# Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 06:13 PM JST

| | | |
|---|---|---|
| PDB ID | : | 7YSG / pdb_00007ysg |
| EMDB ID | : | EMD-34074 |
| Title | : | Cryo-EM structure of human FcmR bound to sIgM |
| Authors | : | Li, Y.; Shen, H.; Xiao, J. |
| Deposited on | : | 2022-08-12 |
| Resolution | : | 3.18 Å(reported) |

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 ⓘ symbol.

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

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

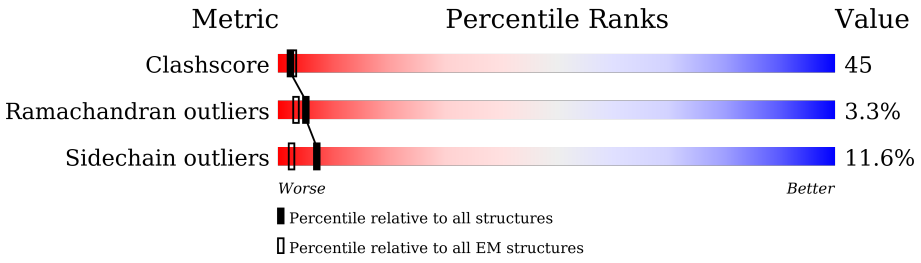
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev118 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0rc1 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.44 |

# 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 3.18 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 | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | 232 | 22% 41% 36% 18% 5% |
| 1 | B | 232 | 21% 36% 36% 22% • • |
| 1 | C | 232 | 31% 48% 36% 9% 5% • |
| 1 | D | 232 | 23% 56% 34% 5% • |
| 1 | E | 232 | 21% 48% 39% 6% • • |
| 1 | F | 232 | 19% 40% 36% 10% 10% • |
| 1 | G | 232 | 21% 56% 34% 5% • • |
| 1 | H | 232 | 24% 55% 32% 9% 5% |

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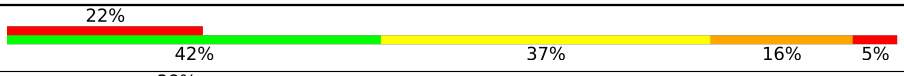
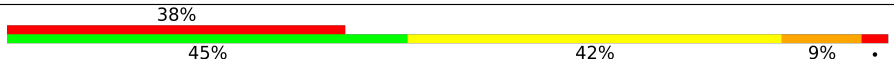
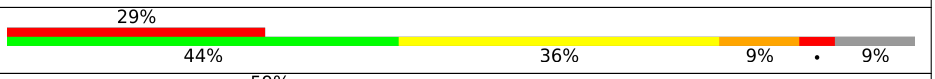
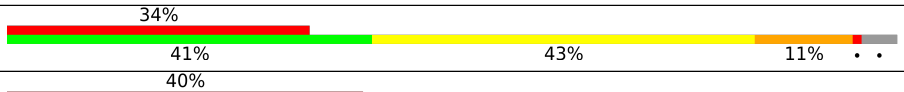
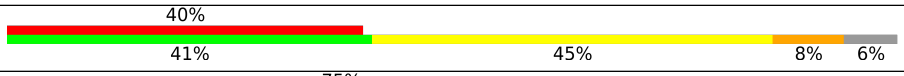
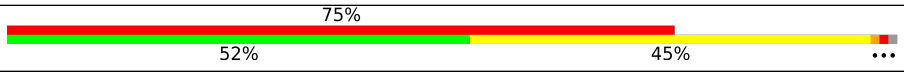
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | K | 232 |   |
| 1 | L | 232 |   |
| 2 | J | 136 |   |
| 3 | P | 541 |   |
| 4 | R | 107 |   |
| 4 | S | 107 |   |
| 4 | U | 107 |   |
| 4 | V | 107 |   |
| 5 | I | 2 |   |

# 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25676 atoms, of which 0 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 Immunoglobulin heavy constant mu.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1786 | 1123 | 303 | 351 | 9 | | |
| 1 | B | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1769 | 1114 | 300 | 347 | 8 | | |
| 1 | C | 227 | Total | C | N | O | S | 0 | 0 |
| | | | 1763 | 1111 | 299 | 345 | 8 | | |
| 1 | D | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1743 | 1100 | 296 | 339 | 8 | | |
| 1 | E | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1743 | 1100 | 296 | 339 | 8 | | |
| 1 | F | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1743 | 1100 | 296 | 339 | 8 | | |
| 1 | G | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1742 | 1100 | 296 | 338 | 8 | | |
| 1 | H | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1798 | 1132 | 304 | 353 | 9 | | |
| 1 | K | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1798 | 1132 | 304 | 353 | 9 | | |
| 1 | L | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1798 | 1132 | 304 | 353 | 9 | | |

- Molecule 2 is a protein called Immunoglobulin J chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | J | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 851 | 528 | 150 | 166 | 7 | | |

- Molecule 3 is a protein called Secretory component.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | P | 495 | Total | C | N | O | S | 0 | 0 |
| | | | 3851 | 2431 | 670 | 731 | 19 | | |

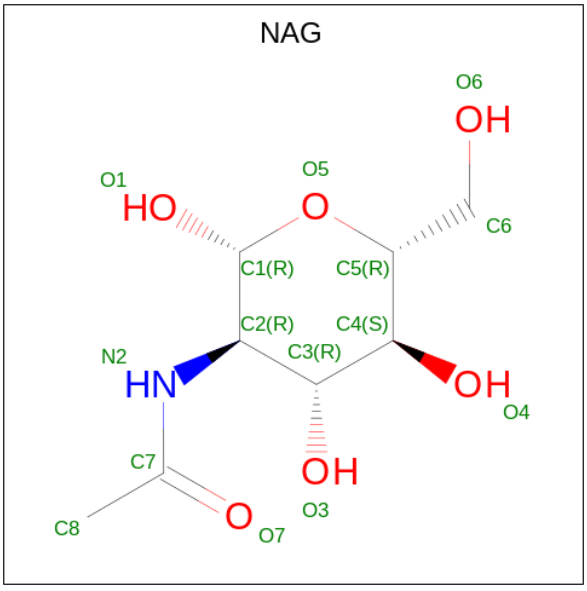
- Molecule 4 is a protein called Fas apoptotic inhibitory molecule 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | R | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 766 | 480 | 132 | 147 | 7 | | |
| 4 | S | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 785 | 492 | 137 | 149 | 7 | | |
| 4 | U | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 766 | 480 | 132 | 147 | 7 | | |
| 4 | V | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 504 | 140 | 154 | 7 | | |

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.


| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 5 | I | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 6 | A | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |

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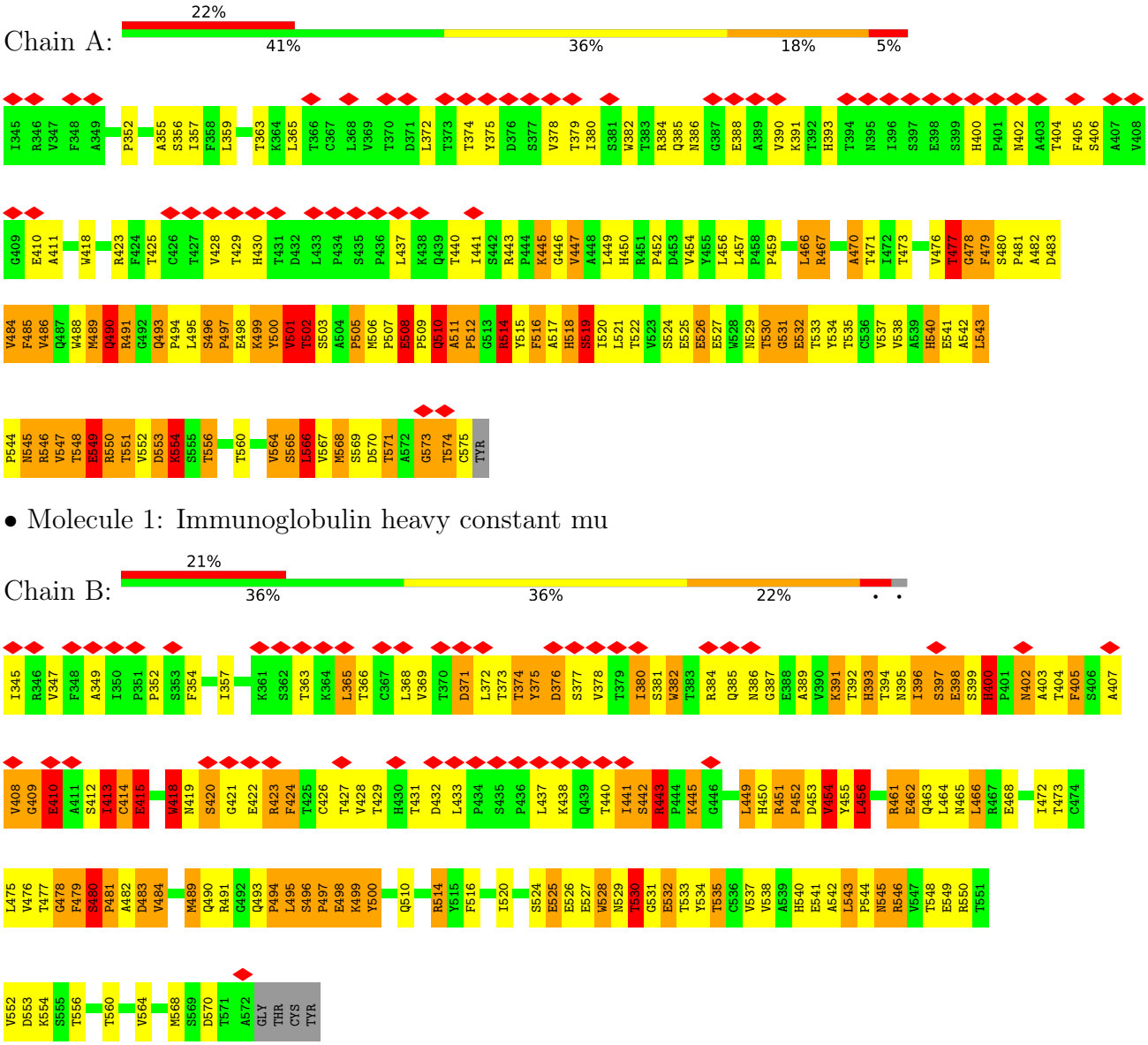
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 6 | B | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 6 | C | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 6 | D | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 6 | E | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 6 | F | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 6 | G | 1 | Total | C | N | O | 0 |
| | | | 15 | 8 | 1 | 6 | |
| 6 | H | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 6 | K | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 6 | L | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |

# 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.

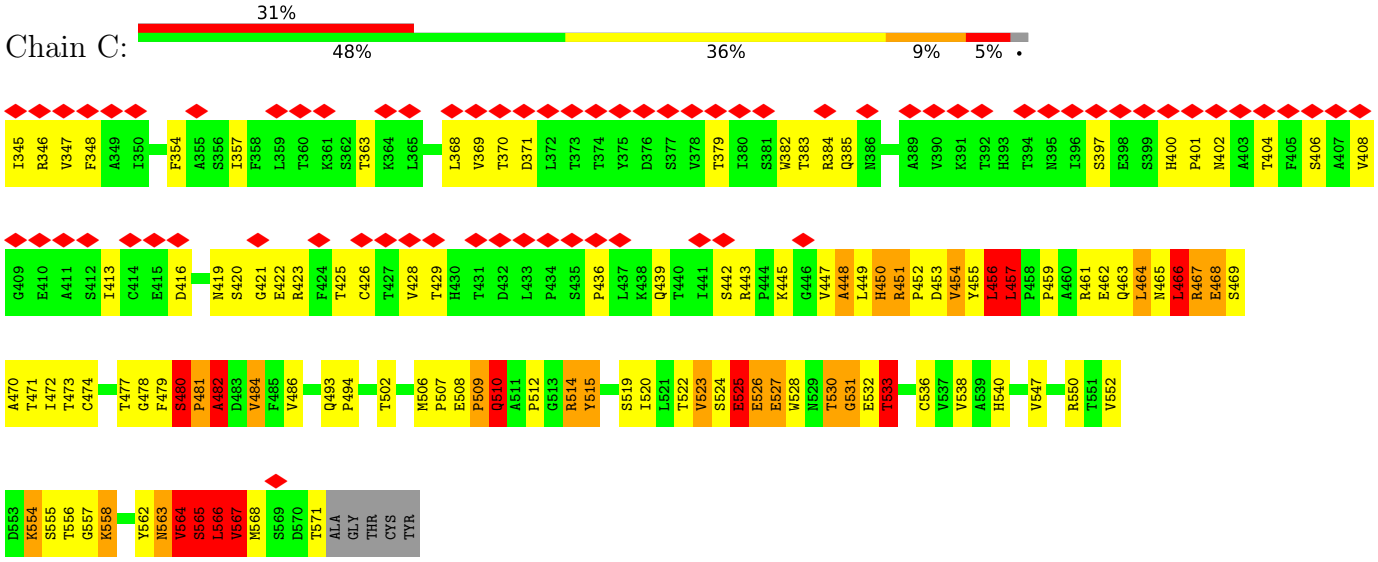
• Molecule 1: Immunoglobulin heavy constant mu



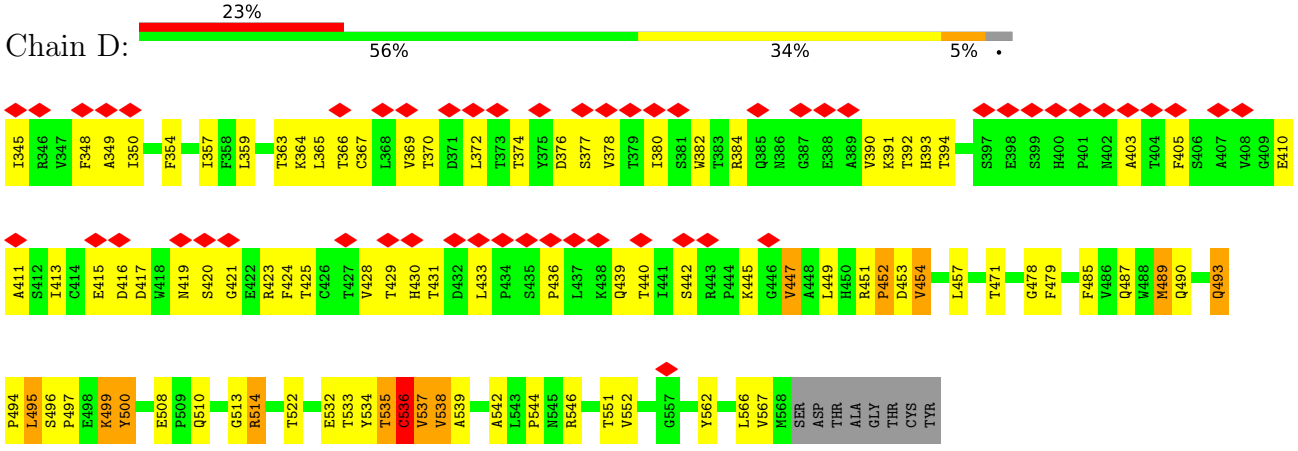

• Molecule 1: Immunoglobulin heavy constant mu



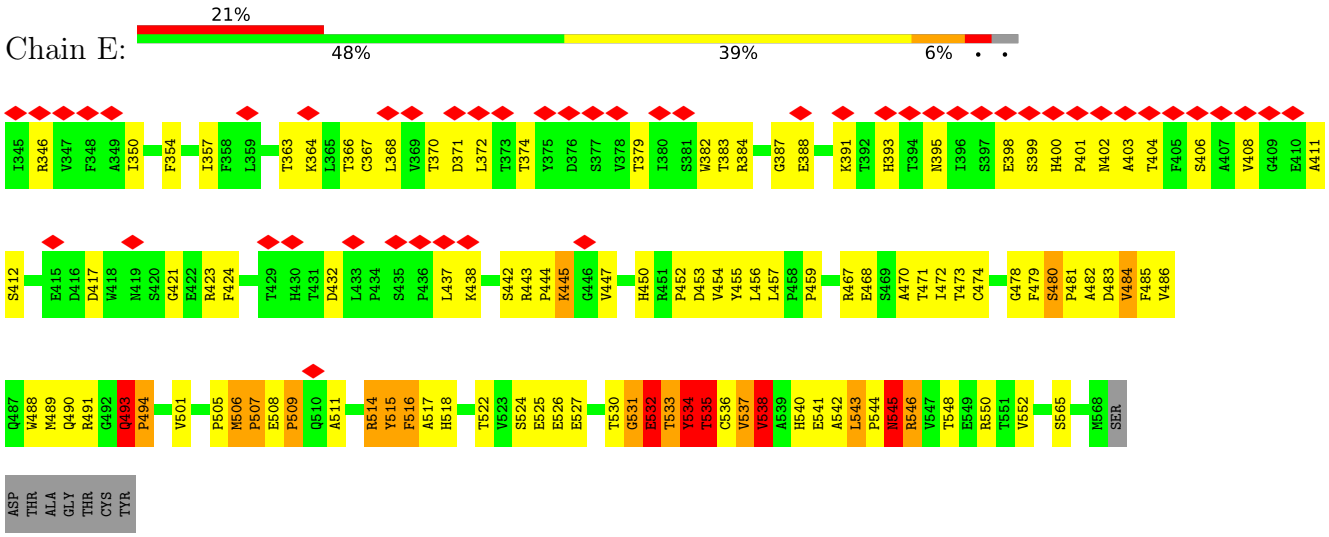

• Molecule 1: Immunoglobulin heavy constant mu




• Molecule 1: Immunoglobulin heavy constant mu

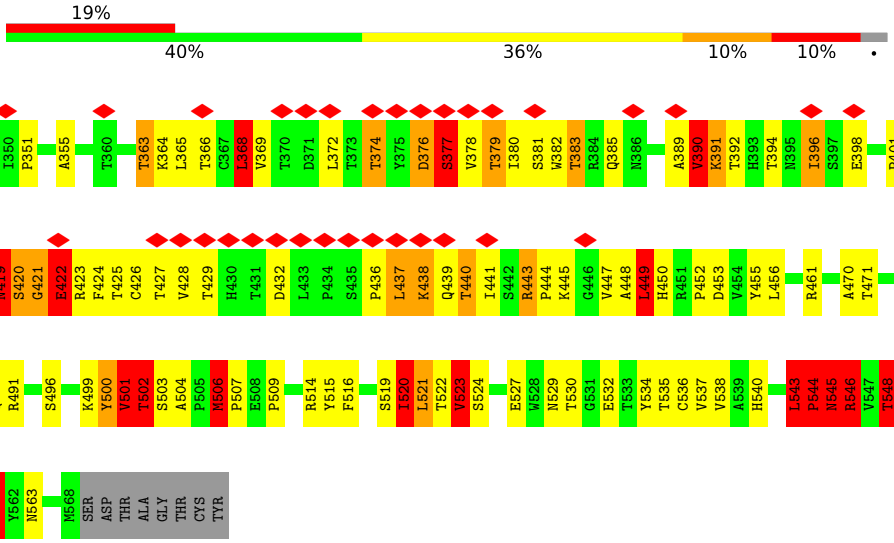



• Molecule 1: Immunoglobulin heavy constant mu



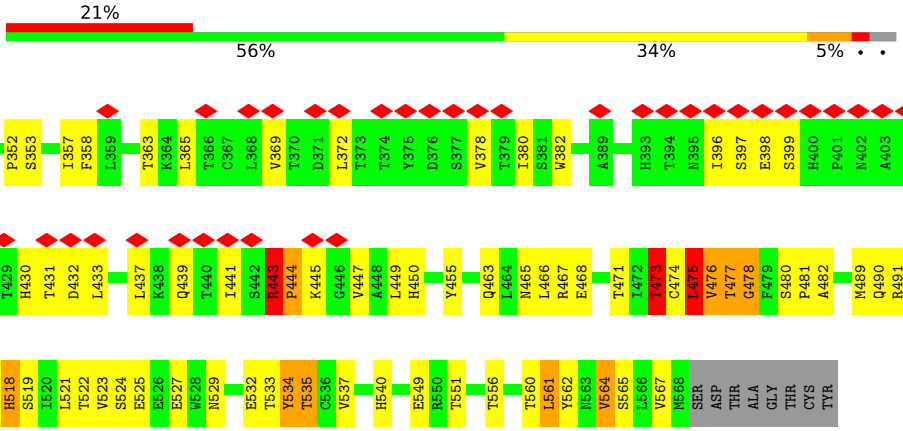

• Molecule 1: Immunoglobulin heavy constant mu

Chain F:



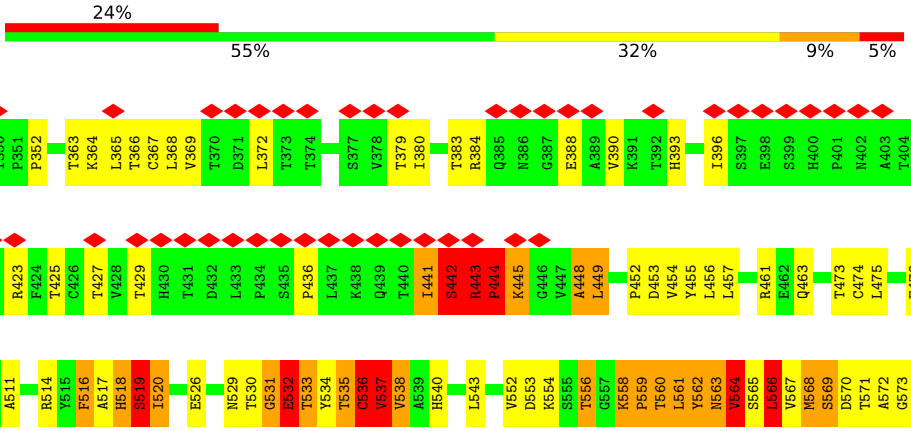

• Molecule 1: Immunoglobulin heavy constant mu

Chain G:



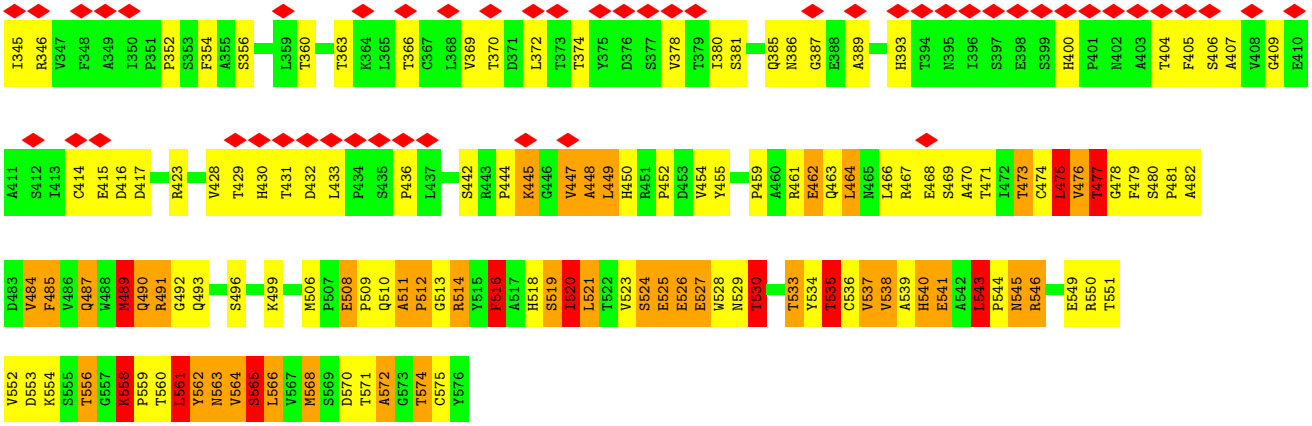

• Molecule 1: Immunoglobulin heavy constant mu

Chain H:

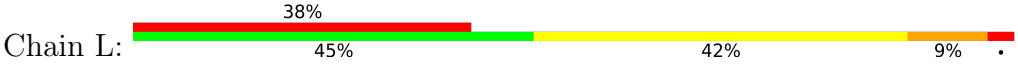


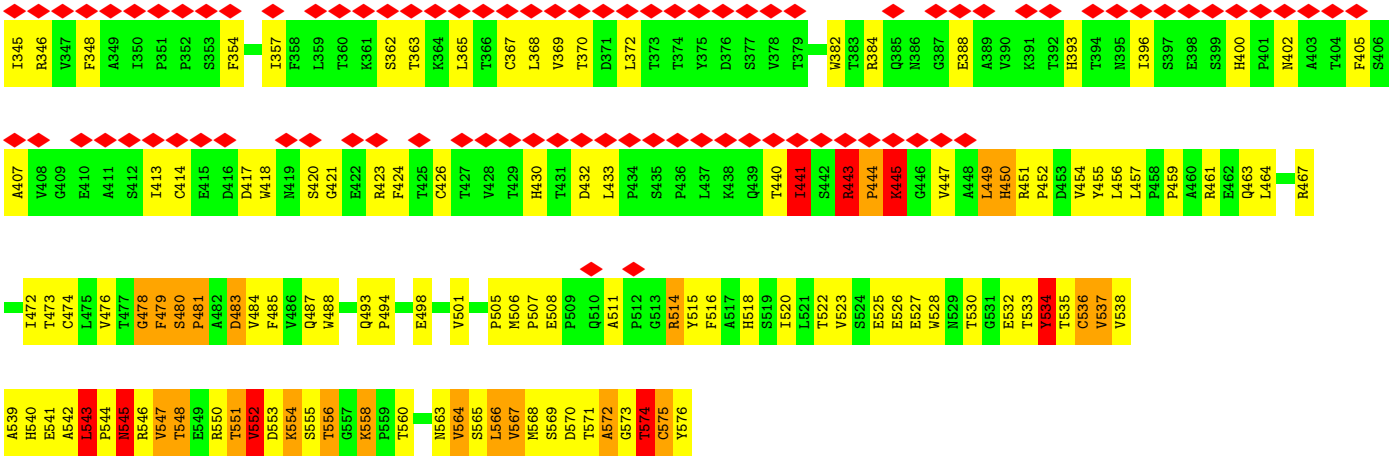

• Molecule 1: Immunoglobulin heavy constant mu

Chain K:

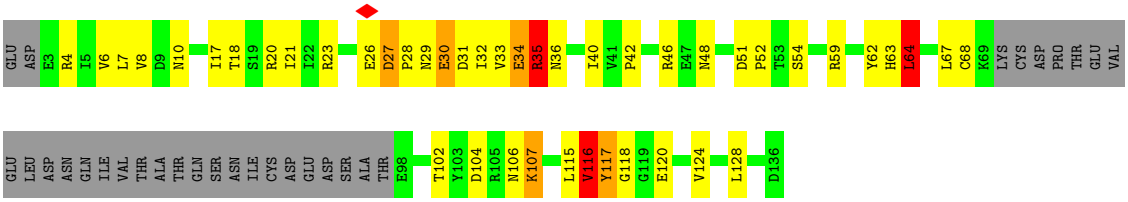


• Molecule 1: Immunoglobulin heavy constant mu

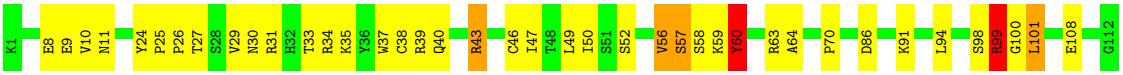


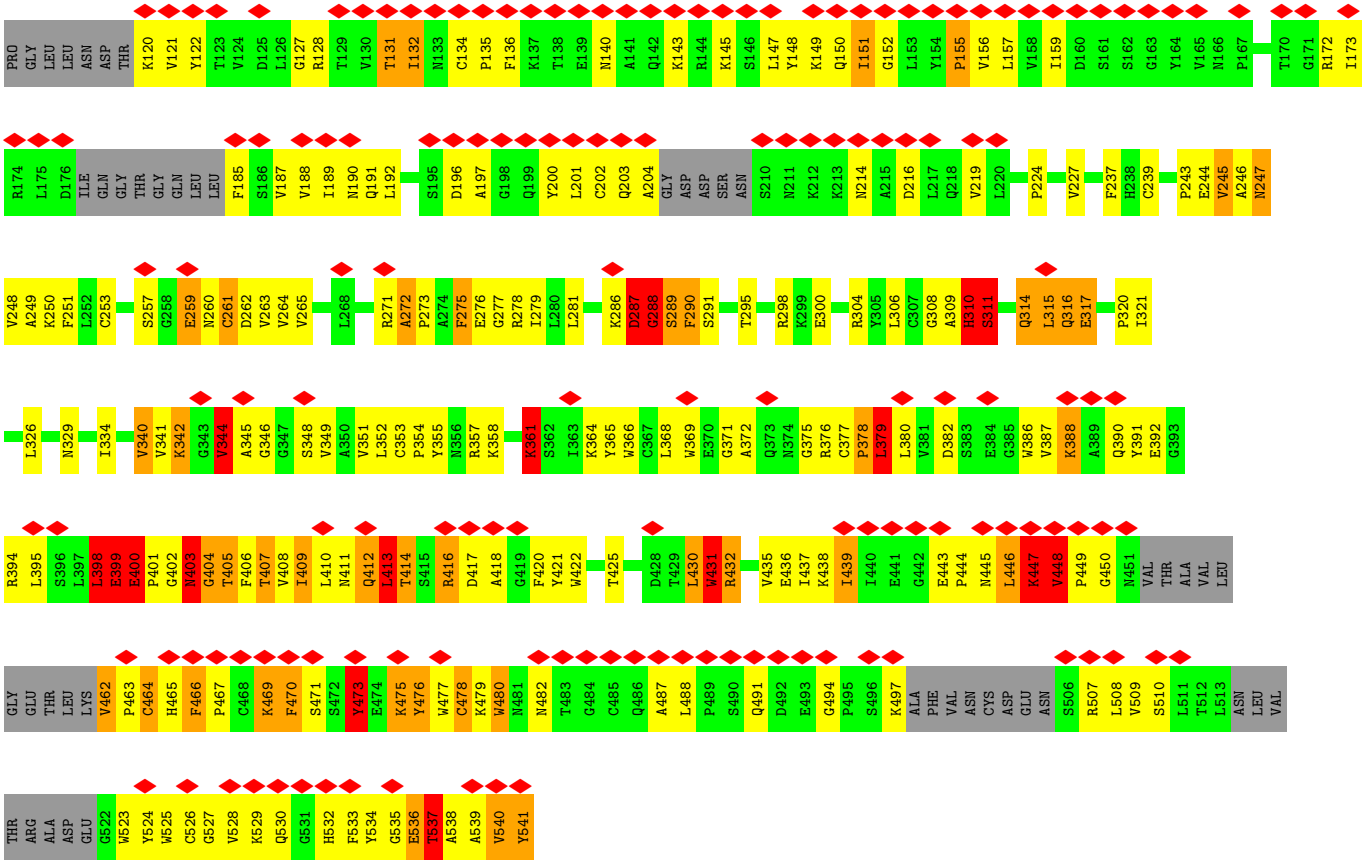



• Molecule 2: Immunoglobulin J chain

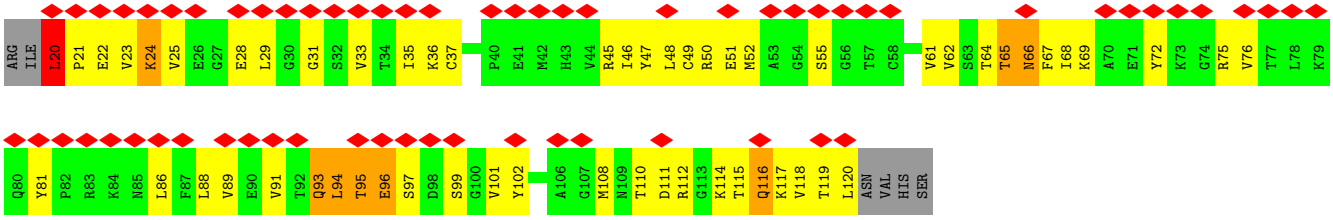
• Molecule 3: Secretory component



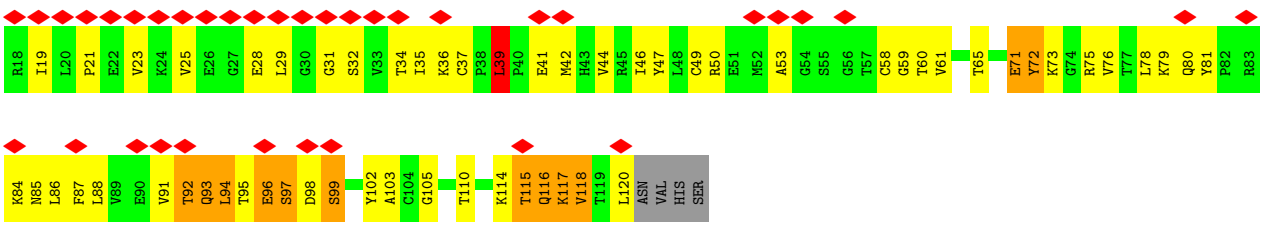
• Molecule 4: Fas apoptotic inhibitory molecule 3

