| 2:D:95:GLY:C | 2:D:97:GLU:H | 2.23 | 0.41 |
| 2:D:184:PRO:HG2 | 2:D:398:MET:CE | 2.40 | 0.41 |
| 2:D:217:LEU:HD13 | 2:D:277:SER:CA | 2.48 | 0.41 |
| 2:D:328:VAL:C | 2:D:330:ALA:N | 2.73 | 0.41 |
| 1:E:20:PHE:CD2 | 1:E:235:MET:CG | 3.04 | 0.41 |
| 1:E:98:GLY:C | 1:E:100:GLY:H | 2.24 | 0.41 |
| 1:E:105:LYS:HG2 | 1:E:110:GLU:HG3 | 2.03 | 0.41 |
| 2:F:242:LEU:HD11 | 2:F:250:VAL:HG23 | 2.02 | 0.41 |
| 2:F:287:SER:O | 2:F:291:ILE:HG12 | 2.21 | 0.41 |
| 2:F:313:MET:O | 2:F:314:ALA:CB | 2.68 | 0.41 |
| 2:F:328:VAL:C | 2:F:330:ALA:N | 2.73 | 0.41 |
| 1:G:70:LEU:HB2 | 1:G:99:ALA:HB2 | 2.03 | 0.41 |
| 1:G:105:LYS:HG2 | 1:G:110:GLU:HG3 | 2.03 | 0.41 |
| 1:G:182:VAL:O | 1:G:184:PRO:N | 2.54 | 0.41 |
| 1:G:262:PHE:HA | 1:G:263:PRO:HD2 | 1.65 | 0.41 |
| 2:H:147:SER:OG | 2:H:148:GLY:N | 2.54 | 0.41 |
| 2:H:273:ALA:HB2 | 2:H:375:VAL:HB | 2.03 | 0.41 |
| 1:A:98:GLY:C | 1:A:100:GLY:H | 2.24 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:114:LEU:HD23 | 1:A:149:MET:HE1 | 2.03 | 0.41 |
| 1:A:135:PHE:CD1 | 1:A:166:MET:SD | 3.14 | 0.41 |
| 1:A:161:TYR:C | 1:A:163:ASP:N | 2.71 | 0.41 |
| 1:A:182:VAL:O | 1:A:184:PRO:N | 2.54 | 0.41 |
| 1:A:210:TYR:O | 1:A:211:ASP:C | 2.57 | 0.41 |
| 1:A:243:ARG:N | 1:A:243:ARG:HD3 | 2.26 | 0.41 |
| 1:A:333:LEU:HD11 | 1:A:337:ASN:HD21 | 1.85 | 0.41 |
| 2:B:149:PHE:CD1 | 2:B:150:THR:N | 2.89 | 0.41 |
| 2:B:152:LEU:C | 2:B:152:LEU:CD1 | 2.89 | 0.41 |
| 2:B:226:ASN:O | 2:B:227:LEU:C | 2.59 | 0.41 |
| 2:B:231:ILE:C | 2:B:233:GLN:N | 2.73 | 0.41 |
| 2:B:318:LEU:HB2 | 2:B:376:CYS:SG | 2.61 | 0.41 |
| 2:B:401:LYS:O | 2:B:402:ARG:HB2 | 2.21 | 0.41 |
| 1:C:98:GLY:C | 1:C:100:GLY:H | 2.24 | 0.41 |
| 1:C:161:TYR:C | 1:C:163:ASP:N | 2.71 | 0.41 |
| 1:C:262:PHE:HA | 1:C:263:PRO:HD2 | 1.65 | 0.41 |
| 1:C:333:LEU:HD11 | 1:C:337:ASN:HD21 | 1.85 | 0.41 |
| 1:C:423:SER:O | 1:C:424:ASN:C | 2.60 | 0.41 |
| 2:D:401:LYS:O | 2:D:402:ARG:HB2 | 2.21 | 0.41 |
| 2:D:414:GLU:C | 2:D:416:GLY:N | 2.74 | 0.41 |
| 1:E:311:ARG:HG2 | 1:E:311:ARG:NH1 | 2.34 | 0.41 |
| 1:E:333:LEU:HD11 | 1:E:337:ASN:HD21 | 1.85 | 0.41 |
| 1:E:380:ASN:HD22 | 1:E:380:ASN:C | 2.24 | 0.41 |
| 1:E:421:ALA:O | 1:E:422:GLU:C | 2.58 | 0.41 |
| 2:F:147:SER:OG | 2:F:148:GLY:N | 2.54 | 0.41 |
| 2:F:152:LEU:C | 2:F:152:LEU:CD1 | 2.89 | 0.41 |
| 2:F:172:TYR:CD1 | 2:F:173:PRO:N | 2.80 | 0.41 |
| 2:F:293:ASN:ND2 | 2:F:338:LYS:HZ1 | 2.16 | 0.41 |
| 2:F:326:LYS:HE2 | 1:G:214:PHE:HB2 | 2.01 | 0.41 |
| 1:G:98:GLY:C | 1:G:100:GLY:H | 2.24 | 0.41 |
| 1:G:135:PHE:CD1 | 1:G:166:MET:SD | 3.14 | 0.41 |
| 1:G:165:ILE:H | 1:G:165:ILE:CD1 | 2.31 | 0.41 |
| 1:G:202:TYR:CE2 | 1:G:268:PHE:HD1 | 2.38 | 0.41 |
| 1:G:308:ARG:HG2 | 3:I:64:TYR:CE2 | 2.56 | 0.41 |
| 1:G:311:ARG:HG2 | 1:G:311:ARG:NH1 | 2.34 | 0.41 |
| 2:H:152:LEU:C | 2:H:152:LEU:CD1 | 2.89 | 0.41 |
| 2:H:313:MET:O | 2:H:314:ALA:CB | 2.68 | 0.41 |
| 2:H:328:VAL:C | 2:H:330:ALA:N | 2.73 | 0.41 |
| 2:H:401:LYS:C | 2:H:403:ALA:H | 2.24 | 0.41 |
| 3:I:65:PHE:CE2 | 3:I:67:GLY:HA2 | 2.56 | 0.41 |
| 1:A:70:LEU:HB2 | 1:A:99:ALA:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:401:LYS:C | 2:B:403:ALA:H | 2.24 | 0.41 |
| 2:B:413:MET:C | 2:B:414:GLU:CG | 2.90 | 0.41 |
| 1:C:12:CYS:C | 1:C:14:ASN:N | 2.71 | 0.41 |
| 1:C:70:LEU:HB2 | 1:C:99:ALA:HB2 | 2.03 | 0.41 |
| 1:C:78:VAL:O | 1:C:84:GLY:HA3 | 2.21 | 0.41 |
| 1:C:114:LEU:HD12 | 1:C:117:SER:OG | 2.21 | 0.41 |
| 1:C:135:PHE:CD1 | 1:C:166:MET:SD | 3.14 | 0.41 |
| 1:C:182:VAL:O | 1:C:184:PRO:N | 2.54 | 0.41 |
| 1:C:238:VAL:HB | 1:C:239:THR:H | 1.66 | 0.41 |
| 1:C:291:LEU:HD21 | 1:C:373:MET:HG2 | 2.03 | 0.41 |
| 1:C:346:TRP:CB | 2:D:401:LYS:CD | 2.93 | 0.41 |
| 2:D:152:LEU:C | 2:D:152:LEU:CD1 | 2.89 | 0.41 |
| 2:D:292:THR:HG21 | 2:D:331:ALA:HB1 | 2.02 | 0.41 |
| 1:E:417:GLU:O | 1:E:420:GLU:HB3 | 2.21 | 0.41 |
| 1:E:435:TYR:C | 1:E:437:ASP:N | 2.72 | 0.41 |
| 2:F:149:PHE:CD1 | 2:F:150:THR:N | 2.89 | 0.41 |
| 2:F:292:THR:HG21 | 2:F:331:ALA:HB1 | 2.02 | 0.41 |
| 2:F:425:MET:O | 2:F:426:ALA:C | 2.60 | 0.41 |
| 2:F:425:MET:O | 2:F:428:LEU:N | 2.45 | 0.41 |
| 1:G:20:PHE:CD2 | 1:G:235:MET:CG | 3.04 | 0.41 |
| 1:G:258:ASN:CA | 2:H:404:PHE:HD2 | 2.26 | 0.41 |
| 1:G:380:ASN:HD22 | 1:G:380:ASN:C | 2.24 | 0.41 |
| 2:H:401:LYS:O | 2:H:402:ARG:HB2 | 2.21 | 0.41 |
| 2:H:425:MET:O | 2:H:426:ALA:C | 2.60 | 0.41 |
| 1:A:20:PHE:CD2 | 1:A:235:MET:CG | 3.04 | 0.40 |
| 1:A:78:VAL:O | 1:A:84:GLY:HA3 | 2.22 | 0.40 |
| 1:A:147:SER:CB | 1:A:190:SER:HB3 | 2.42 | 0.40 |
| 1:A:311:ARG:HG2 | 1:A:311:ARG:NH1 | 2.34 | 0.40 |
| 1:A:423:SER:O | 1:A:424:ASN:C | 2.60 | 0.40 |
| 2:B:11:GLN:HG3 | 2:B:74:VAL:HG21 | 2.04 | 0.40 |
| 2:B:217:LEU:HD13 | 2:B:277:SER:CA | 2.48 | 0.40 |
| 2:B:287:SER:O | 2:B:291:ILE:HG12 | 2.21 | 0.40 |
| 1:C:275:LEU:HD12 | 1:C:275:LEU:HA | 1.78 | 0.40 |
| 2:D:23:LEU:HD11 | 2:D:361:THR:O | 2.21 | 0.40 |
| 2:D:149:PHE:CD1 | 2:D:150:THR:N | 2.89 | 0.40 |
| 1:E:11:GLN:HA | 1:E:74:THR:HG21 | 2.03 | 0.40 |
| 1:E:119:LEU:O | 1:E:122:VAL:HG22 | 2.21 | 0.40 |
| 2:F:401:LYS:O | 2:F:402:ARG:HB2 | 2.21 | 0.40 |
| 1:G:333:LEU:O | 1:G:334:ASN:C | 2.58 | 0.40 |
| 2:H:98:ASP:OD1 | 2:H:98:ASP:N | 2.55 | 0.40 |
| 2:H:149:PHE:CD1 | 2:H:150:THR:N | 2.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:292:THR:HG21 | 2:H:331:ALA:HB1 | 2.02 | 0.40 |
| 2:H:425:MET:O | 2:H:428:LEU:N | 2.45 | 0.40 |
| 1:A:11:GLN:HA | 1:A:74:THR:HG21 | 2.04 | 0.40 |
| 1:A:12:CYS:C | 1:A:14:ASN:N | 2.71 | 0.40 |
| 1:A:114:LEU:HD12 | 1:A:117:SER:OG | 2.21 | 0.40 |
| 1:A:306:ASP:HA | 1:A:307:PRO:HD3 | 1.91 | 0.40 |
| 2:B:251:ASP:CA | 2:B:254:GLU:HG3 | 2.48 | 0.40 |
| 2:B:428:LEU:HD12 | 2:B:428:LEU:HA | 1.79 | 0.40 |
| 1:C:20:PHE:CD2 | 1:C:235:MET:CG | 3.04 | 0.40 |
| 1:C:311:ARG:HG2 | 1:C:311:ARG:NH1 | 2.34 | 0.40 |
| 2:D:11:GLN:HG3 | 2:D:74:VAL:HG21 | 2.04 | 0.40 |
| 2:D:61:HIS:O | 2:D:62:VAL:C | 2.59 | 0.40 |
| 2:F:98:ASP:OD1 | 2:F:98:ASP:N | 2.55 | 0.40 |
| 2:F:401:LYS:C | 2:F:403:ALA:H | 2.24 | 0.40 |
| 1:G:114:LEU:HD12 | 1:G:117:SER:OG | 2.21 | 0.40 |
| 1:G:119:LEU:O | 1:G:122:VAL:HG22 | 2.21 | 0.40 |
| 2:H:297:GLU:HA | 2:H:298:PRO:HD2 | 1.87 | 0.40 |
| 3:I:80:PHE:CZ | 3:I:113:ILE:HB | 2.56 | 0.40 |
| 1:A:202:TYR:CE2 | 1:A:268:PHE:HD1 | 2.38 | 0.40 |
| 1:A:260:VAL:CG2 | 2:B:407:TRP:HE1 | 2.30 | 0.40 |
| 1:A:422:GLU:O | 1:A:426:ASN:CB | 2.67 | 0.40 |
| 2:B:272:TYR:O | 2:B:300:ASN:ND2 | 2.54 | 0.40 |
| 1:C:12:CYS:O | 1:C:14:ASN:N | 2.55 | 0.40 |
| 2:D:100:ALA:HB2 | 2:D:105:ARG:HD3 | 2.02 | 0.40 |
| 2:D:272:TYR:O | 2:D:300:ASN:ND2 | 2.54 | 0.40 |
| 2:D:413:MET:C | 2:D:414:GLU:CG | 2.90 | 0.40 |
| 1:E:2:ARG:NH2 | 2:F:98:ASP:HA | 2.37 | 0.40 |
| 1:E:150:GLY:HA2 | 1:E:153:LEU:CD2 | 2.42 | 0.40 |
| 1:E:161:TYR:C | 1:E:163:ASP:N | 2.71 | 0.40 |
| 1:E:306:ASP:HA | 1:E:307:PRO:HD3 | 1.91 | 0.40 |
| 2:F:325:PRO:HG2 | 1:G:224:TYR:H | 1.85 | 0.40 |
| 2:F:393:HIS:O | 2:F:394:LYS:C | 2.59 | 0.40 |
| 2:F:413:MET:C | 2:F:414:GLU:CG | 2.90 | 0.40 |
| 1:G:11:GLN:HA | 1:G:74:THR:HG21 | 2.04 | 0.40 |
| 1:G:291:LEU:HD21 | 1:G:373:MET:HG2 | 2.03 | 0.40 |
| 1:A:11:GLN:HG3 | 1:A:74:THR:HG23 | 2.04 | 0.40 |
| 1:A:435:TYR:C | 1:A:437:ASP:N | 2.72 | 0.40 |
| 1:C:11:GLN:HG3 | 1:C:74:THR:HG23 | 2.04 | 0.40 |
| 1:C:98:GLY:O | 1:C:100:GLY:N | 2.49 | 0.40 |
| 1:C:139:HIS:HE1 | 1:C:168:THR:CG2 | 2.34 | 0.40 |
| 1:C:422:GLU:O | 1:C:426:ASN:CB | 2.67 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:132:LEU:O | 1:E:164:ARG:HD2 | 2.21 | 0.40 |
| 1:E:333:LEU:O | 1:E:334:ASN:C | 2.58 | 0.40 |
| 2:F:320:ARG:O | 2:F:373:ARG:HA | 2.22 | 0.40 |
| 1:G:133:GLN:CG | 1:G:165:ILE:HD11 | 2.49 | 0.40 |
| 1:G:147:SER:CB | 1:G:190:SER:HB3 | 2.42 | 0.40 |
| 2:H:320:ARG:O | 2:H:373:ARG:HA | 2.22 | 0.40 |
| 2:H:413:MET:C | 2:H:414:GLU:CG | 2.90 | 0.40 |
| 1:A:12:CYS:O | 1:A:14:ASN:N | 2.55 | 0.40 |
| 1:A:291:LEU:HD21 | 1:A:373:MET:HG2 | 2.03 | 0.40 |
| 2:B:23:LEU:HD11 | 2:B:361:THR:O | 2.21 | 0.40 |
| 2:B:98:ASP:OD1 | 2:B:98:ASP:N | 2.55 | 0.40 |
| 2:B:255:PHE:O | 2:B:259:LEU:N | 2.50 | 0.40 |
| 2:B:414:GLU:C | 2:B:416:GLY:N | 2.74 | 0.40 |
| 2:B:434:GLU:C | 2:B:436:GLY:N | 2.74 | 0.40 |
| 1:C:11:GLN:HA | 1:C:74:THR:HG21 | 2.04 | 0.40 |
| 1:C:315:VAL:CG1 | 1:C:377:PHE:CE1 | 3.05 | 0.40 |
| 2:D:100:ALA:O | 2:D:102:ASN:N | 2.49 | 0.40 |
| 2:D:393:HIS:O | 2:D:394:LYS:C | 2.59 | 0.40 |
| 1:E:12:CYS:O | 1:E:14:ASN:N | 2.55 | 0.40 |
| 1:E:114:LEU:HD12 | 1:E:117:SER:OG | 2.21 | 0.40 |
| 1:E:204:ILE:HG23 | 1:E:209:LEU:HD11 | 2.04 | 0.40 |
| 2:F:11:GLN:HG3 | 2:F:74:VAL:HG21 | 2.03 | 0.40 |
| 2:F:11:GLN:N | 5:F:500:GTP:O2B | 2.55 | 0.40 |
| 1:G:132:LEU:O | 1:G:164:ARG:HD2 | 2.21 | 0.40 |
| 1:G:150:GLY:HA2 | 1:G:153:LEU:CD2 | 2.42 | 0.40 |
| 1:G:188:THR:O | 1:G:191:VAL:HG12 | 2.21 | 0.40 |
| 1:G:204:ILE:HG23 | 1:G:209:LEU:HD11 | 2.04 | 0.40 |
| 1:G:421:ALA:O | 1:G:422:GLU:C | 2.58 | 0.40 |
| 2:H:11:GLN:N | 5:H:500:GTP:O2B | 2.55 | 0.40 |
| 2:H:393:HIS:O | 2:H:394:LYS:C | 2.59 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 424/445 (95%) | 274 (65%) | 94 (22%) | 56 (13%) | 0 5 |
| 1 | C | 424/445 (95%) | 274 (65%) | 94 (22%) | 56 (13%) | 0 5 |
| 1 | E | 424/445 (95%) | 274 (65%) | 94 (22%) | 56 (13%) | 0 5 |
| 1 | G | 424/445 (95%) | 274 (65%) | 94 (22%) | 56 (13%) | 0 5 |
| 2 | B | 423/452 (94%) | 279 (66%) | 87 (21%) | 57 (14%) | 0 4 |
| 2 | D | 423/452 (94%) | 281 (66%) | 85 (20%) | 57 (14%) | 0 4 |
| 2 | F | 423/452 (94%) | 279 (66%) | 87 (21%) | 57 (14%) | 0 4 |
| 2 | H | 423/452 (94%) | 278 (66%) | 88 (21%) | 57 (14%) | 0 4 |
| 3 | I | 93/95 (98%) | 72 (77%) | 15 (16%) | 6 (6%) | 1 16 |
| All | All | 3481/3683 (94%) | 2285 (66%) | 738 (21%) | 458 (13%) | 1 5 |

All (458) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 23 | VAL |
| 1 | A | 24 | ILE |
| 1 | A | 32 | PRO |
| 1 | A | 50 | ASN |
| 1 | A | 82 | PRO |
| 1 | A | 97 | SER |
| 1 | A | 128 | SER |
| 1 | A | 176 | LYS |
| 1 | A | 183 | GLU |
| 1 | A | 218 | LYS |
| 1 | A | 238 | VAL |
| 1 | A | 239 | THR |
| 1 | A | 240 | THR |
| 1 | A | 252 | LEU |
| 1 | A | 263 | PRO |
| 1 | A | 266 | HIS |
| 1 | A | 273 | ALA |
| 1 | A | 278 | ARG |
| 1 | A | 280 | SER |
| 1 | A | 281 | GLN |
| 1 | A | 282 | GLN |
| 1 | A | 288 | VAL |
| 1 | A | 294 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 295 | MET |
| 1 | A | 343 | PHE |
| 1 | A | 344 | VAL |
| 1 | A | 346 | TRP |
| 1 | A | 369 | ARG |
| 1 | A | 403 | ALA |
| 2 | B | 56 | THR |
| 2 | B | 58 | ALA |
| 2 | B | 96 | LYS |
| 2 | B | 97 | GLU |
| 2 | B | 108 | TYR |
| 2 | B | 109 | THR |
| 2 | B | 141 | PHE |
| 2 | B | 183 | GLU |
| 2 | B | 217 | LEU |
| 2 | B | 240 | ALA |
| 2 | B | 249 | ASN |
| 2 | B | 255 | PHE |
| 2 | B | 266 | HIS |
| 2 | B | 309 | HIS |
| 2 | B | 346 | TRP |
| 2 | B | 370 | LYS |
| 2 | B | 387 | ALA |
| 2 | B | 403 | ALA |
| 2 | B | 437 | VAL |
| 1 | C | 23 | VAL |
| 1 | C | 24 | ILE |
| 1 | C | 32 | PRO |
| 1 | C | 50 | ASN |
| 1 | C | 82 | PRO |
| 1 | C | 97 | SER |
| 1 | C | 128 | SER |
| 1 | C | 176 | LYS |
| 1 | C | 183 | GLU |
| 1 | C | 218 | LYS |
| 1 | C | 238 | VAL |
| 1 | C | 239 | THR |
| 1 | C | 240 | THR |
| 1 | C | 252 | LEU |
| 1 | C | 263 | PRO |
| 1 | C | 266 | HIS |
| 1 | C | 273 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 278 | ARG |
| 1 | C | 280 | SER |
| 1 | C | 281 | GLN |
| 1 | C | 282 | GLN |
| 1 | C | 288 | VAL |
| 1 | C | 294 | GLN |
| 1 | C | 295 | MET |
| 1 | C | 343 | PHE |
| 1 | C | 344 | VAL |
| 1 | C | 346 | TRP |
| 1 | C | 369 | ARG |
| 1 | C | 403 | ALA |
| 2 | D | 56 | THR |
| 2 | D | 58 | ALA |
| 2 | D | 63 | PRO |
| 2 | D | 96 | LYS |
| 2 | D | 97 | GLU |
| 2 | D | 108 | TYR |
| 2 | D | 109 | THR |
| 2 | D | 141 | PHE |
| 2 | D | 183 | GLU |
| 2 | D | 217 | LEU |
| 2 | D | 240 | ALA |
| 2 | D | 249 | ASN |
| 2 | D | 255 | PHE |
| 2 | D | 266 | HIS |
| 2 | D | 309 | HIS |
| 2 | D | 346 | TRP |
| 2 | D | 370 | LYS |
| 2 | D | 387 | ALA |
| 2 | D | 403 | ALA |
| 2 | D | 437 | VAL |
| 1 | E | 23 | VAL |
| 1 | E | 24 | ILE |
| 1 | E | 32 | PRO |
| 1 | E | 50 | ASN |
| 1 | E | 82 | PRO |
| 1 | E | 97 | SER |
| 1 | E | 128 | SER |
| 1 | E | 176 | LYS |
| 1 | E | 183 | GLU |
| 1 | E | 218 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 238 | VAL |
| 1 | E | 239 | THR |
| 1 | E | 240 | THR |
| 1 | E | 252 | LEU |
| 1 | E | 263 | PRO |
| 1 | E | 266 | HIS |
| 1 | E | 273 | ALA |
| 1 | E | 278 | ARG |
| 1 | E | 280 | SER |
| 1 | E | 281 | GLN |
| 1 | E | 282 | GLN |
| 1 | E | 288 | VAL |
| 1 | E | 294 | GLN |
| 1 | E | 295 | MET |
| 1 | E | 343 | PHE |
| 1 | E | 344 | VAL |
| 1 | E | 346 | TRP |
| 1 | E | 369 | ARG |
| 1 | E | 403 | ALA |
| 2 | F | 63 | PRO |
| 2 | F | 96 | LYS |
| 2 | F | 97 | GLU |
| 2 | F | 108 | TYR |
| 2 | F | 109 | THR |
| 2 | F | 141 | PHE |
| 2 | F | 183 | GLU |
| 2 | F | 217 | LEU |
| 2 | F | 240 | ALA |
| 2 | F | 249 | ASN |
| 2 | F | 255 | PHE |
| 2 | F | 266 | HIS |
| 2 | F | 309 | HIS |
| 2 | F | 346 | TRP |
| 2 | F | 370 | LYS |
| 2 | F | 387 | ALA |
| 2 | F | 403 | ALA |
| 2 | F | 437 | VAL |
| 1 | G | 23 | VAL |
| 1 | G | 24 | ILE |
| 1 | G | 32 | PRO |
| 1 | G | 50 | ASN |
| 1 | G | 82 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 97 | SER |
| 1 | G | 128 | SER |
| 1 | G | 176 | LYS |
| 1 | G | 183 | GLU |
| 1 | G | 218 | LYS |
| 1 | G | 238 | VAL |
| 1 | G | 239 | THR |
| 1 | G | 240 | THR |
| 1 | G | 252 | LEU |
| 1 | G | 263 | PRO |
| 1 | G | 266 | HIS |
| 1 | G | 273 | ALA |
| 1 | G | 278 | ARG |
| 1 | G | 280 | SER |
| 1 | G | 281 | GLN |
| 1 | G | 282 | GLN |
| 1 | G | 288 | VAL |
| 1 | G | 294 | GLN |
| 1 | G | 295 | MET |
| 1 | G | 343 | PHE |
| 1 | G | 344 | VAL |
| 1 | G | 346 | TRP |
| 1 | G | 369 | ARG |
| 1 | G | 403 | ALA |
| 2 | H | 63 | PRO |
| 2 | H | 96 | LYS |
| 2 | H | 97 | GLU |
| 2 | H | 108 | TYR |
| 2 | H | 109 | THR |
| 2 | H | 141 | PHE |
| 2 | H | 183 | GLU |
| 2 | H | 217 | LEU |
| 2 | H | 240 | ALA |
| 2 | H | 249 | ASN |
| 2 | H | 255 | PHE |
| 2 | H | 266 | HIS |
| 2 | H | 309 | HIS |
| 2 | H | 346 | TRP |
| 2 | H | 370 | LYS |
| 2 | H | 387 | ALA |
| 2 | H | 403 | ALA |
| 2 | H | 437 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 38 | GLY |
| 1 | A | 73 | GLY |
| 1 | A | 175 | PRO |
| 1 | A | 265 | LEU |
| 1 | A | 279 | GLY |
| 1 | A | 298 | ALA |
| 1 | A | 300 | ASN |
| 1 | A | 311 | ARG |
| 2 | B | 24 | TYR |
| 2 | B | 73 | THR |
| 2 | B | 83 | TYR |
| 2 | B | 103 | TYR |
| 2 | B | 111 | GLY |
| 2 | B | 131 | GLY |
| 2 | B | 218 | ASP |
| 2 | B | 219 | ILE |
| 2 | B | 238 | ILE |
| 2 | B | 265 | GLY |
| 2 | B | 281 | ALA |
| 2 | B | 314 | ALA |
| 2 | B | 339 | ARG |
| 2 | B | 342 | GLN |
| 2 | B | 373 | ARG |
| 2 | B | 386 | GLU |
| 1 | C | 38 | GLY |
| 1 | C | 73 | GLY |
| 1 | C | 175 | PRO |
| 1 | C | 265 | LEU |
| 1 | C | 279 | GLY |
| 1 | C | 298 | ALA |
| 1 | C | 300 | ASN |
| 1 | C | 311 | ARG |
| 2 | D | 24 | TYR |
| 2 | D | 73 | THR |
| 2 | D | 83 | TYR |
| 2 | D | 103 | TYR |
| 2 | D | 111 | GLY |
| 2 | D | 131 | GLY |
| 2 | D | 218 | ASP |
| 2 | D | 219 | ILE |
| 2 | D | 238 | ILE |
| 2 | D | 265 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 281 | ALA |
| 2 | D | 314 | ALA |
| 2 | D | 339 | ARG |
| 2 | D | 342 | GLN |
| 2 | D | 373 | ARG |
| 2 | D | 386 | GLU |
| 1 | E | 38 | GLY |
| 1 | E | 73 | GLY |
| 1 | E | 175 | PRO |
| 1 | E | 265 | LEU |
| 1 | E | 279 | GLY |
| 1 | E | 298 | ALA |
| 1 | E | 300 | ASN |
| 1 | E | 311 | ARG |
| 2 | F | 24 | TYR |
| 2 | F | 73 | THR |
| 2 | F | 83 | TYR |
| 2 | F | 103 | TYR |
| 2 | F | 111 | GLY |
| 2 | F | 131 | GLY |
| 2 | F | 218 | ASP |
| 2 | F | 219 | ILE |
| 2 | F | 238 | ILE |
| 2 | F | 265 | GLY |
| 2 | F | 281 | ALA |
| 2 | F | 314 | ALA |
| 2 | F | 339 | ARG |
| 2 | F | 342 | GLN |
| 2 | F | 373 | ARG |
| 2 | F | 386 | GLU |
| 1 | G | 38 | GLY |
| 1 | G | 73 | GLY |
| 1 | G | 175 | PRO |
| 1 | G | 265 | LEU |
| 1 | G | 279 | GLY |
| 1 | G | 298 | ALA |
| 1 | G | 300 | ASN |
| 1 | G | 311 | ARG |
| 2 | H | 24 | TYR |
| 2 | H | 73 | THR |
| 2 | H | 83 | TYR |
| 2 | H | 103 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 111 | GLY |
| 2 | H | 131 | GLY |
| 2 | H | 218 | ASP |
| 2 | H | 219 | ILE |
| 2 | H | 238 | ILE |
| 2 | H | 265 | GLY |
| 2 | H | 281 | ALA |
| 2 | H | 314 | ALA |
| 2 | H | 339 | ARG |
| 2 | H | 342 | GLN |
| 2 | H | 373 | ARG |
| 2 | H | 386 | GLU |
| 3 | I | 51 | LYS |
| 3 | I | 135 | LYS |
| 1 | A | 34 | GLY |
| 1 | A | 83 | PHE |
| 1 | A | 99 | ALA |
| 1 | A | 100 | GLY |
| 1 | A | 302 | MET |
| 1 | A | 386 | GLU |
| 2 | B | 48 | SER |
| 2 | B | 104 | ALA |
| 2 | B | 148 | GLY |
| 2 | B | 149 | PHE |
| 2 | B | 173 | PRO |
| 2 | B | 239 | THR |
| 2 | B | 245 | ASP |
| 2 | B | 279 | GLU |
| 2 | B | 330 | ALA |
| 2 | B | 336 | LYS |
| 2 | B | 369 | ALA |
| 1 | C | 34 | GLY |
| 1 | C | 83 | PHE |
| 1 | C | 99 | ALA |
| 1 | C | 100 | GLY |
| 1 | C | 302 | MET |
| 1 | C | 386 | GLU |
| 2 | D | 48 | SER |
| 2 | D | 104 | ALA |
| 2 | D | 148 | GLY |
| 2 | D | 149 | PHE |
| 2 | D | 173 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 239 | THR |
| 2 | D | 245 | ASP |
| 2 | D | 263 | PRO |
| 2 | D | 279 | GLU |
| 2 | D | 330 | ALA |
| 2 | D | 336 | LYS |
| 2 | D | 369 | ALA |
| 1 | E | 34 | GLY |
| 1 | E | 83 | PHE |
| 1 | E | 99 | ALA |
| 1 | E | 100 | GLY |
| 1 | E | 302 | MET |
| 1 | E | 386 | GLU |
| 2 | F | 48 | SER |
| 2 | F | 59 | GLY |
| 2 | F | 104 | ALA |
| 2 | F | 148 | GLY |
| 2 | F | 149 | PHE |
| 2 | F | 173 | PRO |
| 2 | F | 239 | THR |
| 2 | F | 245 | ASP |
| 2 | F | 263 | PRO |
| 2 | F | 279 | GLU |
| 2 | F | 330 | ALA |
| 2 | F | 336 | LYS |
| 2 | F | 369 | ALA |
| 1 | G | 34 | GLY |
| 1 | G | 83 | PHE |
| 1 | G | 99 | ALA |
| 1 | G | 100 | GLY |
| 1 | G | 302 | MET |
| 1 | G | 386 | GLU |
| 2 | H | 48 | SER |
| 2 | H | 59 | GLY |
| 2 | H | 104 | ALA |
| 2 | H | 148 | GLY |
| 2 | H | 149 | PHE |
| 2 | H | 173 | PRO |
| 2 | H | 239 | THR |
| 2 | H | 245 | ASP |
| 2 | H | 263 | PRO |
| 2 | H | 279 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 330 | ALA |
| 2 | H | 336 | LYS |
| 2 | H | 369 | ALA |
| 3 | I | 63 | ARG |
| 3 | I | 67 | GLY |
| 1 | A | 96 | GLN |
| 1 | A | 395 | PHE |
| 2 | B | 129 | CYS |
| 2 | B | 263 | PRO |
| 2 | B | 300 | ASN |
| 2 | B | 348 | PRO |
| 1 | C | 96 | GLN |
| 1 | C | 395 | PHE |
| 2 | D | 129 | CYS |
| 2 | D | 300 | ASN |
| 2 | D | 348 | PRO |
| 1 | E | 96 | GLN |
| 1 | E | 395 | PHE |
| 2 | F | 300 | ASN |
| 2 | F | 348 | PRO |
| 1 | G | 96 | GLN |
| 1 | G | 395 | PHE |
| 2 | H | 300 | ASN |
| 2 | H | 348 | PRO |
| 3 | I | 101 | VAL |
| 1 | A | 57 | ALA |
| 1 | A | 74 | THR |
| 1 | A | 285 | ALA |
| 1 | A | 424 | ASN |
| 2 | B | 256 | GLN |
| 2 | B | 303 | VAL |
| 2 | B | 382 | THR |
| 1 | C | 57 | ALA |
| 1 | C | 74 | THR |
| 1 | C | 285 | ALA |
| 1 | C | 424 | ASN |
| 2 | D | 256 | GLN |
| 2 | D | 303 | VAL |
| 2 | D | 382 | THR |
| 1 | E | 57 | ALA |
| 1 | E | 74 | THR |
| 1 | E | 285 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 424 | ASN |
| 2 | F | 129 | CYS |
| 2 | F | 256 | GLN |
| 2 | F | 303 | VAL |
| 2 | F | 307 | PRO |
| 2 | F | 382 | THR |
| 1 | G | 57 | ALA |
| 1 | G | 74 | THR |
| 1 | G | 285 | ALA |
| 1 | G | 424 | ASN |
| 2 | H | 129 | CYS |
| 2 | H | 256 | GLN |
| 2 | H | 303 | VAL |
| 2 | H | 382 | THR |
| 1 | A | 51 | VAL |
| 1 | A | 58 | GLY |
| 1 | A | 145 | THR |
| 1 | A | 162 | PRO |
| 1 | A | 400 | ARG |
| 2 | B | 62 | VAL |
| 2 | B | 273 | ALA |
| 2 | B | 307 | PRO |
| 1 | C | 51 | VAL |
| 1 | C | 58 | GLY |
| 1 | C | 145 | THR |
| 1 | C | 162 | PRO |
| 1 | C | 400 | ARG |
| 2 | D | 273 | ALA |
| 2 | D | 307 | PRO |
| 1 | E | 51 | VAL |
| 1 | E | 58 | GLY |
| 1 | E | 145 | THR |
| 1 | E | 162 | PRO |
| 1 | E | 400 | ARG |
| 2 | F | 273 | ALA |
| 1 | G | 51 | VAL |
| 1 | G | 58 | GLY |
| 1 | G | 145 | THR |
| 1 | G | 162 | PRO |
| 1 | G | 400 | ARG |
| 2 | H | 273 | ALA |
| 2 | H | 307 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 195 | VAL |
| 1 | C | 195 | VAL |
| 1 | E | 195 | VAL |
| 2 | F | 31 | GLN |
| 1 | G | 195 | VAL |
| 2 | H | 31 | GLN |
| 2 | B | 115 | ILE |
| 1 | C | 72 | PRO |
| 2 | D | 115 | ILE |
| 1 | E | 72 | PRO |
| 2 | F | 115 | ILE |
| 2 | H | 115 | ILE |
| 3 | I | 98 | PRO |
| 1 | A | 72 | PRO |
| 1 | G | 72 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 367/381 (96%) | 307 (84%) | 60 (16%) | 2 13 |
| 1 | C | 367/381 (96%) | 308 (84%) | 59 (16%) | 2 13 |
| 1 | E | 367/381 (96%) | 308 (84%) | 59 (16%) | 2 13 |
| 1 | G | 367/381 (96%) | 308 (84%) | 59 (16%) | 2 13 |
| 2 | B | 354/378 (94%) | 295 (83%) | 59 (17%) | 2 12 |
| 2 | D | 354/378 (94%) | 297 (84%) | 57 (16%) | 2 13 |
| 2 | F | 354/378 (94%) | 296 (84%) | 58 (16%) | 2 12 |
| 2 | H | 354/378 (94%) | 297 (84%) | 57 (16%) | 2 13 |
| 3 | I | 85/85 (100%) | 57 (67%) | 28 (33%) | 0 2 |
| All | All | 2969/3121 (95%) | 2473 (83%) | 496 (17%) | 5 12 |