Chain R:

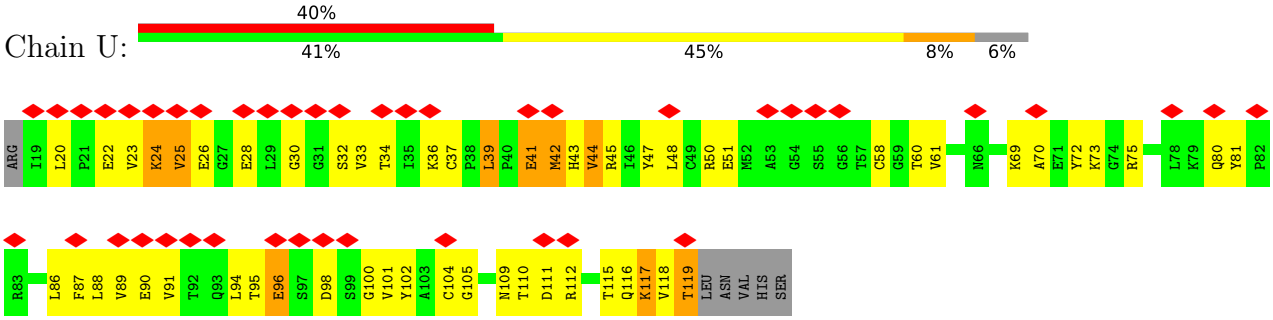
• Molecule 4: Fas apoptotic inhibitory molecule 3

Chain S:

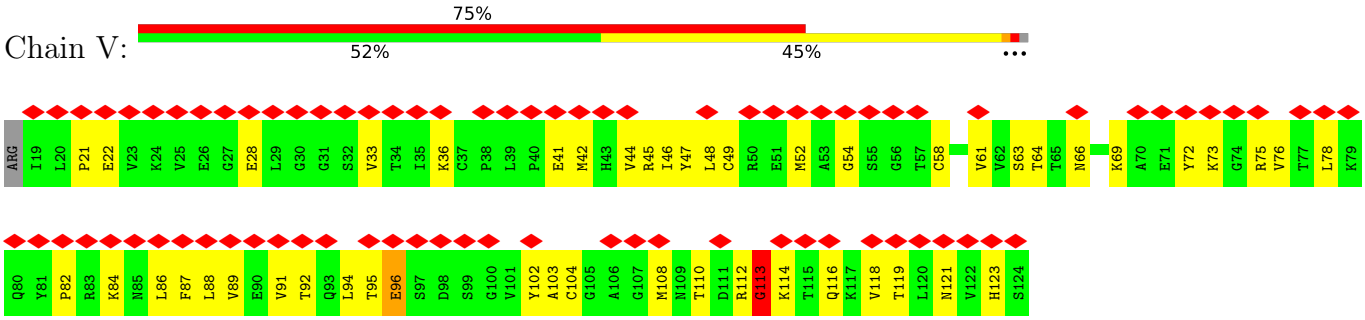
• Molecule 4: Fas apoptotic inhibitory molecule 3

Chain U:



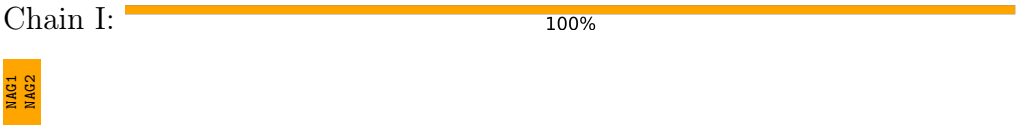

• Molecule 4: Fas apoptotic inhibitory molecule 3

Chain V:




• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 297136 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 1500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 2.308 | Depositor |
| Minimum map value | -1.208 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.048 | Depositor |
| Recommended contour level | 0.27 | Depositor |
| Map size (Å) | 345.6, 345.6, 345.6 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.08, 1.08, 1.08 | 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: NAG

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 | 1.75 | 61/1831 (3.3%) | 1.28 | 27/2508 (1.1%) |
| 1 | B | 1.65 | 53/1814 (2.9%) | 1.47 | 37/2485 (1.5%) |
| 1 | C | 1.17 | 18/1808 (1.0%) | 1.05 | 17/2476 (0.7%) |
| 1 | D | 0.80 | 9/1788 (0.5%) | 0.83 | 7/2449 (0.3%) |
| 1 | E | 0.99 | 20/1788 (1.1%) | 1.07 | 17/2449 (0.7%) |
| 1 | F | 1.16 | 21/1788 (1.2%) | 1.34 | 32/2449 (1.3%) |
| 1 | G | 1.09 | 25/1787 (1.4%) | 0.90 | 11/2447 (0.4%) |
| 1 | H | 1.19 | 26/1844 (1.4%) | 0.97 | 14/2526 (0.6%) |
| 1 | K | 1.35 | 34/1844 (1.8%) | 1.21 | 22/2526 (0.9%) |
| 1 | L | 0.96 | 13/1844 (0.7%) | 1.15 | 23/2526 (0.9%) |
| 2 | J | 0.96 | 8/864 (0.9%) | 0.93 | 8/1173 (0.7%) |
| 3 | P | 0.75 | 13/3935 (0.3%) | 1.02 | 34/5333 (0.6%) |
| 4 | R | 0.44 | 0/776 | 0.83 | 3/1046 (0.3%) |
| 4 | S | 0.57 | 0/795 | 0.92 | 4/1071 (0.4%) |
| 4 | U | 0.46 | 0/776 | 0.92 | 4/1046 (0.4%) |
| 4 | V | 0.30 | 0/816 | 0.53 | 1/1101 (0.1%) |
| All | All | 1.10 | 301/26098 (1.2%) | 1.09 | 261/35611 (0.7%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | C | 0 | 3 |
| 1 | E | 0 | 1 |
| 1 | H | 0 | 1 |
| 3 | P | 0 | 2 |
| All | All | 0 | 7 |

All (301) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | P | 404 | GLY | C-N | 13.60 | 1.52 | 1.33 |
| 1 | H | 536 | CYS | C-O | -9.95 | 1.12 | 1.24 |
| 1 | L | 567 | VAL | C-O | -9.77 | 1.13 | 1.24 |
| 1 | G | 562 | TYR | C-O | -9.72 | 1.13 | 1.23 |
| 1 | B | 477 | THR | CA-C | -9.70 | 1.40 | 1.52 |
| 1 | K | 564 | VAL | C-O | -9.56 | 1.14 | 1.24 |
| 1 | H | 537 | VAL | C-O | -9.54 | 1.13 | 1.24 |
| 1 | A | 477 | THR | CA-C | -9.46 | 1.41 | 1.52 |
| 1 | K | 475 | LEU | C-O | -9.42 | 1.13 | 1.24 |
| 1 | G | 475 | LEU | C-O | -9.37 | 1.12 | 1.24 |
| 1 | H | 517 | ALA | C-O | -9.34 | 1.12 | 1.23 |
| 1 | B | 455 | TYR | C-O | -8.83 | 1.12 | 1.24 |
| 1 | K | 565 | SER | CA-C | -8.73 | 1.43 | 1.53 |
| 1 | H | 487 | GLN | C-O | -8.71 | 1.13 | 1.23 |
| 1 | A | 516 | PHE | C-O | -8.69 | 1.13 | 1.24 |
| 1 | L | 565 | SER | C-O | -8.68 | 1.13 | 1.24 |
| 1 | A | 515 | TYR | C-O | -8.65 | 1.15 | 1.24 |
| 1 | G | 474 | CYS | C-O | -8.64 | 1.13 | 1.24 |
| 1 | L | 564 | VAL | C-O | -8.54 | 1.14 | 1.24 |
| 1 | H | 562 | TYR | C-O | -8.53 | 1.13 | 1.24 |
| 1 | K | 538 | VAL | C-O | -8.44 | 1.15 | 1.24 |
| 1 | F | 501 | VAL | C-O | -8.43 | 1.15 | 1.24 |
| 1 | K | 565 | SER | C-O | -8.42 | 1.13 | 1.23 |
| 1 | L | 574 | THR | C-O | -8.38 | 1.14 | 1.23 |
| 1 | F | 548 | THR | C-O | -8.31 | 1.13 | 1.24 |
| 1 | H | 538 | VAL | C-O | -8.18 | 1.15 | 1.24 |
| 1 | C | 567 | VAL | C-O | -8.18 | 1.15 | 1.24 |
| 1 | H | 486 | VAL | C-O | -8.14 | 1.15 | 1.24 |
| 1 | C | 455 | TYR | C-O | -8.10 | 1.14 | 1.24 |
| 1 | G | 473 | THR | C-O | -8.08 | 1.14 | 1.23 |
| 1 | A | 546 | ARG | C-O | -8.05 | 1.13 | 1.24 |
| 1 | A | 486 | VAL | C-O | -8.04 | 1.14 | 1.24 |
| 1 | H | 516 | PHE | C-O | -7.87 | 1.14 | 1.23 |
| 1 | A | 490 | GLN | CA-C | -7.86 | 1.42 | 1.52 |
| 1 | F | 520 | ILE | C-O | -7.78 | 1.15 | 1.24 |
| 1 | A | 479 | PHE | C-O | -7.78 | 1.13 | 1.23 |
| 1 | H | 536 | CYS | CA-C | -7.71 | 1.43 | 1.52 |
| 3 | P | 59 | LYS | C-O | -7.68 | 1.15 | 1.23 |
| 1 | L | 574 | THR | CA-C | -7.67 | 1.45 | 1.53 |
| 1 | A | 485 | PHE | C-O | -7.66 | 1.14 | 1.24 |
| 1 | H | 564 | VAL | C-O | -7.64 | 1.15 | 1.24 |
| 1 | D | 535 | THR | C-O | -7.63 | 1.15 | 1.23 |
| 1 | H | 518 | HIS | C-O | -7.62 | 1.14 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 489 | MET | CA-C | -7.56 | 1.43 | 1.52 |
| 1 | A | 519 | SER | C-O | -7.54 | 1.15 | 1.24 |
| 1 | K | 519 | SER | CA-C | -7.49 | 1.42 | 1.52 |
| 1 | A | 550 | ARG | C-O | -7.46 | 1.15 | 1.24 |
| 1 | H | 520 | ILE | C-O | -7.45 | 1.16 | 1.24 |
| 1 | B | 484 | VAL | C-O | -7.43 | 1.16 | 1.24 |
| 1 | K | 475 | LEU | CA-C | -7.43 | 1.44 | 1.52 |
| 1 | A | 568 | MET | C-O | -7.40 | 1.14 | 1.23 |
| 1 | C | 456 | LEU | CA-C | -7.34 | 1.44 | 1.52 |
| 1 | B | 535 | THR | C-O | -7.33 | 1.14 | 1.23 |
| 1 | H | 519 | SER | C-O | -7.31 | 1.15 | 1.24 |
| 1 | F | 548 | THR | CA-C | -7.29 | 1.44 | 1.52 |
| 1 | C | 566 | LEU | C-O | -7.29 | 1.15 | 1.23 |
| 1 | F | 521 | LEU | CA-C | -7.28 | 1.44 | 1.52 |
| 3 | P | 56 | VAL | C-O | -7.28 | 1.16 | 1.23 |
| 1 | D | 536 | CYS | C-O | -7.28 | 1.15 | 1.24 |
| 1 | A | 479 | PHE | CA-C | -7.26 | 1.43 | 1.53 |
| 1 | F | 503 | SER | C-O | -7.24 | 1.15 | 1.23 |
| 1 | K | 539 | ALA | CA-C | -7.24 | 1.44 | 1.52 |
| 1 | A | 507 | PRO | C-O | -7.23 | 1.14 | 1.24 |
| 2 | J | 35 | ARG | C-O | -7.23 | 1.14 | 1.23 |
| 1 | A | 502 | THR | CA-C | -7.22 | 1.43 | 1.52 |
| 1 | F | 549 | GLU | C-O | -7.21 | 1.14 | 1.23 |
| 1 | B | 466 | LEU | CA-C | -7.18 | 1.42 | 1.52 |
| 1 | A | 501 | VAL | C-O | -7.14 | 1.15 | 1.24 |
| 1 | B | 527 | GLU | C-O | -7.13 | 1.15 | 1.24 |
| 1 | F | 520 | ILE | CA-C | -7.11 | 1.44 | 1.52 |
| 1 | F | 500 | TYR | C-O | -7.11 | 1.15 | 1.23 |
| 1 | A | 549 | GLU | CA-C | -7.08 | 1.43 | 1.52 |
| 1 | A | 449 | LEU | CA-C | -7.05 | 1.45 | 1.53 |
| 1 | B | 525 | GLU | CA-C | -7.05 | 1.43 | 1.52 |
| 1 | H | 517 | ALA | CA-C | -7.00 | 1.44 | 1.52 |
| 1 | B | 461 | ARG | CA-C | -6.99 | 1.43 | 1.52 |
| 1 | G | 562 | TYR | CA-C | -6.99 | 1.44 | 1.52 |
| 1 | K | 537 | VAL | CA-CB | -6.98 | 1.45 | 1.53 |
| 1 | L | 566 | LEU | C-O | -6.96 | 1.15 | 1.24 |
| 1 | G | 475 | LEU | CA-C | -6.96 | 1.44 | 1.52 |
| 1 | C | 565 | SER | C-O | -6.94 | 1.17 | 1.23 |
| 3 | P | 99 | ARG | C-O | -6.94 | 1.15 | 1.24 |
| 1 | B | 480 | SER | C-O | -6.90 | 1.15 | 1.24 |
| 1 | B | 455 | TYR | CA-C | -6.87 | 1.44 | 1.52 |
| 1 | C | 564 | VAL | C-O | -6.86 | 1.14 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 561 | LEU | C-O | -6.82 | 1.15 | 1.24 |
| 1 | B | 452 | PRO | C-O | -6.81 | 1.16 | 1.23 |
| 1 | B | 544 | PRO | CA-C | -6.79 | 1.42 | 1.52 |
| 1 | F | 546 | ARG | C-O | -6.77 | 1.15 | 1.24 |
| 1 | B | 524 | SER | C-O | -6.75 | 1.15 | 1.23 |
| 1 | A | 508 | GLU | CA-C | -6.72 | 1.45 | 1.53 |
| 1 | A | 477 | THR | C-O | -6.66 | 1.15 | 1.24 |
| 1 | A | 542 | ALA | CA-C | -6.65 | 1.44 | 1.52 |
| 1 | B | 524 | SER | CA-C | -6.62 | 1.44 | 1.52 |
| 1 | B | 534 | TYR | CA-C | -6.59 | 1.44 | 1.52 |
| 1 | A | 496 | SER | CA-C | -6.58 | 1.44 | 1.53 |
| 1 | A | 515 | TYR | CA-CB | -6.57 | 1.44 | 1.53 |
| 1 | D | 536 | CYS | CA-C | -6.56 | 1.44 | 1.52 |
| 1 | A | 542 | ALA | C-O | -6.54 | 1.15 | 1.24 |
| 1 | A | 506 | MET | C-O | -6.53 | 1.15 | 1.25 |
| 3 | P | 99 | ARG | CA-C | -6.53 | 1.43 | 1.52 |
| 1 | K | 566 | LEU | C-O | -6.51 | 1.14 | 1.23 |
| 1 | E | 518 | HIS | C-O | -6.48 | 1.16 | 1.23 |
| 1 | C | 493 | GLN | C-O | -6.47 | 1.19 | 1.25 |
| 1 | G | 503 | SER | C-O | -6.47 | 1.15 | 1.23 |
| 1 | A | 548 | THR | C-O | -6.44 | 1.15 | 1.23 |
| 1 | E | 505 | PRO | C-O | -6.44 | 1.16 | 1.23 |
| 1 | A | 552 | VAL | C-O | -6.43 | 1.17 | 1.23 |
| 1 | A | 489 | MET | CA-C | -6.39 | 1.45 | 1.52 |
| 1 | B | 454 | VAL | C-O | -6.39 | 1.17 | 1.24 |
| 1 | E | 536 | CYS | C-O | -6.39 | 1.16 | 1.24 |
| 1 | C | 484 | VAL | C-O | -6.38 | 1.17 | 1.24 |
| 1 | A | 566 | LEU | C-O | -6.36 | 1.16 | 1.23 |
| 1 | B | 496 | SER | CA-C | -6.34 | 1.45 | 1.52 |
| 1 | B | 463 | GLN | CA-C | -6.33 | 1.44 | 1.52 |
| 1 | B | 532 | GLU | CA-C | -6.33 | 1.44 | 1.52 |
| 2 | J | 62 | TYR | C-O | -6.29 | 1.16 | 1.24 |
| 1 | K | 564 | VAL | CA-C | -6.27 | 1.45 | 1.52 |
| 1 | C | 524 | SER | CA-C | -6.25 | 1.45 | 1.52 |
| 1 | H | 520 | ILE | CA-CB | -6.24 | 1.46 | 1.54 |
| 1 | C | 479 | PHE | CA-C | -6.23 | 1.45 | 1.52 |
| 1 | B | 463 | GLN | C-O | -6.23 | 1.15 | 1.24 |
| 1 | A | 507 | PRO | CA-C | -6.22 | 1.43 | 1.52 |
| 1 | B | 479 | PHE | C-O | -6.20 | 1.15 | 1.23 |
| 1 | D | 453 | ASP | C-O | -6.20 | 1.16 | 1.24 |
| 1 | G | 502 | THR | C-O | -6.19 | 1.16 | 1.23 |
| 1 | A | 553 | ASP | C-O | -6.18 | 1.16 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 486 | VAL | C-O | -6.18 | 1.17 | 1.24 |
| 1 | K | 473 | THR | C-O | -6.18 | 1.17 | 1.24 |
| 1 | A | 505 | PRO | C-O | -6.17 | 1.16 | 1.23 |
| 1 | B | 494 | PRO | CA-C | -6.17 | 1.44 | 1.52 |
| 1 | B | 483 | ASP | CA-C | -6.17 | 1.46 | 1.52 |
| 1 | G | 515 | TYR | C-O | -6.15 | 1.17 | 1.24 |
| 1 | H | 562 | TYR | CA-C | -6.15 | 1.44 | 1.52 |
| 1 | B | 525 | GLU | C-O | -6.14 | 1.16 | 1.24 |
| 1 | L | 554 | LYS | CA-C | -6.13 | 1.44 | 1.52 |
| 1 | A | 517 | ALA | C-O | -6.12 | 1.15 | 1.24 |
| 3 | P | 40 | GLN | N-CA | -6.10 | 1.38 | 1.46 |
| 1 | A | 484 | VAL | CA-CB | -6.09 | 1.46 | 1.55 |
| 1 | C | 515 | TYR | CA-CB | -6.09 | 1.45 | 1.53 |
| 1 | K | 520 | ILE | C-O | -6.08 | 1.17 | 1.24 |
| 1 | A | 506 | MET | CA-C | -6.08 | 1.46 | 1.53 |
| 1 | C | 563 | ASN | CG-ND2 | -6.08 | 1.20 | 1.33 |
| 1 | K | 561 | LEU | CA-C | -6.08 | 1.45 | 1.52 |
| 1 | B | 495 | LEU | CA-C | -6.07 | 1.45 | 1.52 |
| 1 | B | 528 | TRP | C-O | -6.07 | 1.16 | 1.24 |
| 1 | A | 549 | GLU | C-O | -6.06 | 1.16 | 1.23 |
| 3 | P | 40 | GLN | CA-C | -6.06 | 1.45 | 1.52 |
| 1 | A | 505 | PRO | CA-C | -6.05 | 1.45 | 1.52 |
| 1 | C | 455 | TYR | CA-C | -6.02 | 1.45 | 1.52 |
| 1 | A | 502 | THR | C-O | -6.02 | 1.16 | 1.23 |
| 1 | G | 533 | THR | CA-C | -6.02 | 1.44 | 1.52 |
| 1 | B | 480 | SER | CA-C | -6.02 | 1.45 | 1.52 |
| 1 | G | 518 | HIS | C-O | -6.01 | 1.16 | 1.23 |
| 1 | C | 456 | LEU | C-O | -6.01 | 1.16 | 1.24 |
| 1 | H | 563 | ASN | C-O | -6.00 | 1.15 | 1.24 |
| 1 | E | 518 | HIS | CA-C | -6.00 | 1.45 | 1.52 |
| 1 | A | 489 | MET | C-O | -5.99 | 1.16 | 1.24 |
| 1 | F | 481 | PRO | CA-C | -5.99 | 1.45 | 1.52 |
| 1 | B | 453 | ASP | C-O | -5.94 | 1.16 | 1.24 |
| 1 | K | 538 | VAL | CA-C | -5.93 | 1.46 | 1.52 |
| 2 | J | 63 | HIS | C-O | -5.92 | 1.16 | 1.23 |
| 1 | G | 517 | ALA | C-O | -5.92 | 1.16 | 1.23 |
| 1 | H | 485 | PHE | C-O | -5.90 | 1.17 | 1.23 |
| 1 | L | 575 | CYS | C-O | -5.90 | 1.16 | 1.24 |
| 1 | C | 455 | TYR | CB-CG | -5.89 | 1.38 | 1.51 |
| 1 | B | 534 | TYR | C-O | -5.89 | 1.17 | 1.24 |
| 1 | G | 518 | HIS | CA-C | -5.89 | 1.45 | 1.52 |
| 1 | B | 500 | TYR | C-O | -5.88 | 1.16 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | K | 489 | MET | CA-C | -5.88 | 1.45 | 1.52 |
| 1 | B | 493 | GLN | C-O | -5.87 | 1.17 | 1.24 |
| 1 | A | 519 | SER | CA-C | -5.86 | 1.45 | 1.52 |
| 1 | G | 535 | THR | C-O | -5.85 | 1.16 | 1.23 |
| 1 | B | 465 | ASN | C-O | -5.85 | 1.17 | 1.24 |
| 1 | B | 527 | GLU | CA-C | -5.84 | 1.45 | 1.52 |
| 1 | C | 563 | ASN | C-O | -5.81 | 1.15 | 1.23 |
| 1 | B | 462 | GLU | C-O | -5.80 | 1.16 | 1.24 |
| 1 | E | 505 | PRO | CA-C | -5.80 | 1.44 | 1.52 |
| 1 | L | 571 | THR | CA-C | -5.77 | 1.46 | 1.53 |
| 1 | G | 465 | ASN | C-O | -5.77 | 1.16 | 1.24 |
| 1 | K | 516 | PHE | C-O | -5.76 | 1.17 | 1.23 |
| 1 | K | 539 | ALA | C-O | -5.76 | 1.17 | 1.24 |
| 1 | A | 498 | GLU | C-O | -5.75 | 1.17 | 1.24 |
| 1 | E | 536 | CYS | CA-C | -5.74 | 1.45 | 1.52 |
| 1 | G | 561 | LEU | C-O | -5.74 | 1.16 | 1.24 |
| 1 | G | 500 | TYR | C-O | -5.73 | 1.16 | 1.23 |
| 1 | E | 533 | THR | C-O | -5.72 | 1.16 | 1.24 |
| 1 | L | 565 | SER | CA-C | -5.72 | 1.45 | 1.52 |
| 1 | K | 476 | VAL | C-O | -5.71 | 1.16 | 1.23 |
| 1 | B | 478 | GLY | C-O | -5.71 | 1.16 | 1.24 |
| 1 | G | 534 | TYR | C-O | -5.70 | 1.16 | 1.24 |
| 1 | A | 564 | VAL | CA-CB | -5.69 | 1.46 | 1.54 |
| 1 | K | 563 | ASN | C-O | -5.69 | 1.16 | 1.24 |
| 1 | A | 564 | VAL | C-O | -5.68 | 1.17 | 1.24 |
| 1 | G | 565 | SER | CA-C | -5.68 | 1.45 | 1.52 |
| 1 | A | 498 | GLU | CA-C | -5.68 | 1.45 | 1.52 |
| 1 | K | 519 | SER | C-O | -5.67 | 1.16 | 1.24 |
| 1 | A | 499 | LYS | C-O | -5.67 | 1.16 | 1.24 |
| 1 | K | 536 | CYS | C-O | -5.67 | 1.17 | 1.24 |
| 1 | A | 500 | TYR | C-O | -5.67 | 1.16 | 1.23 |
| 1 | B | 500 | TYR | CA-C | -5.66 | 1.45 | 1.53 |
| 1 | E | 486 | VAL | CA-C | -5.66 | 1.46 | 1.52 |
| 1 | A | 485 | PHE | CA-C | -5.66 | 1.46 | 1.52 |
| 1 | K | 485 | PHE | C-O | -5.66 | 1.17 | 1.23 |
| 1 | K | 538 | VAL | N-CA | -5.66 | 1.39 | 1.46 |
| 1 | B | 499 | LYS | CA-C | -5.66 | 1.46 | 1.52 |
| 1 | H | 534 | TYR | C-O | -5.65 | 1.16 | 1.24 |
| 1 | D | 452 | PRO | C-O | -5.65 | 1.17 | 1.23 |
| 1 | F | 521 | LEU | C-O | -5.65 | 1.17 | 1.24 |
| 1 | G | 534 | TYR | CA-C | -5.64 | 1.45 | 1.52 |
| 1 | E | 485 | PHE | C-O | -5.64 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 520 | ILE | CA-CB | -5.64 | 1.47 | 1.54 |
| 1 | E | 507 | PRO | C-O | -5.61 | 1.16 | 1.24 |
| 1 | L | 575 | CYS | CA-C | -5.61 | 1.45 | 1.52 |
| 1 | F | 480 | SER | C-O | -5.61 | 1.17 | 1.24 |
| 1 | A | 569 | SER | C-O | -5.61 | 1.16 | 1.23 |
| 1 | H | 443 | ARG | N-CA | 5.61 | 1.54 | 1.46 |
| 1 | K | 562 | TYR | CA-CB | -5.60 | 1.45 | 1.53 |
| 3 | P | 100 | GLY | CA-C | -5.59 | 1.44 | 1.51 |
| 1 | G | 474 | CYS | CA-C | -5.58 | 1.44 | 1.52 |
| 1 | B | 466 | LEU | C-O | -5.57 | 1.17 | 1.24 |
| 1 | D | 454 | VAL | C-O | -5.56 | 1.16 | 1.23 |
| 2 | J | 34 | GLU | CA-CB | -5.54 | 1.45 | 1.53 |
| 2 | J | 33 | VAL | CA-CB | -5.53 | 1.47 | 1.54 |
| 1 | K | 564 | VAL | CA-CB | -5.53 | 1.47 | 1.54 |
| 1 | E | 538 | VAL | C-O | -5.52 | 1.17 | 1.24 |
| 1 | F | 550 | ARG | C-O | -5.52 | 1.17 | 1.23 |
| 1 | G | 533 | THR | C-O | -5.51 | 1.17 | 1.24 |
| 1 | C | 469 | SER | C-O | -5.50 | 1.17 | 1.23 |
| 1 | A | 541 | GLU | CA-C | -5.50 | 1.44 | 1.52 |
| 1 | K | 487 | GLN | C-O | -5.50 | 1.17 | 1.23 |
| 1 | K | 527 | GLU | C-O | -5.50 | 1.17 | 1.24 |
| 1 | B | 464 | LEU | C-O | -5.49 | 1.17 | 1.24 |
| 1 | E | 506 | MET | C-O | -5.49 | 1.17 | 1.24 |
| 1 | B | 452 | PRO | CA-C | -5.49 | 1.45 | 1.52 |
| 1 | A | 514 | ARG | C-O | -5.48 | 1.16 | 1.23 |
| 1 | B | 461 | ARG | C-O | -5.48 | 1.17 | 1.24 |
| 1 | A | 547 | VAL | C-O | -5.47 | 1.17 | 1.23 |
| 1 | A | 490 | GLN | C-O | -5.47 | 1.17 | 1.24 |
| 3 | P | 404 | GLY | C-O | -5.46 | 1.18 | 1.24 |
| 1 | H | 519 | SER | CA-C | -5.43 | 1.46 | 1.52 |
| 1 | K | 525 | GLU | C-O | -5.42 | 1.17 | 1.24 |
| 1 | B | 491 | ARG | CA-C | -5.41 | 1.48 | 1.53 |
| 1 | K | 524 | SER | CA-C | -5.40 | 1.45 | 1.52 |
| 1 | F | 479 | PHE | CA-C | -5.39 | 1.45 | 1.52 |
| 1 | F | 549 | GLU | CA-C | -5.38 | 1.46 | 1.52 |
| 1 | H | 566 | LEU | C-O | -5.38 | 1.17 | 1.24 |
| 1 | D | 537 | VAL | C-O | -5.38 | 1.17 | 1.24 |
| 1 | A | 503 | SER | C-O | -5.37 | 1.17 | 1.24 |
| 1 | B | 477 | THR | C-O | -5.35 | 1.18 | 1.23 |
| 1 | A | 568 | MET | CA-CB | -5.35 | 1.45 | 1.53 |
| 3 | P | 40 | GLN | C-O | -5.35 | 1.17 | 1.24 |
| 1 | H | 443 | ARG | CA-C | -5.34 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 561 | LEU | C-O | -5.34 | 1.17 | 1.24 |
| 1 | L | 572 | ALA | CA-C | -5.33 | 1.45 | 1.52 |
| 1 | K | 540 | HIS | CA-C | -5.33 | 1.45 | 1.52 |
| 1 | E | 518 | HIS | C-N | -5.29 | 1.26 | 1.33 |
| 1 | K | 534 | TYR | C-O | -5.29 | 1.17 | 1.24 |
| 1 | H | 561 | LEU | C-O | -5.29 | 1.17 | 1.24 |
| 1 | E | 532 | GLU | C-O | -5.28 | 1.20 | 1.23 |
| 1 | G | 476 | VAL | C-O | -5.28 | 1.15 | 1.23 |
| 1 | A | 511 | ALA | C-O | -5.27 | 1.18 | 1.24 |
| 1 | G | 516 | PHE | C-O | -5.27 | 1.17 | 1.23 |
| 1 | F | 481 | PRO | C-O | -5.26 | 1.17 | 1.23 |
| 1 | E | 535 | THR | C-O | -5.25 | 1.16 | 1.23 |
| 1 | D | 489 | MET | CA-C | -5.25 | 1.46 | 1.52 |
| 1 | E | 484 | VAL | C-O | -5.24 | 1.18 | 1.23 |
| 1 | H | 518 | HIS | CA-C | -5.24 | 1.46 | 1.53 |
| 1 | E | 546 | ARG | C-O | -5.23 | 1.17 | 1.24 |
| 1 | A | 478 | GLY | C-O | -5.22 | 1.16 | 1.24 |
| 1 | G | 564 | VAL | C-O | -5.21 | 1.18 | 1.24 |
| 1 | B | 482 | ALA | C-O | -5.20 | 1.17 | 1.24 |
| 1 | E | 517 | ALA | C-O | -5.18 | 1.17 | 1.23 |
| 1 | H | 535 | THR | C-O | -5.18 | 1.17 | 1.23 |
| 1 | B | 534 | TYR | CA-CB | -5.16 | 1.44 | 1.53 |
| 2 | J | 34 | GLU | C-O | -5.16 | 1.17 | 1.23 |
| 1 | L | 573 | GLY | C-O | -5.16 | 1.17 | 1.23 |
| 1 | B | 533 | THR | C-O | -5.16 | 1.17 | 1.23 |
| 1 | A | 551 | THR | C-O | -5.15 | 1.17 | 1.23 |
| 1 | A | 565 | SER | C-O | -5.14 | 1.17 | 1.24 |
| 1 | B | 484 | VAL | CA-CB | -5.13 | 1.48 | 1.54 |
| 1 | B | 466 | LEU | N-CA | -5.12 | 1.39 | 1.46 |
| 1 | A | 486 | VAL | CA-CB | -5.11 | 1.48 | 1.54 |
| 1 | C | 523 | VAL | N-CA | -5.11 | 1.40 | 1.46 |
| 1 | A | 541 | GLU | C-O | -5.11 | 1.16 | 1.24 |
| 1 | E | 516 | PHE | C-O | -5.11 | 1.17 | 1.23 |
| 1 | D | 500 | TYR | CA-C | -5.09 | 1.46 | 1.52 |
| 1 | B | 528 | TRP | CA-C | -5.09 | 1.45 | 1.52 |
| 2 | J | 116 | VAL | C-O | -5.07 | 1.18 | 1.23 |
| 3 | P | 98 | SER | CA-C | -5.07 | 1.44 | 1.52 |
| 1 | A | 470 | ALA | CA-C | -5.06 | 1.46 | 1.52 |
| 1 | F | 549 | GLU | CA-CB | -5.05 | 1.45 | 1.53 |
| 1 | B | 489 | MET | C-O | -5.04 | 1.17 | 1.23 |
| 1 | B | 545 | ASN | CA-CB | -5.03 | 1.46 | 1.53 |
| 3 | P | 100 | GLY | C-O | -5.02 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 550 | ARG | CA-C | -5.02 | 1.46 | 1.52 |
| 2 | J | 35 | ARG | CA-CB | -5.01 | 1.44 | 1.53 |
| 1 | K | 535 | THR | C-O | -5.00 | 1.17 | 1.23 |
| 3 | P | 289 | SER | CA-C | -5.00 | 1.48 | 1.53 |
| 1 | B | 454 | VAL | CA-C | -5.00 | 1.46 | 1.52 |
| 1 | F | 506 | MET | C-O | -5.00 | 1.17 | 1.24 |

All (261) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 493 | GLN | CA-C-N | 18.52 | 142.99 | 119.84 |
| 1 | E | 493 | GLN | C-N-CA | 18.52 | 142.99 | 119.84 |
| 1 | L | 551 | THR | N-CA-C | 16.42 | 136.17 | 109.40 |
| 3 | P | 404 | GLY | CA-C-N | 14.64 | 149.50 | 121.54 |
| 3 | P | 404 | GLY | C-N-CA | 14.64 | 149.50 | 121.54 |
| 1 | B | 496 | SER | CA-C-N | 14.20 | 137.59 | 119.84 |
| 1 | B | 496 | SER | C-N-CA | 14.20 | 137.59 | 119.84 |
| 1 | L | 552 | VAL | N-CA-C | 13.67 | 125.56 | 108.06 |
| 1 | L | 543 | LEU | CA-C-N | 13.02 | 134.16 | 119.32 |
| 1 | L | 543 | LEU | C-N-CA | 13.02 | 134.16 | 119.32 |
| 1 | F | 558 | LYS | CA-C-N | 12.77 | 135.81 | 119.84 |
| 1 | F | 558 | LYS | C-N-CA | 12.77 | 135.81 | 119.84 |
| 1 | C | 564 | VAL | CB-CA-C | -12.39 | 97.57 | 111.45 |
| 1 | F | 448 | ALA | N-CA-C | 12.32 | 126.76 | 112.72 |
| 1 | B | 414 | CYS | N-CA-C | 12.04 | 129.35 | 109.24 |
| 1 | A | 480 | SER | C-N-CD | -11.81 | 94.61 | 120.60 |
| 1 | E | 537 | VAL | N-CA-C | 11.42 | 122.64 | 106.53 |
| 1 | K | 543 | LEU | CA-C-N | 11.25 | 133.91 | 119.84 |
| 1 | K | 543 | LEU | C-N-CA | 11.25 | 133.91 | 119.84 |
| 3 | P | 272 | ALA | CA-C-N | 11.18 | 131.46 | 119.05 |
| 3 | P | 272 | ALA | C-N-CA | 11.18 | 131.46 | 119.05 |
| 1 | K | 477 | THR | N-CA-C | 11.18 | 126.63 | 108.41 |
| 1 | L | 552 | VAL | CB-CA-C | -11.12 | 94.68 | 111.80 |
| 1 | K | 537 | VAL | N-CA-C | 11.06 | 124.31 | 106.72 |
| 1 | G | 443 | ARG | CA-C-N | 11.06 | 133.67 | 119.84 |
| 1 | G | 443 | ARG | C-N-CA | 11.06 | 133.67 | 119.84 |
| 1 | A | 493 | GLN | CA-C-N | 11.03 | 133.63 | 119.84 |
| 1 | A | 493 | GLN | C-N-CA | 11.03 | 133.63 | 119.84 |
| 3 | P | 404 | GLY | CA-C-O | -10.82 | 106.23 | 120.29 |
| 1 | F | 506 | MET | CA-C-N | 10.59 | 133.08 | 119.84 |
| 1 | F | 506 | MET | C-N-CA | 10.59 | 133.08 | 119.84 |
| 1 | D | 496 | SER | CA-C-N | 10.31 | 132.73 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 496 | SER | C-N-CA | 10.31 | 132.73 | 119.84 |
| 3 | P | 448 | VAL | CA-C-N | 9.86 | 130.64 | 119.99 |
| 3 | P | 448 | VAL | C-N-CA | 9.86 | 130.64 | 119.99 |
| 1 | C | 493 | GLN | CA-C-N | 9.80 | 132.09 | 119.84 |
| 1 | C | 493 | GLN | C-N-CA | 9.80 | 132.09 | 119.84 |
| 1 | A | 480 | SER | CA-C-N | 9.78 | 150.47 | 127.00 |
| 1 | A | 480 | SER | C-N-CA | 9.78 | 150.47 | 127.00 |
| 1 | B | 479 | PHE | N-CA-C | 9.71 | 123.16 | 110.43 |
| 1 | A | 498 | GLU | N-CA-C | -9.60 | 99.69 | 111.40 |
| 4 | S | 39 | LEU | CA-C-N | 9.54 | 131.76 | 119.84 |
| 4 | S | 39 | LEU | C-N-CA | 9.54 | 131.76 | 119.84 |
| 1 | A | 511 | ALA | CA-C-N | 9.52 | 131.74 | 119.84 |
| 1 | A | 511 | ALA | C-N-CA | 9.52 | 131.74 | 119.84 |
| 1 | E | 533 | THR | N-CA-C | 9.39 | 130.80 | 110.80 |
| 1 | F | 543 | LEU | CA-C-N | 9.18 | 131.31 | 119.84 |
| 1 | F | 543 | LEU | C-N-CA | 9.18 | 131.31 | 119.84 |
| 1 | L | 533 | THR | N-CA-C | 9.17 | 123.72 | 112.54 |
| 1 | F | 414 | CYS | N-CA-C | 9.12 | 124.29 | 112.26 |
| 4 | R | 66 | ASN | N-CA-C | 8.90 | 129.76 | 110.80 |
| 1 | F | 417 | ASP | N-CA-C | -8.78 | 99.94 | 113.02 |
| 1 | F | 406 | SER | N-CA-C | -8.73 | 100.31 | 112.45 |
| 1 | B | 381 | SER | N-CA-C | -8.73 | 93.68 | 107.73 |
| 1 | B | 385 | GLN | N-CA-C | -8.68 | 101.82 | 111.28 |
| 1 | K | 449 | LEU | N-CA-C | 8.64 | 129.21 | 110.80 |
| 1 | H | 443 | ARG | N-CA-CB | 8.55 | 125.60 | 110.37 |
| 1 | A | 530 | THR | N-CA-C | -8.51 | 101.95 | 111.14 |
| 1 | L | 443 | ARG | CA-C-N | 8.49 | 130.45 | 119.84 |
| 1 | L | 443 | ARG | C-N-CA | 8.49 | 130.45 | 119.84 |
| 1 | B | 514 | ARG | N-CA-C | 8.48 | 121.26 | 110.33 |
| 1 | C | 480 | SER | CA-C-N | 8.38 | 130.32 | 119.84 |
| 1 | C | 480 | SER | C-N-CA | 8.38 | 130.32 | 119.84 |
| 1 | E | 543 | LEU | CA-C-N | 8.37 | 130.30 | 119.84 |
| 1 | E | 543 | LEU | C-N-CA | 8.37 | 130.30 | 119.84 |
| 1 | G | 478 | GLY | N-CA-C | 8.32 | 132.90 | 113.18 |
| 1 | K | 566 | LEU | N-CA-C | 8.27 | 123.46 | 108.17 |
| 1 | A | 506 | MET | CA-C-N | 8.26 | 130.17 | 119.84 |
| 1 | A | 506 | MET | C-N-CA | 8.26 | 130.17 | 119.84 |
| 1 | D | 493 | GLN | CA-C-N | 8.21 | 130.10 | 119.84 |
| 1 | D | 493 | GLN | C-N-CA | 8.21 | 130.10 | 119.84 |
| 1 | A | 479 | PHE | N-CA-C | 8.07 | 120.95 | 110.53 |
| 1 | L | 564 | VAL | CB-CA-C | -8.00 | 99.42 | 111.33 |
| 1 | B | 443 | ARG | N-CA-C | -7.98 | 94.33 | 108.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 499 | LYS | N-CA-C | -7.92 | 102.58 | 112.72 |
| 1 | B | 418 | TRP | N-CA-C | -7.86 | 94.05 | 110.80 |
| 4 | U | 24 | LYS | N-CA-C | 7.82 | 121.33 | 107.80 |
| 1 | K | 537 | VAL | CB-CA-C | -7.72 | 101.98 | 111.32 |
| 1 | A | 496 | SER | CA-C-N | 7.66 | 129.42 | 119.84 |
| 1 | A | 496 | SER | C-N-CA | 7.66 | 129.42 | 119.84 |
| 2 | J | 34 | GLU | N-CA-C | 7.63 | 121.69 | 110.17 |
| 1 | G | 476 | VAL | N-CA-CB | -7.45 | 104.14 | 111.89 |
| 3 | P | 58 | SER | N-CA-C | -7.35 | 103.20 | 111.14 |
| 1 | K | 564 | VAL | CB-CA-C | -7.32 | 99.66 | 111.59 |
| 1 | B | 398 | GLU | N-CA-C | 7.30 | 120.41 | 110.55 |
| 1 | B | 400 | HIS | N-CA-C | 7.30 | 121.03 | 109.64 |
| 1 | A | 554 | LYS | N-CA-C | 7.30 | 126.34 | 110.80 |
| 2 | J | 118 | GLY | N-CA-C | -7.29 | 95.91 | 113.18 |
| 1 | H | 441 | ILE | CA-C-N | 7.27 | 135.43 | 121.54 |
| 1 | H | 441 | ILE | C-N-CA | 7.27 | 135.43 | 121.54 |
| 3 | P | 448 | VAL | N-CA-C | 7.26 | 124.57 | 108.88 |
| 1 | D | 538 | VAL | CB-CA-C | -7.18 | 100.00 | 110.63 |
| 1 | F | 428 | VAL | N-CA-C | 7.15 | 118.16 | 107.51 |
| 1 | K | 473 | THR | N-CA-C | 7.11 | 120.67 | 108.02 |
| 1 | K | 566 | LEU | N-CA-CB | -7.08 | 100.41 | 110.46 |
| 1 | C | 482 | ALA | N-CA-C | 7.08 | 125.87 | 110.80 |
| 1 | A | 445 | LYS | N-CA-C | 7.05 | 118.94 | 110.19 |
| 1 | K | 476 | VAL | N-CA-CB | -7.02 | 103.18 | 111.60 |
| 1 | H | 448 | ALA | N-CA-C | -7.01 | 102.02 | 108.75 |
| 1 | E | 534 | TYR | N-CA-C | 6.97 | 125.65 | 110.80 |
| 1 | F | 520 | ILE | CB-CA-C | -6.95 | 100.47 | 110.83 |
| 1 | G | 565 | SER | N-CA-C | -6.94 | 99.94 | 110.14 |
| 1 | F | 419 | ASN | N-CA-C | -6.94 | 96.02 | 110.80 |
| 1 | L | 572 | ALA | N-CA-C | -6.92 | 96.06 | 110.80 |
| 1 | H | 443 | ARG | CA-C-N | 6.88 | 128.44 | 119.84 |
| 1 | H | 443 | ARG | C-N-CA | 6.88 | 128.44 | 119.84 |
| 1 | K | 476 | VAL | N-CA-C | 6.88 | 117.33 | 106.88 |
| 1 | A | 486 | VAL | CB-CA-C | -6.86 | 101.52 | 110.84 |
| 1 | B | 543 | LEU | CA-C-N | 6.81 | 128.35 | 119.84 |
| 1 | B | 543 | LEU | C-N-CA | 6.81 | 128.35 | 119.84 |
| 1 | E | 546 | ARG | N-CA-C | 6.77 | 125.23 | 110.80 |
| 1 | B | 493 | GLN | CA-C-N | 6.76 | 126.52 | 119.76 |
| 1 | B | 493 | GLN | C-N-CA | 6.76 | 126.52 | 119.76 |
| 1 | A | 447 | VAL | CB-CA-C | -6.76 | 100.20 | 111.29 |
| 3 | P | 404 | GLY | N-CA-C | 6.76 | 123.34 | 113.48 |
| 1 | K | 546 | ARG | N-CA-C | 6.74 | 123.97 | 113.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | H | 563 | ASN | CB-CA-C | 6.74 | 121.48 | 111.17 |
| 1 | G | 476 | VAL | N-CA-C | 6.73 | 117.16 | 106.32 |
| 1 | G | 477 | THR | N-CA-C | 6.72 | 119.62 | 110.35 |
| 1 | F | 394 | THR | N-CA-C | -6.69 | 99.40 | 110.17 |
| 1 | A | 556 | THR | N-CA-C | -6.68 | 104.77 | 113.12 |
| 1 | B | 371 | ASP | N-CA-C | 6.67 | 120.74 | 112.47 |
| 3 | P | 532 | HIS | N-CA-C | -6.66 | 103.72 | 110.97 |
| 1 | B | 409 | GLY | N-CA-C | -6.65 | 97.41 | 113.18 |
| 1 | C | 525 | GLU | N-CA-C | 6.63 | 124.93 | 110.80 |
| 1 | B | 397 | SER | N-CA-C | 6.62 | 119.07 | 110.53 |
| 1 | B | 382 | TRP | N-CA-C | -6.60 | 96.31 | 107.99 |
| 3 | P | 353 | CYS | CB-CA-C | -6.60 | 103.64 | 110.17 |
| 1 | B | 415 | GLU | N-CA-C | 6.54 | 124.74 | 110.80 |
| 1 | K | 527 | GLU | N-CA-C | -6.54 | 104.07 | 111.14 |
| 1 | H | 520 | ILE | CB-CA-C | -6.54 | 100.95 | 110.63 |
| 2 | J | 33 | VAL | CB-CA-C | -6.53 | 102.81 | 110.91 |
| 3 | P | 447 | LYS | N-CA-C | 6.52 | 119.57 | 109.60 |
| 1 | F | 504 | ALA | CA-C-N | 6.51 | 126.49 | 119.78 |
| 1 | F | 504 | ALA | C-N-CA | 6.51 | 126.49 | 119.78 |
| 1 | L | 547 | VAL | CB-CA-C | -6.51 | 105.62 | 111.74 |
| 3 | P | 99 | ARG | N-CA-C | 6.50 | 123.81 | 114.39 |
| 1 | F | 482 | ALA | N-CA-C | 6.49 | 119.81 | 108.52 |
| 1 | L | 537 | VAL | N-CA-C | 6.47 | 117.23 | 108.17 |
| 1 | F | 449 | LEU | N-CA-C | 6.45 | 124.53 | 110.80 |
| 1 | H | 564 | VAL | CB-CA-C | -6.44 | 100.72 | 111.29 |
| 1 | C | 449 | LEU | N-CA-C | 6.41 | 117.89 | 107.32 |
| 1 | A | 505 | PRO | CA-C-O | -6.41 | 114.38 | 121.23 |
| 1 | L | 545 | ASN | O-C-N | 6.38 | 129.72 | 122.20 |
| 3 | P | 310 | HIS | N-CA-C | -6.38 | 97.22 | 110.80 |
| 1 | E | 493 | GLN | N-CA-C | 6.30 | 118.38 | 108.55 |
| 1 | B | 525 | GLU | N-CA-C | 6.28 | 118.93 | 111.71 |
| 1 | D | 452 | PRO | CB-CA-C | -6.27 | 101.95 | 110.60 |
| 1 | B | 432 | ASP | N-CA-C | -6.23 | 105.50 | 113.23 |
| 3 | P | 57 | SER | N-CA-C | 6.22 | 124.05 | 110.80 |
| 1 | F | 479 | PHE | N-CA-CB | 6.20 | 119.10 | 110.17 |
| 1 | F | 379 | THR | N-CA-C | 6.20 | 119.20 | 109.96 |
| 3 | P | 311 | SER | N-CA-C | 6.20 | 124.00 | 110.80 |
| 1 | B | 375 | TYR | N-CA-C | -6.12 | 97.76 | 110.80 |
| 1 | F | 479 | PHE | N-CA-C | 6.12 | 119.13 | 110.50 |
| 1 | E | 532 | GLU | N-CA-C | 6.10 | 121.75 | 113.21 |
| 3 | P | 480 | TRP | N-CA-C | 6.10 | 118.55 | 109.59 |
| 4 | U | 95 | THR | N-CA-C | -6.08 | 104.93 | 113.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 27 | ASP | CA-C-N | 6.07 | 127.40 | 120.85 |
| 2 | J | 27 | ASP | C-N-CA | 6.07 | 127.40 | 120.85 |
| 2 | J | 34 | GLU | CB-CA-C | -6.01 | 99.57 | 111.60 |
| 1 | G | 473 | THR | N-CA-C | 5.98 | 121.18 | 107.48 |
| 1 | K | 530 | THR | N-CA-C | -5.97 | 104.46 | 110.97 |
| 1 | L | 558 | LYS | CA-C-N | 5.94 | 126.44 | 120.14 |
| 1 | L | 558 | LYS | C-N-CA | 5.94 | 126.44 | 120.14 |
| 1 | K | 558 | LYS | CA-C-N | 5.93 | 125.95 | 119.90 |
| 1 | K | 558 | LYS | C-N-CA | 5.93 | 125.95 | 119.90 |
| 2 | J | 116 | VAL | CB-CA-C | -5.92 | 104.84 | 111.23 |
| 1 | C | 467 | ARG | N-CA-C | 5.89 | 123.34 | 110.80 |
| 1 | A | 514 | ARG | CB-CA-C | -5.89 | 99.88 | 110.36 |
| 1 | F | 502 | THR | N-CA-C | 5.87 | 117.97 | 108.41 |
| 1 | H | 538 | VAL | CB-CA-C | -5.86 | 102.10 | 110.83 |
| 3 | P | 353 | CYS | N-CA-C | 5.82 | 119.16 | 108.69 |
| 1 | H | 532 | GLU | N-CA-C | 5.81 | 118.86 | 109.86 |
| 4 | S | 99 | SER | N-CA-C | 5.80 | 118.12 | 109.59 |
| 1 | K | 538 | VAL | CB-CA-C | -5.79 | 103.57 | 111.33 |
| 1 | E | 515 | TYR | CB-CA-C | -5.78 | 102.00 | 113.45 |
| 1 | B | 481 | PRO | N-CA-C | -5.75 | 100.62 | 112.47 |
| 1 | K | 519 | SER | N-CA-C | -5.74 | 98.58 | 110.80 |
| 1 | G | 478 | GLY | CA-C-N | 5.73 | 131.09 | 123.00 |
| 1 | G | 478 | GLY | C-N-CA | 5.73 | 131.09 | 123.00 |
| 1 | G | 518 | HIS | CB-CA-C | -5.71 | 98.04 | 109.35 |
| 1 | F | 560 | THR | N-CA-C | 5.70 | 122.95 | 110.80 |
| 1 | E | 531 | GLY | N-CA-C | -5.68 | 99.73 | 113.18 |
| 1 | F | 398 | GLU | N-CA-C | 5.67 | 118.91 | 110.52 |
| 1 | A | 510 | GLN | N-CA-C | 5.66 | 119.39 | 111.30 |
| 3 | P | 398 | LEU | N-CA-C | 5.66 | 117.23 | 110.44 |
| 1 | F | 366 | THR | N-CA-C | 5.65 | 117.60 | 108.34 |
| 1 | A | 477 | THR | CB-CA-C | -5.64 | 98.59 | 109.37 |
| 1 | B | 483 | ASP | N-CA-C | -5.64 | 97.80 | 107.61 |
| 1 | C | 531 | GLY | N-CA-C | 5.64 | 126.54 | 113.18 |
| 3 | P | 288 | GLY | N-CA-C | -5.62 | 99.86 | 113.18 |
| 1 | K | 448 | ALA | N-CA-C | 5.62 | 115.98 | 108.23 |
| 3 | P | 277 | GLY | CA-C-N | 5.62 | 132.27 | 121.54 |
| 3 | P | 277 | GLY | C-N-CA | 5.62 | 132.27 | 121.54 |
| 1 | A | 489 | MET | CB-CG-SD | -5.60 | 95.89 | 112.70 |
| 1 | F | 402 | ASN | N-CA-C | -5.58 | 103.61 | 110.65 |
| 1 | L | 553 | ASP | O-C-N | 5.58 | 129.38 | 123.42 |
| 1 | B | 489 | MET | CB-CA-C | -5.57 | 98.64 | 109.68 |
| 1 | K | 536 | CYS | N-CA-CB | -5.56 | 101.18 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 486 | VAL | CB-CA-C | -5.55 | 102.38 | 110.81 |
| 3 | P | 537 | THR | N-CA-C | 5.55 | 118.72 | 109.96 |
| 1 | L | 483 | ASP | N-CA-C | 5.54 | 122.60 | 110.80 |
| 1 | F | 415 | GLU | N-CA-C | 5.52 | 122.55 | 110.80 |
| 4 | U | 39 | LEU | CA-C-N | 5.50 | 125.17 | 119.56 |
| 4 | U | 39 | LEU | C-N-CA | 5.50 | 125.17 | 119.56 |
| 1 | H | 442 | SER | N-CA-C | 5.49 | 122.50 | 110.80 |
| 4 | V | 113 | GLY | N-CA-C | 5.49 | 126.19 | 113.18 |
| 2 | J | 64 | LEU | N-CA-C | 5.48 | 122.48 | 110.80 |
| 1 | E | 537 | VAL | CB-CA-C | -5.48 | 105.23 | 111.59 |
| 1 | H | 533 | THR | N-CA-C | 5.47 | 119.96 | 112.68 |
| 1 | L | 440 | THR | O-C-N | 5.46 | 129.45 | 123.22 |
| 3 | P | 9 | GLU | CB-CA-C | -5.46 | 104.66 | 111.43 |
| 3 | P | 476 | TYR | N-CA-C | 5.46 | 118.16 | 109.81 |
| 3 | P | 156 | VAL | N-CA-C | -5.45 | 102.02 | 109.37 |
| 1 | F | 422 | GLU | CB-CA-C | -5.44 | 107.60 | 114.40 |
| 1 | C | 566 | LEU | CB-CA-C | -5.42 | 100.59 | 109.53 |
| 3 | P | 413 | LEU | N-CA-C | 5.39 | 122.28 | 110.80 |
| 3 | P | 361 | LYS | N-CA-C | 5.37 | 118.07 | 110.50 |
| 1 | B | 365 | LEU | N-CA-C | 5.37 | 118.91 | 107.70 |
| 1 | E | 538 | VAL | N-CA-C | 5.37 | 120.50 | 109.34 |
| 3 | P | 407 | THR | CB-CA-C | -5.36 | 103.62 | 111.23 |
| 1 | B | 452 | PRO | CA-C-O | -5.35 | 114.89 | 121.31 |
| 1 | B | 494 | PRO | CB-CA-C | -5.35 | 104.10 | 111.21 |
| 1 | E | 545 | ASN | N-CA-C | -5.33 | 104.05 | 110.44 |
| 1 | A | 540 | HIS | O-C-N | -5.32 | 117.10 | 123.27 |
| 1 | F | 484 | VAL | N-CA-CB | -5.32 | 101.70 | 111.91 |
| 1 | L | 440 | THR | CA-C-N | 5.31 | 131.53 | 121.97 |
| 1 | L | 440 | THR | C-N-CA | 5.31 | 131.53 | 121.97 |
| 1 | H | 564 | VAL | N-CA-C | 5.31 | 120.38 | 109.34 |
| 4 | R | 20 | LEU | CA-C-N | 5.27 | 126.43 | 119.84 |
| 4 | R | 20 | LEU | C-N-CA | 5.27 | 126.43 | 119.84 |
| 1 | A | 526 | GLU | O-C-N | 5.25 | 127.69 | 122.12 |
| 3 | P | 60 | TYR | N-CA-CB | 5.25 | 120.10 | 112.28 |
| 1 | B | 477 | THR | CB-CA-C | -5.24 | 100.48 | 109.65 |
| 1 | A | 486 | VAL | N-CA-C | 5.24 | 115.85 | 108.36 |
| 3 | P | 431 | TRP | N-CA-C | -5.23 | 101.94 | 110.20 |
| 1 | B | 373 | THR | N-CA-C | 5.21 | 117.44 | 110.35 |
| 1 | E | 533 | THR | CA-C-O | -5.21 | 113.06 | 120.51 |
| 1 | C | 533 | THR | CB-CA-C | 5.20 | 118.93 | 110.24 |
| 1 | B | 414 | CYS | CA-CB-SG | -5.20 | 102.44 | 114.40 |
| 1 | C | 454 | VAL | CB-CA-C | -5.20 | 102.76 | 111.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 530 | THR | N-CA-C | -5.19 | 106.53 | 112.92 |
| 4 | S | 97 | SER | N-CA-C | -5.17 | 98.49 | 107.49 |
| 1 | L | 445 | LYS | N-CA-C | -5.17 | 106.82 | 113.23 |
| 1 | D | 452 | PRO | CA-C-O | -5.16 | 115.72 | 122.12 |
| 3 | P | 344 | VAL | N-CA-C | 5.16 | 116.34 | 109.37 |
| 1 | F | 368 | LEU | N-CA-C | -5.14 | 102.03 | 109.59 |
| 1 | C | 524 | SER | N-CA-C | -5.12 | 99.92 | 108.32 |
| 1 | K | 473 | THR | CB-CA-C | -5.12 | 102.89 | 110.62 |
| 1 | C | 566 | LEU | N-CA-C | 5.08 | 118.50 | 109.96 |
| 1 | F | 545 | ASN | N-CA-C | -5.06 | 104.37 | 110.44 |
| 1 | B | 452 | PRO | CB-CA-C | -5.05 | 104.49 | 111.21 |
| 1 | L | 567 | VAL | N-CA-C | 5.05 | 116.19 | 109.37 |
| 1 | B | 402 | ASN | N-CA-C | -5.04 | 106.72 | 112.92 |
| 1 | F | 408 | VAL | N-CA-C | 5.02 | 116.43 | 109.45 |
| 3 | P | 9 | GLU | N-CA-C | 5.01 | 115.72 | 107.20 |
| 1 | B | 456 | LEU | N-CA-CB | -5.01 | 102.70 | 110.57 |
| 1 | C | 457 | LEU | CA-C-N | 5.01 | 125.54 | 120.38 |
| 1 | C | 457 | LEU | C-N-CA | 5.01 | 125.54 | 120.38 |
| 1 | L | 575 | CYS | N-CA-C | 5.01 | 121.47 | 110.80 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | C | 452 | PRO | Mainchain |
| 1 | C | 464 | LEU | Mainchain |
| 1 | C | 480 | SER | Peptide |
| 1 | E | 480 | SER | Peptide |
| 1 | H | 441 | ILE | Mainchain |
| 3 | P | 376 | ARG | Mainchain |
| 3 | P | 400 | GLU | Peptide |

## 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 | 1786 | 0 | 1741 | 177 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | B | 1769 | 0 | 1729 | 167 | 0 |
| 1 | C | 1763 | 0 | 1724 | 140 | 0 |
| 1 | D | 1743 | 0 | 1708 | 95 | 0 |
| 1 | E | 1743 | 0 | 1710 | 143 | 0 |
| 1 | F | 1743 | 0 | 1706 | 154 | 0 |
| 1 | G | 1742 | 0 | 1709 | 93 | 0 |
| 1 | H | 1798 | 0 | 1751 | 108 | 0 |
| 1 | K | 1798 | 0 | 1753 | 200 | 0 |
| 1 | L | 1798 | 0 | 1751 | 274 | 0 |
| 2 | J | 851 | 0 | 842 | 82 | 0 |
| 3 | P | 3851 | 0 | 3755 | 535 | 0 |
| 4 | R | 766 | 0 | 784 | 93 | 0 |
| 4 | S | 785 | 0 | 808 | 93 | 0 |
| 4 | U | 766 | 0 | 784 | 60 | 0 |
| 4 | V | 805 | 0 | 821 | 53 | 0 |
| 5 | I | 28 | 0 | 25 | 6 | 0 |
| 6 | A | 14 | 0 | 13 | 1 | 0 |
| 6 | B | 14 | 0 | 13 | 1 | 0 |
| 6 | C | 14 | 0 | 13 | 2 | 0 |
| 6 | D | 14 | 0 | 13 | 0 | 0 |
| 6 | E | 14 | 0 | 13 | 1 | 0 |
| 6 | F | 14 | 0 | 13 | 1 | 0 |
| 6 | G | 15 | 0 | 15 | 0 | 0 |
| 6 | H | 14 | 0 | 13 | 3 | 0 |
| 6 | K | 14 | 0 | 13 | 4 | 0 |
| 6 | L | 14 | 0 | 13 | 0 | 0 |
| All | All | 25676 | 0 | 25233 | 2288 | 0 |