All (496) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 14 | ASN |
| 1 | A | 24 | ILE |
| 1 | A | 26 | ASP |
| 1 | A | 32 | PRO |
| 1 | A | 41 | ASP |
| 1 | A | 68 | VAL |
| 1 | A | 76 | ASP |
| 1 | A | 90 | ASP |
| 1 | A | 94 | PHE |
| 1 | A | 101 | ASN |
| 1 | A | 122 | VAL |
| 1 | A | 129 | CYS |
| 1 | A | 135 | PHE |
| 1 | A | 141 | LEU |
| 1 | A | 145 | THR |
| 1 | A | 149 | MET |
| 1 | A | 153 | LEU |
| 1 | A | 161 | TYR |
| 1 | A | 163 | ASP |
| 1 | A | 165 | ILE |
| 1 | A | 174 | SER |
| 1 | A | 198 | THR |
| 1 | A | 201 | THR |
| 1 | A | 203 | CYS |
| 1 | A | 207 | GLU |
| 1 | A | 211 | ASP |
| 1 | A | 214 | PHE |
| 1 | A | 215 | ARG |
| 1 | A | 224 | TYR |
| 1 | A | 227 | LEU |
| 1 | A | 230 | LEU |
| 1 | A | 236 | SER |
| 1 | A | 240 | THR |
| 1 | A | 244 | PHE |
| 1 | A | 265 | LEU |
| 1 | A | 267 | PHE |
| 1 | A | 275 | LEU |
| 1 | A | 282 | GLN |
| 1 | A | 283 | TYR |
| 1 | A | 284 | ARG |
| 1 | A | 289 | PRO |
| 1 | A | 299 | LYS |
| 1 | A | 306 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 309 | HIS |
| 1 | A | 322 | ARG |
| 1 | A | 324 | SER |
| 1 | A | 325 | MET |
| 1 | A | 343 | PHE |
| 1 | A | 344 | VAL |
| 1 | A | 349 | ASN |
| 1 | A | 369 | ARG |
| 1 | A | 380 | ASN |
| 1 | A | 387 | LEU |
| 1 | A | 413 | MET |
| 1 | A | 414 | ASP |
| 1 | A | 424 | ASN |
| 1 | A | 427 | ASP |
| 1 | A | 431 | GLU |
| 1 | A | 432 | TYR |
| 1 | A | 437 | ASP |
| 2 | B | 6 | SER |
| 2 | B | 20 | CYS |
| 2 | B | 21 | TRP |
| 2 | B | 31 | GLN |
| 2 | B | 48 | SER |
| 2 | B | 50 | ASN |
| 2 | B | 60 | LYS |
| 2 | B | 61 | HIS |
| 2 | B | 74 | VAL |
| 2 | B | 79 | ARG |
| 2 | B | 82 | THR |
| 2 | B | 84 | ARG |
| 2 | B | 87 | PHE |
| 2 | B | 88 | HIS |
| 2 | B | 90 | GLU |
| 2 | B | 98 | ASP |
| 2 | B | 115 | ILE |
| 2 | B | 120 | ASP |
| 2 | B | 125 | LEU |
| 2 | B | 127 | ASP |
| 2 | B | 130 | THR |
| 2 | B | 135 | PHE |
| 2 | B | 141 | PHE |
| 2 | B | 150 | THR |
| 2 | B | 152 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 155 | GLU |
| 2 | B | 169 | PHE |
| 2 | B | 172 | TYR |
| 2 | B | 173 | PRO |
| 2 | B | 183 | GLU |
| 2 | B | 192 | HIS |
| 2 | B | 204 | VAL |
| 2 | B | 219 | ILE |
| 2 | B | 224 | TYR |
| 2 | B | 231 | ILE |
| 2 | B | 234 | ILE |
| 2 | B | 243 | ARG |
| 2 | B | 244 | PHE |
| 2 | B | 253 | THR |
| 2 | B | 260 | VAL |
| 2 | B | 267 | PHE |
| 2 | B | 269 | LEU |
| 2 | B | 279 | GLU |
| 2 | B | 280 | LYS |
| 2 | B | 290 | GLU |
| 2 | B | 303 | VAL |
| 2 | B | 325 | PRO |
| 2 | B | 334 | THR |
| 2 | B | 345 | ASP |
| 2 | B | 352 | LYS |
| 2 | B | 368 | LEU |
| 2 | B | 376 | CYS |
| 2 | B | 378 | LEU |
| 2 | B | 380 | ASN |
| 2 | B | 404 | PHE |
| 2 | B | 415 | GLU |
| 2 | B | 417 | GLU |
| 2 | B | 431 | ASP |
| 2 | B | 432 | TYR |
| 1 | C | 14 | ASN |
| 1 | C | 24 | ILE |
| 1 | C | 26 | ASP |
| 1 | C | 32 | PRO |
| 1 | C | 41 | ASP |
| 1 | C | 68 | VAL |
| 1 | C | 76 | ASP |
| 1 | C | 90 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 94 | PHE |
| 1 | C | 101 | ASN |
| 1 | C | 122 | VAL |
| 1 | C | 129 | CYS |
| 1 | C | 135 | PHE |
| 1 | C | 141 | LEU |
| 1 | C | 145 | THR |
| 1 | C | 149 | MET |
| 1 | C | 153 | LEU |
| 1 | C | 161 | TYR |
| 1 | C | 163 | ASP |
| 1 | C | 165 | ILE |
| 1 | C | 174 | SER |
| 1 | C | 198 | THR |
| 1 | C | 201 | THR |
| 1 | C | 203 | CYS |
| 1 | C | 207 | GLU |
| 1 | C | 211 | ASP |
| 1 | C | 214 | PHE |
| 1 | C | 215 | ARG |
| 1 | C | 224 | TYR |
| 1 | C | 227 | LEU |
| 1 | C | 230 | LEU |
| 1 | C | 236 | SER |
| 1 | C | 240 | THR |
| 1 | C | 244 | PHE |
| 1 | C | 265 | LEU |
| 1 | C | 267 | PHE |
| 1 | C | 275 | LEU |
| 1 | C | 282 | GLN |
| 1 | C | 283 | TYR |
| 1 | C | 284 | ARG |
| 1 | C | 299 | LYS |
| 1 | C | 306 | ASP |
| 1 | C | 309 | HIS |
| 1 | C | 322 | ARG |
| 1 | C | 324 | SER |
| 1 | C | 325 | MET |
| 1 | C | 343 | PHE |
| 1 | C | 344 | VAL |
| 1 | C | 349 | ASN |
| 1 | C | 369 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 380 | ASN |
| 1 | C | 387 | LEU |
| 1 | C | 413 | MET |
| 1 | C | 414 | ASP |
| 1 | C | 424 | ASN |
| 1 | C | 427 | ASP |
| 1 | C | 431 | GLU |
| 1 | C | 432 | TYR |
| 1 | C | 437 | ASP |
| 2 | D | 6 | SER |
| 2 | D | 20 | CYS |
| 2 | D | 21 | TRP |
| 2 | D | 31 | GLN |
| 2 | D | 48 | SER |
| 2 | D | 50 | ASN |
| 2 | D | 60 | LYS |
| 2 | D | 74 | VAL |
| 2 | D | 79 | ARG |
| 2 | D | 82 | THR |
| 2 | D | 84 | ARG |
| 2 | D | 87 | PHE |
| 2 | D | 88 | HIS |
| 2 | D | 90 | GLU |
| 2 | D | 98 | ASP |
| 2 | D | 115 | ILE |
| 2 | D | 120 | ASP |
| 2 | D | 125 | LEU |
| 2 | D | 127 | ASP |
| 2 | D | 130 | THR |
| 2 | D | 135 | PHE |
| 2 | D | 141 | PHE |
| 2 | D | 150 | THR |
| 2 | D | 152 | LEU |
| 2 | D | 155 | GLU |
| 2 | D | 169 | PHE |
| 2 | D | 172 | TYR |
| 2 | D | 173 | PRO |
| 2 | D | 183 | GLU |
| 2 | D | 192 | HIS |
| 2 | D | 204 | VAL |
| 2 | D | 219 | ILE |
| 2 | D | 224 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 231 | ILE |
| 2 | D | 234 | ILE |
| 2 | D | 243 | ARG |
| 2 | D | 244 | PHE |
| 2 | D | 253 | THR |
| 2 | D | 260 | VAL |
| 2 | D | 267 | PHE |
| 2 | D | 269 | LEU |
| 2 | D | 279 | GLU |
| 2 | D | 290 | GLU |
| 2 | D | 303 | VAL |
| 2 | D | 325 | PRO |
| 2 | D | 334 | THR |
| 2 | D | 345 | ASP |
| 2 | D | 352 | LYS |
| 2 | D | 368 | LEU |
| 2 | D | 376 | CYS |
| 2 | D | 378 | LEU |
| 2 | D | 380 | ASN |
| 2 | D | 404 | PHE |
| 2 | D | 415 | GLU |
| 2 | D | 417 | GLU |
| 2 | D | 431 | ASP |
| 2 | D | 432 | TYR |
| 1 | E | 14 | ASN |
| 1 | E | 24 | ILE |
| 1 | E | 26 | ASP |
| 1 | E | 32 | PRO |
| 1 | E | 41 | ASP |
| 1 | E | 68 | VAL |
| 1 | E | 76 | ASP |
| 1 | E | 90 | ASP |
| 1 | E | 94 | PHE |
| 1 | E | 101 | ASN |
| 1 | E | 122 | VAL |
| 1 | E | 129 | CYS |
| 1 | E | 135 | PHE |
| 1 | E | 141 | LEU |
| 1 | E | 145 | THR |
| 1 | E | 149 | MET |
| 1 | E | 153 | LEU |
| 1 | E | 161 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 163 | ASP |
| 1 | E | 165 | ILE |
| 1 | E | 174 | SER |
| 1 | E | 198 | THR |
| 1 | E | 201 | THR |
| 1 | E | 203 | CYS |
| 1 | E | 207 | GLU |
| 1 | E | 211 | ASP |
| 1 | E | 214 | PHE |
| 1 | E | 215 | ARG |
| 1 | E | 224 | TYR |
| 1 | E | 227 | LEU |
| 1 | E | 230 | LEU |
| 1 | E | 236 | SER |
| 1 | E | 240 | THR |
| 1 | E | 244 | PHE |
| 1 | E | 265 | LEU |
| 1 | E | 267 | PHE |
| 1 | E | 275 | LEU |
| 1 | E | 282 | GLN |
| 1 | E | 283 | TYR |
| 1 | E | 284 | ARG |
| 1 | E | 299 | LYS |
| 1 | E | 306 | ASP |
| 1 | E | 309 | HIS |
| 1 | E | 322 | ARG |
| 1 | E | 324 | SER |
| 1 | E | 325 | MET |
| 1 | E | 343 | PHE |
| 1 | E | 344 | VAL |
| 1 | E | 349 | ASN |
| 1 | E | 369 | ARG |
| 1 | E | 380 | ASN |
| 1 | E | 387 | LEU |
| 1 | E | 413 | MET |
| 1 | E | 414 | ASP |
| 1 | E | 424 | ASN |
| 1 | E | 427 | ASP |
| 1 | E | 431 | GLU |
| 1 | E | 432 | TYR |
| 1 | E | 437 | ASP |
| 2 | F | 6 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F | 20 | CYS |
| 2 | F | 21 | TRP |
| 2 | F | 31 | GLN |
| 2 | F | 48 | SER |
| 2 | F | 50 | ASN |
| 2 | F | 60 | LYS |
| 2 | F | 74 | VAL |
| 2 | F | 79 | ARG |
| 2 | F | 82 | THR |
| 2 | F | 84 | ARG |
| 2 | F | 87 | PHE |
| 2 | F | 88 | HIS |
| 2 | F | 90 | GLU |
| 2 | F | 98 | ASP |
| 2 | F | 115 | ILE |
| 2 | F | 120 | ASP |
| 2 | F | 125 | LEU |
| 2 | F | 127 | ASP |
| 2 | F | 130 | THR |
| 2 | F | 135 | PHE |
| 2 | F | 141 | PHE |
| 2 | F | 150 | THR |
| 2 | F | 152 | LEU |
| 2 | F | 155 | GLU |
| 2 | F | 169 | PHE |
| 2 | F | 172 | TYR |
| 2 | F | 173 | PRO |
| 2 | F | 183 | GLU |
| 2 | F | 192 | HIS |
| 2 | F | 204 | VAL |
| 2 | F | 219 | ILE |
| 2 | F | 224 | TYR |
| 2 | F | 231 | ILE |
| 2 | F | 234 | ILE |
| 2 | F | 243 | ARG |
| 2 | F | 244 | PHE |
| 2 | F | 253 | THR |
| 2 | F | 260 | VAL |
| 2 | F | 267 | PHE |
| 2 | F | 269 | LEU |
| 2 | F | 279 | GLU |
| 2 | F | 280 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F | 290 | GLU |
| 2 | F | 303 | VAL |
| 2 | F | 325 | PRO |
| 2 | F | 334 | THR |
| 2 | F | 345 | ASP |
| 2 | F | 352 | LYS |
| 2 | F | 368 | LEU |
| 2 | F | 376 | CYS |
| 2 | F | 378 | LEU |
| 2 | F | 380 | ASN |
| 2 | F | 404 | PHE |
| 2 | F | 415 | GLU |
| 2 | F | 417 | GLU |
| 2 | F | 431 | ASP |
| 2 | F | 432 | TYR |
| 1 | G | 14 | ASN |
| 1 | G | 24 | ILE |
| 1 | G | 26 | ASP |
| 1 | G | 32 | PRO |
| 1 | G | 41 | ASP |
| 1 | G | 68 | VAL |
| 1 | G | 76 | ASP |
| 1 | G | 90 | ASP |
| 1 | G | 94 | PHE |
| 1 | G | 101 | ASN |
| 1 | G | 122 | VAL |
| 1 | G | 129 | CYS |
| 1 | G | 135 | PHE |
| 1 | G | 141 | LEU |
| 1 | G | 145 | THR |
| 1 | G | 149 | MET |
| 1 | G | 153 | LEU |
| 1 | G | 161 | TYR |
| 1 | G | 163 | ASP |
| 1 | G | 165 | ILE |
| 1 | G | 174 | SER |
| 1 | G | 198 | THR |
| 1 | G | 201 | THR |
| 1 | G | 203 | CYS |
| 1 | G | 207 | GLU |
| 1 | G | 211 | ASP |
| 1 | G | 214 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 215 | ARG |
| 1 | G | 224 | TYR |
| 1 | G | 227 | LEU |
| 1 | G | 230 | LEU |
| 1 | G | 236 | SER |
| 1 | G | 240 | THR |
| 1 | G | 244 | PHE |
| 1 | G | 265 | LEU |
| 1 | G | 267 | PHE |
| 1 | G | 275 | LEU |
| 1 | G | 282 | GLN |
| 1 | G | 283 | TYR |
| 1 | G | 284 | ARG |
| 1 | G | 299 | LYS |
| 1 | G | 306 | ASP |
| 1 | G | 309 | HIS |
| 1 | G | 322 | ARG |
| 1 | G | 324 | SER |
| 1 | G | 325 | MET |
| 1 | G | 343 | PHE |
| 1 | G | 344 | VAL |
| 1 | G | 349 | ASN |
| 1 | G | 369 | ARG |
| 1 | G | 380 | ASN |
| 1 | G | 387 | LEU |
| 1 | G | 413 | MET |
| 1 | G | 414 | ASP |
| 1 | G | 424 | ASN |
| 1 | G | 427 | ASP |
| 1 | G | 431 | GLU |
| 1 | G | 432 | TYR |
| 1 | G | 437 | ASP |
| 2 | H | 6 | SER |
| 2 | H | 20 | CYS |
| 2 | H | 21 | TRP |
| 2 | H | 31 | GLN |
| 2 | H | 48 | SER |
| 2 | H | 50 | ASN |
| 2 | H | 74 | VAL |
| 2 | H | 79 | ARG |
| 2 | H | 82 | THR |
| 2 | H | 84 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 87 | PHE |
| 2 | H | 88 | HIS |
| 2 | H | 90 | GLU |
| 2 | H | 98 | ASP |
| 2 | H | 115 | ILE |
| 2 | H | 120 | ASP |
| 2 | H | 125 | LEU |
| 2 | H | 127 | ASP |
| 2 | H | 130 | THR |
| 2 | H | 135 | PHE |
| 2 | H | 141 | PHE |
| 2 | H | 150 | THR |
| 2 | H | 152 | LEU |
| 2 | H | 155 | GLU |
| 2 | H | 169 | PHE |
| 2 | H | 172 | TYR |
| 2 | H | 173 | PRO |
| 2 | H | 183 | GLU |
| 2 | H | 192 | HIS |
| 2 | H | 204 | VAL |
| 2 | H | 219 | ILE |
| 2 | H | 224 | TYR |
| 2 | H | 231 | ILE |
| 2 | H | 234 | ILE |
| 2 | H | 243 | ARG |
| 2 | H | 244 | PHE |
| 2 | H | 253 | THR |
| 2 | H | 260 | VAL |
| 2 | H | 267 | PHE |
| 2 | H | 269 | LEU |
| 2 | H | 279 | GLU |
| 2 | H | 280 | LYS |
| 2 | H | 290 | GLU |
| 2 | H | 303 | VAL |
| 2 | H | 325 | PRO |
| 2 | H | 334 | THR |
| 2 | H | 345 | ASP |
| 2 | H | 352 | LYS |
| 2 | H | 368 | LEU |
| 2 | H | 376 | CYS |
| 2 | H | 378 | LEU |
| 2 | H | 380 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 404 | PHE |
| 2 | H | 415 | GLU |
| 2 | H | 417 | GLU |
| 2 | H | 431 | ASP |
| 2 | H | 432 | TYR |
| 3 | I | 47 | SER |
| 3 | I | 49 | GLU |
| 3 | I | 50 | LYS |
| 3 | I | 51 | LYS |
| 3 | I | 54 | LYS |
| 3 | I | 56 | ARG |
| 3 | I | 59 | ARG |
| 3 | I | 70 | TYR |
| 3 | I | 75 | ASP |
| 3 | I | 76 | ARG |
| 3 | I | 78 | ARG |
| 3 | I | 79 | SER |
| 3 | I | 80 | PHE |
| 3 | I | 86 | ASP |
| 3 | I | 88 | THR |
| 3 | I | 89 | ARG |
| 3 | I | 90 | SER |
| 3 | I | 93 | ASP |
| 3 | I | 102 | ARG |
| 3 | I | 106 | THR |
| 3 | I | 108 | ASP |
| 3 | I | 112 | LYS |
| 3 | I | 117 | ASP |
| 3 | I | 120 | GLU |
| 3 | I | 131 | ASN |
| 3 | I | 132 | PHE |
| 3 | I | 136 | VAL |
| 3 | I | 140 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 14 | ASN |
| 1 | A | 91 | ASN |
| 1 | A | 101 | ASN |
| 1 | A | 102 | ASN |
| 1 | A | 107 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 136 | GLN |
| 1 | A | 139 | HIS |
| 1 | A | 197 | ASN |
| 1 | A | 282 | GLN |
| 1 | A | 331 | GLN |
| 1 | A | 334 | ASN |
| 1 | A | 337 | ASN |
| 1 | A | 349 | ASN |
| 1 | A | 380 | ASN |
| 1 | A | 406 | HIS |
| 1 | A | 436 | GLN |
| 2 | B | 11 | GLN |
| 2 | B | 15 | GLN |
| 2 | B | 28 | HIS |
| 2 | B | 50 | ASN |
| 2 | B | 61 | HIS |
| 2 | B | 91 | GLN |
| 2 | B | 101 | ASN |
| 2 | B | 128 | GLN |
| 2 | B | 133 | GLN |
| 2 | B | 139 | HIS |
| 2 | B | 197 | HIS |
| 2 | B | 216 | ASN |
| 2 | B | 226 | ASN |
| 2 | B | 256 | GLN |
| 2 | B | 258 | ASN |
| 2 | B | 309 | HIS |
| 2 | B | 380 | ASN |
| 1 | C | 14 | ASN |
| 1 | C | 91 | ASN |
| 1 | C | 101 | ASN |
| 1 | C | 102 | ASN |
| 1 | C | 107 | HIS |
| 1 | C | 136 | GLN |
| 1 | C | 139 | HIS |
| 1 | C | 197 | ASN |
| 1 | C | 206 | ASN |
| 1 | C | 282 | GLN |
| 1 | C | 331 | GLN |
| 1 | C | 334 | ASN |
| 1 | C | 337 | ASN |
| 1 | C | 349 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 380 | ASN |
| 1 | C | 406 | HIS |
| 1 | C | 436 | GLN |
| 2 | D | 11 | GLN |
| 2 | D | 15 | GLN |
| 2 | D | 28 | HIS |
| 2 | D | 50 | ASN |
| 2 | D | 61 | HIS |
| 2 | D | 91 | GLN |
| 2 | D | 128 | GLN |
| 2 | D | 133 | GLN |
| 2 | D | 139 | HIS |
| 2 | D | 197 | HIS |
| 2 | D | 216 | ASN |
| 2 | D | 226 | ASN |
| 2 | D | 256 | GLN |
| 2 | D | 309 | HIS |
| 2 | D | 380 | ASN |
| 1 | E | 14 | ASN |
| 1 | E | 91 | ASN |
| 1 | E | 101 | ASN |
| 1 | E | 102 | ASN |
| 1 | E | 107 | HIS |
| 1 | E | 136 | GLN |
| 1 | E | 139 | HIS |
| 1 | E | 197 | ASN |
| 1 | E | 282 | GLN |
| 1 | E | 331 | GLN |
| 1 | E | 334 | ASN |
| 1 | E | 337 | ASN |
| 1 | E | 349 | ASN |
| 1 | E | 380 | ASN |
| 1 | E | 406 | HIS |
| 1 | E | 436 | GLN |
| 2 | F | 11 | GLN |
| 2 | F | 15 | GLN |
| 2 | F | 28 | HIS |
| 2 | F | 50 | ASN |
| 2 | F | 61 | HIS |
| 2 | F | 91 | GLN |
| 2 | F | 128 | GLN |
| 2 | F | 133 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F | 139 | HIS |
| 2 | F | 197 | HIS |
| 2 | F | 216 | ASN |
| 2 | F | 226 | ASN |
| 2 | F | 256 | GLN |
| 2 | F | 309 | HIS |
| 2 | F | 380 | ASN |
| 1 | G | 14 | ASN |
| 1 | G | 91 | ASN |
| 1 | G | 102 | ASN |
| 1 | G | 107 | HIS |
| 1 | G | 136 | GLN |
| 1 | G | 139 | HIS |
| 1 | G | 197 | ASN |
| 1 | G | 258 | ASN |
| 1 | G | 282 | GLN |
| 1 | G | 309 | HIS |
| 1 | G | 331 | GLN |
| 1 | G | 334 | ASN |
| 1 | G | 337 | ASN |
| 1 | G | 349 | ASN |
| 1 | G | 380 | ASN |
| 1 | G | 406 | HIS |
| 1 | G | 436 | GLN |
| 2 | H | 11 | GLN |
| 2 | H | 15 | GLN |
| 2 | H | 28 | HIS |
| 2 | H | 50 | ASN |
| 2 | H | 91 | GLN |
| 2 | H | 101 | ASN |
| 2 | H | 128 | GLN |
| 2 | H | 133 | GLN |
| 2 | H | 197 | HIS |
| 2 | H | 216 | ASN |
| 2 | H | 226 | ASN |
| 2 | H | 256 | GLN |
| 2 | H | 309 | HIS |
| 2 | H | 380 | ASN |
| 2 | H | 406 | HIS |