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

All (2288) 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:F:482:ALA:HB2 | 1:F:515:TYR:CD2 | 1.29 | 1.63 |
| 4:R:20:LEU:HD21 | 4:R:117:LYS:CG | 1.17 | 1.62 |
| 1:A:359:LEU:HD12 | 2:J:117:TYR:CD2 | 1.09 | 1.58 |
| 4:R:20:LEU:CD2 | 4:R:117:LYS:HG3 | 1.16 | 1.57 |
| 3:P:395:LEU:CD1 | 3:P:410:LEU:HD13 | 1.29 | 1.56 |
| 1:L:540:HIS:CB | 1:L:543:LEU:HD21 | 1.18 | 1.56 |
| 3:P:395:LEU:HD13 | 3:P:410:LEU:CD1 | 1.36 | 1.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:131:THR:CG2 | 3:P:188:VAL:HG22 | 1.23 | 1.54 |
| 1:L:450:HIS:H | 1:L:480:SER:CB | 1.19 | 1.54 |
| 1:A:359:LEU:CD1 | 2:J:117:TYR:HD2 | 1.14 | 1.53 |
| 3:P:131:THR:HG21 | 3:P:188:VAL:CG2 | 1.34 | 1.53 |
| 3:P:466:PHE:CE2 | 3:P:507:ARG:HG3 | 1.39 | 1.51 |
| 1:L:540:HIS:CA | 1:L:543:LEU:CD2 | 1.86 | 1.51 |
| 1:F:482:ALA:CB | 1:F:515:TYR:CD2 | 1.92 | 1.51 |
| 1:C:563:ASN:ND2 | 6:C:601:NAG:C1 | 1.70 | 1.50 |
| 4:S:31:GLY:C | 4:S:94:LEU:HD23 | 1.09 | 1.49 |
| 4:S:39:LEU:HD13 | 4:S:87:PHE:CD1 | 1.46 | 1.49 |
| 3:P:278:ARG:O | 3:P:422:TRP:CZ2 | 1.66 | 1.45 |
| 1:F:535:THR:HG22 | 1:F:551:THR:CG2 | 1.43 | 1.45 |
| 3:P:448:VAL:HB | 3:P:449:PRO:CD | 1.14 | 1.45 |
| 3:P:477:TRP:CH2 | 3:P:524:TYR:CD1 | 2.02 | 1.45 |
| 1:L:540:HIS:CB | 1:L:543:LEU:CD2 | 1.95 | 1.45 |
| 3:P:345:ALA:C | 3:P:413:LEU:HD12 | 1.34 | 1.45 |
| 1:L:540:HIS:HB3 | 1:L:543:LEU:CD2 | 1.46 | 1.43 |
| 3:P:446:LEU:CA | 3:P:465:HIS:O | 1.66 | 1.43 |
| 1:K:450:HIS:CD2 | 1:K:514:ARG:HH12 | 1.36 | 1.43 |
| 1:K:464:LEU:CD1 | 1:K:525:GLU:OE2 | 1.64 | 1.43 |
| 1:L:511:ALA:HB3 | 1:L:514:ARG:CD | 1.51 | 1.41 |
| 1:L:540:HIS:N | 1:L:543:LEU:HD23 | 1.35 | 1.40 |
| 4:S:31:GLY:C | 4:S:94:LEU:CD2 | 1.95 | 1.40 |
| 1:H:554:LYS:HZ3 | 1:H:558:LYS:NZ | 1.03 | 1.38 |
| 1:E:489:MET:SD | 1:E:494:PRO:HD3 | 1.65 | 1.37 |
| 1:H:554:LYS:NZ | 1:H:558:LYS:NZ | 1.71 | 1.37 |
| 1:L:424:PHE:N | 1:L:441:ILE:HD11 | 1.36 | 1.36 |
| 3:P:477:TRP:HH2 | 3:P:524:TYR:CD1 | 1.36 | 1.36 |
| 1:L:424:PHE:CB | 1:L:441:ILE:HD11 | 1.54 | 1.35 |
| 1:F:560:THR:O | 1:G:560:THR:HG22 | 1.25 | 1.35 |
| 3:P:131:THR:CG2 | 3:P:188:VAL:CG2 | 1.97 | 1.35 |
| 1:E:450:HIS:CG | 1:E:514:ARG:NH2 | 1.95 | 1.34 |
| 3:P:340:VAL:CG1 | 3:P:436:GLU:HB3 | 1.54 | 1.34 |
| 4:S:39:LEU:CD1 | 4:S:87:PHE:CE1 | 2.08 | 1.34 |
| 3:P:346:GLY:N | 3:P:413:LEU:CG | 1.88 | 1.34 |
| 1:L:421:GLY:O | 1:L:443:ARG:NH1 | 1.59 | 1.33 |
| 1:A:356:SER:CA | 2:J:117:TYR:OH | 1.77 | 1.32 |
| 1:F:482:ALA:CB | 1:F:515:TYR:HD2 | 1.29 | 1.32 |
| 3:P:446:LEU:HD21 | 3:P:537:THR:O | 1.17 | 1.32 |
| 3:P:368:LEU:N | 3:P:378:PRO:HD2 | 1.46 | 1.31 |
| 1:L:424:PHE:CB | 1:L:441:ILE:CD1 | 2.09 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:450:HIS:N | 1:L:480:SER:CB | 1.94 | 1.30 |
| 1:L:424:PHE:HB2 | 1:L:441:ILE:CD1 | 1.61 | 1.30 |
| 1:L:511:ALA:HB3 | 1:L:514:ARG:CG | 1.60 | 1.30 |
| 3:P:448:VAL:CB | 3:P:449:PRO:CD | 2.01 | 1.30 |
| 1:E:450:HIS:ND1 | 1:E:514:ARG:NH2 | 1.75 | 1.30 |
| 3:P:446:LEU:CD2 | 3:P:537:THR:O | 1.79 | 1.30 |
| 3:P:466:PHE:HE2 | 3:P:507:ARG:CG | 1.46 | 1.29 |
| 4:S:31:GLY:O | 4:S:94:LEU:HD23 | 1.25 | 1.29 |
| 1:L:424:PHE:CA | 1:L:441:ILE:HD11 | 1.62 | 1.29 |
| 1:L:540:HIS:C | 1:L:543:LEU:CD2 | 2.05 | 1.28 |
| 3:P:251:PHE:CE1 | 3:P:308:GLY:O | 1.86 | 1.28 |
| 1:C:508:GLU:HG2 | 1:C:509:PRO:CD | 1.61 | 1.28 |
| 3:P:477:TRP:CZ2 | 3:P:524:TYR:HB3 | 1.67 | 1.27 |
| 1:D:421:GLY:HA2 | 1:D:445:LYS:CE | 1.66 | 1.26 |
| 1:L:424:PHE:N | 1:L:441:ILE:CD1 | 1.99 | 1.26 |
| 3:P:261:CYS:CB | 3:P:315:LEU:HD23 | 1.66 | 1.25 |
| 4:S:29:LEU:CD2 | 4:S:95:THR:HG23 | 1.66 | 1.24 |
| 3:P:447:LYS:HG2 | 3:P:465:HIS:CB | 1.68 | 1.23 |
| 1:G:523:VAL:HG21 | 1:G:534:TYR:OH | 1.32 | 1.22 |
| 1:L:450:HIS:HB2 | 1:L:480:SER:OG | 1.07 | 1.22 |
| 1:L:450:HIS:CB | 1:L:480:SER:OG | 1.87 | 1.22 |
| 1:L:479:PHE:CB | 1:L:515:TYR:O | 1.87 | 1.22 |
| 3:P:278:ARG:O | 3:P:422:TRP:HZ2 | 0.94 | 1.22 |
| 1:F:535:THR:CG2 | 1:F:551:THR:HG22 | 1.69 | 1.22 |
| 1:L:456:LEU:HD23 | 1:L:552:VAL:CG2 | 1.68 | 1.22 |
| 4:S:39:LEU:CD1 | 4:S:87:PHE:CD1 | 2.22 | 1.21 |
| 1:A:356:SER:CB | 2:J:117:TYR:OH | 1.87 | 1.21 |
| 1:K:509:PRO:CG | 1:L:501:VAL:HG21 | 1.69 | 1.21 |
| 1:L:479:PHE:HB2 | 1:L:515:TYR:O | 1.05 | 1.20 |
| 3:P:345:ALA:C | 3:P:413:LEU:CD1 | 2.13 | 1.20 |
| 4:S:37:CYS:CB | 4:S:116:GLN:OE1 | 1.88 | 1.20 |
| 3:P:448:VAL:CB | 3:P:449:PRO:HD2 | 1.64 | 1.20 |
| 1:L:540:HIS:C | 1:L:543:LEU:HD22 | 1.63 | 1.20 |
| 1:D:490:GLN:OE1 | 1:D:532:GLU:HB3 | 1.41 | 1.20 |
| 1:L:540:HIS:N | 1:L:543:LEU:CD2 | 1.94 | 1.20 |
| 1:C:461:ARG:NH1 | 1:C:465:ASN:HD21 | 1.40 | 1.19 |
| 2:J:21:ILE:CD1 | 1:L:555:SER:HB3 | 1.71 | 1.19 |
| 1:K:463:GLN:HB2 | 1:L:455:TYR:CZ | 1.77 | 1.18 |
| 3:P:466:PHE:CE2 | 3:P:507:ARG:CG | 2.24 | 1.17 |
| 1:K:354:PHE:HE1 | 1:K:541:GLU:N | 1.42 | 1.16 |
| 3:P:261:CYS:SG | 3:P:315:LEU:HD23 | 0.64 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:421:TYR:CE1 | 3:P:437:ILE:HD12 | 1.79 | 1.16 |
| 4:S:37:CYS:HA | 4:S:116:GLN:OE1 | 1.45 | 1.16 |
| 3:P:368:LEU:H | 3:P:378:PRO:CD | 1.59 | 1.16 |
| 1:B:413:ILE:CD1 | 1:B:414:CYS:H | 1.58 | 1.15 |
| 1:E:493:GLN:HB2 | 1:E:494:PRO:HD2 | 1.20 | 1.15 |
| 1:L:540:HIS:CA | 1:L:543:LEU:HD21 | 1.59 | 1.15 |
| 1:L:511:ALA:HB3 | 1:L:514:ARG:HD2 | 1.26 | 1.15 |
| 1:K:511:ALA:HB1 | 1:K:512:PRO:CD | 1.72 | 1.15 |
| 1:B:414:CYS:SG | 1:C:416:ASP:HB2 | 1.87 | 1.14 |
| 1:B:461:ARG:HH21 | 1:L:570:ASP:CG | 1.54 | 1.14 |
| 3:P:261:CYS:SG | 3:P:315:LEU:CG | 2.35 | 1.14 |
| 1:B:413:ILE:HD13 | 1:B:414:CYS:N | 1.62 | 1.14 |
| 1:F:482:ALA:CB | 1:F:515:TYR:CE2 | 2.30 | 1.13 |
| 1:L:424:PHE:H | 1:L:441:ILE:CD1 | 1.58 | 1.13 |
| 1:E:543:LEU:HD23 | 1:E:544:PRO:HD3 | 1.30 | 1.13 |
| 1:K:509:PRO:HG3 | 1:L:501:VAL:HG21 | 1.17 | 1.13 |
| 3:P:450:GLY:HA3 | 3:P:540:VAL:HG12 | 1.29 | 1.13 |
| 1:B:480:SER:OG | 1:B:481:PRO:HD3 | 1.47 | 1.12 |
| 1:A:514:ARG:HB3 | 1:A:514:ARG:HH11 | 1.11 | 1.12 |
| 4:S:37:CYS:CA | 4:S:116:GLN:OE1 | 1.97 | 1.12 |
| 1:D:420:SER:C | 1:D:445:LYS:HZ2 | 1.56 | 1.11 |
| 1:G:506:MET:HE3 | 1:G:516:PHE:HE2 | 1.09 | 1.11 |
| 3:P:345:ALA:HA | 3:P:413:LEU:HB2 | 1.17 | 1.11 |
| 3:P:261:CYS:SG | 3:P:315:LEU:CD2 | 1.19 | 1.11 |
| 1:C:508:GLU:HG2 | 1:C:509:PRO:HD3 | 1.33 | 1.10 |
| 3:P:250:LYS:HG2 | 3:P:309:ALA:HB2 | 1.33 | 1.10 |
| 3:P:346:GLY:N | 3:P:413:LEU:CB | 2.14 | 1.10 |
| 4:R:75:ARG:NH2 | 4:R:95:THR:OG1 | 1.84 | 1.10 |
| 1:F:524:SER:HG | 1:F:527:GLU:HB2 | 1.16 | 1.10 |
| 1:K:464:LEU:HD12 | 1:K:525:GLU:OE2 | 1.44 | 1.10 |
| 4:U:22:GLU:HB2 | 4:U:119:THR:O | 1.51 | 1.10 |
| 1:A:478:GLY:O | 1:A:514:ARG:NH1 | 1.83 | 1.10 |
| 1:L:540:HIS:H | 1:L:543:LEU:CD2 | 1.57 | 1.10 |
| 3:P:411:ASN:HB3 | 3:P:537:THR:OG1 | 1.47 | 1.10 |
| 3:P:445:ASN:O | 3:P:466:PHE:HA | 1.51 | 1.10 |
| 4:R:116:GLN:HE22 | 4:R:118:VAL:CG2 | 1.64 | 1.10 |
| 3:P:475:LYS:HB2 | 3:P:507:ARG:HD2 | 1.20 | 1.09 |
| 1:A:493:GLN:HB2 | 1:A:494:PRO:HD2 | 1.25 | 1.09 |
| 1:K:464:LEU:HD11 | 1:K:525:GLU:OE2 | 1.47 | 1.09 |
| 1:A:356:SER:HB2 | 2:J:117:TYR:OH | 1.44 | 1.09 |
| 1:C:508:GLU:HG2 | 1:C:509:PRO:HD2 | 1.27 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:563:ASN:HD21 | 6:K:601:NAG:C1 | 1.63 | 1.09 |
| 4:R:61:VAL:HG21 | 4:R:72:TYR:CD2 | 1.87 | 1.08 |
| 1:B:480:SER:HG | 1:B:481:PRO:HD3 | 1.00 | 1.08 |
| 1:L:540:HIS:O | 1:L:543:LEU:CD2 | 2.01 | 1.08 |
| 3:P:448:VAL:CG2 | 3:P:449:PRO:HD2 | 1.82 | 1.08 |
| 3:P:447:LYS:HG2 | 3:P:465:HIS:HB3 | 1.30 | 1.08 |
| 1:K:450:HIS:CD2 | 1:K:514:ARG:NH1 | 2.20 | 1.07 |
| 3:P:131:THR:HG23 | 3:P:188:VAL:HA | 1.32 | 1.07 |
| 4:R:61:VAL:HG21 | 4:R:72:TYR:HD2 | 1.11 | 1.07 |
| 1:D:421:GLY:CA | 1:D:445:LYS:CE | 2.33 | 1.07 |
| 3:P:251:PHE:CD1 | 3:P:308:GLY:O | 2.07 | 1.07 |
| 4:S:39:LEU:HD13 | 4:S:87:PHE:CE1 | 1.82 | 1.07 |
| 1:L:450:HIS:N | 1:L:480:SER:HB2 | 1.58 | 1.07 |
| 1:F:482:ALA:HB2 | 1:F:515:TYR:CE2 | 1.88 | 1.07 |
| 4:R:22:GLU:HA | 4:R:117:LYS:O | 1.54 | 1.07 |
| 1:A:356:SER:HA | 2:J:117:TYR:OH | 1.55 | 1.07 |
| 1:E:421:GLY:HA3 | 1:E:445:LYS:HE3 | 1.36 | 1.07 |
| 1:F:482:ALA:HB1 | 1:F:515:TYR:HD2 | 1.16 | 1.06 |
| 1:L:511:ALA:CB | 1:L:514:ARG:CD | 2.31 | 1.06 |
| 1:K:527:GLU:HA | 1:K:530:THR:OG1 | 1.55 | 1.06 |
| 1:L:450:HIS:N | 1:L:480:SER:OG | 1.85 | 1.06 |
| 1:L:424:PHE:H | 1:L:441:ILE:CG1 | 1.69 | 1.06 |
| 4:R:50:ARG:HD2 | 4:R:72:TYR:OH | 1.56 | 1.06 |
| 1:K:354:PHE:CE1 | 1:K:541:GLU:N | 2.24 | 1.06 |
| 3:P:340:VAL:CG1 | 3:P:436:GLU:CB | 2.34 | 1.06 |
| 1:E:454:VAL:HG21 | 1:E:538:VAL:HG21 | 1.37 | 1.05 |
| 1:E:450:HIS:CG | 1:E:514:ARG:HH22 | 1.68 | 1.05 |
| 1:E:508:GLU:OE1 | 1:E:509:PRO:HD2 | 1.55 | 1.05 |
| 1:K:454:VAL:CG2 | 1:K:538:VAL:HG21 | 1.85 | 1.05 |
| 1:L:511:ALA:CB | 1:L:514:ARG:HD2 | 1.86 | 1.05 |
| 3:P:243:PRO:O | 3:P:246:ALA:CB | 2.04 | 1.05 |
| 3:P:261:CYS:SG | 3:P:315:LEU:HD21 | 1.91 | 1.05 |
| 1:F:450:HIS:HD2 | 1:F:514:ARG:CZ | 1.68 | 1.05 |
| 1:L:443:ARG:N | 1:L:444:PRO:HD3 | 1.67 | 1.04 |
| 3:P:477:TRP:CZ2 | 3:P:524:TYR:CB | 2.40 | 1.04 |
| 1:C:508:GLU:CG | 1:C:509:PRO:HD3 | 1.87 | 1.04 |
| 1:L:456:LEU:CD2 | 1:L:552:VAL:CG2 | 2.34 | 1.04 |
| 1:E:450:HIS:CE1 | 1:E:514:ARG:HH12 | 1.75 | 1.04 |
| 3:P:448:VAL:HB | 3:P:449:PRO:HD2 | 1.07 | 1.04 |
| 3:P:345:ALA:CA | 3:P:413:LEU:HB2 | 1.87 | 1.03 |
| 2:J:21:ILE:HD11 | 1:L:555:SER:HB3 | 1.08 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:395:LEU:HB2 | 3:P:410:LEU:HD11 | 1.40 | 1.03 |
| 3:P:346:GLY:H | 3:P:413:LEU:CB | 1.69 | 1.03 |
| 4:R:22:GLU:OE1 | 4:R:101:VAL:HG13 | 1.57 | 1.03 |
| 4:R:46:ILE:H | 4:R:64:THR:CG2 | 1.72 | 1.03 |
| 1:B:478:GLY:O | 1:B:514:ARG:HG3 | 1.59 | 1.02 |
| 1:K:509:PRO:CG | 1:L:501:VAL:CG2 | 2.35 | 1.02 |
| 1:L:456:LEU:CD2 | 1:L:552:VAL:HG22 | 1.89 | 1.02 |
| 1:E:489:MET:SD | 1:E:494:PRO:CD | 2.47 | 1.02 |
| 1:E:543:LEU:HD23 | 1:E:544:PRO:CD | 1.89 | 1.02 |
| 1:C:566:LEU:H | 1:C:566:LEU:HD12 | 1.23 | 1.02 |
| 3:P:368:LEU:H | 3:P:378:PRO:HD2 | 0.89 | 1.02 |
| 3:P:368:LEU:HB2 | 3:P:378:PRO:CG | 1.90 | 1.02 |
| 4:R:116:GLN:NE2 | 4:R:118:VAL:HG23 | 1.74 | 1.02 |
| 1:C:451:ARG:HB3 | 1:C:451:ARG:HH11 | 1.20 | 1.02 |
| 1:G:501:VAL:HG21 | 1:H:509:PRO:HD3 | 1.42 | 1.01 |
| 2:J:27:ASP:HB2 | 2:J:28:PRO:CD | 1.90 | 1.01 |
| 3:P:418:ALA:HB2 | 3:P:439:ILE:HD13 | 1.43 | 1.01 |
| 3:P:462:VAL:HG12 | 3:P:540:VAL:HG11 | 1.36 | 1.01 |
| 1:F:524:SER:OG | 1:F:527:GLU:HB2 | 1.61 | 1.01 |
| 3:P:340:VAL:HG12 | 3:P:436:GLU:O | 1.60 | 1.01 |
| 1:K:354:PHE:HZ | 1:K:546:ARG:HD3 | 1.26 | 1.01 |
| 1:L:421:GLY:O | 1:L:443:ARG:CZ | 2.06 | 1.01 |
| 4:S:29:LEU:HD23 | 4:S:95:THR:HG23 | 1.42 | 1.01 |
| 1:C:461:ARG:NH1 | 1:C:465:ASN:ND2 | 2.08 | 1.01 |
| 2:J:115:LEU:HD12 | 2:J:124:VAL:HG21 | 1.38 | 1.01 |
| 1:K:509:PRO:HG2 | 1:L:501:VAL:CG2 | 1.90 | 1.01 |
| 3:P:446:LEU:CD2 | 3:P:538:ALA:HB2 | 1.89 | 1.01 |
| 1:E:450:HIS:CD2 | 1:E:514:ARG:NH1 | 2.29 | 1.00 |
| 1:F:450:HIS:CD2 | 1:F:514:ARG:CZ | 2.42 | 1.00 |
| 1:K:484:VAL:HG23 | 1:K:540:HIS:HB2 | 1.43 | 1.00 |
| 1:K:511:ALA:HB1 | 1:K:512:PRO:HD3 | 1.01 | 1.00 |
| 4:R:20:LEU:CD2 | 4:R:117:LYS:CG | 1.96 | 1.00 |
| 3:P:447:LYS:H | 3:P:465:HIS:H | 1.03 | 1.00 |
| 1:L:424:PHE:CG | 1:L:441:ILE:HD11 | 1.96 | 1.00 |
| 1:A:456:LEU:HD11 | 1:A:550:ARG:O | 1.59 | 1.00 |
| 3:P:414:THR:OG1 | 3:P:417:ASP:OD2 | 1.80 | 1.00 |
| 3:P:447:LYS:HG2 | 3:P:465:HIS:HB2 | 1.42 | 1.00 |
| 1:C:457:LEU:HD12 | 1:C:473:THR:OG1 | 1.62 | 1.00 |
| 3:P:391:TYR:OH | 3:P:416:ARG:NH1 | 1.95 | 0.99 |
| 3:P:450:GLY:CA | 3:P:540:VAL:HG12 | 1.92 | 0.99 |
| 3:P:131:THR:CG2 | 3:P:188:VAL:HA | 1.92 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:451:ARG:HG2 | 1:B:542:ALA:O | 1.60 | 0.99 |
| 1:K:527:GLU:O | 1:K:530:THR:OG1 | 1.80 | 0.99 |
| 1:D:421:GLY:HA2 | 1:D:445:LYS:HE2 | 1.42 | 0.99 |
| 1:E:421:GLY:HA3 | 1:E:445:LYS:CE | 1.91 | 0.99 |
| 1:K:527:GLU:C | 1:K:530:THR:HG1 | 1.70 | 0.99 |
| 1:E:493:GLN:CB | 1:E:494:PRO:HD2 | 1.77 | 0.99 |
| 1:L:424:PHE:CG | 1:L:441:ILE:CD1 | 2.46 | 0.99 |
| 1:B:413:ILE:HD13 | 1:B:414:CYS:H | 0.82 | 0.99 |
| 1:D:421:GLY:CA | 1:D:445:LYS:NZ | 2.26 | 0.99 |
| 1:L:456:LEU:HD23 | 1:L:552:VAL:HG22 | 1.01 | 0.99 |
| 1:E:450:HIS:CG | 1:E:514:ARG:CZ | 2.46 | 0.98 |
| 3:P:131:THR:HG23 | 3:P:188:VAL:HG22 | 1.42 | 0.98 |
| 4:S:29:LEU:HD22 | 4:S:95:THR:HG23 | 1.43 | 0.98 |
| 1:C:508:GLU:CG | 1:C:509:PRO:CD | 2.40 | 0.98 |
| 1:E:508:GLU:OE1 | 1:E:509:PRO:CD | 2.11 | 0.98 |
| 1:K:511:ALA:CB | 1:K:512:PRO:HD3 | 1.89 | 0.98 |
| 3:P:447:LYS:CG | 3:P:465:HIS:HB3 | 1.92 | 0.98 |
| 1:C:482:ALA:HB2 | 1:C:515:TYR:CD1 | 1.97 | 0.98 |
| 1:B:450:HIS:O | 1:B:542:ALA:CB | 2.12 | 0.98 |
| 1:D:421:GLY:N | 1:D:445:LYS:NZ | 2.12 | 0.98 |
| 1:A:502:THR:HB | 1:A:519:SER:HB2 | 1.46 | 0.97 |
| 4:R:116:GLN:HE22 | 4:R:118:VAL:HG23 | 1.23 | 0.97 |
| 3:P:446:LEU:HA | 3:P:465:HIS:C | 1.88 | 0.97 |
| 1:H:526:GLU:O | 1:H:530:THR:HG23 | 1.64 | 0.97 |
| 3:P:368:LEU:HB2 | 3:P:378:PRO:CD | 1.94 | 0.97 |
| 3:P:447:LYS:H | 3:P:465:HIS:N | 1.62 | 0.97 |
| 1:A:355:ALA:O | 2:J:117:TYR:HE2 | 1.48 | 0.97 |
| 1:K:527:GLU:CA | 1:K:530:THR:OG1 | 2.12 | 0.97 |
| 2:J:21:ILE:HD11 | 1:L:555:SER:CB | 1.93 | 0.97 |
| 4:S:31:GLY:HA3 | 4:S:94:LEU:HD21 | 1.47 | 0.97 |
| 1:K:450:HIS:CG | 1:K:514:ARG:HH12 | 1.82 | 0.96 |
| 3:P:340:VAL:HG13 | 3:P:436:GLU:CB | 1.92 | 0.96 |
| 3:P:243:PRO:O | 3:P:246:ALA:HB3 | 1.63 | 0.96 |
| 4:U:50:ARG:NH1 | 4:U:100:GLY:HA3 | 1.79 | 0.96 |
| 3:P:395:LEU:CD1 | 3:P:410:LEU:CD1 | 2.13 | 0.96 |
| 1:E:450:HIS:CE1 | 1:E:514:ARG:HH22 | 1.83 | 0.96 |
| 3:P:345:ALA:O | 3:P:413:LEU:HD12 | 1.65 | 0.95 |
| 3:P:477:TRP:CH2 | 3:P:524:TYR:HD1 | 1.62 | 0.95 |
| 3:P:342:LYS:HB3 | 3:P:438:LYS:HB3 | 1.45 | 0.95 |
| 3:P:445:ASN:O | 3:P:467:PRO:HD3 | 1.66 | 0.95 |
| 4:R:61:VAL:CG2 | 4:R:72:TYR:HD2 | 1.77 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:454:VAL:CG2 | 1:E:538:VAL:HG21 | 1.96 | 0.95 |
| 1:E:450:HIS:NE2 | 1:E:514:ARG:NH1 | 2.13 | 0.95 |
| 4:U:22:GLU:CG | 4:U:119:THR:HG23 | 1.96 | 0.95 |
| 1:K:510:GLN:CG | 1:L:522:THR:HG21 | 1.97 | 0.95 |
| 1:L:543:LEU:HB2 | 1:L:546:ARG:HA | 1.46 | 0.95 |
| 3:P:477:TRP:CZ2 | 3:P:524:TYR:CG | 2.54 | 0.95 |
| 3:P:477:TRP:CZ2 | 3:P:524:TYR:CD1 | 2.54 | 0.94 |
| 1:D:420:SER:C | 1:D:445:LYS:NZ | 2.26 | 0.94 |
| 1:L:487:GLN:O | 1:L:537:VAL:HG12 | 1.66 | 0.94 |
| 1:B:451:ARG:HG2 | 1:B:542:ALA:C | 1.93 | 0.94 |
| 1:L:540:HIS:O | 1:L:543:LEU:HD23 | 1.67 | 0.94 |
| 4:S:29:LEU:CD2 | 4:S:95:THR:CG2 | 2.44 | 0.94 |
| 1:F:450:HIS:HD2 | 1:F:514:ARG:NH2 | 1.64 | 0.94 |
| 1:L:424:PHE:HB2 | 1:L:441:ILE:HD13 | 1.46 | 0.94 |
| 3:P:366:TRP:CE2 | 3:P:408:VAL:HG21 | 2.03 | 0.94 |
| 3:P:450:GLY:HA3 | 3:P:540:VAL:CG1 | 1.97 | 0.94 |
| 3:P:340:VAL:HG13 | 3:P:436:GLU:HB3 | 0.96 | 0.94 |
| 1:A:355:ALA:C | 2:J:117:TYR:HE2 | 1.75 | 0.93 |
| 1:L:443:ARG:H | 1:L:444:PRO:HD3 | 1.34 | 0.93 |
| 1:C:526:GLU:O | 1:C:530:THR:HG23 | 1.67 | 0.93 |
| 1:G:506:MET:HE3 | 1:G:516:PHE:CE2 | 2.01 | 0.93 |
| 1:K:563:ASN:ND2 | 6:K:601:NAG:C1 | 2.31 | 0.93 |
| 1:K:454:VAL:HG21 | 1:K:538:VAL:HG21 | 1.47 | 0.93 |
| 1:C:457:LEU:CD1 | 1:C:473:THR:OG1 | 2.17 | 0.93 |
| 1:E:450:HIS:HD1 | 1:E:514:ARG:HH22 | 1.11 | 0.93 |
| 3:P:446:LEU:HA | 3:P:465:HIS:O | 0.75 | 0.93 |
| 3:P:477:TRP:HZ2 | 3:P:524:TYR:CB | 1.81 | 0.93 |
| 1:C:461:ARG:HH12 | 1:C:465:ASN:ND2 | 1.63 | 0.93 |
| 4:S:31:GLY:CA | 4:S:94:LEU:CD2 | 2.47 | 0.92 |
| 3:P:278:ARG:O | 3:P:422:TRP:CH2 | 2.21 | 0.92 |
| 3:P:446:LEU:H | 3:P:446:LEU:HD12 | 1.33 | 0.92 |
| 1:B:450:HIS:O | 1:B:542:ALA:HB3 | 1.68 | 0.92 |
| 4:R:111:ASP:O | 4:R:114:LYS:CE | 2.18 | 0.92 |
| 4:S:39:LEU:CD1 | 4:S:87:PHE:HE1 | 1.77 | 0.92 |
| 1:A:359:LEU:CD1 | 2:J:117:TYR:CD2 | 2.04 | 0.92 |
| 1:H:554:LYS:NZ | 1:H:558:LYS:HZ2 | 1.50 | 0.92 |
| 1:K:516:PHE:CE2 | 1:L:520:ILE:HD13 | 2.04 | 0.92 |
| 1:L:424:PHE:H | 1:L:441:ILE:HG13 | 1.32 | 0.92 |
| 4:R:116:GLN:NE2 | 4:R:118:VAL:CG2 | 2.32 | 0.92 |
| 1:A:359:LEU:HD13 | 2:J:117:TYR:HB3 | 1.50 | 0.92 |
| 3:P:448:VAL:HB | 3:P:449:PRO:HD3 | 0.92 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:479:LYS:HG2 | 3:P:524:TYR:CE1 | 2.05 | 0.91 |
| 1:L:479:PHE:CZ | 1:L:484:VAL:HG11 | 2.05 | 0.91 |
| 1:L:540:HIS:O | 1:L:543:LEU:HD22 | 1.65 | 0.91 |
| 4:S:39:LEU:HD12 | 4:S:87:PHE:CE1 | 2.04 | 0.91 |
| 1:K:510:GLN:HG2 | 1:L:522:THR:HG21 | 1.52 | 0.91 |
| 3:P:131:THR:HG23 | 3:P:188:VAL:CA | 1.99 | 0.91 |
| 3:P:278:ARG:C | 3:P:422:TRP:HZ2 | 1.78 | 0.91 |
| 3:P:529:LYS:CE | 3:P:534:TYR:HE2 | 1.82 | 0.91 |
| 3:P:411:ASN:ND2 | 3:P:525:TRP:CZ2 | 2.39 | 0.91 |
| 1:B:414:CYS:SG | 1:C:416:ASP:CB | 2.58 | 0.91 |
| 1:F:502:THR:OG1 | 1:F:519:SER:CB | 2.18 | 0.91 |
| 2:J:28:PRO:HG3 | 1:L:467:ARG:CZ | 1.99 | 0.91 |
| 1:E:482:ALA:CB | 1:E:515:TYR:HE2 | 1.83 | 0.90 |
| 4:S:31:GLY:CA | 4:S:94:LEU:HD23 | 2.01 | 0.90 |
| 1:K:445:LYS:HA | 1:K:445:LYS:CE | 2.02 | 0.90 |
| 3:P:475:LYS:CB | 3:P:507:ARG:HD2 | 2.00 | 0.90 |
| 4:R:46:ILE:H | 4:R:64:THR:HG23 | 1.35 | 0.90 |
| 1:K:450:HIS:CG | 1:K:514:ARG:NH1 | 2.38 | 0.90 |
| 1:L:450:HIS:H | 1:L:480:SER:HB2 | 0.76 | 0.90 |
| 1:B:461:ARG:NH2 | 1:L:570:ASP:OD2 | 2.05 | 0.90 |