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | GTP | D | 500 | - | 26,34,34 | 1.32 | 5 (19%) | 32,54,54 | 1.16 | 3 (9%) |
| 5 | GTP | B | 500 | - | 26,34,34 | 1.55 | 5 (19%) | 32,54,54 | 1.59 | 4 (12%) |
| 5 | GTP | F | 500 | - | 26,34,34 | 1.33 | 4 (15%) | 32,54,54 | 1.15 | 3 (9%) |
| 4 | GDP | G | 600 | - | 24,30,30 | 2.59 | 9 (37%) | 30,47,47 | 2.92 | 8 (26%) |
| 4 | GDP | C | 600 | - | 24,30,30 | 2.58 | 9 (37%) | 30,47,47 | 2.92 | 8 (26%) |
| 4 | GDP | A | 600 | - | 24,30,30 | 2.59 | 9 (37%) | 30,47,47 | 2.92 | 8 (26%) |
| 5 | GTP | H | 500 | - | 26,34,34 | 1.32 | 5 (19%) | 32,54,54 | 1.15 | 3 (9%) |
| 4 | GDP | E | 600 | - | 24,30,30 | 2.59 | 9 (37%) | 30,47,47 | 2.92 | 8 (26%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 5 | GTP | D | 500 | - | - | 3/18/38/38 | 0/3/3/3 |
| 5 | GTP | B | 500 | - | - | 3/18/38/38 | 0/3/3/3 |
| 5 | GTP | F | 500 | - | - | 3/18/38/38 | 0/3/3/3 |
| 4 | GDP | G | 600 | - | - | 4/12/32/32 | 0/3/3/3 |
| 4 | GDP | C | 600 | - | - | 4/12/32/32 | 0/3/3/3 |
| 4 | GDP | A | 600 | - | - | 4/12/32/32 | 0/3/3/3 |
| 5 | GTP | H | 500 | - | - | 3/18/38/38 | 0/3/3/3 |
| 4 | GDP | E | 600 | - | - | 4/12/32/32 | 0/3/3/3 |

All (55) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | A | 600 | GDP | O4'-C1' | 6.29 | 1.49 | 1.41 |
| 4 | C | 600 | GDP | O4'-C1' | 6.26 | 1.49 | 1.41 |
| 4 | G | 600 | GDP | O4'-C1' | 6.24 | 1.49 | 1.41 |
| 4 | E | 600 | GDP | O4'-C1' | 6.21 | 1.49 | 1.41 |
| 4 | C | 600 | GDP | O6-C6 | 5.64 | 1.34 | 1.23 |
| 4 | G | 600 | GDP | O6-C6 | 5.64 | 1.34 | 1.23 |
| 4 | E | 600 | GDP | O6-C6 | 5.63 | 1.34 | 1.23 |
| 4 | A | 600 | GDP | O6-C6 | 5.61 | 1.34 | 1.23 |
| 4 | E | 600 | GDP | C2-N1 | 4.67 | 1.49 | 1.37 |
| 4 | A | 600 | GDP | C2-N1 | 4.66 | 1.49 | 1.37 |
| 4 | G | 600 | GDP | C2-N1 | 4.65 | 1.49 | 1.37 |
| 4 | C | 600 | GDP | C2-N1 | 4.64 | 1.49 | 1.37 |
| 4 | G | 600 | GDP | PB-O2B | -3.80 | 1.40 | 1.54 |
| 4 | A | 600 | GDP | PB-O2B | -3.80 | 1.40 | 1.54 |
| 4 | C | 600 | GDP | PB-O2B | -3.79 | 1.40 | 1.54 |
| 4 | E | 600 | GDP | PB-O2B | -3.78 | 1.40 | 1.54 |
| 5 | B | 500 | GTP | C5-C6 | -3.71 | 1.39 | 1.47 |
| 5 | D | 500 | GTP | C5-C6 | -3.71 | 1.39 | 1.47 |
| 5 | F | 500 | GTP | C5-C6 | -3.69 | 1.39 | 1.47 |
| 5 | H | 500 | GTP | C5-C6 | -3.67 | 1.39 | 1.47 |
| 5 | B | 500 | GTP | PG-O1G | 3.63 | 1.62 | 1.50 |
| 4 | G | 600 | GDP | C8-N7 | 3.55 | 1.41 | 1.35 |
| 4 | A | 600 | GDP | C8-N7 | 3.53 | 1.41 | 1.35 |
| 4 | E | 600 | GDP | C8-N7 | 3.48 | 1.40 | 1.35 |
| 4 | C | 600 | GDP | C8-N7 | 3.46 | 1.40 | 1.35 |
| 4 | E | 600 | GDP | C5-C6 | -2.88 | 1.41 | 1.47 |
| 4 | A | 600 | GDP | C5-C6 | -2.87 | 1.41 | 1.47 |
| 4 | C | 600 | GDP | C5-C6 | -2.87 | 1.41 | 1.47 |
| 4 | G | 600 | GDP | C5-C6 | -2.84 | 1.41 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | D | 500 | GTP | C6-N1 | 2.59 | 1.41 | 1.37 |
| 5 | H | 500 | GTP | C6-N1 | 2.58 | 1.41 | 1.37 |
| 5 | F | 500 | GTP | C6-N1 | 2.58 | 1.41 | 1.37 |
| 5 | B | 500 | GTP | C6-N1 | 2.58 | 1.41 | 1.37 |
| 5 | B | 500 | GTP | C8-N7 | -2.43 | 1.30 | 1.35 |
| 4 | E | 600 | GDP | C2-N3 | -2.41 | 1.27 | 1.33 |
| 5 | D | 500 | GTP | C8-N7 | -2.41 | 1.30 | 1.35 |
| 5 | F | 500 | GTP | C8-N7 | -2.40 | 1.30 | 1.35 |
| 4 | A | 600 | GDP | C2-N3 | -2.39 | 1.27 | 1.33 |
| 5 | H | 500 | GTP | C8-N7 | -2.39 | 1.31 | 1.35 |
| 4 | G | 600 | GDP | C2-N3 | -2.38 | 1.27 | 1.33 |
| 4 | C | 600 | GDP | C2-N3 | -2.38 | 1.27 | 1.33 |
| 4 | G | 600 | GDP | PB-O3B | 2.37 | 1.64 | 1.54 |
| 4 | E | 600 | GDP | PB-O3B | 2.37 | 1.64 | 1.54 |
| 4 | C | 600 | GDP | PB-O3B | 2.35 | 1.63 | 1.54 |
| 4 | A | 600 | GDP | PB-O3B | 2.35 | 1.63 | 1.54 |
| 5 | F | 500 | GTP | O4'-C1' | 2.26 | 1.44 | 1.41 |
| 5 | B | 500 | GTP | O4'-C1' | 2.24 | 1.44 | 1.41 |
| 5 | H | 500 | GTP | O4'-C1' | 2.21 | 1.44 | 1.41 |
| 5 | D | 500 | GTP | O4'-C1' | 2.21 | 1.44 | 1.41 |
| 4 | G | 600 | GDP | O3'-C3' | 2.07 | 1.47 | 1.43 |
| 4 | E | 600 | GDP | O3'-C3' | 2.07 | 1.47 | 1.43 |
| 4 | A | 600 | GDP | O3'-C3' | 2.06 | 1.47 | 1.43 |
| 4 | C | 600 | GDP | O3'-C3' | 2.05 | 1.47 | 1.43 |
| 5 | H | 500 | GTP | PB-O2B | -2.01 | 1.45 | 1.55 |
| 5 | D | 500 | GTP | PB-O2B | -2.00 | 1.45 | 1.55 |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 600 | GDP | C8-N7-C5 | 9.30 | 120.70 | 102.99 |
| 4 | C | 600 | GDP | C8-N7-C5 | 9.29 | 120.68 | 102.99 |
| 4 | E | 600 | GDP | C8-N7-C5 | 9.28 | 120.66 | 102.99 |
| 4 | G | 600 | GDP | C8-N7-C5 | 9.28 | 120.66 | 102.99 |
| 4 | E | 600 | GDP | N2-C2-N3 | 6.30 | 131.99 | 119.74 |
| 4 | C | 600 | GDP | N2-C2-N3 | 6.28 | 131.97 | 119.74 |
| 4 | A | 600 | GDP | N2-C2-N3 | 6.28 | 131.96 | 119.74 |
| 4 | G | 600 | GDP | N2-C2-N3 | 6.25 | 131.91 | 119.74 |
| 4 | G | 600 | GDP | C5-C6-N1 | 6.06 | 124.66 | 113.95 |
| 4 | A | 600 | GDP | C5-C6-N1 | 6.06 | 124.65 | 113.95 |
| 4 | E | 600 | GDP | C5-C6-N1 | 6.06 | 124.65 | 113.95 |
| 4 | C | 600 | GDP | C5-C6-N1 | 6.06 | 124.64 | 113.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | B | 500 | GTP | O2G-PG-O3B | 5.04 | 121.55 | 104.64 |
| 5 | B | 500 | GTP | O3G-PG-O3B | 4.41 | 119.42 | 104.64 |
| 4 | C | 600 | GDP | O6-C6-C5 | -4.24 | 116.09 | 124.37 |
| 4 | G | 600 | GDP | O6-C6-C5 | -4.23 | 116.10 | 124.37 |
| 4 | E | 600 | GDP | O6-C6-C5 | -4.22 | 116.12 | 124.37 |
| 4 | A | 600 | GDP | O6-C6-C5 | -4.22 | 116.13 | 124.37 |
| 4 | E | 600 | GDP | N2-C2-N1 | -4.20 | 107.78 | 116.71 |
| 4 | A | 600 | GDP | N2-C2-N1 | -4.20 | 107.78 | 116.71 |
| 4 | C | 600 | GDP | N2-C2-N1 | -4.19 | 107.80 | 116.71 |
| 4 | G | 600 | GDP | N2-C2-N1 | -4.17 | 107.83 | 116.71 |
| 4 | A | 600 | GDP | C2-N1-C6 | -3.72 | 118.25 | 125.10 |
| 4 | E | 600 | GDP | C2-N1-C6 | -3.72 | 118.25 | 125.10 |
| 4 | C | 600 | GDP | C2-N1-C6 | -3.70 | 118.28 | 125.10 |
| 4 | G | 600 | GDP | C2-N1-C6 | -3.70 | 118.29 | 125.10 |
| 4 | C | 600 | GDP | C2'-C3'-C4' | 3.40 | 109.24 | 102.64 |
| 4 | E | 600 | GDP | C2'-C3'-C4' | 3.38 | 109.21 | 102.64 |
| 4 | G | 600 | GDP | C2'-C3'-C4' | 3.37 | 109.19 | 102.64 |
| 4 | A | 600 | GDP | C2'-C3'-C4' | 3.36 | 109.17 | 102.64 |
| 5 | D | 500 | GTP | O2G-PG-O3B | 2.98 | 114.63 | 104.64 |
| 5 | F | 500 | GTP | O2G-PG-O3B | 2.93 | 114.45 | 104.64 |
| 5 | H | 500 | GTP | O2G-PG-O3B | 2.92 | 114.43 | 104.64 |
| 5 | B | 500 | GTP | O3G-PG-O2G | -2.57 | 97.80 | 107.64 |
| 5 | D | 500 | GTP | O3G-PG-O3B | 2.53 | 113.14 | 104.64 |
| 5 | H | 500 | GTP | O3G-PG-O3B | 2.49 | 112.99 | 104.64 |
| 5 | F | 500 | GTP | O3G-PG-O3B | 2.48 | 112.96 | 104.64 |
| 4 | C | 600 | GDP | O2'-C2'-C3' | 2.26 | 119.12 | 111.82 |
| 4 | G | 600 | GDP | O2'-C2'-C3' | 2.26 | 119.12 | 111.82 |
| 4 | A | 600 | GDP | O2'-C2'-C3' | 2.25 | 119.09 | 111.82 |
| 4 | E | 600 | GDP | O2'-C2'-C3' | 2.24 | 119.06 | 111.82 |
| 5 | H | 500 | GTP | O5'-C5'-C4' | 2.06 | 116.08 | 108.99 |
| 5 | D | 500 | GTP | O5'-C5'-C4' | 2.05 | 116.06 | 108.99 |
| 5 | F | 500 | GTP | O5'-C5'-C4' | 2.05 | 116.03 | 108.99 |
| 5 | B | 500 | GTP | O5'-C5'-C4' | 2.04 | 116.02 | 108.99 |

There are no chirality outliers.