| 3:P:346:GLY:N | 3:P:413:LEU:HB2 | 1.86 | 0.90 |
| 1:G:450:HIS:HD2 | 1:G:514:ARG:NH2 | 1.68 | 0.90 |
| 1:L:424:PHE:HB2 | 1:L:441:ILE:CG1 | 2.01 | 0.90 |
| 3:P:448:VAL:CB | 3:P:449:PRO:HD3 | 1.81 | 0.90 |
| 4:U:22:GLU:CB | 4:U:119:THR:HG23 | 2.01 | 0.90 |
| 1:L:540:HIS:HB3 | 1:L:543:LEU:HD21 | 0.90 | 0.90 |
| 3:P:477:TRP:HH2 | 3:P:524:TYR:CE1 | 1.89 | 0.89 |
| 1:H:554:LYS:CE | 1:H:558:LYS:HZ2 | 1.85 | 0.89 |
| 3:P:395:LEU:HB2 | 3:P:410:LEU:CD1 | 2.02 | 0.89 |
| 3:P:445:ASN:OD1 | 3:P:467:PRO:HG2 | 1.71 | 0.89 |
| 1:E:526:GLU:O | 1:E:530:THR:HG23 | 1.73 | 0.89 |
| 4:R:25:VAL:HG11 | 4:R:33:VAL:HG13 | 1.54 | 0.89 |
| 1:K:511:ALA:CB | 1:K:512:PRO:CD | 2.46 | 0.89 |
| 4:S:117:LYS:HD3 | 4:S:117:LYS:N | 1.87 | 0.89 |
| 3:P:447:LYS:HB2 | 3:P:464:CYS:C | 1.98 | 0.89 |
| 3:P:529:LYS:HG3 | 3:P:534:TYR:CE2 | 2.08 | 0.89 |
| 1:F:450:HIS:ND1 | 1:F:480:SER:CB | 2.30 | 0.88 |
| 1:K:510:GLN:HG3 | 1:L:522:THR:CG2 | 2.03 | 0.88 |
| 1:L:540:HIS:H | 1:L:543:LEU:HD23 | 0.84 | 0.88 |
| 1:F:482:ALA:HB3 | 1:F:515:TYR:CE2 | 2.08 | 0.88 |
| 1:K:510:GLN:CG | 1:L:522:THR:CG2 | 2.50 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:366:TRP:CZ3 | 3:P:380:LEU:HD12 | 2.08 | 0.88 |
| 1:B:481:PRO:HD2 | 1:B:540:HIS:NE2 | 1.89 | 0.88 |
| 1:L:511:ALA:CB | 1:L:514:ARG:CG | 2.50 | 0.88 |
| 3:P:345:ALA:CA | 3:P:413:LEU:HD12 | 1.98 | 0.88 |
| 1:A:356:SER:HB2 | 2:J:117:TYR:HH | 1.37 | 0.87 |
| 1:E:527:GLU:O | 1:E:530:THR:OG1 | 1.92 | 0.87 |
| 1:A:554:LYS:O | 1:A:554:LYS:NZ | 2.08 | 0.87 |
| 1:B:545:ASN:O | 1:B:545:ASN:ND2 | 2.06 | 0.87 |
| 3:P:529:LYS:NZ | 3:P:534:TYR:CE2 | 2.43 | 0.87 |
| 1:H:554:LYS:CE | 1:H:558:LYS:NZ | 2.37 | 0.87 |
| 3:P:357:ARG:NH2 | 3:P:403:ASN:HD22 | 1.72 | 0.87 |
| 3:P:470:PHE:HE2 | 3:P:528:VAL:HG11 | 1.39 | 0.87 |
| 4:S:39:LEU:HD11 | 4:S:87:PHE:HE1 | 1.38 | 0.87 |
| 3:P:131:THR:CG2 | 3:P:188:VAL:CA | 2.52 | 0.87 |
| 4:S:39:LEU:HD13 | 4:S:87:PHE:HD1 | 1.07 | 0.87 |
| 1:A:493:GLN:OE1 | 1:A:493:GLN:N | 2.07 | 0.87 |
| 1:F:450:HIS:CD2 | 1:F:514:ARG:NH1 | 2.43 | 0.87 |
| 4:S:37:CYS:HB2 | 4:S:116:GLN:OE1 | 1.72 | 0.87 |
| 1:A:493:GLN:CB | 1:A:494:PRO:HD2 | 1.94 | 0.87 |
| 1:C:564:VAL:HG21 | 1:H:566:LEU:HD21 | 1.55 | 0.87 |
| 1:L:545:ASN:ND2 | 1:L:545:ASN:O | 2.07 | 0.87 |
| 1:L:540:HIS:CA | 1:L:543:LEU:HD23 | 1.74 | 0.87 |
| 1:K:445:LYS:HA | 1:K:445:LYS:HE3 | 1.57 | 0.86 |
| 1:F:480:SER:HB2 | 1:F:481:PRO:HD2 | 1.56 | 0.86 |
| 3:P:411:ASN:ND2 | 3:P:525:TRP:CE2 | 2.42 | 0.86 |
| 3:P:529:LYS:HG3 | 3:P:534:TYR:CD2 | 2.09 | 0.86 |
| 1:F:535:THR:CG2 | 1:F:551:THR:CG2 | 2.37 | 0.86 |
| 3:P:418:ALA:HB2 | 3:P:439:ILE:CD1 | 2.03 | 0.86 |
| 1:A:355:ALA:C | 2:J:117:TYR:CE2 | 2.53 | 0.86 |
| 1:F:363:THR:HG21 | 1:F:419:ASN:HB2 | 1.57 | 0.86 |
| 1:G:357:ILE:HD12 | 1:G:363:THR:HG22 | 1.57 | 0.86 |
| 3:P:412:GLN:NE2 | 3:P:412:GLN:O | 2.08 | 0.86 |
| 3:P:357:ARG:HH21 | 3:P:403:ASN:HD22 | 1.20 | 0.86 |
| 1:B:451:ARG:CG | 1:B:542:ALA:O | 2.24 | 0.86 |
| 1:C:451:ARG:HH11 | 1:C:451:ARG:CB | 1.87 | 0.86 |
| 3:P:418:ALA:HA | 3:P:439:ILE:HD11 | 1.56 | 0.86 |
| 3:P:446:LEU:HD22 | 3:P:538:ALA:HB2 | 1.56 | 0.86 |
| 1:E:506:MET:HG2 | 1:E:507:PRO:HD2 | 1.58 | 0.85 |
| 1:K:354:PHE:CZ | 1:K:546:ARG:HD3 | 2.10 | 0.85 |
| 4:R:111:ASP:O | 4:R:114:LYS:HE3 | 1.76 | 0.85 |
| 3:P:264:VAL:HG13 | 3:P:275:PHE:CD2 | 2.11 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:471:SER:O | 3:P:475:LYS:NZ | 2.09 | 0.85 |
| 3:P:395:LEU:HD12 | 3:P:409:ILE:O | 1.76 | 0.85 |
| 1:A:456:LEU:CD1 | 1:A:550:ARG:O | 2.25 | 0.85 |
| 1:E:511:ALA:HB1 | 1:E:514:ARG:HG3 | 1.57 | 0.85 |
| 1:B:478:GLY:O | 1:B:514:ARG:CG | 2.25 | 0.85 |
| 3:P:253:CYS:SG | 3:P:315:LEU:HB3 | 2.16 | 0.85 |
| 3:P:357:ARG:HH21 | 3:P:403:ASN:ND2 | 1.74 | 0.85 |
| 1:K:516:PHE:CE2 | 1:L:520:ILE:CD1 | 2.59 | 0.85 |
| 1:C:482:ALA:HB2 | 1:C:515:TYR:CE1 | 2.11 | 0.84 |
| 1:C:525:GLU:N | 1:C:525:GLU:OE1 | 2.10 | 0.84 |
| 1:K:527:GLU:C | 1:K:530:THR:OG1 | 2.17 | 0.84 |
| 6:H:601:NAG:H61 | 6:K:601:NAG:H61 | 1.58 | 0.84 |
| 1:D:421:GLY:CA | 1:D:445:LYS:HE3 | 2.07 | 0.84 |
| 1:E:493:GLN:HB2 | 1:E:494:PRO:CD | 2.08 | 0.84 |
| 1:G:443:ARG:O | 1:G:443:ARG:NE | 2.09 | 0.84 |
| 1:H:554:LYS:NZ | 1:H:558:LYS:HZ1 | 1.53 | 0.84 |
| 1:G:525:GLU:OE2 | 1:G:529:ASN:ND2 | 2.10 | 0.84 |
| 2:J:27:ASP:HB2 | 2:J:28:PRO:HD3 | 1.57 | 0.84 |
| 1:K:463:GLN:HB2 | 1:L:455:TYR:CE2 | 2.13 | 0.84 |
| 1:F:502:THR:OG1 | 1:F:519:SER:HA | 1.77 | 0.84 |
| 1:D:421:GLY:N | 1:D:445:LYS:HZ1 | 1.76 | 0.84 |
| 4:R:29:LEU:O | 4:R:94:LEU:O | 1.96 | 0.84 |
| 1:E:491:ARG:HD3 | 4:V:44:VAL:HG11 | 1.59 | 0.83 |
| 1:H:475:LEU:HD13 | 1:H:518:HIS:CE1 | 2.13 | 0.83 |
| 1:L:479:PHE:HZ | 1:L:484:VAL:HG11 | 1.43 | 0.83 |
| 1:A:518:HIS:HE1 | 1:B:520:ILE:CG2 | 1.91 | 0.83 |
| 1:A:491:ARG:HH11 | 1:A:491:ARG:HG2 | 1.42 | 0.83 |
| 1:C:480:SER:O | 1:C:540:HIS:CE1 | 2.31 | 0.83 |
| 1:E:421:GLY:CA | 1:E:445:LYS:HE2 | 2.09 | 0.83 |
| 1:L:540:HIS:HB2 | 1:L:543:LEU:HD21 | 1.57 | 0.83 |
| 1:L:511:ALA:HB3 | 1:L:514:ARG:HG3 | 1.59 | 0.83 |
| 3:P:131:THR:HG21 | 3:P:188:VAL:HG23 | 1.57 | 0.83 |
| 1:K:509:PRO:HG2 | 1:L:501:VAL:HG23 | 1.60 | 0.83 |
| 3:P:439:ILE:H | 3:P:439:ILE:HD12 | 1.42 | 0.83 |
| 1:L:443:ARG:N | 1:L:444:PRO:CD | 2.42 | 0.82 |
| 1:L:540:HIS:HB3 | 1:L:543:LEU:HD22 | 1.60 | 0.82 |
| 3:P:395:LEU:CB | 3:P:410:LEU:CD1 | 2.55 | 0.82 |
| 1:K:509:PRO:HG3 | 1:L:501:VAL:CG2 | 2.01 | 0.82 |
| 1:C:526:GLU:O | 1:C:530:THR:CG2 | 2.27 | 0.82 |
| 1:K:516:PHE:CD2 | 1:L:520:ILE:HD13 | 2.15 | 0.82 |
| 4:R:20:LEU:HD23 | 4:R:117:LYS:CG | 2.10 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:514:ARG:HH11 | 1:A:514:ARG:CB | 1.91 | 0.82 |
| 1:B:443:ARG:H | 1:B:443:ARG:HD3 | 1.44 | 0.82 |
| 1:B:443:ARG:HG2 | 1:B:443:ARG:HH11 | 1.43 | 0.82 |
| 1:L:481:PRO:HD2 | 1:L:540:HIS:HE2 | 1.45 | 0.82 |
| 1:C:527:GLU:O | 1:C:532:GLU:HG2 | 1.80 | 0.82 |
| 3:P:475:LYS:CE | 3:P:475:LYS:H | 1.93 | 0.82 |
| 1:A:356:SER:N | 2:J:117:TYR:OH | 2.13 | 0.82 |
| 2:J:27:ASP:CB | 2:J:28:PRO:CD | 2.55 | 0.82 |
| 3:P:366:TRP:CE3 | 3:P:380:LEU:HD12 | 2.15 | 0.82 |
| 1:L:450:HIS:HB2 | 1:L:480:SER:HG | 0.85 | 0.81 |
| 1:B:451:ARG:NH1 | 1:B:451:ARG:HB2 | 1.95 | 0.81 |
| 3:P:525:TRP:CZ3 | 3:P:537:THR:HG21 | 2.14 | 0.81 |
| 1:F:480:SER:HB2 | 1:F:481:PRO:CD | 2.10 | 0.81 |
| 3:P:446:LEU:HD23 | 3:P:538:ALA:HB2 | 1.62 | 0.81 |
| 3:P:523:TRP:CZ3 | 3:P:539:ALA:HB1 | 2.14 | 0.81 |
| 3:P:529:LYS:HE2 | 3:P:534:TYR:HE2 | 1.43 | 0.81 |
| 1:E:421:GLY:CA | 1:E:445:LYS:CE | 2.58 | 0.81 |
| 1:B:449:LEU:HA | 1:B:480:SER:OG | 1.81 | 0.81 |
| 3:P:344:VAL:HG22 | 3:P:413:LEU:CD1 | 2.10 | 0.81 |
| 3:P:345:ALA:HA | 3:P:413:LEU:CB | 2.06 | 0.81 |
| 1:F:535:THR:HG22 | 1:F:551:THR:HG21 | 1.58 | 0.81 |
| 1:K:510:GLN:HG3 | 1:L:522:THR:HG23 | 1.63 | 0.81 |
| 1:L:479:PHE:O | 1:L:515:TYR:HB2 | 1.81 | 0.81 |
| 3:P:525:TRP:CE3 | 3:P:537:THR:HG21 | 2.16 | 0.81 |
| 4:R:46:ILE:H | 4:R:64:THR:HG21 | 1.46 | 0.81 |
| 1:D:493:GLN:OE1 | 1:D:493:GLN:N | 2.14 | 0.81 |
| 1:E:543:LEU:CD2 | 1:E:544:PRO:HD2 | 2.11 | 0.81 |
| 1:E:543:LEU:CD2 | 1:E:544:PRO:CD | 2.58 | 0.81 |
| 1:F:523:VAL:HG11 | 1:F:534:TYR:CZ | 2.15 | 0.81 |
| 1:K:454:VAL:HG22 | 1:K:538:VAL:HG21 | 1.61 | 0.81 |
| 1:A:533:THR:HA | 1:A:553:ASP:HB3 | 1.62 | 0.81 |
| 1:F:450:HIS:CD2 | 1:F:514:ARG:NH2 | 2.47 | 0.81 |
| 3:P:462:VAL:HB | 3:P:509:VAL:HB | 1.62 | 0.81 |
| 1:D:421:GLY:HA2 | 1:D:445:LYS:NZ | 1.93 | 0.81 |
| 4:S:39:LEU:HD11 | 4:S:87:PHE:CE1 | 2.10 | 0.81 |
| 1:A:482:ALA:O | 1:A:505:PRO:HG2 | 1.79 | 0.80 |
| 3:P:345:ALA:C | 3:P:413:LEU:CG | 2.47 | 0.80 |
| 3:P:446:LEU:HD23 | 3:P:537:THR:O | 1.79 | 0.80 |
| 3:P:412:GLN:HE22 | 3:P:414:THR:HG23 | 1.47 | 0.80 |
| 4:R:61:VAL:CG2 | 4:R:72:TYR:CD2 | 2.59 | 0.80 |
| 1:A:510:GLN:NE2 | 1:A:510:GLN:H | 1.78 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:27:ASP:HB2 | 2:J:28:PRO:HD2 | 1.61 | 0.80 |
| 1:F:524:SER:OG | 1:F:527:GLU:CB | 2.29 | 0.80 |
| 1:K:563:ASN:HB3 | 1:L:563:ASN:HA | 1.64 | 0.80 |
| 1:A:356:SER:HA | 2:J:117:TYR:CZ | 2.15 | 0.80 |
| 3:P:411:ASN:HB3 | 3:P:537:THR:CB | 2.12 | 0.80 |
| 3:P:418:ALA:CA | 3:P:439:ILE:HD11 | 2.12 | 0.80 |
| 3:P:479:LYS:CG | 3:P:524:TYR:CE1 | 2.65 | 0.80 |
| 1:B:461:ARG:NH2 | 1:L:570:ASP:CG | 2.38 | 0.80 |
| 1:L:479:PHE:CZ | 1:L:484:VAL:CG1 | 2.64 | 0.80 |
| 3:P:261:CYS:SG | 3:P:315:LEU:HD22 | 1.36 | 0.80 |
| 4:S:32:SER:N | 4:S:94:LEU:HD23 | 1.95 | 0.80 |
| 3:P:348:SER:CB | 3:P:537:THR:OG1 | 2.30 | 0.80 |
| 1:B:480:SER:CB | 1:B:481:PRO:HD3 | 2.12 | 0.79 |
| 1:G:450:HIS:CD2 | 1:G:514:ARG:CZ | 2.65 | 0.79 |
| 1:L:450:HIS:CA | 1:L:480:SER:OG | 2.29 | 0.79 |
| 1:L:479:PHE:HB3 | 1:L:515:TYR:CB | 2.12 | 0.79 |
| 3:P:131:THR:HG22 | 3:P:187:VAL:O | 1.81 | 0.79 |
| 1:A:514:ARG:HB3 | 1:A:514:ARG:NH1 | 1.95 | 0.79 |
| 1:L:424:PHE:CB | 1:L:441:ILE:HD13 | 2.07 | 0.79 |
| 1:L:443:ARG:H | 1:L:444:PRO:CD | 1.93 | 0.79 |
| 3:P:248:VAL:CG1 | 3:P:311:SER:H | 1.95 | 0.79 |
| 1:B:382:TRP:CZ3 | 1:B:441:ILE:HD11 | 2.18 | 0.79 |
| 1:E:482:ALA:HB2 | 1:E:515:TYR:HE2 | 1.46 | 0.78 |
| 3:P:355:TYR:CE1 | 3:P:405:THR:N | 2.51 | 0.78 |
| 1:A:489:MET:HE1 | 1:A:537:VAL:HG21 | 1.65 | 0.78 |
| 1:E:454:VAL:HG21 | 1:E:538:VAL:CG2 | 2.13 | 0.78 |
| 3:P:131:THR:HG23 | 3:P:188:VAL:CB | 2.12 | 0.78 |
| 3:P:340:VAL:HG12 | 3:P:436:GLU:C | 2.07 | 0.78 |
| 1:G:501:VAL:CG2 | 1:H:509:PRO:HD3 | 2.13 | 0.78 |
| 1:K:543:LEU:HD12 | 1:K:543:LEU:H | 1.48 | 0.78 |
| 3:P:475:LYS:H | 3:P:475:LYS:CD | 1.96 | 0.78 |
| 1:B:354:PHE:HZ | 1:B:546:ARG:HG2 | 1.46 | 0.78 |
| 1:B:461:ARG:NH2 | 1:L:570:ASP:OD1 | 2.17 | 0.78 |
| 1:A:535:THR:HG22 | 1:A:551:THR:HB | 1.65 | 0.78 |
| 1:L:479:PHE:HB3 | 1:L:515:TYR:HB2 | 1.64 | 0.78 |
| 3:P:342:LYS:CE | 3:P:438:LYS:HE2 | 2.14 | 0.78 |
| 4:S:75:ARG:O | 4:S:92:THR:HG23 | 1.84 | 0.78 |
| 1:A:359:LEU:CD1 | 2:J:117:TYR:HB3 | 2.13 | 0.78 |
| 1:B:454:VAL:HG22 | 1:B:550:ARG:HG3 | 1.66 | 0.78 |
| 1:G:450:HIS:HD2 | 1:G:514:ARG:CZ | 1.95 | 0.78 |
| 6:H:601:NAG:H83 | 6:H:601:NAG:O3 | 1.84 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:413:LEU:HD23 | 3:P:413:LEU:H | 1.49 | 0.77 |
| 3:P:471:SER:HA | 3:P:475:LYS:HZ3 | 1.49 | 0.77 |
| 1:L:479:PHE:CZ | 1:L:484:VAL:HB | 2.19 | 0.77 |
| 3:P:287:ASP:OD1 | 3:P:287:ASP:N | 2.17 | 0.77 |
| 3:P:479:LYS:CG | 3:P:524:TYR:HE1 | 1.96 | 0.77 |
| 1:G:523:VAL:CG2 | 1:G:534:TYR:OH | 2.26 | 0.77 |
| 3:P:346:GLY:N | 3:P:413:LEU:CD1 | 2.41 | 0.77 |
| 4:R:20:LEU:HD21 | 4:R:117:LYS:CB | 2.14 | 0.77 |
| 4:S:31:GLY:CA | 4:S:94:LEU:HD21 | 2.13 | 0.77 |
| 1:L:540:HIS:C | 1:L:543:LEU:HD23 | 1.88 | 0.77 |
| 3:P:131:THR:CG2 | 3:P:188:VAL:CB | 2.63 | 0.77 |
| 3:P:346:GLY:H | 3:P:413:LEU:HB2 | 1.45 | 0.77 |
| 3:P:446:LEU:HD22 | 3:P:538:ALA:CB | 2.15 | 0.77 |
| 3:P:348:SER:OG | 3:P:537:THR:OG1 | 2.02 | 0.77 |
| 3:P:361:LYS:HG2 | 3:P:364:LYS:HE2 | 1.64 | 0.77 |
| 1:F:396:ILE:HA | 1:F:408:VAL:HG22 | 1.67 | 0.77 |
| 3:P:132:ILE:HD13 | 3:P:187:VAL:HG23 | 1.66 | 0.77 |
| 3:P:529:LYS:CE | 3:P:534:TYR:CE2 | 2.67 | 0.77 |
| 1:A:491:ARG:NH1 | 1:A:491:ARG:O | 2.19 | 0.77 |
| 3:P:134:CYS:HB2 | 3:P:185:PHE:HD2 | 1.50 | 0.77 |
| 1:E:346:ARG:HE | 1:E:371:ASP:HB2 | 1.49 | 0.76 |
| 1:E:516:PHE:CZ | 1:F:520:ILE:HD11 | 2.20 | 0.76 |
| 1:H:365:LEU:HD11 | 1:H:418:TRP:HZ2 | 1.50 | 0.76 |
| 1:K:510:GLN:HG2 | 1:L:522:THR:CG2 | 2.12 | 0.76 |
| 1:D:364:LYS:HD2 | 1:D:410:GLU:HG3 | 1.65 | 0.76 |
| 1:L:514:ARG:HB3 | 1:L:514:ARG:HH11 | 1.48 | 0.76 |
| 3:P:348:SER:HB3 | 3:P:536:GLU:HB2 | 1.66 | 0.76 |
| 1:L:424:PHE:N | 1:L:441:ILE:CG1 | 2.42 | 0.76 |
| 4:R:20:LEU:CD2 | 4:R:117:LYS:CB | 2.63 | 0.76 |
| 3:P:466:PHE:CD2 | 3:P:507:ARG:HG3 | 2.16 | 0.76 |
| 3:P:425:THR:O | 3:P:430:LEU:HD21 | 1.85 | 0.76 |
| 4:R:23:VAL:HB | 4:R:118:VAL:HG13 | 1.66 | 0.76 |
| 1:L:514:ARG:HH11 | 1:L:514:ARG:CB | 1.98 | 0.76 |
| 3:P:450:GLY:N | 3:P:540:VAL:HG12 | 2.00 | 0.76 |
| 1:E:450:HIS:CE1 | 1:E:514:ARG:NH1 | 2.49 | 0.76 |
| 1:F:450:HIS:HE2 | 1:F:514:ARG:HH12 | 1.34 | 0.76 |
| 3:P:43:ARG:HG2 | 3:P:43:ARG:HH11 | 1.50 | 0.76 |
| 1:G:471:THR:HG22 | 1:G:522:THR:HG22 | 1.67 | 0.76 |
| 1:F:348:PHE:H | 1:F:369:VAL:HG13 | 1.51 | 0.75 |
| 1:A:550:ARG:HG2 | 1:A:550:ARG:HH11 | 1.51 | 0.75 |
| 3:P:243:PRO:HA | 3:P:246:ALA:HB2 | 1.66 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:421:GLY:HA3 | 1:D:445:LYS:HE3 | 1.67 | 0.75 |
| 1:H:554:LYS:HZ3 | 1:H:558:LYS:HZ3 | 1.26 | 0.75 |
| 3:P:462:VAL:CG2 | 3:P:509:VAL:O | 2.35 | 0.75 |
| 1:L:467:ARG:NH1 | 1:L:525:GLU:OE1 | 2.20 | 0.75 |
| 3:P:368:LEU:N | 3:P:378:PRO:CD | 2.28 | 0.75 |
| 3:P:525:TRP:CE3 | 3:P:537:THR:CG2 | 2.68 | 0.75 |
| 1:A:524:SER:OG | 1:A:527:GLU:HB2 | 1.87 | 0.75 |
| 1:L:450:HIS:HB2 | 1:L:480:SER:CB | 2.15 | 0.75 |
| 1:L:532:GLU:HB2 | 1:L:534:TYR:CE2 | 2.22 | 0.75 |
| 4:S:71:GLU:N | 4:S:71:GLU:OE1 | 2.19 | 0.75 |
| 1:G:537:VAL:HG22 | 1:G:549:GLU:HG2 | 1.68 | 0.75 |
| 1:H:554:LYS:HZ3 | 1:H:558:LYS:HZ1 | 0.76 | 0.75 |
| 1:A:355:ALA:O | 2:J:117:TYR:CE2 | 2.39 | 0.75 |
| 3:P:357:ARG:NH2 | 3:P:403:ASN:ND2 | 2.32 | 0.75 |
| 1:A:359:LEU:HD12 | 2:J:117:TYR:CG | 2.07 | 0.75 |
| 1:E:483:ASP:O | 1:E:540:HIS:ND1 | 2.19 | 0.75 |
| 1:F:449:LEU:HA | 1:F:481:PRO:HD3 | 1.67 | 0.75 |
| 1:F:502:THR:OG1 | 1:F:519:SER:CA | 2.35 | 0.75 |
| 4:S:29:LEU:HD23 | 4:S:95:THR:CG2 | 2.14 | 0.75 |
| 1:F:560:THR:O | 1:G:560:THR:CG2 | 2.21 | 0.74 |
| 3:P:131:THR:HG22 | 3:P:187:VAL:C | 2.12 | 0.74 |
| 3:P:411:ASN:CB | 3:P:537:THR:OG1 | 2.32 | 0.74 |
| 1:B:454:VAL:HG11 | 1:B:538:VAL:HG11 | 1.68 | 0.74 |
| 1:E:471:THR:HG22 | 1:E:522:THR:HG22 | 1.68 | 0.74 |
| 4:S:31:GLY:O | 4:S:94:LEU:CD2 | 2.17 | 0.74 |
| 4:S:37:CYS:HB3 | 4:S:116:GLN:OE1 | 1.84 | 0.74 |
| 5:I:1:NAG:C1 | 5:I:1:NAG:H82 | 2.18 | 0.74 |
| 1:L:424:PHE:CG | 1:L:441:ILE:HD13 | 2.18 | 0.74 |
| 3:P:361:LYS:O | 3:P:361:LYS:HE3 | 1.87 | 0.74 |
| 3:P:450:GLY:CA | 3:P:540:VAL:CG1 | 2.61 | 0.74 |
| 3:P:466:PHE:HE2 | 3:P:507:ARG:CB | 2.00 | 0.74 |
| 5:I:1:NAG:O4 | 5:I:1:NAG:N2 | 2.17 | 0.74 |
| 1:B:466:LEU:HB3 | 1:B:468:GLU:HG3 | 1.70 | 0.74 |
| 1:K:463:GLN:CB | 1:L:455:TYR:CZ | 2.67 | 0.74 |
| 3:P:43:ARG:HG2 | 3:P:43:ARG:NH1 | 2.01 | 0.74 |
| 1:B:443:ARG:H | 1:B:443:ARG:CD | 2.01 | 0.74 |
| 1:D:514:ARG:HH11 | 4:V:66:ASN:ND2 | 1.85 | 0.74 |
| 1:E:450:HIS:CD2 | 1:E:514:ARG:CZ | 2.68 | 0.74 |
| 3:P:342:LYS:HB3 | 3:P:438:LYS:CB | 2.18 | 0.74 |
| 1:L:424:PHE:HB2 | 1:L:441:ILE:HG12 | 1.69 | 0.74 |
| 3:P:446:LEU:CD2 | 3:P:538:ALA:CB | 2.65 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:477:TRP:HZ2 | 3:P:524:TYR:CG | 1.96 | 0.74 |
| 1:K:464:LEU:CD1 | 1:K:525:GLU:CD | 2.59 | 0.73 |
| 3:P:264:VAL:HG12 | 3:P:265:VAL:HG23 | 1.69 | 0.73 |
| 3:P:395:LEU:HA | 3:P:410:LEU:HD12 | 1.70 | 0.73 |
| 3:P:446:LEU:HD21 | 3:P:537:THR:C | 2.12 | 0.73 |
| 4:V:21:PRO:HD2 | 4:V:116:GLN:HG3 | 1.69 | 0.73 |
| 1:E:450:HIS:CB | 1:E:514:ARG:NH2 | 2.51 | 0.73 |
| 3:P:368:LEU:CB | 3:P:378:PRO:CD | 2.66 | 0.73 |
| 4:R:25:VAL:HG11 | 4:R:33:VAL:CG1 | 2.16 | 0.73 |
| 3:P:243:PRO:O | 3:P:246:ALA:HB2 | 1.84 | 0.73 |
| 1:F:482:ALA:HB3 | 1:F:515:TYR:HE2 | 1.50 | 0.73 |
| 1:L:479:PHE:HZ | 1:L:484:VAL:CG1 | 1.99 | 0.73 |
| 3:P:281:LEU:HD11 | 3:P:290:PHE:HE2 | 1.52 | 0.73 |
| 3:P:446:LEU:HD12 | 3:P:446:LEU:N | 2.03 | 0.73 |
| 1:L:421:GLY:O | 1:L:443:ARG:NH2 | 2.22 | 0.73 |
| 3:P:361:LYS:HG2 | 3:P:364:LYS:CE | 2.17 | 0.73 |
| 1:F:450:HIS:NE2 | 1:F:514:ARG:NH1 | 2.35 | 0.73 |
| 3:P:348:SER:HB2 | 3:P:537:THR:OG1 | 1.88 | 0.73 |
| 1:A:485:PHE:HE2 | 2:J:115:LEU:HD22 | 1.53 | 0.73 |
| 1:B:490:GLN:HG3 | 1:B:490:GLN:O | 1.88 | 0.73 |
| 1:K:518:HIS:CE1 | 1:L:518:HIS:ND1 | 2.57 | 0.73 |
| 3:P:265:VAL:HG21 | 3:P:279:ILE:HG21 | 1.71 | 0.73 |
| 4:R:31:GLY:O | 4:R:94:LEU:HD13 | 1.88 | 0.73 |
| 1:C:456:LEU:HD12 | 1:C:550:ARG:HB2 | 1.71 | 0.73 |
| 1:D:514:ARG:HD3 | 1:D:514:ARG:N | 2.02 | 0.73 |
| 1:D:514:ARG:NH2 | 1:D:514:ARG:HG2 | 2.02 | 0.73 |
| 1:E:543:LEU:HD22 | 1:E:544:PRO:HD2 | 1.70 | 0.73 |
| 3:P:398:LEU:HD11 | 3:P:409:ILE:HG13 | 1.69 | 0.73 |
| 4:R:75:ARG:HG2 | 4:R:75:ARG:O | 1.89 | 0.73 |
| 4:S:35:ILE:HG12 | 4:S:118:VAL:HG21 | 1.70 | 0.73 |
| 1:B:480:SER:OG | 1:B:481:PRO:CD | 2.34 | 0.73 |
| 1:C:467:ARG:HD3 | 1:C:467:ARG:N | 2.03 | 0.73 |
| 3:P:345:ALA:C | 3:P:413:LEU:HB2 | 2.13 | 0.73 |
| 4:S:72:TYR:HB3 | 4:S:76:VAL:HG21 | 1.70 | 0.73 |
| 1:F:535:THR:HG22 | 1:F:551:THR:HG22 | 0.75 | 0.72 |
| 3:P:342:LYS:HE2 | 3:P:438:LYS:HE2 | 1.69 | 0.72 |
| 3:P:471:SER:CA | 3:P:475:LYS:HZ3 | 2.02 | 0.72 |
| 1:C:461:ARG:HH12 | 1:C:465:ASN:HD21 | 0.78 | 0.72 |
| 1:E:493:GLN:NE2 | 1:E:493:GLN:H | 1.87 | 0.72 |
| 3:P:244:GLU:H | 3:P:244:GLU:CD | 1.97 | 0.72 |
| 1:L:479:PHE:CZ | 1:L:484:VAL:CB | 2.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:554:LYS:O | 1:C:554:LYS:HG2 | 1.89 | 0.72 |
| 4:S:71:GLU:CD | 4:S:71:GLU:H | 1.95 | 0.72 |
| 1:C:421:GLY:O | 1:C:423:ARG:NH2 | 2.23 | 0.72 |
| 1:C:454:VAL:HG22 | 1:C:538:VAL:HG21 | 1.71 | 0.72 |
| 2:J:64:LEU:HD22 | 2:J:64:LEU:N | 2.04 | 0.72 |
| 3:P:479:LYS:HG2 | 3:P:524:TYR:CD1 | 2.24 | 0.72 |
| 4:S:32:SER:N | 4:S:94:LEU:CD2 | 2.51 | 0.72 |
| 1:L:540:HIS:N | 1:L:543:LEU:HD21 | 1.85 | 0.72 |
| 3:P:450:GLY:N | 3:P:540:VAL:CG1 | 2.53 | 0.72 |
| 4:U:22:GLU:O | 4:U:22:GLU:HG2 | 1.89 | 0.72 |
| 1:A:554:LYS:HZ2 | 1:A:554:LYS:C | 1.96 | 0.72 |
| 1:K:471:THR:HG23 | 1:K:520:ILE:HG13 | 1.71 | 0.72 |
| 3:P:132:ILE:N | 3:P:132:ILE:HD12 | 2.05 | 0.71 |
| 4:S:39:LEU:HD22 | 4:S:86:LEU:N | 2.04 | 0.71 |
| 1:B:450:HIS:C | 1:B:542:ALA:CB | 2.63 | 0.71 |
| 3:P:439:ILE:HD12 | 3:P:439:ILE:N | 2.05 | 0.71 |
| 3:P:447:LYS:HB2 | 3:P:465:HIS:N | 2.04 | 0.71 |
| 1:E:506:MET:CG | 1:E:507:PRO:HD2 | 2.19 | 0.71 |
| 1:K:484:VAL:HG23 | 1:K:540:HIS:CB | 2.20 | 0.71 |
| 4:V:76:VAL:HG12 | 4:V:91:VAL:HG22 | 1.72 | 0.71 |
| 1:L:527:GLU:HB3 | 1:L:534:TYR:OH | 1.89 | 0.71 |
| 1:L:479:PHE:HZ | 1:L:484:VAL:CB | 2.03 | 0.71 |
| 1:G:430:HIS:CD2 | 1:G:431:THR:H | 2.09 | 0.71 |
| 1:H:365:LEU:HD22 | 1:H:413:ILE:HD13 | 1.73 | 0.71 |
| 1:K:553:ASP:OD2 | 1:K:554:LYS:N | 2.23 | 0.71 |
| 1:C:371:ASP:H | 1:C:404:THR:HG23 | 1.55 | 0.71 |
| 1:G:428:VAL:H | 1:G:437:LEU:HB3 | 1.55 | 0.71 |
| 3:P:340:VAL:HG12 | 3:P:436:GLU:CB | 2.20 | 0.71 |
| 1:B:421:GLY:H | 1:B:443:ARG:HH21 | 1.37 | 0.71 |
| 1:C:568:MET:HE2 | 1:H:562:TYR:CD1 | 2.26 | 0.71 |
| 1:K:540:HIS:O | 1:K:543:LEU:HD12 | 1.91 | 0.71 |
| 3:P:418:ALA:CB | 3:P:439:ILE:CD1 | 2.69 | 0.71 |
| 1:K:354:PHE:CE1 | 1:K:541:GLU:HB3 | 2.26 | 0.71 |
| 1:D:478:GLY:HA2 | 1:D:514:ARG:HB3 | 1.72 | 0.70 |
| 1:F:449:LEU:HA | 1:F:481:PRO:CD | 2.20 | 0.70 |
| 1:L:456:LEU:HG | 1:L:552:VAL:HG21 | 1.73 | 0.70 |
| 1:A:356:SER:HA | 2:J:117:TYR:CE2 | 2.26 | 0.70 |
| 1:A:550:ARG:HG2 | 1:A:550:ARG:NH1 | 2.03 | 0.70 |
| 4:U:22:GLU:CB | 4:U:119:THR:CG2 | 2.68 | 0.70 |
| 1:A:357:ILE:HG12 | 1:A:363:THR:HG22 | 1.73 | 0.70 |
| 1:B:454:VAL:HG11 | 1:B:538:VAL:CG1 | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:368:LEU:HD12 | 3:P:378:PRO:HG2 | 1.72 | 0.70 |
| 3:P:529:LYS:CG | 3:P:534:TYR:CE2 | 2.73 | 0.70 |
| 1:E:372:LEU:HD12 | 1:E:432:ASP:HB3 | 1.74 | 0.70 |
| 3:P:421:TYR:CD1 | 3:P:437:ILE:HD12 | 2.26 | 0.70 |
| 4:U:37:CYS:HB3 | 4:U:87:PHE:HB3 | 1.73 | 0.70 |
| 1:F:543:LEU:HD23 | 1:F:544:PRO:HD2 | 1.71 | 0.70 |
| 3:P:466:PHE:CD2 | 3:P:507:ARG:CG | 2.74 | 0.70 |
| 4:S:99:SER:HB2 | 4:S:120:LEU:O | 1.91 | 0.70 |
| 1:H:418:TRP:HB3 | 1:H:443:ARG:HB2 | 1.72 | 0.70 |
| 2:J:21:ILE:HD13 | 1:L:554:LYS:HG2 | 1.74 | 0.70 |
| 3:P:529:LYS:HE2 | 3:P:534:TYR:CE2 | 2.26 | 0.70 |
| 1:C:566:LEU:HD12 | 1:C:566:LEU:N | 2.01 | 0.70 |
| 1:F:550:ARG:HG2 | 1:F:550:ARG:NH1 | 2.05 | 0.70 |
| 3:P:134:CYS:HB2 | 3:P:185:PHE:CD2 | 2.26 | 0.70 |
| 3:P:471:SER:HB2 | 3:P:475:LYS:NZ | 2.07 | 0.70 |
| 1:B:374:THR:HB | 1:B:399:SER:HA | 1.72 | 0.70 |
| 1:K:381:SER:HB3 | 1:K:389:ALA:HB1 | 1.74 | 0.70 |
| 3:P:479:LYS:HB2 | 3:P:488:LEU:HD13 | 1.74 | 0.70 |
| 1:G:532:GLU:OE1 | 1:G:532:GLU:HA | 1.90 | 0.70 |
| 1:C:566:LEU:HD13 | 1:D:566:LEU:HD23 | 1.74 | 0.69 |
| 3:P:247:ASN:OD1 | 3:P:247:ASN:N | 2.24 | 0.69 |
| 4:V:45:ARG:NH2 | 4:V:110:THR:OG1 | 2.25 | 0.69 |
| 3:P:418:ALA:CA | 3:P:439:ILE:CD1 | 2.69 | 0.69 |
| 3:P:471:SER:CA | 3:P:475:LYS:NZ | 2.55 | 0.69 |
| 1:A:356:SER:CB | 2:J:117:TYR:HH | 1.97 | 0.69 |
| 3:P:306:LEU:HD22 | 3:P:321:ILE:HD12 | 1.74 | 0.69 |
| 4:U:22:GLU:HG3 | 4:U:119:THR:HG23 | 1.72 | 0.69 |
| 4:U:33:VAL:HG12 | 4:U:94:LEU:HD11 | 1.75 | 0.69 |
| 3:P:413:LEU:HD23 | 3:P:413:LEU:N | 2.06 | 0.69 |
| 1:L:354:PHE:HA | 1:L:357:ILE:HG12 | 1.75 | 0.69 |
| 1:L:508:GLU:OE1 | 1:L:508:GLU:HA | 1.92 | 0.69 |
| 4:R:116:GLN:HE22 | 4:R:118:VAL:HG22 | 1.53 | 0.69 |
| 1:E:508:GLU:OE1 | 1:E:509:PRO:HD3 | 1.93 | 0.69 |
| 4:S:61:VAL:CG1 | 4:S:72:TYR:CD1 | 2.76 | 0.69 |
| 3:P:446:LEU:HB3 | 3:P:466:PHE:CD1 | 2.27 | 0.69 |
| 3:P:462:VAL:HB | 3:P:509:VAL:O | 1.92 | 0.69 |
| 4:R:47:TYR:HE2 | 4:R:49:CYS:HB2 | 1.57 | 0.69 |
| 1:C:564:VAL:CG2 | 1:H:566:LEU:HD21 | 2.23 | 0.69 |
| 3:P:149:LYS:HD2 | 3:P:151:ILE:CG2 | 2.22 | 0.69 |
| 3:P:340:VAL:HG12 | 3:P:436:GLU:HB3 | 1.69 | 0.69 |
| 3:P:447:LYS:CG | 3:P:465:HIS:CB | 2.55 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:451:ARG:HB3 | 1:C:451:ARG:NH1 | 2.03 | 0.69 |
| 1:H:456:LEU:HD22 | 1:H:552:VAL:HB | 1.75 | 0.68 |
| 4:S:61:VAL:HG11 | 4:S:72:TYR:CD1 | 2.27 | 0.68 |
| 1:B:443:ARG:HH11 | 1:B:443:ARG:CG | 2.06 | 0.68 |
| 2:J:30:GLU:OE1 | 2:J:30:GLU:HA | 1.92 | 0.68 |
| 4:S:72:TYR:HB3 | 4:S:76:VAL:CG2 | 2.24 | 0.68 |
| 1:C:457:LEU:HD13 | 1:D:457:LEU:HD23 | 1.75 | 0.68 |
| 1:K:454:VAL:HG21 | 1:K:538:VAL:CG2 | 2.21 | 0.68 |
| 1:L:424:PHE:O | 1:L:441:ILE:HG12 | 1.93 | 0.68 |
| 1:K:566:LEU:HD23 | 1:K:566:LEU:O | 1.94 | 0.68 |
| 4:R:75:ARG:HH22 | 4:R:95:THR:HG1 | 1.36 | 0.68 |
| 1:L:487:GLN:HB3 | 1:L:537:VAL:CG1 | 2.24 | 0.68 |
| 3:P:476:TYR:CD1 | 3:P:527:GLY:O | 2.46 | 0.68 |
| 2:J:64:LEU:HD22 | 2:J:64:LEU:H | 1.59 | 0.68 |
| 1:K:509:PRO:HG2 | 1:L:501:VAL:HG21 | 1.54 | 0.68 |
| 1:K:561:LEU:HG | 1:K:561:LEU:O | 1.93 | 0.68 |
| 1:F:543:LEU:HD13 | 1:F:548:THR:HG22 | 1.75 | 0.68 |
| 3:P:526:CYS:O | 3:P:538:ALA:CB | 2.42 | 0.68 |
| 4:S:76:VAL:HG22 | 4:S:91:VAL:HG22 | 1.75 | 0.68 |
| 1:E:357:ILE:HG22 | 1:E:363:THR:HA | 1.76 | 0.67 |
| 1:F:549:GLU:O | 1:F:549:GLU:HG2 | 1.94 | 0.67 |
| 3:P:149:LYS:HD2 | 3:P:151:ILE:HG22 | 1.75 | 0.67 |
| 3:P:151:ILE:C | 3:P:151:ILE:HD12 | 2.19 | 0.67 |
| 1:A:518:HIS:CE1 | 1:B:520:ILE:CG2 | 2.76 | 0.67 |
| 1:L:384:ARG:HD3 | 1:L:388:GLU:HB3 | 1.77 | 0.67 |
| 1:L:511:ALA:HB3 | 1:L:514:ARG:HG2 | 1.71 | 0.67 |
| 3:P:344:VAL:HG22 | 3:P:413:LEU:HD11 | 1.74 | 0.67 |
| 4:U:41:GLU:C | 4:U:43:HIS:H | 2.02 | 0.67 |
| 4:U:70:ALA:HA | 4:U:73:LYS:HE2 | 1.76 | 0.67 |
| 1:E:452:PRO:HD2 | 1:E:543:LEU:HG | 1.76 | 0.67 |
| 1:L:540:HIS:CB | 1:L:543:LEU:HD22 | 2.08 | 0.67 |
| 3:P:526:CYS:O | 3:P:538:ALA:HB3 | 1.94 | 0.67 |
| 1:C:480:SER:O | 1:C:540:HIS:NE2 | 2.26 | 0.67 |
| 3:P:395:LEU:CG | 3:P:410:LEU:CD1 | 2.71 | 0.67 |
| 4:V:28:GLU:C | 4:V:96:GLU:OE1 | 2.37 | 0.67 |
| 1:A:471:THR:HG22 | 1:A:522:THR:HG22 | 1.75 | 0.67 |
| 6:A:601:NAG:H5 | 6:B:601:NAG:H4 | 1.76 | 0.67 |
| 1:C:456:LEU:CD1 | 1:C:550:ARG:HB2 | 2.25 | 0.67 |
| 2:J:4:ARG:HG2 | 2:J:20:ARG:HD3 | 1.76 | 0.67 |
| 3:P:261:CYS:SG | 3:P:315:LEU:CB | 2.82 | 0.67 |
| 3:P:342:LYS:CB | 3:P:438:LYS:O | 2.43 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:346:GLY:H | 3:P:413:LEU:CA | 2.08 | 0.67 |
| 3:P:348:SER:HB3 | 3:P:537:THR:H | 1.57 | 0.67 |
| 1:G:450:HIS:CD2 | 1:G:514:ARG:NH2 | 2.59 | 0.67 |
| 1:G:516:PHE:CE1 | 1:H:520:ILE:HD12 | 2.30 | 0.67 |
| 3:P:135:PRO:O | 3:P:204:ALA:HB3 | 1.94 | 0.67 |
| 1:F:450:HIS:HB2 | 1:F:480:SER:N | 2.10 | 0.67 |
| 3:P:131:THR:CG2 | 3:P:188:VAL:HG23 | 2.18 | 0.67 |
| 1:G:524:SER:HB3 | 1:G:527:GLU:HG3 | 1.75 | 0.66 |
| 4:U:102:TYR:HB2 | 4:U:118:VAL:HG23 | 1.77 | 0.66 |
| 3:P:352:LEU:HD23 | 3:P:406:PHE:O | 1.96 | 0.66 |
| 3:P:395:LEU:CG | 3:P:410:LEU:HD13 | 2.22 | 0.66 |
| 1:B:382:TRP:HZ3 | 1:B:441:ILE:HD11 | 1.59 | 0.66 |
| 1:L:473:THR:HG22 | 1:L:520:ILE:HG22 | 1.75 | 0.66 |
| 3:P:261:CYS:SG | 3:P:315:LEU:HB3 | 2.34 | 0.66 |
| 1:C:345:ILE:N | 1:C:370:THR:O | 2.29 | 0.66 |
| 1:L:479:PHE:CE2 | 1:L:484:VAL:HG11 | 2.30 | 0.66 |
| 3:P:480:TRP:CH2 | 3:P:482:ASN:HB3 | 2.31 | 0.66 |
| 1:B:354:PHE:CZ | 1:B:546:ARG:HG2 | 2.28 | 0.66 |
| 3:P:368:LEU:HB2 | 3:P:378:PRO:HG2 | 1.76 | 0.66 |
| 4:U:22:GLU:HB3 | 4:U:119:THR:CG2 | 2.26 | 0.66 |
| 1:C:466:LEU:HD21 | 4:V:45:ARG:NE | 2.11 | 0.66 |
| 3:P:132:ILE:HD12 | 3:P:132:ILE:H | 1.60 | 0.66 |
| 1:A:538:VAL:CG2 | 1:A:548:THR:CG2 | 2.74 | 0.66 |
| 3:P:475:LYS:H | 3:P:475:LYS:HE2 | 1.59 | 0.66 |
| 1:H:368:LEU:HB2 | 1:H:406:SER:HB2 | 1.76 | 0.66 |
| 1:F:374:THR:H | 1:F:401:PRO:HB3 | 1.61 | 0.66 |
| 1:F:502:THR:OG1 | 1:F:519:SER:OG | 2.06 | 0.66 |
| 1:B:564:VAL:HG22 | 1:C:564:VAL:HA | 1.78 | 0.65 |
| 1:E:482:ALA:HB2 | 1:E:515:TYR:CE2 | 2.29 | 0.65 |
| 1:E:482:ALA:HA | 1:E:515:TYR:CE2 | 2.30 | 0.65 |
| 4:U:94:LEU:C | 4:U:96:GLU:H | 2.04 | 0.65 |
| 1:G:380:ILE:HD13 | 1:G:409:GLY:HA3 | 1.78 | 0.65 |
| 3:P:368:LEU:CA | 3:P:378:PRO:CD | 2.74 | 0.65 |
| 1:K:535:THR:HG22 | 1:K:551:THR:OG1 | 1.96 | 0.65 |
| 1:A:483:ASP:O | 1:A:540:HIS:HD2 | 1.79 | 0.65 |
| 1:B:451:ARG:HA | 1:B:542:ALA:HB3 | 1.77 | 0.65 |
| 1:C:568:MET:CE | 1:H:562:TYR:HD1 | 2.09 | 0.65 |
| 1:E:545:ASN:OD1 | 1:E:545:ASN:N | 2.25 | 0.65 |
| 1:F:523:VAL:CG1 | 1:F:534:TYR:CZ | 2.80 | 0.65 |
| 2:J:21:ILE:CG1 | 1:L:555:SER:HB3 | 2.25 | 0.65 |
| 1:A:564:VAL:HG11 | 1:L:568:MET:HE1 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:514:ARG:HG2 | 1:D:514:ARG:HH21 | 1.62 | 0.65 |
| 1:L:443:ARG:HD3 | 1:L:443:ARG:C | 2.21 | 0.65 |
| 1:B:480:SER:CB | 1:B:481:PRO:CD | 2.70 | 0.65 |
| 3:P:529:LYS:CG | 3:P:534:TYR:CD2 | 2.79 | 0.65 |
| 1:E:421:GLY:CA | 1:E:445:LYS:HE3 | 2.21 | 0.65 |
| 1:F:347:VAL:HG13 | 1:F:437:LEU:HB3 | 1.77 | 0.65 |
| 1:L:424:PHE:O | 1:L:441:ILE:CG1 | 2.45 | 0.65 |
| 3:P:368:LEU:CA | 3:P:378:PRO:HD2 | 2.25 | 0.65 |
| 3:P:462:VAL:CG1 | 3:P:540:VAL:HG11 | 2.21 | 0.65 |
| 3:P:477:TRP:CE2 | 3:P:524:TYR:HB3 | 2.30 | 0.65 |
| 3:P:471:SER:C | 3:P:475:LYS:HZ1 | 2.05 | 0.65 |
| 1:B:397:SER:HB2 | 1:B:408:VAL:HG12 | 1.78 | 0.65 |
| 1:D:391:LYS:NZ | 1:D:392:THR:O | 2.29 | 0.65 |
| 1:C:508:GLU:HG3 | 1:C:509:PRO:HD3 | 1.79 | 0.64 |
| 1:L:546:ARG:HG2 | 1:L:546:ARG:O | 1.97 | 0.64 |
| 3:P:340:VAL:CG1 | 3:P:436:GLU:CG | 2.74 | 0.64 |
| 4:U:22:GLU:HB2 | 4:U:119:THR:N | 2.12 | 0.64 |
| 1:A:540:HIS:HB3 | 1:A:543:LEU:HD12 | 1.78 | 0.64 |
| 1:G:397:SER:HB3 | 1:G:408:VAL:HG23 | 1.79 | 0.64 |
| 3:P:394:ARG:NH1 | 3:P:414:THR:OG1 | 2.30 | 0.64 |
| 3:P:462:VAL:HG23 | 3:P:509:VAL:O | 1.96 | 0.64 |
| 4:S:39:LEU:CD2 | 4:S:85:ASN:HA | 2.27 | 0.64 |
| 4:U:22:GLU:HA | 4:U:118:VAL:HA | 1.77 | 0.64 |
| 1:B:347:VAL:HG11 | 1:B:428:VAL:HG21 | 1.79 | 0.64 |
| 1:B:568:MET:HE2 | 1:K:562:TYR:CD2 | 2.32 | 0.64 |
| 1:A:459:PRO:CG | 1:A:470:ALA:HB1 | 2.28 | 0.64 |
| 1:F:546:ARG:HH11 | 1:F:546:ARG:CG | 2.10 | 0.64 |
| 1:H:372:LEU:HD11 | 1:H:405:PHE:HB2 | 1.80 | 0.64 |
| 2:J:27:ASP:CB | 2:J:28:PRO:HD2 | 2.26 | 0.64 |
| 3:P:264:VAL:CG2 | 3:P:275:PHE:HE2 | 2.10 | 0.64 |
| 3:P:470:PHE:HE2 | 3:P:528:VAL:CG1 | 2.10 | 0.64 |
| 1:E:450:HIS:CE1 | 1:E:514:ARG:NH2 | 2.54 | 0.64 |
| 1:G:346:ARG:NH1 | 1:G:347:VAL:O | 2.31 | 0.64 |
| 1:G:556:THR:O | 1:H:461:ARG:NH2 | 2.30 | 0.64 |
| 1:K:464:LEU:HD13 | 1:K:525:GLU:OE2 | 1.91 | 0.64 |
| 3:P:471:SER:HB2 | 3:P:475:LYS:HZ2 | 1.62 | 0.64 |
| 1:F:383:THR:HA | 1:F:389:ALA:HA | 1.79 | 0.64 |
| 1:K:452:PRO:HG3 | 1:K:479:PHE:HB3 | 1.78 | 0.64 |
| 1:K:518:HIS:ND1 | 1:L:518:HIS:ND1 | 2.45 | 0.64 |
| 3:P:448:VAL:HG23 | 3:P:449:PRO:HD2 | 1.75 | 0.64 |
| 4:U:22:GLU:CB | 4:U:119:THR:O | 2.37 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:482:ALA:HA | 1:E:515:TYR:CD2 | 2.33 | 0.64 |
| 1:L:367:CYS:HB2 | 1:L:382:TRP:HE3 | 1.63 | 0.64 |
| 3:P:526:CYS:HB3 | 3:P:538:ALA:HB3 | 1.79 | 0.64 |
| 1:B:413:ILE:CD1 | 1:B:414:CYS:N | 2.40 | 0.64 |
| 1:L:527:GLU:O | 1:L:530:THR:OG1 | 2.15 | 0.64 |
| 4:U:50:ARG:HH12 | 4:U:100:GLY:HA3 | 1.62 | 0.64 |
| 1:A:485:PHE:HE2 | 2:J:115:LEU:CD2 | 2.11 | 0.64 |
| 1:E:516:PHE:CE2 | 1:F:520:ILE:HD11 | 2.33 | 0.64 |
| 1:F:482:ALA:HB1 | 1:F:515:TYR:CD2 | 1.99 | 0.64 |
| 1:K:521:LEU:HD23 | 1:K:521:LEU:O | 1.97 | 0.64 |
| 3:P:314:GLN:CA | 3:P:314:GLN:HE21 | 2.09 | 0.64 |
| 4:R:48:LEU:HD11 | 4:R:102:TYR:HB3 | 1.79 | 0.64 |
| 1:C:419:ASN:O | 1:C:443:ARG:NH1 | 2.30 | 0.63 |
| 1:K:516:PHE:CD2 | 1:L:520:ILE:CD1 | 2.79 | 0.63 |
| 3:P:250:LYS:HG2 | 3:P:309:ALA:CB | 2.20 | 0.63 |
| 1:L:537:VAL:HA | 1:L:548:THR:O | 1.99 | 0.63 |
| 3:P:525:TRP:HA | 3:P:538:ALA:O | 1.98 | 0.63 |
| 4:R:21:PRO:O | 4:R:117:LYS:O | 2.14 | 0.63 |
| 4:R:46:ILE:HG22 | 4:R:64:THR:CG2 | 2.28 | 0.63 |
| 5:I:2:NAG:O7 | 5:I:2:NAG:O3 | 2.12 | 0.63 |
| 1:H:384:ARG:HH21 | 1:H:390:VAL:HG22 | 1.61 | 0.63 |
| 1:K:469:SER:CA | 1:K:525:GLU:HB2 | 2.29 | 0.63 |
| 1:L:451:ARG:NH1 | 1:L:544:PRO:HG3 | 2.13 | 0.63 |
| 1:A:566:LEU:HD13 | 1:A:566:LEU:N | 2.13 | 0.63 |
| 3:P:494:GLY:O | 3:P:507:ARG:NH2 | 2.30 | 0.63 |
| 1:A:502:THR:HA | 1:A:519:SER:HA | 1.80 | 0.63 |
| 1:C:457:LEU:HD11 | 1:C:473:THR:OG1 | 1.98 | 0.63 |
| 1:D:471:THR:HG22 | 1:D:522:THR:HG22 | 1.79 | 0.63 |
| 1:C:369:VAL:O | 1:C:406:SER:HA | 1.99 | 0.63 |
| 1:K:518:HIS:ND1 | 1:L:518:HIS:CE1 | 2.66 | 0.63 |
| 1:K:540:HIS:O | 1:K:543:LEU:CD1 | 2.47 | 0.63 |
| 3:P:131:THR:HG21 | 3:P:188:VAL:HG22 | 0.63 | 0.63 |
| 1:F:346:ARG:HH21 | 1:F:348:PHE:HA | 1.64 | 0.63 |
| 1:A:493:GLN:HB2 | 1:A:494:PRO:CD | 2.15 | 0.63 |
| 2:J:35:ARG:HG2 | 2:J:35:ARG:HH11 | 1.64 | 0.63 |
| 1:L:511:ALA:CB | 1:L:514:ARG:NE | 2.62 | 0.63 |
| 3:P:131:THR:HG23 | 3:P:188:VAL:CG2 | 2.02 | 0.63 |
| 3:P:264:VAL:HG22 | 3:P:275:PHE:HE2 | 1.64 | 0.63 |
| 3:P:334:ILE:HG23 | 3:P:431:TRP:CZ3 | 2.34 | 0.63 |
| 1:L:538:VAL:HG13 | 1:L:548:THR:OG1 | 1.98 | 0.62 |
| 3:P:345:ALA:CA | 3:P:413:LEU:CB | 2.72 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:S:41:GLU:HA | 4:S:41:GLU:OE2 | 1.99 | 0.62 |
| 2:J:10:ASN:HD22 | 2:J:67:LEU:HD22 | 1.65 | 0.62 |
| 3:P:398:LEU:N | 3:P:398:LEU:HD12 | 2.13 | 0.62 |
| 4:R:20:LEU:CD2 | 4:R:117:LYS:HG2 | 2.20 | 0.62 |
| 4:U:25:VAL:HG23 | 4:U:25:VAL:O | 1.99 | 0.62 |
| 1:C:451:ARG:HH11 | 1:C:451:ARG:CG | 2.11 | 0.62 |
| 1:A:537:VAL:HG22 | 1:A:549:GLU:HB3 | 1.81 | 0.62 |
| 1:A:570:ASP:HB2 | 4:R:112:ARG:HH22 | 1.64 | 0.62 |
| 1:C:568:MET:CE | 1:H:562:TYR:CD1 | 2.81 | 0.62 |
| 1:F:449:LEU:HD22 | 1:F:449:LEU:H | 1.64 | 0.62 |
| 3:P:361:LYS:CG | 3:P:364:LYS:HE2 | 2.30 | 0.62 |
| 1:D:354:PHE:HA | 1:D:357:ILE:HG22 | 1.81 | 0.62 |
| 1:F:543:LEU:HD22 | 1:F:548:THR:CG2 | 2.28 | 0.62 |
| 3:P:43:ARG:HH11 | 3:P:43:ARG:CG | 2.13 | 0.62 |
| 3:P:464:CYS:O | 3:P:507:ARG:O | 2.17 | 0.62 |
| 3:P:466:PHE:CE2 | 3:P:507:ARG:CB | 2.79 | 0.62 |
| 1:E:482:ALA:CB | 1:E:515:TYR:CE2 | 2.76 | 0.62 |
| 1:H:560:THR:HB | 1:K:560:THR:O | 1.99 | 0.62 |
| 1:C:454:VAL:CG2 | 1:C:538:VAL:HG21 | 2.29 | 0.62 |
| 1:A:538:VAL:HG23 | 1:A:548:THR:HG22 | 1.80 | 0.62 |
| 1:F:450:HIS:ND1 | 1:F:480:SER:HB3 | 2.11 | 0.62 |
| 1:F:545:ASN:HB3 | 1:G:358:PHE:HZ | 1.64 | 0.62 |
| 1:K:378:VAL:HG12 | 1:K:431:THR:HG23 | 1.81 | 0.62 |
| 1:A:566:LEU:HD13 | 1:A:566:LEU:H | 1.64 | 0.62 |
| 1:C:563:ASN:HD22 | 6:C:601:NAG:C1 | 2.03 | 0.62 |
| 1:K:521:LEU:HD23 | 1:K:521:LEU:C | 2.25 | 0.62 |
| 3:P:471:SER:CB | 3:P:475:LYS:NZ | 2.63 | 0.62 |
| 1:B:345:ILE:HA | 1:B:372:LEU:HB2 | 1.82 | 0.62 |
| 1:E:450:HIS:HB3 | 1:E:514:ARG:NH2 | 2.15 | 0.62 |
| 1:L:543:LEU:HD22 | 1:L:543:LEU:H | 1.64 | 0.62 |
| 4:R:111:ASP:O | 4:R:114:LYS:CD | 2.47 | 0.62 |
| 3:P:398:LEU:HD11 | 3:P:409:ILE:CG1 | 2.30 | 0.61 |
| 4:R:86:LEU:HD23 | 4:R:88:LEU:HD21 | 1.82 | 0.61 |
| 2:J:8:VAL:HG11 | 2:J:68:CYS:HA | 1.81 | 0.61 |
| 3:P:366:TRP:NE1 | 3:P:408:VAL:HG21 | 2.14 | 0.61 |
| 3:P:418:ALA:CB | 3:P:439:ILE:HD13 | 2.25 | 0.61 |
| 1:B:354:PHE:HA | 1:B:357:ILE:HG22 | 1.82 | 0.61 |
| 1:B:418:TRP:CE2 | 1:B:443:ARG:HB3 | 2.35 | 0.61 |
| 1:K:469:SER:N | 1:K:525:GLU:HB2 | 2.15 | 0.61 |
| 3:P:529:LYS:HG3 | 3:P:534:TYR:HD2 | 1.65 | 0.61 |
| 4:S:31:GLY:HA3 | 4:S:94:LEU:CD2 | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:U:22:GLU:HB2 | 4:U:119:THR:C | 2.22 | 0.61 |
| 1:A:508:GLU:HG2 | 1:A:509:PRO:HD2 | 1.80 | 0.61 |
| 1:B:445:LYS:CA | 1:B:445:LYS:HZ3 | 2.13 | 0.61 |
| 3:P:529:LYS:HG3 | 3:P:534:TYR:HE2 | 1.62 | 0.61 |
| 1:E:459:PRO:HG3 | 1:E:470:ALA:HB1 | 1.82 | 0.61 |
| 4:R:46:ILE:O | 4:R:64:THR:HG23 | 2.00 | 0.61 |
| 4:R:76:VAL:HG12 | 4:R:91:VAL:HG22 | 1.82 | 0.61 |
| 1:H:481:PRO:HB2 | 1:H:540:HIS:HE2 | 1.66 | 0.61 |
| 2:J:6:VAL:HA | 2:J:18:THR:HG22 | 1.83 | 0.61 |
| 1:E:483:ASP:O | 1:E:540:HIS:CE1 | 2.54 | 0.61 |
| 1:E:491:ARG:CD | 4:V:44:VAL:HG11 | 2.29 | 0.61 |
| 1:C:566:LEU:HD21 | 1:H:564:VAL:HG11 | 1.81 | 0.61 |
| 3:P:264:VAL:HG13 | 3:P:275:PHE:CE2 | 2.35 | 0.61 |
| 3:P:462:VAL:HB | 3:P:509:VAL:CB | 2.30 | 0.61 |
| 3:P:466:PHE:CD1 | 3:P:470:PHE:CZ | 2.83 | 0.61 |
| 1:A:356:SER:CA | 2:J:117:TYR:CZ | 2.76 | 0.61 |
| 1:A:518:HIS:CE1 | 1:B:520:ILE:HG21 | 2.36 | 0.61 |
| 2:J:106:ASN:HA | 3:P:29:VAL:HG21 | 1.83 | 0.61 |
| 3:P:342:LYS:HA | 3:P:438:LYS:O | 2.00 | 0.61 |
| 3:P:342:LYS:HE3 | 3:P:438:LYS:HE2 | 1.82 | 0.61 |
| 1:B:510:GLN:HA | 1:B:510:GLN:OE1 | 2.01 | 0.61 |
| 1:K:540:HIS:HB3 | 1:K:543:LEU:HD11 | 1.83 | 0.61 |
| 3:P:418:ALA:HA | 3:P:439:ILE:CD1 | 2.27 | 0.61 |
| 1:A:490:GLN:HB3 | 1:A:495:LEU:HD21 | 1.83 | 0.60 |
| 1:A:518:HIS:HE1 | 1:B:520:ILE:HG21 | 1.63 | 0.60 |
| 1:B:363:THR:HG23 | 1:B:415:GLU:HA | 1.82 | 0.60 |
| 1:H:384:ARG:HE | 1:H:390:VAL:HG22 | 1.66 | 0.60 |
| 2:J:115:LEU:HD12 | 2:J:124:VAL:CG2 | 2.24 | 0.60 |
| 3:P:286:LYS:C | 3:P:286:LYS:HD3 | 2.26 | 0.60 |
| 4:V:112:ARG:HB3 | 4:V:112:ARG:CZ | 2.31 | 0.60 |
| 1:A:567:VAL:O | 1:A:567:VAL:HG12 | 2.02 | 0.60 |
| 3:P:276:GLU:OE1 | 3:P:372:ALA:HB2 | 2.01 | 0.60 |
| 4:S:49:CYS:N | 4:S:103:ALA:O | 2.33 | 0.60 |
| 1:C:467:ARG:HD3 | 1:C:467:ARG:H | 1.66 | 0.60 |
| 1:C:482:ALA:HB2 | 1:C:515:TYR:CG | 2.35 | 0.60 |
| 1:F:524:SER:OG | 1:F:527:GLU:CG | 2.50 | 0.60 |
| 1:G:352:PRO:HB2 | 1:G:357:ILE:HD11 | 1.83 | 0.60 |
| 1:K:484:VAL:CG2 | 1:K:540:HIS:HB2 | 2.25 | 0.60 |
| 3:P:471:SER:C | 3:P:475:LYS:NZ | 2.59 | 0.60 |