All (28) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 600 | GDP | PA-O3A-PB-O2B |
| 4 | A | 600 | GDP | C5'-O5'-PA-O3A |
| 4 | A | 600 | GDP | C5'-O5'-PA-O1A |
| 4 | C | 600 | GDP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | C | 600 | GDP | C5'-O5'-PA-O3A |
| 4 | C | 600 | GDP | C5'-O5'-PA-O1A |
| 4 | E | 600 | GDP | PA-O3A-PB-O2B |
| 4 | E | 600 | GDP | C5'-O5'-PA-O3A |
| 4 | E | 600 | GDP | C5'-O5'-PA-O1A |
| 4 | G | 600 | GDP | PA-O3A-PB-O2B |
| 4 | G | 600 | GDP | C5'-O5'-PA-O3A |
| 4 | G | 600 | GDP | C5'-O5'-PA-O1A |
| 5 | D | 500 | GTP | C3'-C4'-C5'-O5' |
| 5 | F | 500 | GTP | C3'-C4'-C5'-O5' |
| 5 | B | 500 | GTP | C3'-C4'-C5'-O5' |
| 5 | H | 500 | GTP | C3'-C4'-C5'-O5' |
| 5 | B | 500 | GTP | O4'-C4'-C5'-O5' |
| 5 | D | 500 | GTP | O4'-C4'-C5'-O5' |
| 5 | F | 500 | GTP | O4'-C4'-C5'-O5' |
| 5 | H | 500 | GTP | O4'-C4'-C5'-O5' |
| 4 | A | 600 | GDP | PA-O3A-PB-O3B |
| 4 | C | 600 | GDP | PA-O3A-PB-O3B |
| 4 | E | 600 | GDP | PA-O3A-PB-O3B |
| 4 | G | 600 | GDP | PA-O3A-PB-O3B |
| 5 | B | 500 | GTP | PG-O3B-PB-O1B |
| 5 | D | 500 | GTP | PG-O3B-PB-O1B |
| 5 | F | 500 | GTP | PG-O3B-PB-O1B |
| 5 | H | 500 | GTP | PG-O3B-PB-O1B |

There are no ring outliers.

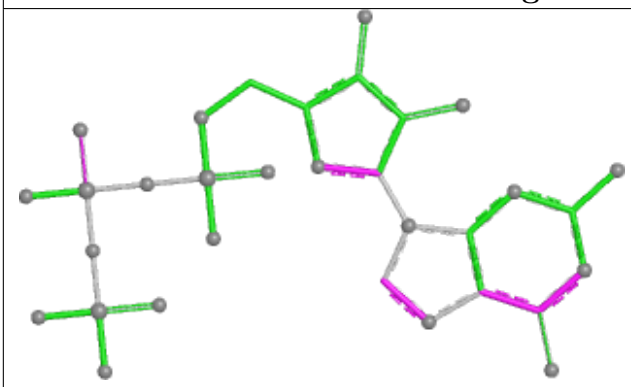
8 monomers are involved in 26 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | D | 500 | GTP | 4 | 0 |
| 5 | B | 500 | GTP | 5 | 0 |
| 5 | F | 500 | GTP | 5 | 0 |
| 4 | G | 600 | GDP | 4 | 0 |
| 4 | C | 600 | GDP | 1 | 0 |
| 4 | A | 600 | GDP | 1 | 0 |
| 5 | H | 500 | GTP | 5 | 0 |
| 4 | E | 600 | GDP | 1 | 0 |

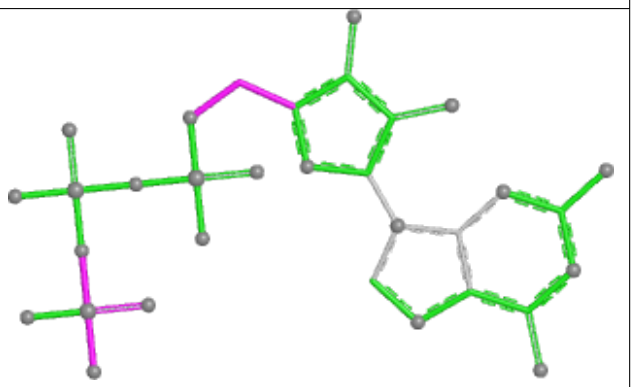
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

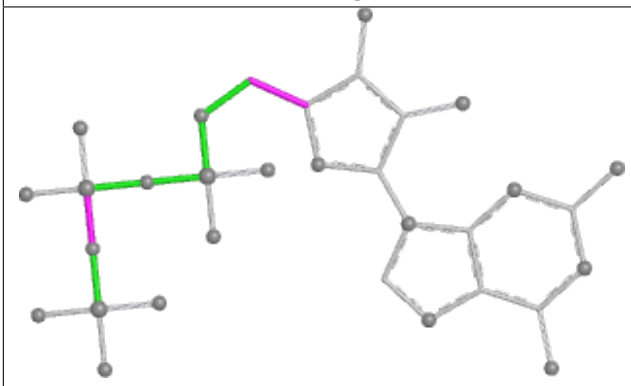
**Ligand GTP D 500**



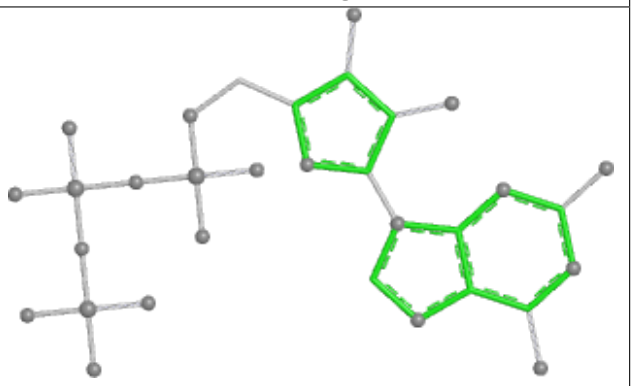
**Bond lengths**



**Bond angles**

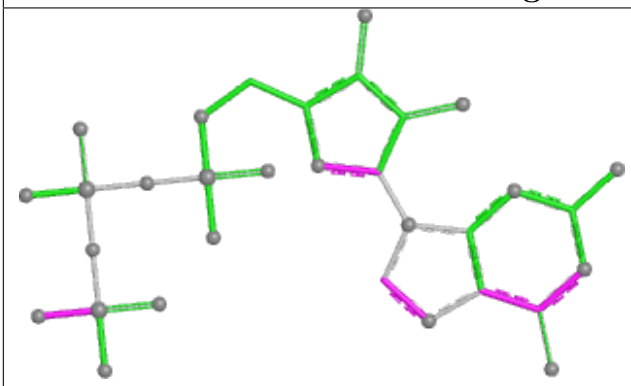


**Torsions**

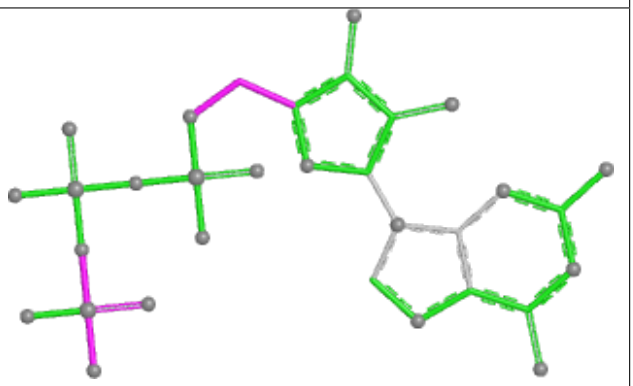


**Rings**

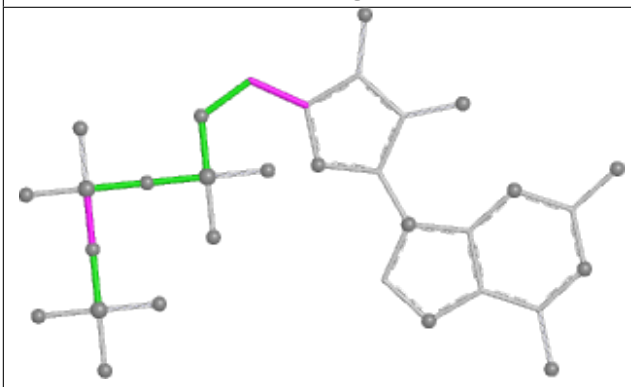
## Ligand GTP B 500



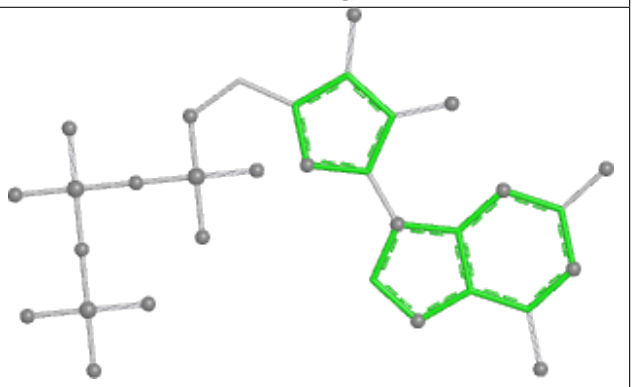
Bond lengths



Bond angles

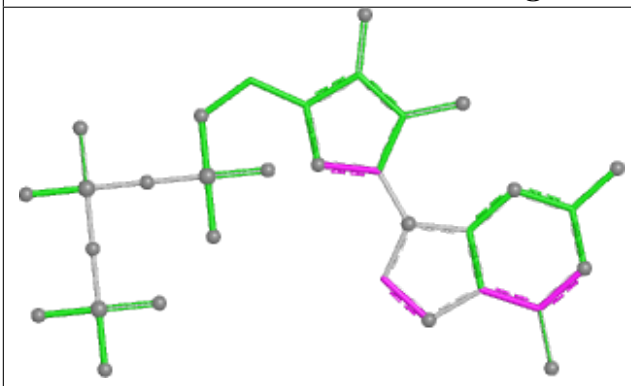


Torsions

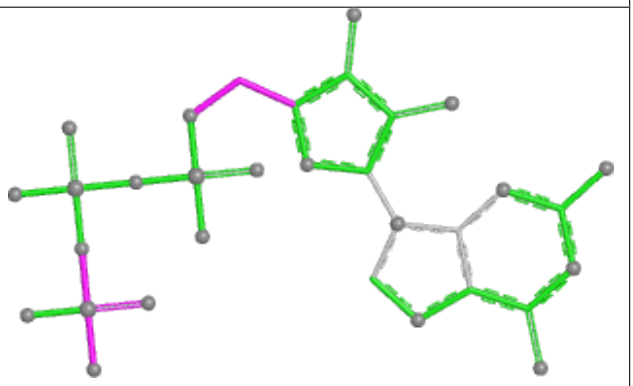


Rings

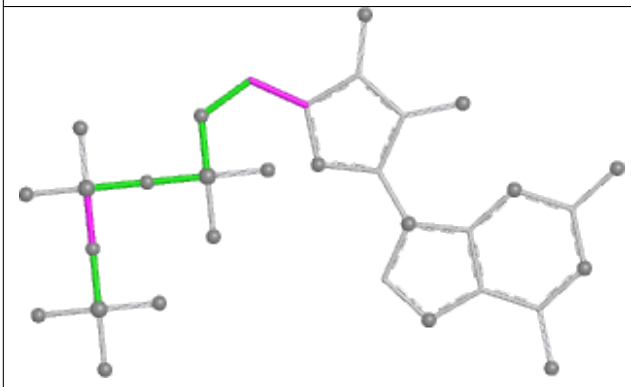
## Ligand GTP F 500



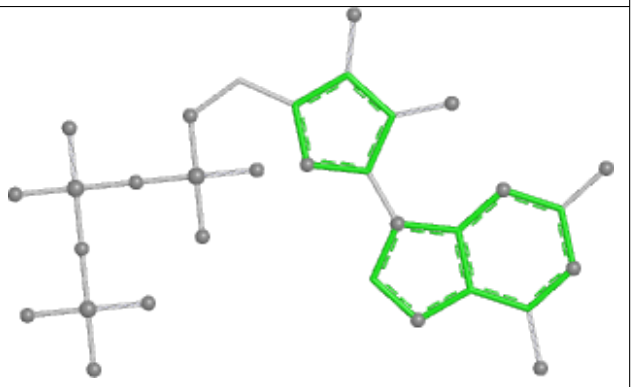
Bond lengths



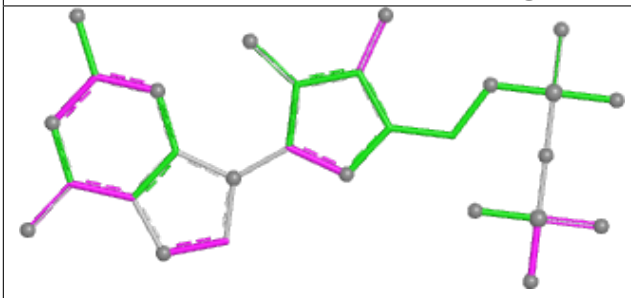
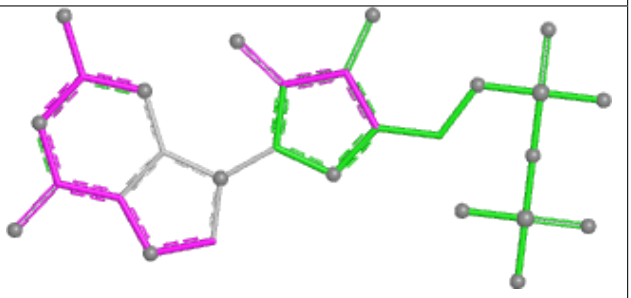
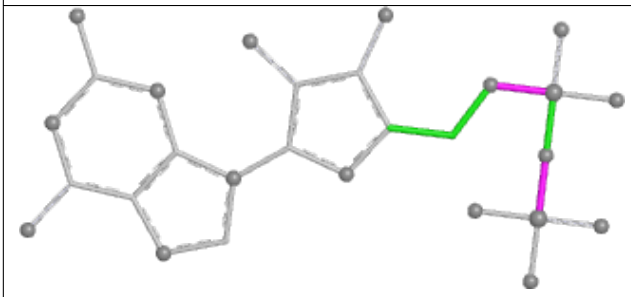
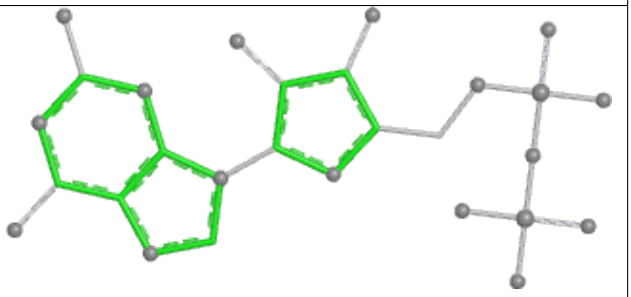
Bond angles

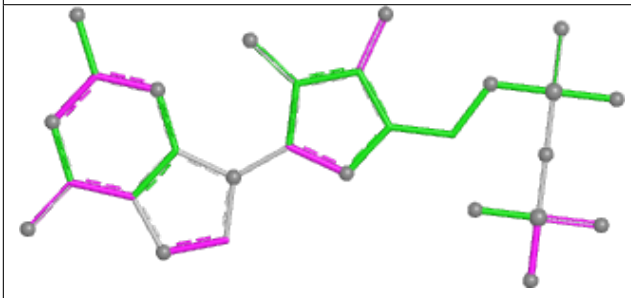
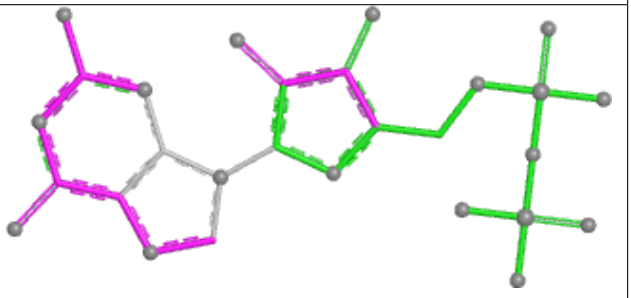
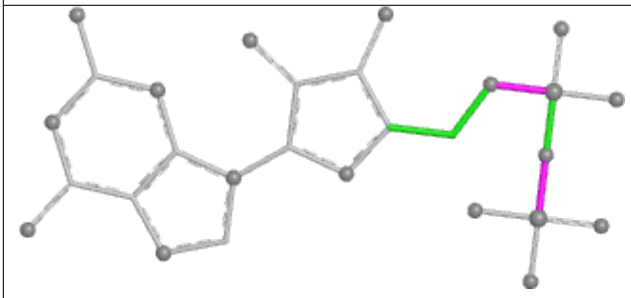
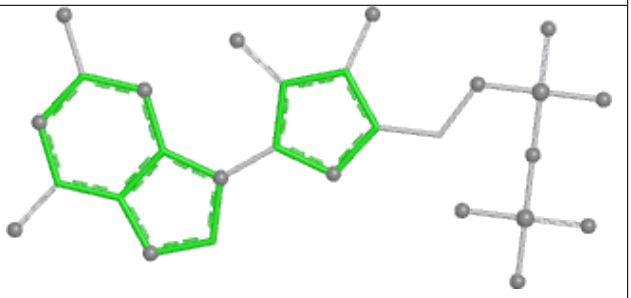


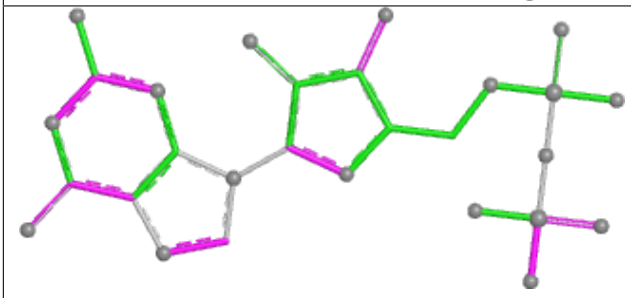
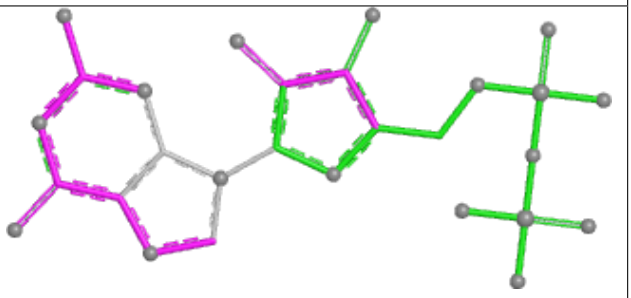
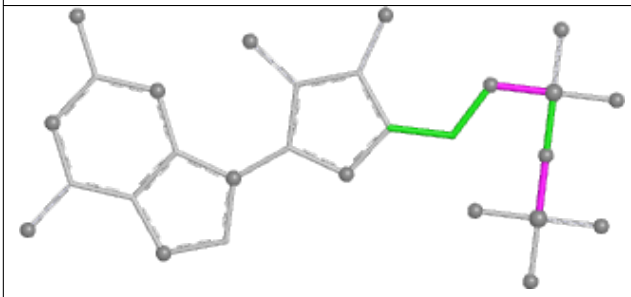
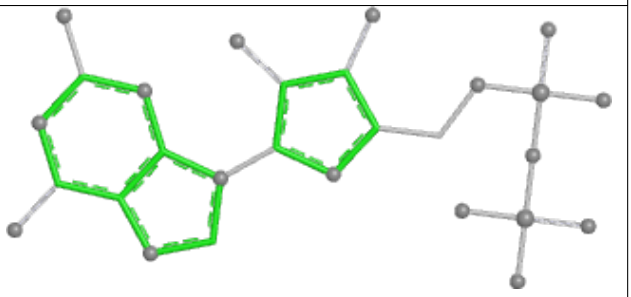
Torsions

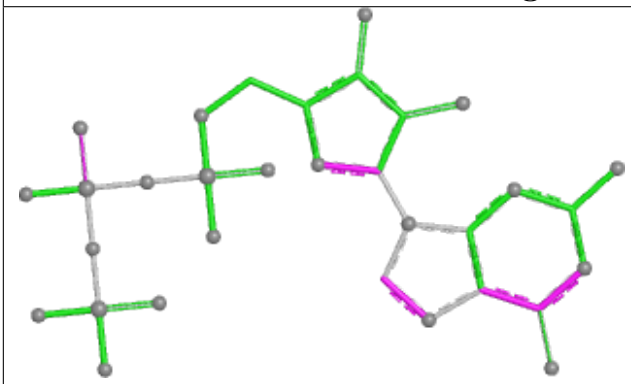
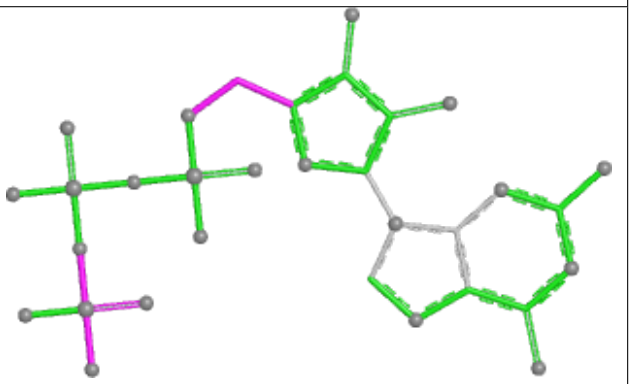
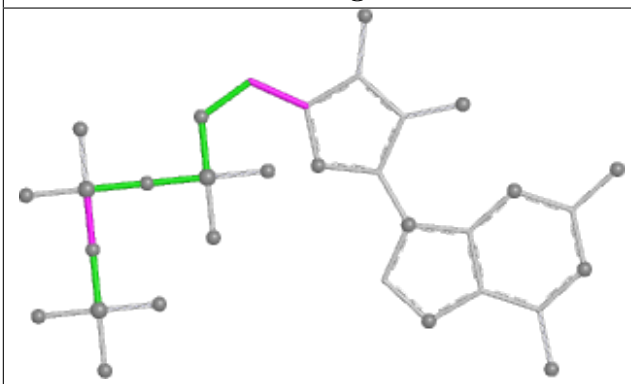
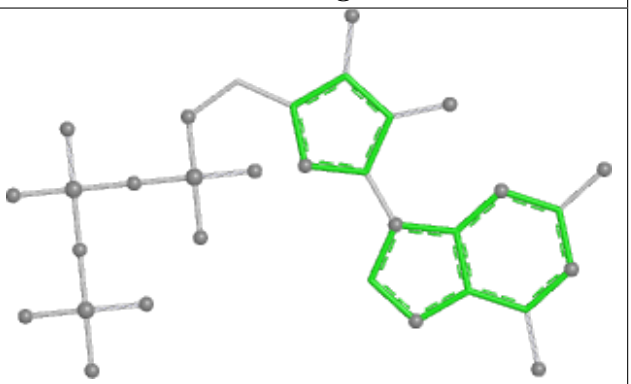


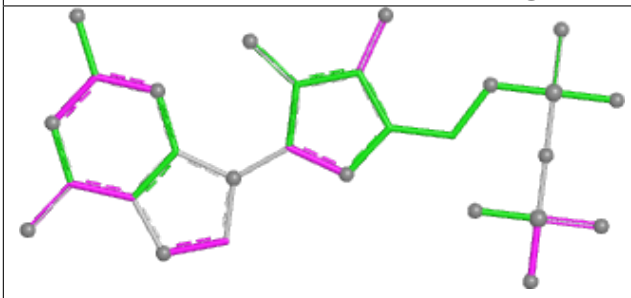
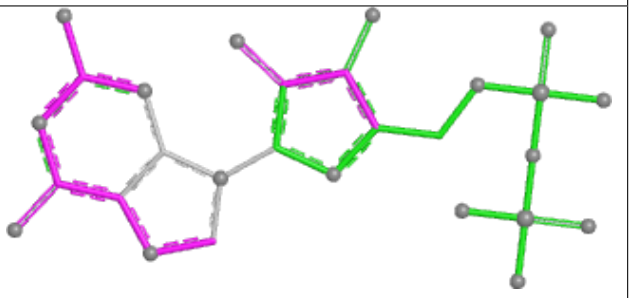
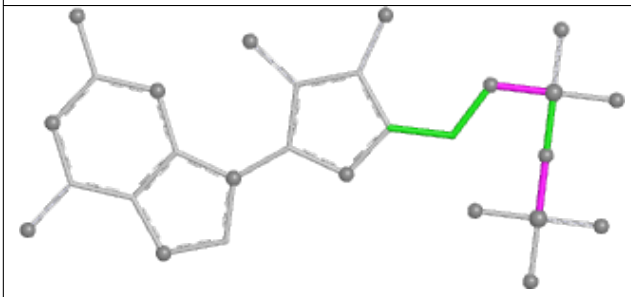
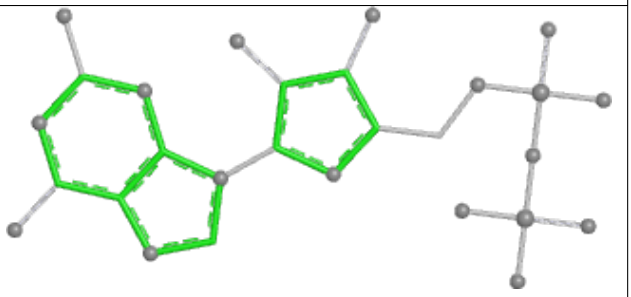
Rings

| Ligand GDP G 600 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP C 600 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP A 600 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GTP H 500 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP E 600 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 2 | B | 4 |
| 2 | D | 4 |
| 2 | F | 4 |
| 2 | H | 4 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | B | 274:PRO | C | 275:VAL | N | 2.09 |
| 1 | D | 274:PRO | C | 275:VAL | N | 2.09 |
| 1 | F | 274:PRO | C | 275:VAL | N | 2.09 |
| 1 | H | 274:PRO | C | 275:VAL | N | 2.09 |
| 1 | B | 92:LEU | C | 93:ILE | N | 1.98 |
| 1 | D | 92:LEU | C | 93:ILE | N | 1.98 |
| 1 | F | 92:LEU | C | 93:ILE | N | 1.98 |
| 1 | H | 92:LEU | C | 93:ILE | N | 1.98 |

*Continued on next page...*

*Continued from previous page...*

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | B | 298:PRO | C | 299:ALA | N | 1.73 |
| 1 | D | 298:PRO | C | 299:ALA | N | 1.73 |
| 1 | F | 298:PRO | C | 299:ALA | N | 1.73 |
| 1 | H | 298:PRO | C | 299:ALA | N | 1.73 |
| 1 | B | 68:VAL | C | 69:ASP | N | 1.67 |
| 1 | D | 68:VAL | C | 69:ASP | N | 1.67 |
| 1 | F | 68:VAL | C | 69:ASP | N | 1.67 |
| 1 | H | 68:VAL | C | 69:ASP | N | 1.67 |

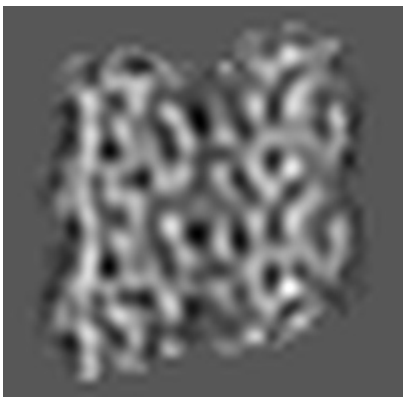
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1788. These allow visual inspection of the internal detail of the map and identification of artifacts.

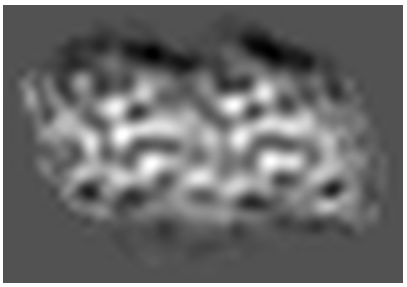
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

### 6.1.1 Primary map



X



Y

Z

The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

### 6.2.1 Primary map

X Index: 17

Y Index: 25

Z Index: 24

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

### 6.3.1 Primary map

X Index: 17

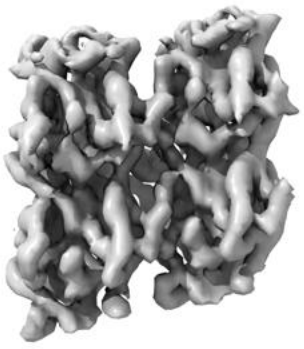
Y Index: 10

Z Index: 32

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.92. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