| 4:R:20:LEU:HD22 | 4:R:20:LEU:C | 2.26 | 0.60 |
| 1:K:546:ARG:O | 1:K:546:ARG:HG2 | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:537:VAL:HG23 | 1:L:548:THR:O | 2.01 | 0.60 |
| 4:U:39:LEU:O | 4:U:39:LEU:HD23 | 2.02 | 0.60 |
| 1:D:493:GLN:H | 1:D:493:GLN:CD | 2.09 | 0.60 |
| 1:H:532:GLU:O | 1:H:553:ASP:CB | 2.49 | 0.60 |
| 1:L:538:VAL:CG1 | 1:L:548:THR:OG1 | 2.50 | 0.60 |
| 1:E:447:VAL:O | 1:E:447:VAL:HG13 | 2.01 | 0.60 |
| 1:F:490:GLN:NE2 | 1:F:532:GLU:OE1 | 2.33 | 0.60 |
| 1:G:467:ARG:HH11 | 1:G:467:ARG:HG3 | 1.67 | 0.60 |
| 1:G:516:PHE:C | 1:G:516:PHE:CD2 | 2.80 | 0.60 |
| 1:H:418:TRP:O | 1:H:442:SER:O | 2.18 | 0.60 |
| 3:P:466:PHE:HE2 | 3:P:507:ARG:HG3 | 0.72 | 0.60 |
| 1:A:516:PHE:CE1 | 1:B:520:ILE:HD11 | 2.37 | 0.60 |
| 1:L:479:PHE:CE2 | 1:L:484:VAL:CG1 | 2.85 | 0.60 |
| 3:P:462:VAL:CB | 3:P:509:VAL:O | 2.49 | 0.60 |
| 1:C:347:VAL:O | 1:C:439:GLN:NE2 | 2.34 | 0.60 |
| 1:C:471:THR:HG22 | 1:C:522:THR:HG22 | 1.82 | 0.60 |
| 1:H:529:ASN:C | 1:H:531:GLY:H | 2.10 | 0.60 |
| 1:L:424:PHE:CA | 1:L:441:ILE:CG1 | 2.78 | 0.60 |
| 1:L:480:SER:CB | 1:L:481:PRO:HD3 | 2.32 | 0.60 |
| 1:L:543:LEU:CB | 1:L:546:ARG:HA | 2.27 | 0.60 |
| 3:P:366:TRP:O | 3:P:379:LEU:HA | 2.02 | 0.60 |
| 4:R:21:PRO:O | 4:R:117:LYS:HB2 | 2.01 | 0.60 |
| 4:U:81:TYR:HD1 | 4:U:86:LEU:HB2 | 1.65 | 0.60 |
| 1:D:449:LEU:HB3 | 1:D:542:ALA:HB2 | 1.82 | 0.60 |
| 1:L:423:ARG:NH2 | 1:L:444:PRO:HB3 | 2.17 | 0.60 |
| 4:S:39:LEU:HD12 | 4:S:87:PHE:CD1 | 2.31 | 0.60 |
| 1:E:399:SER:HB3 | 1:E:403:ALA:HA | 1.82 | 0.60 |
| 1:F:480:SER:CB | 1:F:481:PRO:CD | 2.80 | 0.60 |
| 1:L:417:ASP:OD2 | 1:L:418:TRP:N | 2.35 | 0.60 |
| 2:J:48:ASN:HB3 | 2:J:51:ASP:HB3 | 1.84 | 0.59 |
| 1:L:484:VAL:HG13 | 1:L:484:VAL:O | 2.00 | 0.59 |
| 3:P:348:SER:CB | 3:P:537:THR:H | 2.15 | 0.59 |
| 1:A:489:MET:HE1 | 1:A:537:VAL:CG2 | 2.31 | 0.59 |
| 1:A:491:ARG:HG2 | 1:A:491:ARG:NH1 | 2.14 | 0.59 |
| 4:S:61:VAL:HG11 | 4:S:72:TYR:HD1 | 1.67 | 0.59 |
| 1:A:532:GLU:O | 1:A:553:ASP:HB2 | 2.02 | 0.59 |
| 3:P:391:TYR:HH | 3:P:416:ARG:HH12 | 1.42 | 0.59 |
| 3:P:447:LYS:N | 3:P:465:HIS:H | 1.86 | 0.59 |
| 4:U:50:ARG:HH11 | 4:U:100:GLY:HA3 | 1.65 | 0.59 |
| 1:E:493:GLN:H | 1:E:493:GLN:HE21 | 1.50 | 0.59 |
| 3:P:122:TYR:CE2 | 3:P:132:ILE:HG23 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:131:THR:HG22 | 3:P:188:VAL:HA | 1.83 | 0.59 |
| 3:P:341:VAL:HG23 | 3:P:341:VAL:O | 2.01 | 0.59 |
| 1:E:478:GLY:HA2 | 1:E:514:ARG:HB3 | 1.83 | 0.59 |
| 1:H:568:MET:O | 1:H:569:SER:C | 2.45 | 0.59 |
| 1:K:571:THR:O | 1:K:572:ALA:C | 2.45 | 0.59 |
| 3:P:128:ARG:HE | 3:P:320:PRO:HB3 | 1.67 | 0.59 |
| 3:P:248:VAL:HG12 | 3:P:311:SER:H | 1.66 | 0.59 |
| 4:V:95:THR:HG22 | 4:V:95:THR:O | 2.02 | 0.59 |
| 1:A:551:THR:HG23 | 1:A:551:THR:O | 2.02 | 0.59 |
| 1:D:421:GLY:N | 1:D:445:LYS:HZ2 | 1.80 | 0.59 |
| 1:F:543:LEU:CD2 | 1:F:548:THR:HG21 | 2.32 | 0.59 |
| 2:J:42:PRO:HG3 | 2:J:102:THR:HG22 | 1.85 | 0.59 |
| 1:L:574:THR:HG23 | 1:L:574:THR:O | 2.01 | 0.59 |
| 3:P:281:LEU:HD11 | 3:P:290:PHE:CE2 | 2.35 | 0.59 |
| 3:P:342:LYS:HE2 | 3:P:438:LYS:CE | 2.32 | 0.59 |
| 3:P:342:LYS:CA | 3:P:438:LYS:O | 2.51 | 0.59 |
| 3:P:523:TRP:CH2 | 3:P:539:ALA:HB1 | 2.37 | 0.59 |
| 1:B:384:ARG:HB3 | 1:B:387:GLY:H | 1.68 | 0.59 |
| 1:C:567:VAL:O | 1:C:567:VAL:HG22 | 2.03 | 0.59 |
| 1:F:550:ARG:HG2 | 1:F:550:ARG:HH11 | 1.66 | 0.59 |
| 1:K:464:LEU:HD11 | 1:K:525:GLU:CD | 2.24 | 0.59 |
| 3:P:132:ILE:CD1 | 3:P:187:VAL:HG23 | 2.33 | 0.59 |
| 1:B:443:ARG:HD3 | 1:B:443:ARG:O | 2.02 | 0.59 |
| 1:E:374:THR:OG1 | 1:E:398:GLU:O | 2.18 | 0.59 |
| 1:E:493:GLN:CB | 1:E:494:PRO:CD | 2.64 | 0.59 |
| 1:L:537:VAL:HG13 | 1:L:537:VAL:O | 2.02 | 0.59 |
| 3:P:43:ARG:HG2 | 3:P:43:ARG:O | 2.03 | 0.59 |
| 3:P:361:LYS:CB | 3:P:364:LYS:HE2 | 2.33 | 0.59 |
| 3:P:446:LEU:C | 3:P:465:HIS:O | 2.41 | 0.59 |
| 4:V:28:GLU:CA | 4:V:96:GLU:OE1 | 2.51 | 0.59 |
| 1:A:493:GLN:CB | 1:A:494:PRO:CD | 2.73 | 0.59 |
| 1:L:363:THR:HG21 | 1:L:418:TRP:HB2 | 1.85 | 0.59 |
| 4:S:23:VAL:HB | 4:S:35:ILE:HD13 | 1.85 | 0.59 |
| 4:U:101:VAL:O | 4:U:101:VAL:HG13 | 2.02 | 0.59 |
| 1:E:456:LEU:HD23 | 1:E:552:VAL:HG12 | 1.83 | 0.58 |
| 1:G:468:GLU:HG2 | 4:S:60:THR:HG21 | 1.85 | 0.58 |
| 2:J:40:ILE:HD13 | 1:K:574:THR:HG21 | 1.83 | 0.58 |
| 3:P:159:ILE:HD11 | 3:P:173:ILE:HG21 | 1.85 | 0.58 |
| 4:R:20:LEU:CD2 | 4:R:117:LYS:HB2 | 2.33 | 0.58 |
| 4:V:94:LEU:HD23 | 4:V:96:GLU:HG2 | 1.84 | 0.58 |
| 1:C:368:LEU:HD11 | 1:C:406:SER:HB3 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:565:SER:HB3 | 6:E:601:NAG:H62 | 1.85 | 0.58 |
| 1:F:545:ASN:HB3 | 1:G:358:PHE:CZ | 2.38 | 0.58 |
| 3:P:149:LYS:O | 3:P:155:PRO:HA | 2.03 | 0.58 |
| 1:C:565:SER:O | 1:C:565:SER:OG | 2.17 | 0.58 |
| 1:E:354:PHE:HA | 1:E:357:ILE:HG12 | 1.85 | 0.58 |
| 1:G:467:ARG:HH11 | 1:G:467:ARG:CG | 2.16 | 0.58 |
| 3:P:445:ASN:O | 3:P:467:PRO:CD | 2.48 | 0.58 |
| 3:P:35:LYS:HB2 | 3:P:52:SER:HB2 | 1.85 | 0.58 |
| 3:P:122:TYR:HE2 | 3:P:132:ILE:HG23 | 1.68 | 0.58 |
| 3:P:131:THR:HG22 | 3:P:188:VAL:CA | 2.33 | 0.58 |
| 3:P:528:VAL:HG13 | 3:P:535:GLY:HA3 | 1.85 | 0.58 |
| 4:R:20:LEU:CG | 4:R:117:LYS:HG3 | 2.22 | 0.58 |
| 4:R:111:ASP:O | 4:R:114:LYS:HD2 | 2.03 | 0.58 |
| 4:S:94:LEU:HD12 | 4:S:94:LEU:O | 2.02 | 0.58 |
| 1:B:451:ARG:HB2 | 1:B:451:ARG:HH11 | 1.68 | 0.58 |
| 1:G:378:VAL:HG21 | 1:G:405:PHE:CE2 | 2.38 | 0.58 |
| 3:P:398:LEU:CD1 | 3:P:407:THR:O | 2.52 | 0.58 |
| 4:R:45:ARG:NH2 | 4:R:110:THR:OG1 | 2.37 | 0.58 |
| 4:U:104:CYS:HB2 | 4:U:116:GLN:HG2 | 1.84 | 0.58 |
| 1:L:400:HIS:CE1 | 1:L:405:PHE:HA | 2.38 | 0.58 |
| 3:P:189:ILE:HG23 | 3:P:192:LEU:HD11 | 1.85 | 0.58 |
| 3:P:476:TYR:CD1 | 3:P:529:LYS:HB2 | 2.38 | 0.58 |
| 1:F:372:LEU:H | 1:F:404:THR:HA | 1.69 | 0.58 |
| 1:F:449:LEU:HA | 1:F:480:SER:HB2 | 1.84 | 0.58 |
| 1:H:562:TYR:CD2 | 1:H:562:TYR:N | 2.71 | 0.58 |
| 1:K:520:ILE:O | 1:K:520:ILE:HG23 | 2.03 | 0.58 |
| 1:L:430:HIS:CE1 | 1:L:432:ASP:HB3 | 2.37 | 0.58 |
| 4:U:41:GLU:OE1 | 4:U:41:GLU:HA | 2.03 | 0.58 |
| 4:V:22:GLU:HA | 4:V:118:VAL:HA | 1.84 | 0.58 |
| 1:A:393:HIS:HA | 1:A:410:GLU:HB3 | 1.84 | 0.58 |
| 1:B:454:VAL:HB | 1:B:476:VAL:HG12 | 1.85 | 0.58 |
| 1:C:459:PRO:HD3 | 1:C:472:ILE:HG12 | 1.85 | 0.58 |
| 1:F:563:ASN:OD1 | 6:F:601:NAG:N2 | 2.36 | 0.58 |
| 1:G:523:VAL:HG21 | 1:G:534:TYR:HH | 1.63 | 0.58 |
| 2:J:31:ASP:HB2 | 1:L:554:LYS:NZ | 2.19 | 0.58 |
| 1:K:545:ASN:ND2 | 1:K:545:ASN:H | 2.00 | 0.58 |
| 1:L:424:PHE:CA | 1:L:441:ILE:CD1 | 2.45 | 0.58 |
| 1:L:540:HIS:ND1 | 1:L:542:ALA:HB3 | 2.18 | 0.58 |
| 1:A:356:SER:N | 2:J:117:TYR:HH | 2.00 | 0.58 |
| 1:E:537:VAL:O | 1:E:537:VAL:HG12 | 2.03 | 0.58 |
| 1:H:393:HIS:HB2 | 1:H:396:ILE:HD11 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:448:ALA:HB1 | 1:K:481:PRO:HG3 | 1.85 | 0.58 |
| 3:P:314:GLN:HE21 | 3:P:314:GLN:HA | 1.69 | 0.58 |
| 4:R:47:TYR:CE2 | 4:R:49:CYS:HB2 | 2.38 | 0.58 |
| 4:S:99:SER:CB | 4:S:120:LEU:HB3 | 2.34 | 0.58 |
| 4:V:84:LYS:HE3 | 4:V:86:LEU:HD23 | 1.86 | 0.58 |
| 1:C:567:VAL:HB | 1:D:567:VAL:HG13 | 1.86 | 0.57 |
| 2:J:116:VAL:O | 2:J:116:VAL:HG22 | 2.04 | 0.57 |
| 1:K:354:PHE:CE1 | 1:K:541:GLU:CA | 2.87 | 0.57 |
| 1:L:367:CYS:HB2 | 1:L:382:TRP:CE3 | 2.38 | 0.57 |
| 1:L:450:HIS:CA | 1:L:480:SER:CB | 2.81 | 0.57 |
| 1:L:450:HIS:NE2 | 4:R:65:THR:HG22 | 2.18 | 0.57 |
| 3:P:398:LEU:HD13 | 3:P:407:THR:O | 2.03 | 0.57 |
| 1:B:450:HIS:O | 1:B:542:ALA:HB2 | 2.03 | 0.57 |
| 1:F:351:PRO:HB3 | 1:F:443:ARG:HD2 | 1.85 | 0.57 |
| 1:H:445:LYS:HA | 1:H:445:LYS:HE3 | 1.86 | 0.57 |
| 3:P:314:GLN:HE21 | 3:P:314:GLN:N | 2.02 | 0.57 |
| 4:R:46:ILE:N | 4:R:64:THR:HG21 | 2.18 | 0.57 |
| 1:B:423:ARG:HA | 1:B:442:SER:HB2 | 1.85 | 0.57 |
| 1:E:524:SER:OG | 1:E:527:GLU:OE1 | 2.22 | 0.57 |
| 1:E:535:THR:CG2 | 1:E:550:ARG:O | 2.52 | 0.57 |
| 1:H:364:LYS:HE3 | 1:H:410:GLU:HB3 | 1.87 | 0.57 |
| 1:D:349:ALA:HB2 | 1:D:439:GLN:HG3 | 1.85 | 0.57 |
| 2:J:36:ASN:ND2 | 1:L:563:ASN:OD1 | 2.37 | 0.57 |
| 3:P:340:VAL:HG11 | 3:P:436:GLU:CD | 2.29 | 0.57 |
| 4:U:102:TYR:HB2 | 4:U:118:VAL:CG2 | 2.34 | 0.57 |
| 2:J:52:PRO:HG3 | 2:J:128:LEU:HD21 | 1.86 | 0.57 |
| 1:L:540:HIS:ND1 | 1:L:542:ALA:CB | 2.67 | 0.57 |
| 1:K:366:THR:HG23 | 1:K:409:GLY:H | 1.69 | 0.57 |
| 1:K:476:VAL:O | 1:K:476:VAL:HG12 | 2.04 | 0.57 |
| 1:A:491:ARG:HG2 | 1:A:491:ARG:O | 2.04 | 0.57 |
| 3:P:475:LYS:HE2 | 3:P:475:LYS:N | 2.20 | 0.57 |
| 1:A:488:TRP:NE1 | 1:A:519:SER:OG | 2.24 | 0.57 |
| 1:A:491:ARG:HH11 | 1:A:491:ARG:CG | 2.16 | 0.57 |
| 1:B:568:MET:HE1 | 1:L:564:VAL:HG21 | 1.86 | 0.57 |
| 1:D:534:TYR:N | 1:D:534:TYR:CD1 | 2.73 | 0.57 |
| 1:E:400:HIS:HB3 | 1:E:404:THR:H | 1.69 | 0.57 |
| 1:L:543:LEU:HD13 | 1:L:543:LEU:N | 2.19 | 0.57 |
| 3:P:201:LEU:HD13 | 3:P:214:ASN:HA | 1.86 | 0.57 |
| 3:P:541:TYR:N | 3:P:541:TYR:CD1 | 2.73 | 0.57 |
| 1:A:501:VAL:HG13 | 1:A:501:VAL:O | 2.04 | 0.57 |
| 1:F:452:PRO:HD2 | 1:F:543:LEU:HG | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:398:GLU:HG3 | 1:G:399:SER:H | 1.70 | 0.57 |
| 1:G:475:LEU:HG | 1:G:475:LEU:O | 2.04 | 0.57 |
| 1:L:534:TYR:CD2 | 1:L:534:TYR:N | 2.73 | 0.57 |
| 3:P:147:LEU:HB3 | 3:P:159:ILE:HB | 1.86 | 0.57 |
| 3:P:368:LEU:HB2 | 3:P:378:PRO:HD3 | 1.83 | 0.57 |
| 4:S:39:LEU:CD2 | 4:S:85:ASN:C | 2.78 | 0.57 |
| 1:A:359:LEU:CD1 | 2:J:117:TYR:CB | 2.82 | 0.57 |
| 1:A:489:MET:CE | 1:A:537:VAL:CG2 | 2.83 | 0.57 |
| 1:C:566:LEU:H | 1:C:566:LEU:CD1 | 2.01 | 0.57 |
| 1:F:548:THR:HG23 | 1:F:548:THR:O | 2.05 | 0.57 |
| 1:D:374:THR:HG22 | 1:D:403:ALA:HB1 | 1.85 | 0.56 |
| 1:G:363:THR:HG21 | 1:G:418:TRP:HB3 | 1.86 | 0.56 |
| 4:V:108:MET:HA | 4:V:108:MET:HE3 | 1.85 | 0.56 |
| 1:A:520:ILE:HD13 | 1:B:475:LEU:HD11 | 1.87 | 0.56 |
| 1:C:383:THR:HG1 | 1:C:425:THR:HG1 | 1.53 | 0.56 |
| 1:D:454:VAL:HG21 | 1:D:538:VAL:HG21 | 1.87 | 0.56 |
| 1:E:489:MET:SD | 1:E:493:GLN:HA | 2.45 | 0.56 |
| 1:H:568:MET:O | 1:H:570:ASP:N | 2.38 | 0.56 |
| 1:K:452:PRO:HD2 | 1:K:543:LEU:HG | 1.86 | 0.56 |
| 5:I:2:NAG:O6 | 5:I:2:NAG:O4 | 2.02 | 0.56 |
| 1:B:484:VAL:HG13 | 1:B:484:VAL:O | 2.05 | 0.56 |
| 1:E:364:LYS:NZ | 1:E:412:SER:OG | 2.31 | 0.56 |
| 1:K:477:THR:HG22 | 1:K:516:PHE:HB2 | 1.86 | 0.56 |
| 3:P:523:TRP:HZ3 | 3:P:539:ALA:HB1 | 1.68 | 0.56 |
| 4:R:35:ILE:HD12 | 4:R:118:VAL:HG11 | 1.87 | 0.56 |
| 4:S:72:TYR:HD2 | 4:S:72:TYR:N | 2.03 | 0.56 |
| 4:U:22:GLU:HB3 | 4:U:119:THR:HG22 | 1.86 | 0.56 |
| 4:U:118:VAL:HG23 | 4:U:118:VAL:O | 2.04 | 0.56 |
| 1:A:501:VAL:O | 1:A:501:VAL:HG22 | 2.03 | 0.56 |
| 1:C:486:VAL:HG22 | 1:C:538:VAL:HG22 | 1.87 | 0.56 |
| 1:E:437:LEU:HG | 1:E:438:LYS:H | 1.69 | 0.56 |
| 1:G:396:ILE:HD11 | 1:G:407:ALA:HB1 | 1.88 | 0.56 |
| 1:G:467:ARG:O | 4:S:60:THR:HG22 | 2.06 | 0.56 |
| 1:H:456:LEU:HD12 | 1:H:536:CYS:HB3 | 1.86 | 0.56 |
| 3:P:149:LYS:CD | 3:P:151:ILE:HG22 | 2.34 | 0.56 |
| 3:P:361:LYS:HD2 | 3:P:361:LYS:C | 2.30 | 0.56 |
| 1:H:479:PHE:HB2 | 1:H:540:HIS:CE1 | 2.41 | 0.56 |
| 1:K:478:GLY:HA2 | 1:K:514:ARG:HB3 | 1.86 | 0.56 |
| 1:C:508:GLU:CG | 1:C:509:PRO:HD2 | 2.17 | 0.56 |
| 1:C:556:THR:O | 1:C:556:THR:HG22 | 2.04 | 0.56 |
| 1:D:367:CYS:HB3 | 1:D:382:TRP:CZ2 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:452:PRO:HD2 | 1:H:543:LEU:HG | 1.88 | 0.56 |
| 1:K:560:THR:O | 1:K:560:THR:HG23 | 2.05 | 0.56 |
| 3:P:407:THR:O | 3:P:407:THR:HG22 | 2.06 | 0.56 |
| 1:B:564:VAL:CG2 | 1:C:564:VAL:HA | 2.35 | 0.56 |
| 1:D:369:VAL:HG11 | 1:D:378:VAL:HG21 | 1.87 | 0.56 |
| 1:D:429:THR:HB | 1:D:436:PRO:HA | 1.87 | 0.56 |
| 1:E:367:CYS:H | 1:E:382:TRP:HH2 | 1.52 | 0.56 |
| 4:U:51:GLU:HA | 4:U:58:CYS:HA | 1.88 | 0.56 |
| 1:A:450:HIS:N | 1:A:450:HIS:CD2 | 2.72 | 0.56 |
| 1:A:489:MET:CE | 1:A:537:VAL:HG21 | 2.33 | 0.56 |
| 1:G:501:VAL:O | 1:G:501:VAL:HG12 | 2.06 | 0.56 |
| 1:G:502:THR:HG23 | 1:G:502:THR:O | 2.04 | 0.56 |
| 2:J:64:LEU:H | 2:J:64:LEU:CD2 | 2.18 | 0.56 |
| 3:P:366:TRP:CZ2 | 3:P:408:VAL:HG21 | 2.41 | 0.56 |
| 3:P:431:TRP:N | 3:P:431:TRP:CD1 | 2.72 | 0.56 |
| 3:P:462:VAL:CB | 3:P:509:VAL:HB | 2.34 | 0.56 |
| 4:R:91:VAL:HG12 | 4:R:93:GLN:O | 2.06 | 0.56 |
| 1:D:380:ILE:HD12 | 1:D:393:HIS:CD2 | 2.41 | 0.56 |
| 1:K:510:GLN:CG | 1:L:522:THR:HG23 | 2.27 | 0.56 |
| 1:L:487:GLN:HB3 | 1:L:537:VAL:HG11 | 1.88 | 0.56 |
| 4:S:34:THR:HB | 4:S:88:LEU:HD11 | 1.88 | 0.56 |
| 1:A:564:VAL:HG22 | 1:B:564:VAL:HA | 1.88 | 0.56 |
| 1:K:535:THR:HA | 1:K:550:ARG:O | 2.06 | 0.56 |
| 1:L:452:PRO:HB3 | 1:L:479:PHE:HD1 | 1.71 | 0.56 |
| 2:J:21:ILE:CD1 | 1:L:555:SER:CB | 2.65 | 0.55 |
| 3:P:250:LYS:HA | 3:P:309:ALA:HA | 1.87 | 0.55 |
| 4:S:61:VAL:HG13 | 4:S:72:TYR:CD1 | 2.41 | 0.55 |
| 1:B:449:LEU:HA | 1:B:480:SER:HG | 1.72 | 0.55 |
| 1:G:516:PHE:C | 1:G:516:PHE:HD2 | 2.14 | 0.55 |
| 1:H:532:GLU:O | 1:H:553:ASP:HB3 | 2.05 | 0.55 |
| 2:J:17:ILE:HD11 | 2:J:64:LEU:HD12 | 1.87 | 0.55 |
| 1:K:380:ILE:HB | 1:K:393:HIS:HD2 | 1.71 | 0.55 |
| 1:K:496:SER:HG | 1:K:499:LYS:HZ3 | 1.48 | 0.55 |
| 3:P:421:TYR:CZ | 3:P:437:ILE:HD12 | 2.37 | 0.55 |
| 1:B:451:ARG:CB | 1:B:451:ARG:CZ | 2.84 | 0.55 |
| 1:C:478:GLY:HA2 | 1:C:514:ARG:HG2 | 1.89 | 0.55 |
| 1:E:491:ARG:HG2 | 4:V:44:VAL:HG11 | 1.88 | 0.55 |
| 1:H:443:ARG:N | 1:H:444:PRO:HD3 | 2.22 | 0.55 |
| 1:H:554:LYS:HE2 | 1:H:558:LYS:NZ | 2.21 | 0.55 |
| 3:P:469:LYS:HG2 | 3:P:469:LYS:O | 2.05 | 0.55 |
| 4:R:61:VAL:HG21 | 4:R:72:TYR:CE2 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:116:VAL:O | 2:J:116:VAL:HG13 | 2.05 | 0.55 |
| 1:L:369:VAL:HG12 | 1:L:372:LEU:HD21 | 1.88 | 0.55 |
| 3:P:317:GLU:N | 3:P:317:GLU:OE2 | 2.39 | 0.55 |
| 3:P:491:GLN:HE22 | 3:P:510:SER:HB2 | 1.72 | 0.55 |
| 1:B:553:ASP:OD1 | 1:B:554:LYS:N | 2.36 | 0.55 |
| 3:P:395:LEU:CA | 3:P:410:LEU:HD12 | 2.35 | 0.55 |
| 4:S:23:VAL:HG22 | 4:S:25:VAL:HG23 | 1.89 | 0.55 |
| 1:A:356:SER:N | 2:J:117:TYR:CE2 | 2.75 | 0.55 |
| 1:A:574:THR:HA | 1:K:461:ARG:NH1 | 2.21 | 0.55 |
| 1:B:461:ARG:CZ | 1:L:570:ASP:OD2 | 2.55 | 0.55 |
| 1:C:423:ARG:HE | 1:C:442:SER:HB3 | 1.71 | 0.55 |
| 2:J:21:ILE:CD1 | 1:L:554:LYS:HG2 | 2.37 | 0.55 |
| 1:L:424:PHE:N | 1:L:441:ILE:HG13 | 2.10 | 0.55 |
| 1:L:424:PHE:CD2 | 1:L:441:ILE:HD13 | 2.41 | 0.55 |
| 1:L:450:HIS:CB | 1:L:480:SER:CB | 2.78 | 0.55 |
| 1:L:511:ALA:O | 1:L:514:ARG:CG | 2.55 | 0.55 |
| 3:P:38:CYS:SG | 3:P:91:LYS:HB2 | 2.47 | 0.55 |
| 3:P:315:LEU:HG | 3:P:315:LEU:O | 2.05 | 0.55 |
| 3:P:450:GLY:H | 3:P:540:VAL:HG12 | 1.67 | 0.55 |
| 1:B:454:VAL:CG1 | 1:B:538:VAL:HG11 | 2.36 | 0.55 |
| 1:H:443:ARG:N | 1:H:444:PRO:CD | 2.68 | 0.55 |
| 1:L:508:GLU:CG | 1:L:514:ARG:HB2 | 2.36 | 0.55 |
| 1:L:508:GLU:HG3 | 1:L:514:ARG:HB2 | 1.89 | 0.55 |
| 1:L:511:ALA:CB | 1:L:514:ARG:HG2 | 2.34 | 0.55 |
| 3:P:249:ALA:O | 3:P:309:ALA:HA | 2.06 | 0.55 |
| 3:P:371:GLY:H | 3:P:375:GLY:HA2 | 1.72 | 0.55 |
| 1:A:516:PHE:C | 1:A:516:PHE:CD2 | 2.85 | 0.55 |
| 1:B:420:SER:CB | 1:B:422:GLU:OE1 | 2.54 | 0.55 |
| 1:B:445:LYS:HZ3 | 1:B:445:LYS:N | 2.05 | 0.55 |
| 1:D:384:ARG:NH1 | 1:D:390:VAL:HA | 2.22 | 0.55 |
| 4:S:72:TYR:N | 4:S:72:TYR:CD2 | 2.72 | 0.55 |
| 1:A:423:ARG:HE | 1:A:440:THR:HG23 | 1.71 | 0.55 |
| 1:C:454:VAL:HG13 | 1:C:474:CYS:SG | 2.46 | 0.55 |
| 1:D:369:VAL:HB | 1:D:428:VAL:HG11 | 1.89 | 0.55 |
| 1:E:450:HIS:CE1 | 1:E:514:ARG:CZ | 2.90 | 0.55 |
| 1:F:520:ILE:O | 1:F:520:ILE:HG13 | 2.05 | 0.55 |
| 1:K:563:ASN:HB3 | 1:L:563:ASN:CA | 2.35 | 0.55 |
| 3:P:30:ASN:O | 3:P:35:LYS:NZ | 2.34 | 0.55 |
| 3:P:39:ARG:HB2 | 3:P:49:LEU:HD11 | 1.87 | 0.55 |
| 5:I:1:NAG:C1 | 5:I:1:NAG:C8 | 2.85 | 0.55 |
| 1:B:380:ILE:HB | 1:B:393:HIS:CD2 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:454:VAL:HG21 | 1:H:538:VAL:HG21 | 1.89 | 0.55 |
| 2:J:35:ARG:HH11 | 2:J:35:ARG:CG | 2.19 | 0.55 |
| 1:K:354:PHE:CE1 | 1:K:541:GLU:CB | 2.90 | 0.55 |
| 3:P:464:CYS:O | 3:P:507:ARG:C | 2.50 | 0.55 |
| 1:F:537:VAL:HG22 | 1:F:549:GLU:HB3 | 1.89 | 0.54 |
| 1:K:535:THR:CG2 | 1:K:551:THR:OG1 | 2.54 | 0.54 |
| 1:A:400:HIS:ND1 | 1:A:402:ASN:OD1 | 2.39 | 0.54 |
| 1:G:476:VAL:O | 1:G:476:VAL:HG12 | 2.06 | 0.54 |
| 4:S:39:LEU:O | 4:S:39:LEU:HD23 | 2.07 | 0.54 |
| 1:A:391:LYS:HA | 1:A:391:LYS:HE3 | 1.90 | 0.54 |
| 1:E:454:VAL:HG22 | 1:E:538:VAL:HG21 | 1.87 | 0.54 |
| 1:E:479:PHE:HB2 | 1:E:540:HIS:CE1 | 2.41 | 0.54 |
| 2:J:31:ASP:HB2 | 1:L:554:LYS:HZ1 | 1.72 | 0.54 |
| 1:B:393:HIS:CD2 | 1:B:409:GLY:HA3 | 2.43 | 0.54 |
| 1:B:568:MET:HE2 | 1:K:562:TYR:CE2 | 2.42 | 0.54 |
| 1:C:346:ARG:HG2 | 1:C:371:ASP:OD1 | 2.08 | 0.54 |
| 1:D:500:TYR:C | 1:D:500:TYR:CD1 | 2.85 | 0.54 |
| 1:F:500:TYR:CD1 | 1:F:500:TYR:C | 2.84 | 0.54 |
| 1:G:463:GLN:HG2 | 1:H:455:TYR:CZ | 2.42 | 0.54 |
| 2:J:117:TYR:CD1 | 2:J:117:TYR:C | 2.85 | 0.54 |
| 1:K:481:PRO:HG2 | 1:K:541:GLU:OE2 | 2.06 | 0.54 |
| 3:P:290:PHE:CD1 | 3:P:290:PHE:C | 2.85 | 0.54 |
| 3:P:425:THR:O | 3:P:430:LEU:CD2 | 2.54 | 0.54 |
| 1:C:419:ASN:OD1 | 1:C:420:SER:N | 2.40 | 0.54 |
| 1:L:523:VAL:HG11 | 1:L:534:TYR:HE1 | 1.71 | 0.54 |
| 3:P:361:LYS:HB3 | 3:P:364:LYS:HE2 | 1.90 | 0.54 |
| 3:P:369:TRP:CD1 | 3:P:420:PHE:H | 2.26 | 0.54 |
| 3:P:447:LYS:N | 3:P:465:HIS:N | 2.46 | 0.54 |
| 3:P:450:GLY:H | 3:P:540:VAL:CG1 | 2.20 | 0.54 |
| 4:R:99:SER:HB2 | 4:R:120:LEU:HB2 | 1.89 | 0.54 |