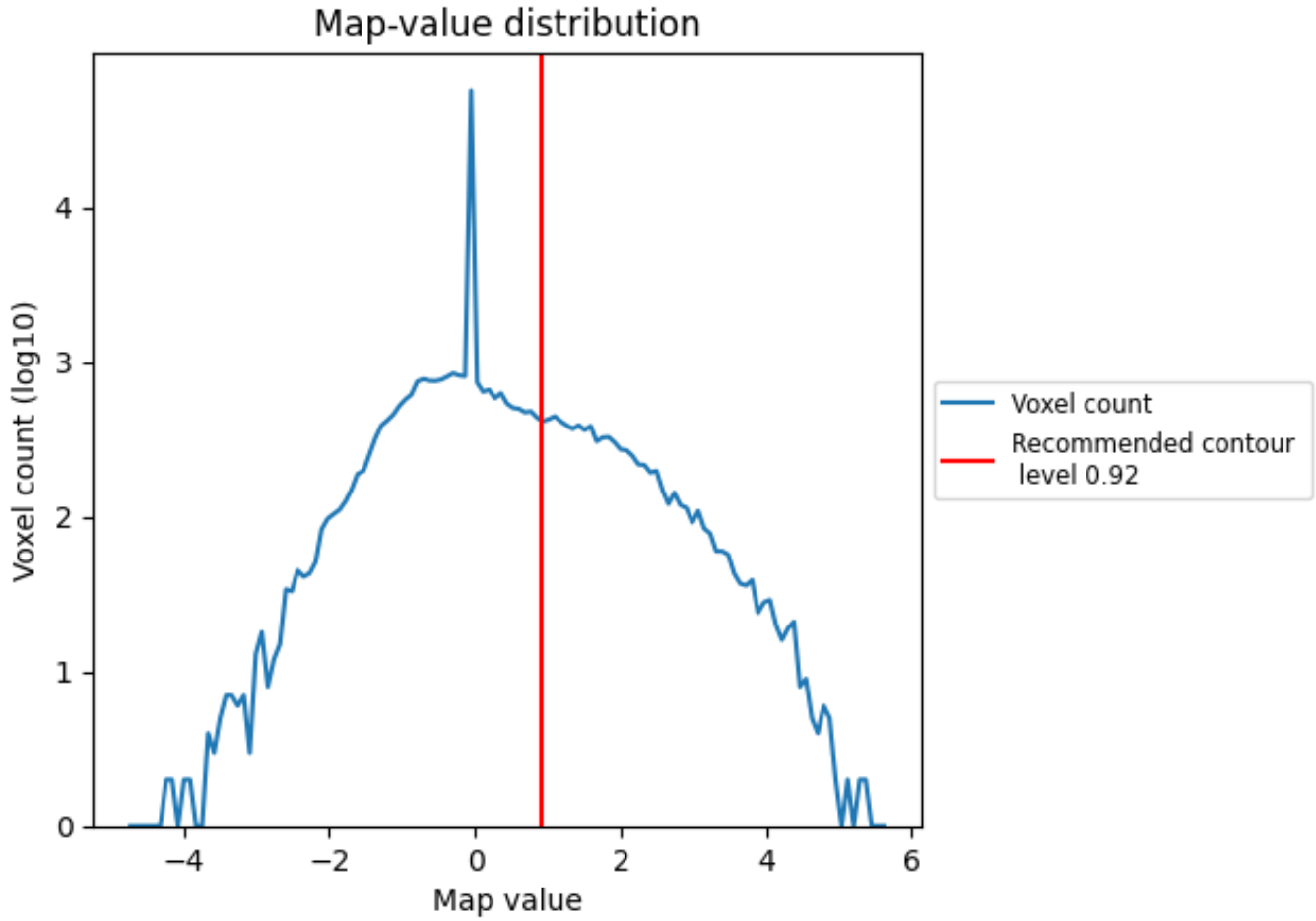
## 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

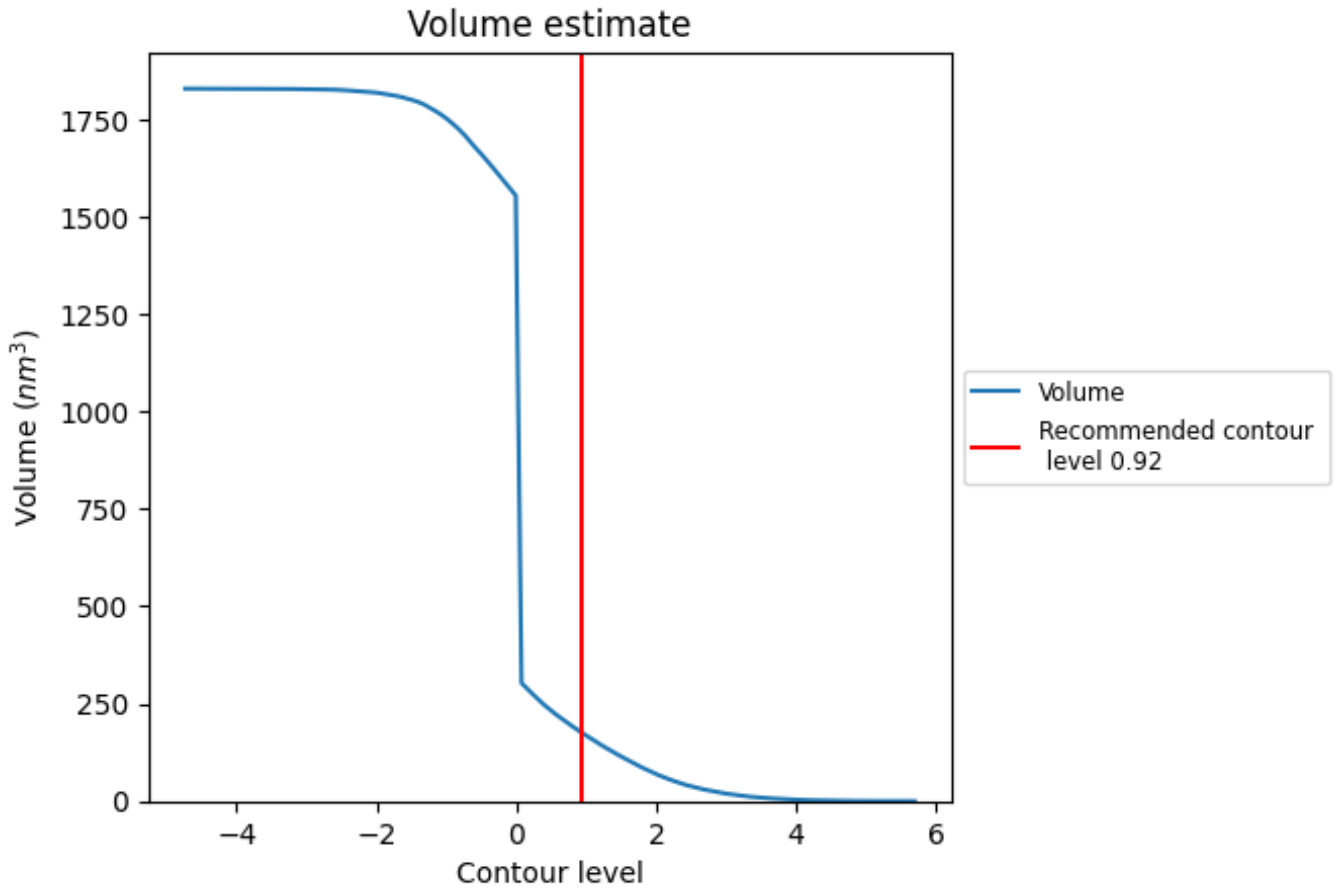
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate




The volume at the recommended contour level is 178 $nm^3$; this corresponds to an approximate mass of 160 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

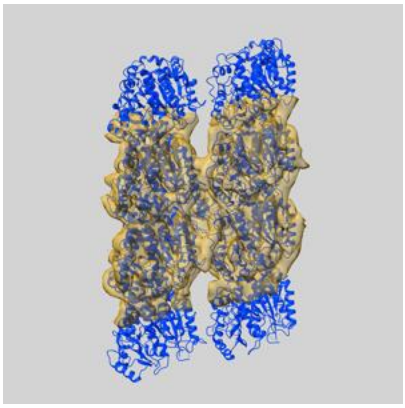
# 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

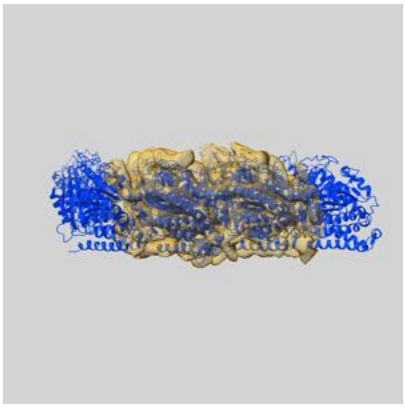
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1788 and PDB model 2XRP. Per-residue inclusion information can be found in section 3 on page 8.

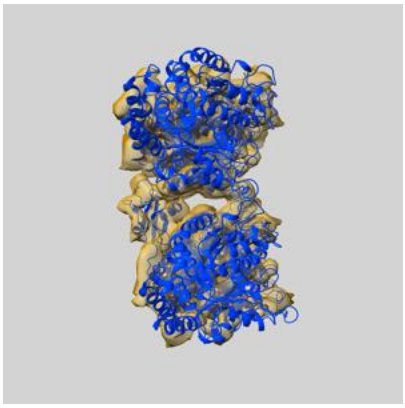
## 9.1 Map-model overlay



X



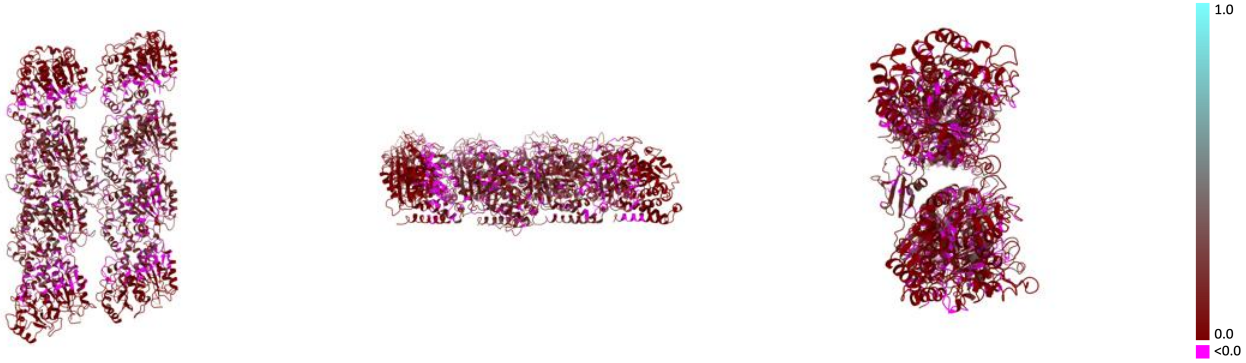
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.92 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

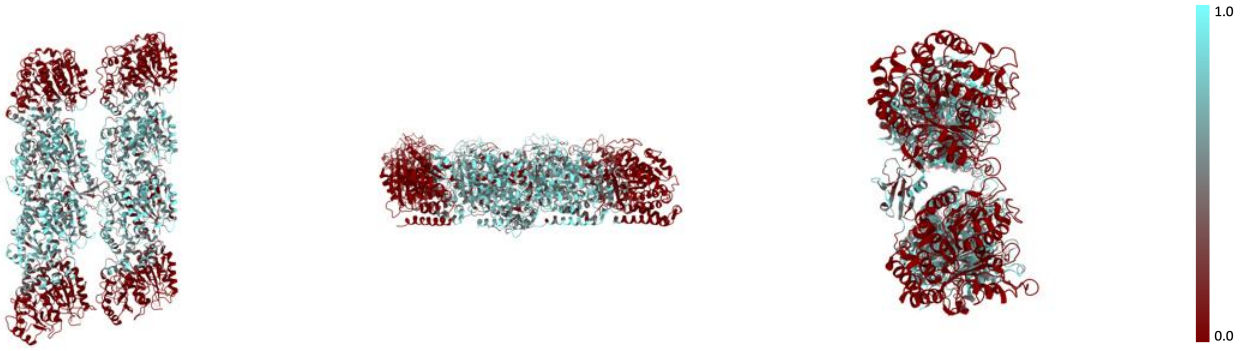
## 9.2 Q-score mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

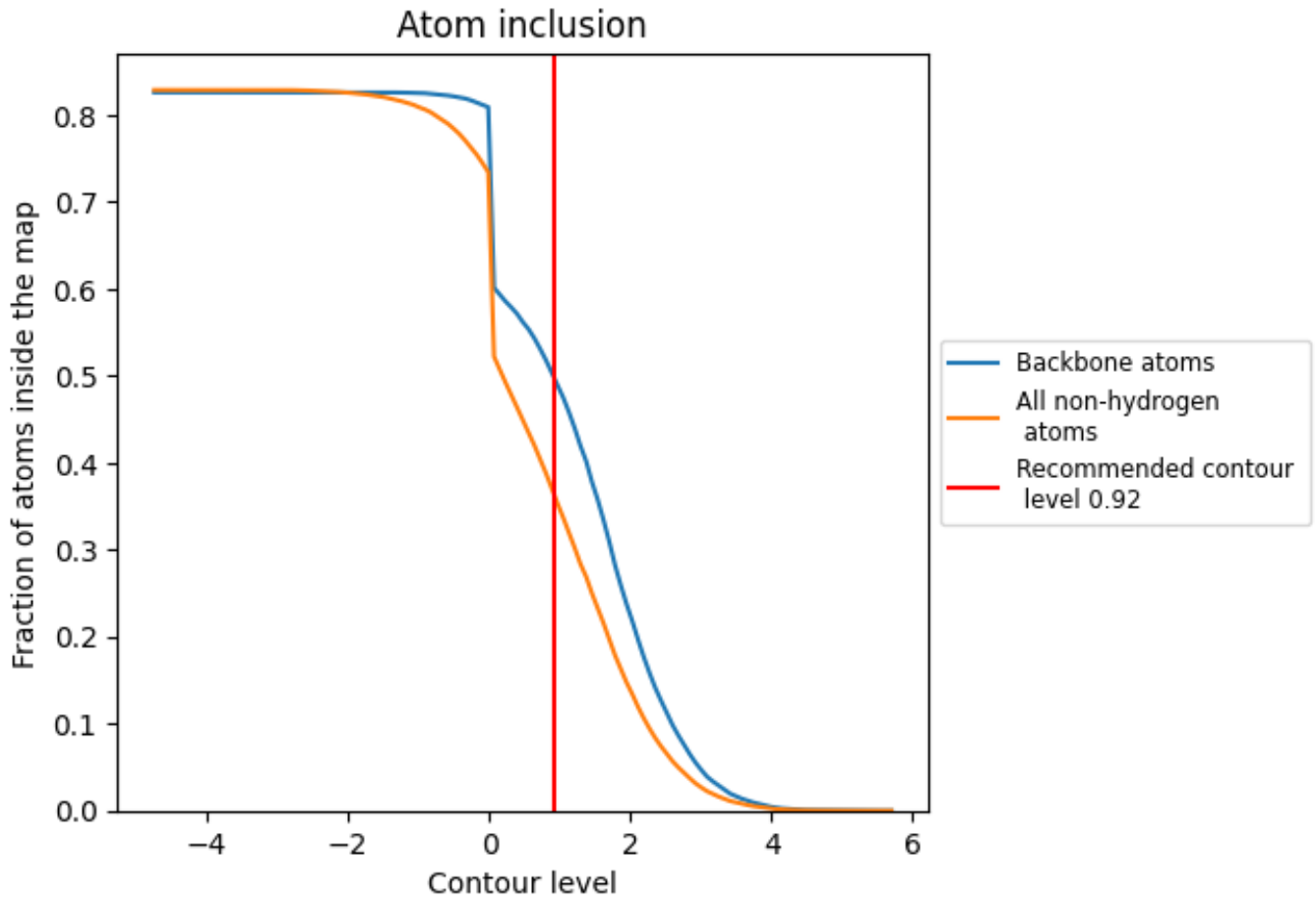
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.92).

## 9.4 Atom inclusion (i)




At the recommended contour level, 50% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.92) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.3643 | 0.0680 |
| A | 0.1219 | 0.0180 |
| B | 0.6069 | 0.1210 |
| C | 0.6287 | 0.1220 |
| D | 0.1190 | 0.0140 |
| E | 0.1158 | 0.0180 |
| F | 0.6102 | 0.1240 |
| G | 0.5810 | 0.1040 |
| H | 0.1263 | 0.0140 |
| I | 0.4303 | 0.1140 |