| 1:B:369:VAL:HG23 | 1:B:407:ALA:HB2 | 1.89 | 0.54 |
| 1:B:400:HIS:HB3 | 1:B:403:ALA:HA | 1.90 | 0.54 |
| 1:K:512:PRO:HD2 | 1:K:514:ARG:HG2 | 1.90 | 0.54 |
| 1:L:354:PHE:CD2 | 1:L:546:ARG:NH2 | 2.75 | 0.54 |
| 1:L:414:CYS:SG | 3:P:497:LYS:NZ | 2.75 | 0.54 |
| 3:P:263:VAL:HG21 | 3:P:314:GLN:NE2 | 2.23 | 0.54 |
| 3:P:399:GLU:O | 3:P:406:PHE:HA | 2.08 | 0.54 |
| 3:P:450:GLY:HA2 | 3:P:463:PRO:HD2 | 1.90 | 0.54 |
| 4:R:116:GLN:NE2 | 4:R:116:GLN:O | 2.41 | 0.54 |
| 1:A:566:LEU:N | 1:A:566:LEU:CD1 | 2.70 | 0.54 |
| 1:B:476:VAL:HG23 | 1:B:479:PHE:HE1 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:364:LYS:HA | 1:D:411:ALA:O | 2.08 | 0.54 |
| 1:E:482:ALA:CA | 1:E:515:TYR:CE2 | 2.91 | 0.54 |
| 1:L:481:PRO:HD2 | 1:L:540:HIS:NE2 | 2.20 | 0.54 |
| 3:P:289:SER:O | 3:P:289:SER:OG | 2.20 | 0.54 |
| 4:V:61:VAL:HA | 4:V:69:LYS:HB2 | 1.90 | 0.54 |
| 1:F:486:VAL:HG22 | 1:F:538:VAL:HG22 | 1.90 | 0.54 |
| 1:L:456:LEU:CG | 1:L:552:VAL:HG21 | 2.35 | 0.54 |
| 3:P:462:VAL:HG11 | 3:P:509:VAL:CG1 | 2.37 | 0.54 |
| 1:A:524:SER:HG | 1:A:527:GLU:HB2 | 1.70 | 0.54 |
| 1:B:443:ARG:HD3 | 1:B:443:ARG:N | 2.15 | 0.54 |
| 1:D:454:VAL:CG2 | 1:D:538:VAL:HG21 | 2.38 | 0.54 |
| 3:P:473:TYR:CD2 | 3:P:473:TYR:N | 2.76 | 0.54 |
| 1:B:531:GLY:HA2 | 1:B:554:LYS:HB2 | 1.90 | 0.54 |
| 1:C:448:ALA:O | 1:C:481:PRO:HD3 | 2.08 | 0.54 |
| 1:L:456:LEU:CG | 1:L:552:VAL:CG2 | 2.85 | 0.54 |
| 3:P:314:GLN:HA | 3:P:314:GLN:NE2 | 2.23 | 0.54 |
| 1:D:487:GLN:NE2 | 1:D:494:PRO:HB3 | 2.22 | 0.53 |
| 1:K:354:PHE:HE1 | 1:K:540:HIS:C | 2.13 | 0.53 |
| 1:B:473:THR:HG22 | 1:B:520:ILE:HG22 | 1.90 | 0.53 |
| 1:F:502:THR:O | 1:F:502:THR:HG22 | 2.08 | 0.53 |
| 1:H:445:LYS:HA | 1:H:445:LYS:CE | 2.38 | 0.53 |
| 1:L:346:ARG:HG2 | 1:L:370:THR:H | 1.73 | 0.53 |
| 3:P:264:VAL:HG13 | 3:P:275:PHE:HD2 | 1.66 | 0.53 |
| 3:P:264:VAL:CG1 | 3:P:275:PHE:CE2 | 2.91 | 0.53 |
| 3:P:366:TRP:CZ3 | 3:P:380:LEU:CD1 | 2.87 | 0.53 |
| 4:R:22:GLU:HG3 | 4:R:119:THR:HG22 | 1.90 | 0.53 |
| 1:A:538:VAL:HG22 | 1:A:548:THR:CG2 | 2.38 | 0.53 |
| 1:C:457:LEU:CD1 | 1:D:457:LEU:HD23 | 2.38 | 0.53 |
| 1:K:463:GLN:HB2 | 1:L:455:TYR:CE1 | 2.37 | 0.53 |
| 3:P:445:ASN:OD1 | 3:P:467:PRO:CG | 2.51 | 0.53 |
| 3:P:121:VAL:HA | 3:P:216:ASP:HB3 | 1.90 | 0.53 |
| 3:P:541:TYR:N | 3:P:541:TYR:HD1 | 2.06 | 0.53 |
| 4:U:105:GLY:HA2 | 4:U:115:THR:HG23 | 1.90 | 0.53 |
| 3:P:24:TYR:CD2 | 3:P:30:ASN:HB3 | 2.43 | 0.53 |
| 3:P:355:TYR:CD1 | 3:P:405:THR:HA | 2.44 | 0.53 |
| 3:P:447:LYS:HE2 | 3:P:465:HIS:CG | 2.44 | 0.53 |
| 1:A:384:ARG:NH1 | 1:A:388:GLU:OE2 | 2.42 | 0.53 |
| 1:A:483:ASP:O | 1:A:540:HIS:CD2 | 2.62 | 0.53 |
| 1:B:421:GLY:N | 1:B:443:ARG:HH21 | 2.04 | 0.53 |
| 1:C:473:THR:HG22 | 1:C:520:ILE:HG22 | 1.91 | 0.53 |
| 1:D:377:SER:O | 1:D:431:THR:OG1 | 2.22 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:562:TYR:N | 1:K:562:TYR:HD1 | 2.06 | 0.53 |
| 3:P:37:TRP:HB3 | 3:P:50:ILE:HG22 | 1.89 | 0.53 |
| 3:P:134:CYS:O | 3:P:185:PHE:HB3 | 2.09 | 0.53 |
| 3:P:197:ALA:HB2 | 3:P:219:VAL:HG13 | 1.91 | 0.53 |
| 3:P:477:TRP:HD1 | 3:P:526:CYS:HB2 | 1.74 | 0.53 |
| 1:C:457:LEU:CD1 | 1:C:473:THR:HG1 | 2.21 | 0.53 |
| 1:E:383:THR:HB | 1:E:387:GLY:HA2 | 1.91 | 0.53 |
| 1:E:482:ALA:CA | 1:E:515:TYR:HE2 | 2.22 | 0.53 |
| 3:P:355:TYR:HE1 | 3:P:405:THR:O | 1.92 | 0.53 |
| 1:C:477:THR:OG1 | 1:C:508:GLU:OE2 | 2.26 | 0.53 |
| 1:G:482:ALA:HB2 | 1:G:515:TYR:CE2 | 2.44 | 0.53 |
| 1:K:491:ARG:O | 1:K:493:GLN:N | 2.41 | 0.53 |
| 3:P:447:LYS:CD | 3:P:465:HIS:HB3 | 2.37 | 0.53 |
| 1:C:506:MET:HG3 | 1:C:507:PRO:HD2 | 1.91 | 0.53 |
| 1:K:480:SER:HB2 | 1:K:481:PRO:HD3 | 1.91 | 0.53 |
| 3:P:479:LYS:HG3 | 3:P:524:TYR:HE1 | 1.73 | 0.53 |
| 1:A:459:PRO:HG2 | 1:A:470:ALA:HB1 | 1.90 | 0.53 |
| 1:A:538:VAL:CG2 | 1:A:548:THR:HG22 | 2.38 | 0.53 |
| 1:F:471:THR:HG22 | 1:F:522:THR:HG23 | 1.91 | 0.53 |
| 4:R:46:ILE:N | 4:R:64:THR:HG23 | 2.15 | 0.53 |
| 1:B:489:MET:HG2 | 1:B:494:PRO:HA | 1.91 | 0.52 |
| 1:C:426:CYS:HB3 | 1:C:439:GLN:HB2 | 1.91 | 0.52 |
| 1:E:480:SER:O | 1:E:480:SER:OG | 2.25 | 0.52 |
| 1:G:481:PRO:HD2 | 1:G:540:HIS:CE1 | 2.44 | 0.52 |
| 1:G:482:ALA:HB2 | 1:G:515:TYR:CZ | 2.44 | 0.52 |
| 1:L:511:ALA:HB2 | 1:L:514:ARG:HD2 | 1.81 | 0.52 |
| 3:P:8:GLU:OE1 | 3:P:8:GLU:N | 2.42 | 0.52 |
| 3:P:446:LEU:CD2 | 3:P:537:THR:C | 2.75 | 0.52 |
| 3:P:463:PRO:HA | 3:P:508:LEU:HD12 | 1.91 | 0.52 |
| 4:R:22:GLU:OE1 | 4:R:101:VAL:CG1 | 2.44 | 0.52 |
| 4:S:75:ARG:HG3 | 4:S:91:VAL:HG13 | 1.90 | 0.52 |
| 4:U:36:LYS:HA | 4:U:88:LEU:HD23 | 1.90 | 0.52 |
| 1:A:466:LEU:N | 1:A:466:LEU:CD1 | 2.72 | 0.52 |
| 1:A:489:MET:HG2 | 1:A:494:PRO:HA | 1.91 | 0.52 |
| 1:A:538:VAL:HG22 | 1:A:548:THR:HG23 | 1.91 | 0.52 |
| 1:B:384:ARG:HA | 1:B:424:PHE:CE2 | 2.45 | 0.52 |
| 1:E:535:THR:HG22 | 1:E:550:ARG:O | 2.10 | 0.52 |
| 1:K:356:SER:O | 1:K:360:THR:OG1 | 2.25 | 0.52 |
| 1:K:508:GLU:HG3 | 1:K:514:ARG:HB2 | 1.89 | 0.52 |
| 1:K:562:TYR:N | 1:K:562:TYR:CD1 | 2.71 | 0.52 |
| 3:P:27:THR:OG1 | 3:P:30:ASN:OD1 | 2.27 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:508:GLU:HG2 | 1:A:509:PRO:CD | 2.40 | 0.52 |
| 1:F:456:LEU:HD11 | 1:F:536:CYS:HB3 | 1.91 | 0.52 |
| 1:K:480:SER:HA | 1:K:513:GLY:O | 2.09 | 0.52 |
| 1:L:449:LEU:HA | 1:L:480:SER:HB3 | 1.89 | 0.52 |
| 1:B:568:MET:HE2 | 1:K:562:TYR:HD2 | 1.75 | 0.52 |
| 1:C:466:LEU:HD21 | 4:V:45:ARG:CZ | 2.39 | 0.52 |
| 1:L:556:THR:O | 1:L:556:THR:HG23 | 2.10 | 0.52 |
| 3:P:196:ASP:O | 3:P:200:TYR:OH | 2.25 | 0.52 |
| 3:P:344:VAL:HG21 | 3:P:444:PRO:HA | 1.92 | 0.52 |
| 3:P:470:PHE:CZ | 3:P:528:VAL:HB | 2.43 | 0.52 |
| 3:P:491:GLN:NE2 | 3:P:510:SER:HB2 | 2.24 | 0.52 |
| 4:R:52:MET:CE | 4:R:69:LYS:HZ2 | 2.22 | 0.52 |
| 1:F:449:LEU:N | 1:F:449:LEU:CD2 | 2.73 | 0.52 |
| 1:F:453:ASP:OD2 | 1:F:455:TYR:OH | 2.21 | 0.52 |
| 2:J:35:ARG:CG | 2:J:35:ARG:NH1 | 2.70 | 0.52 |
| 1:L:430:HIS:HE1 | 1:L:432:ASP:HB3 | 1.74 | 0.52 |
| 4:U:48:LEU:HB2 | 4:U:89:VAL:HG11 | 1.91 | 0.52 |
| 1:K:558:LYS:NZ | 1:L:461:ARG:HE | 2.06 | 0.52 |
| 1:L:505:PRO:O | 1:L:506:MET:HE2 | 2.10 | 0.52 |
| 4:R:37:CYS:HA | 4:R:116:GLN:HG3 | 1.91 | 0.52 |
| 1:A:510:GLN:H | 1:A:510:GLN:CD | 2.18 | 0.52 |
| 1:B:420:SER:HB2 | 1:B:422:GLU:OE1 | 2.10 | 0.52 |
| 1:F:414:CYS:HB3 | 1:G:414:CYS:SG | 2.50 | 0.52 |
| 1:L:456:LEU:CD2 | 1:L:552:VAL:HG21 | 2.32 | 0.52 |
| 4:R:25:VAL:HB | 4:R:120:LEU:HG | 1.91 | 0.52 |
| 4:R:95:THR:C | 4:R:97:SER:H | 2.17 | 0.52 |
| 1:B:454:VAL:HG22 | 1:B:550:ARG:CG | 2.38 | 0.52 |
| 1:C:451:ARG:NH1 | 1:C:451:ARG:CG | 2.72 | 0.52 |
| 1:L:450:HIS:CE1 | 4:R:65:THR:HG22 | 2.45 | 0.52 |
| 3:P:261:CYS:O | 3:P:263:VAL:N | 2.43 | 0.52 |
| 2:J:40:ILE:CD1 | 1:K:574:THR:HG21 | 2.39 | 0.52 |
| 1:K:565:SER:O | 1:K:565:SER:OG | 2.19 | 0.52 |
| 4:U:22:GLU:CB | 4:U:119:THR:N | 2.72 | 0.52 |
| 4:U:22:GLU:CD | 4:U:119:THR:HG23 | 2.33 | 0.52 |
| 1:E:493:GLN:NE2 | 1:E:493:GLN:N | 2.58 | 0.52 |
| 1:F:449:LEU:HD22 | 1:F:449:LEU:N | 2.25 | 0.52 |
| 1:L:526:GLU:O | 1:L:530:THR:HG23 | 2.10 | 0.52 |
| 1:A:356:SER:CA | 2:J:117:TYR:CE2 | 2.92 | 0.51 |
| 1:E:368:LEU:HD21 | 1:E:406:SER:HB2 | 1.92 | 0.51 |
| 1:F:474:CYS:HB2 | 1:F:488:TRP:CZ2 | 2.45 | 0.51 |
| 1:K:450:HIS:NE2 | 1:K:514:ARG:NH1 | 2.54 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:227:VAL:HG23 | 3:P:326:LEU:HA | 1.92 | 0.51 |
| 1:A:518:HIS:HE1 | 1:B:520:ILE:HG23 | 1.70 | 0.51 |
| 1:A:535:THR:HG22 | 1:A:551:THR:CB | 2.37 | 0.51 |
| 1:C:526:GLU:H | 1:C:526:GLU:CD | 2.17 | 0.51 |
| 1:E:467:ARG:HD3 | 1:E:525:GLU:HG3 | 1.92 | 0.51 |
| 1:L:354:PHE:HD2 | 1:L:546:ARG:HH21 | 1.55 | 0.51 |
| 3:P:63:ARG:NH2 | 3:P:86:ASP:OD2 | 2.41 | 0.51 |
| 3:P:355:TYR:CE1 | 3:P:405:THR:CA | 2.93 | 0.51 |
| 3:P:525:TRP:CE3 | 3:P:537:THR:HG22 | 2.44 | 0.51 |
| 4:S:79:LYS:HD3 | 4:S:80:GLN:H | 1.75 | 0.51 |
| 1:A:564:VAL:CG2 | 1:B:564:VAL:HA | 2.40 | 0.51 |
| 1:C:429:THR:HG22 | 1:C:436:PRO:HB3 | 1.92 | 0.51 |
| 1:H:495:LEU:HD22 | 1:H:499:LYS:HE3 | 1.92 | 0.51 |
| 1:K:518:HIS:ND1 | 1:L:518:HIS:CG | 2.78 | 0.51 |
| 1:A:467:ARG:HG3 | 1:A:525:GLU:OE1 | 2.11 | 0.51 |
| 1:C:466:LEU:CD2 | 4:V:45:ARG:CZ | 2.88 | 0.51 |
| 1:D:562:TYR:CE1 | 1:H:568:MET:SD | 3.04 | 0.51 |
| 3:P:361:LYS:HG2 | 3:P:364:LYS:HE3 | 1.91 | 0.51 |
| 3:P:450:GLY:N | 3:P:540:VAL:HG13 | 2.26 | 0.51 |
| 1:F:543:LEU:HD22 | 1:F:548:THR:HG21 | 1.92 | 0.51 |
| 1:G:518:HIS:NE2 | 1:H:520:ILE:HD11 | 2.25 | 0.51 |
| 3:P:295:THR:HG22 | 3:P:432:ARG:HB2 | 1.93 | 0.51 |
| 3:P:525:TRP:CZ3 | 3:P:537:THR:CG2 | 2.92 | 0.51 |
| 4:V:112:ARG:CB | 4:V:112:ARG:NH1 | 2.73 | 0.51 |
| 1:C:482:ALA:CB | 1:C:515:TYR:CE1 | 2.91 | 0.51 |
| 1:F:546:ARG:CG | 1:F:546:ARG:NH1 | 2.72 | 0.51 |
| 2:J:28:PRO:HG3 | 1:L:467:ARG:NH2 | 2.24 | 0.51 |
| 1:K:423:ARG:HG3 | 1:K:442:SER:HB2 | 1.93 | 0.51 |
| 3:P:127:GLY:N | 3:P:192:LEU:O | 2.35 | 0.51 |
| 4:U:39:LEU:HD23 | 4:U:39:LEU:C | 2.35 | 0.51 |
| 1:B:445:LYS:CB | 1:B:445:LYS:NZ | 2.72 | 0.51 |
| 1:B:498:GLU:O | 1:B:498:GLU:HG2 | 2.11 | 0.51 |
| 1:H:453:ASP:OD1 | 1:H:455:TYR:OH | 2.18 | 0.51 |
| 1:K:510:GLN:OE1 | 1:K:510:GLN:HA | 2.09 | 0.51 |
| 3:P:368:LEU:CD1 | 3:P:378:PRO:HG2 | 2.39 | 0.51 |
| 1:A:380:ILE:H | 1:A:393:HIS:CD2 | 2.29 | 0.51 |
| 1:G:352:PRO:HD3 | 1:G:365:LEU:HD13 | 1.92 | 0.51 |
| 3:P:132:ILE:HD12 | 3:P:187:VAL:O | 2.11 | 0.51 |
| 3:P:239:CYS:HB2 | 3:P:290:PHE:CE1 | 2.46 | 0.51 |
| 3:P:248:VAL:HG12 | 3:P:311:SER:N | 2.26 | 0.51 |
| 1:F:427:THR:HG23 | 1:F:438:LYS:HB3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:514:ARG:CA | 1:L:514:ARG:NH1 | 2.73 | 0.51 |
| 3:P:60:TYR:HB3 | 3:P:64:ALA:HB3 | 1.93 | 0.51 |
| 3:P:368:LEU:CG | 3:P:378:PRO:HG2 | 2.40 | 0.51 |
| 3:P:391:TYR:N | 3:P:391:TYR:CD1 | 2.79 | 0.51 |
| 4:S:29:LEU:HD22 | 4:S:95:THR:CG2 | 2.27 | 0.51 |
| 4:U:72:TYR:HA | 4:U:75:ARG:HD3 | 1.92 | 0.51 |
| 1:A:400:HIS:HD2 | 1:A:406:SER:HB2 | 1.76 | 0.51 |
| 1:L:365:LEU:HD23 | 1:L:413:ILE:HD11 | 1.93 | 0.51 |
| 3:P:314:GLN:CA | 3:P:314:GLN:NE2 | 2.72 | 0.51 |
| 1:D:393:HIS:CD2 | 1:D:393:HIS:H | 2.27 | 0.50 |
| 1:G:502:THR:HA | 1:G:519:SER:HA | 1.93 | 0.50 |
| 1:L:523:VAL:HG11 | 1:L:534:TYR:CE1 | 2.46 | 0.50 |
| 1:L:540:HIS:HB3 | 1:L:543:LEU:CG | 2.32 | 0.50 |
| 3:P:446:LEU:CD2 | 3:P:538:ALA:CA | 2.90 | 0.50 |
| 3:P:470:PHE:O | 3:P:473:TYR:CE2 | 2.64 | 0.50 |
| 1:G:443:ARG:C | 1:G:443:ARG:CD | 2.84 | 0.50 |
| 1:K:537:VAL:HG12 | 1:K:549:GLU:HG2 | 1.93 | 0.50 |
| 3:P:253:CYS:HB2 | 3:P:306:LEU:HB2 | 1.93 | 0.50 |
| 4:U:41:GLU:C | 4:U:43:HIS:N | 2.69 | 0.50 |
| 1:A:477:THR:HG22 | 1:A:508:GLU:OE2 | 2.12 | 0.50 |
| 1:G:450:HIS:CD2 | 1:G:514:ARG:NH1 | 2.80 | 0.50 |
| 2:J:21:ILE:CG1 | 1:L:555:SER:CB | 2.90 | 0.50 |
| 1:K:516:PHE:CD1 | 1:K:516:PHE:C | 2.88 | 0.50 |
| 3:P:243:PRO:CA | 3:P:246:ALA:HB2 | 2.37 | 0.50 |
| 3:P:368:LEU:C | 3:P:378:PRO:HD3 | 2.36 | 0.50 |
| 3:P:529:LYS:CG | 3:P:534:TYR:HE2 | 2.17 | 0.50 |
| 4:R:28:GLU:HG3 | 4:R:29:LEU:H | 1.76 | 0.50 |
| 4:U:48:LEU:HD22 | 4:U:89:VAL:HG21 | 1.93 | 0.50 |
| 1:C:384:ARG:NH2 | 1:C:422:GLU:O | 2.44 | 0.50 |
| 1:D:421:GLY:CA | 1:D:445:LYS:HZ1 | 2.11 | 0.50 |
| 1:E:484:VAL:O | 1:E:484:VAL:HG13 | 2.12 | 0.50 |
| 1:F:523:VAL:CG1 | 1:F:534:TYR:OH | 2.60 | 0.50 |
| 1:H:365:LEU:HD11 | 1:H:418:TRP:CZ2 | 2.40 | 0.50 |
| 1:K:477:THR:CG2 | 1:K:516:PHE:HB2 | 2.41 | 0.50 |
| 3:P:414:THR:HG1 | 3:P:417:ASP:CG | 2.10 | 0.50 |
| 1:A:384:ARG:HG2 | 1:A:385:GLN:H | 1.77 | 0.50 |
| 1:A:459:PRO:CB | 1:A:470:ALA:HB1 | 2.41 | 0.50 |
| 4:S:97:SER:O | 4:S:97:SER:OG | 2.29 | 0.50 |
| 1:F:545:ASN:N | 1:F:545:ASN:ND2 | 2.58 | 0.50 |
| 1:K:430:HIS:CD2 | 1:K:432:ASP:HB2 | 2.47 | 0.50 |
| 1:K:490:GLN:O | 1:K:490:GLN:HG3 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:448:VAL:HG23 | 3:P:463:PRO:CG | 2.41 | 0.50 |
| 3:P:470:PHE:O | 3:P:473:TYR:CD2 | 2.64 | 0.50 |
| 4:V:48:LEU:HD21 | 4:V:102:TYR:CG | 2.47 | 0.50 |
| 1:A:560:THR:O | 1:B:560:THR:N | 2.43 | 0.50 |
| 1:L:511:ALA:O | 1:L:514:ARG:HG2 | 2.11 | 0.50 |
| 3:P:148:TYR:HD2 | 3:P:202:CYS:HA | 1.77 | 0.50 |
| 3:P:478:CYS:HA | 3:P:487:ALA:HA | 1.93 | 0.50 |
| 1:A:402:ASN:OD1 | 1:A:404:THR:OG1 | 2.22 | 0.50 |
| 1:F:427:THR:HG22 | 1:F:436:PRO:HB2 | 1.94 | 0.50 |
| 2:J:115:LEU:CD1 | 2:J:124:VAL:HG21 | 2.25 | 0.50 |
| 3:P:245:VAL:HG11 | 3:P:320:PRO:HG2 | 1.93 | 0.50 |
| 3:P:351:VAL:HG11 | 3:P:435:VAL:HG11 | 1.94 | 0.50 |
| 1:B:445:LYS:HZ3 | 1:B:445:LYS:CB | 2.25 | 0.50 |
| 1:D:514:ARG:HH11 | 4:V:66:ASN:HD21 | 1.60 | 0.50 |
| 3:P:526:CYS:O | 3:P:538:ALA:HB2 | 2.11 | 0.50 |
| 4:R:36:LYS:HE2 | 4:R:86:LEU:HG | 1.93 | 0.50 |
| 1:A:359:LEU:CD1 | 2:J:117:TYR:CG | 2.81 | 0.49 |
| 1:C:456:LEU:HD11 | 1:C:536:CYS:HB3 | 1.93 | 0.49 |
| 1:G:467:ARG:HD3 | 1:G:525:GLU:OE1 | 2.12 | 0.49 |
| 1:K:510:GLN:HG3 | 1:L:522:THR:HG21 | 1.72 | 0.49 |
| 3:P:476:TYR:O | 3:P:527:GLY:N | 2.45 | 0.49 |
| 1:C:484:VAL:O | 1:C:484:VAL:HG13 | 2.11 | 0.49 |
| 1:H:480:SER:HB3 | 1:H:481:PRO:HD3 | 1.94 | 0.49 |
| 1:K:464:LEU:HD13 | 1:K:525:GLU:CG | 2.42 | 0.49 |
| 1:K:473:THR:O | 1:K:473:THR:HG22 | 2.12 | 0.49 |
| 1:K:479:PHE:HB2 | 1:K:540:HIS:CE1 | 2.47 | 0.49 |
| 3:P:24:TYR:HD2 | 3:P:30:ASN:HB3 | 1.75 | 0.49 |
| 3:P:368:LEU:CA | 3:P:378:PRO:HD3 | 2.42 | 0.49 |
| 4:U:34:THR:HG22 | 4:U:90:GLU:HG3 | 1.94 | 0.49 |
| 1:A:489:MET:HB2 | 1:A:535:THR:OG1 | 2.13 | 0.49 |
| 1:F:449:LEU:CA | 1:F:480:SER:HB2 | 2.37 | 0.49 |
| 1:K:459:PRO:HG3 | 1:K:470:ALA:HB1 | 1.95 | 0.49 |
| 4:R:81:TYR:HB2 | 4:R:86:LEU:HB2 | 1.95 | 0.49 |
| 1:A:485:PHE:CE2 | 2:J:115:LEU:HD22 | 2.41 | 0.49 |
| 1:L:484:VAL:HA | 1:L:539:ALA:O | 2.12 | 0.49 |
| 3:P:466:PHE:CE2 | 3:P:507:ARG:HB2 | 2.47 | 0.49 |
| 1:A:457:LEU:HB2 | 1:A:473:THR:CG2 | 2.42 | 0.49 |
| 1:B:496:SER:HB2 | 1:B:497:PRO:HD2 | 1.95 | 0.49 |
| 1:C:480:SER:O | 1:C:540:HIS:HE1 | 1.93 | 0.49 |
| 1:K:566:LEU:HD23 | 1:K:566:LEU:C | 2.37 | 0.49 |
| 3:P:310:HIS:CE1 | 3:P:316:GLN:HB2 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:U:50:ARG:NH1 | 4:U:100:GLY:CA | 2.64 | 0.49 |
| 1:B:543:LEU:HD11 | 1:B:548:THR:HG22 | 1.95 | 0.49 |
| 1:E:514:ARG:NH1 | 1:E:514:ARG:HG2 | 2.27 | 0.49 |
| 1:G:489:MET:HA | 1:G:494:PRO:HA | 1.94 | 0.49 |
| 1:L:514:ARG:CB | 1:L:514:ARG:NH1 | 2.72 | 0.49 |
| 3:P:351:VAL:HB | 3:P:408:VAL:HG22 | 1.95 | 0.49 |
| 3:P:361:LYS:C | 3:P:361:LYS:CD | 2.85 | 0.49 |
| 4:V:78:LEU:HB2 | 4:V:87:PHE:CE1 | 2.47 | 0.49 |
| 1:H:573:GLY:O | 1:H:574:THR:C | 2.56 | 0.49 |
| 1:K:463:GLN:O | 1:K:463:GLN:HG2 | 2.09 | 0.49 |
| 4:R:50:ARG:NH1 | 4:R:51:GLU:O | 2.45 | 0.49 |
| 4:S:46:ILE:HD13 | 4:S:87:PHE:CD2 | 2.47 | 0.49 |
| 4:V:75:ARG:NH2 | 4:V:95:THR:H | 2.11 | 0.49 |
| 1:C:363:THR:OG1 | 1:C:413:ILE:O | 2.30 | 0.49 |
| 1:C:502:THR:HA | 1:C:519:SER:HA | 1.94 | 0.49 |
| 1:D:376:ASP:HB3 | 1:D:430:HIS:NE2 | 2.28 | 0.49 |
| 1:D:376:ASP:OD1 | 1:D:377:SER:N | 2.45 | 0.49 |
| 1:E:514:ARG:HG2 | 1:E:514:ARG:HH11 | 1.78 | 0.49 |
| 1:G:378:VAL:HG21 | 1:G:405:PHE:HE2 | 1.77 | 0.49 |
| 1:K:380:ILE:HB | 1:K:393:HIS:CD2 | 2.48 | 0.49 |
| 4:U:32:SER:HA | 4:U:91:VAL:O | 2.13 | 0.49 |
| 1:A:423:ARG:CZ | 1:A:425:THR:HB | 2.43 | 0.49 |
| 1:B:481:PRO:HD2 | 1:B:540:HIS:CE1 | 2.48 | 0.49 |
| 1:B:537:VAL:HG12 | 1:B:549:GLU:HG2 | 1.95 | 0.49 |
| 1:C:463:GLN:O | 1:C:466:LEU:HB2 | 2.12 | 0.49 |
| 1:E:511:ALA:CB | 1:E:514:ARG:HG3 | 2.38 | 0.49 |
| 3:P:99:ARG:HG3 | 3:P:99:ARG:O | 2.11 | 0.49 |
| 3:P:340:VAL:HG11 | 3:P:436:GLU:CG | 2.43 | 0.49 |
| 3:P:368:LEU:CB | 3:P:378:PRO:CG | 2.78 | 0.49 |
| 3:P:400:GLU:HA | 3:P:402:GLY:N | 2.27 | 0.49 |
| 4:U:94:LEU:C | 4:U:96:GLU:N | 2.69 | 0.49 |
| 1:B:354:PHE:CZ | 1:B:546:ARG:CG | 2.96 | 0.49 |
| 1:F:554:LYS:C | 1:F:554:LYS:CD | 2.85 | 0.49 |
| 1:K:533:THR:HG22 | 1:K:551:THR:CG2 | 2.43 | 0.49 |
| 4:R:20:LEU:CD2 | 4:R:20:LEU:C | 2.86 | 0.49 |
| 1:K:346:ARG:O | 1:K:370:THR:OG1 | 2.24 | 0.48 |
| 1:K:487:GLN:HB3 | 1:K:537:VAL:HG23 | 1.95 | 0.48 |
| 3:P:263:VAL:HG21 | 3:P:314:GLN:HE22 | 1.78 | 0.48 |
| 3:P:286:LYS:C | 3:P:286:LYS:CD | 2.85 | 0.48 |
| 1:F:561:LEU:HD12 | 1:F:561:LEU:HA | 1.52 | 0.48 |
| 1:H:572:ALA:HB3 | 1:H:574:THR:HG22 | 1.93 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:463:GLN:HA | 1:K:466:LEU:HD23 | 1.93 | 0.48 |
| 4:S:50:ARG:N | 4:S:59:GLY:O | 2.45 | 0.48 |
| 1:C:481:PRO:O | 1:C:481:PRO:HG2 | 2.13 | 0.48 |
| 1:D:510:GLN:OE1 | 1:D:510:GLN:HA | 2.14 | 0.48 |
| 1:K:386:ASN:OD1 | 1:K:387:GLY:N | 2.46 | 0.48 |
| 1:K:545:ASN:ND2 | 1:K:545:ASN:N | 2.60 | 0.48 |
| 3:P:29:VAL:O | 3:P:33:THR:HG23 | 2.13 | 0.48 |
| 3:P:395:LEU:CB | 3:P:410:LEU:HD11 | 2.20 | 0.48 |
| 3:P:411:ASN:ND2 | 3:P:525:TRP:CH2 | 2.81 | 0.48 |
| 4:S:39:LEU:HD23 | 4:S:85:ASN:HA | 1.94 | 0.48 |
| 4:S:49:CYS:HB3 | 4:S:58:CYS:HB2 | 1.44 | 0.48 |
| 1:A:428:VAL:HG22 | 1:A:437:LEU:H | 1.78 | 0.48 |
| 1:B:389:ALA:C | 1:B:391:LYS:H | 2.21 | 0.48 |
| 1:E:459:PRO:HD3 | 1:E:472:ILE:HG13 | 1.96 | 0.48 |
| 1:G:491:ARG:HD2 | 4:U:44:VAL:HG11 | 1.95 | 0.48 |
| 1:L:538:VAL:HG12 | 1:L:548:THR:HB | 1.94 | 0.48 |
| 3:P:251:PHE:CZ | 3:P:308:GLY:O | 2.58 | 0.48 |
| 4:U:50:ARG:HH12 | 4:U:100:GLY:CA | 2.24 | 0.48 |
| 1:B:414:CYS:SG | 1:C:416:ASP:HB3 | 2.49 | 0.48 |
| 1:F:470:ALA:HB3 | 1:F:523:VAL:HG23 | 1.95 | 0.48 |
| 1:F:554:LYS:O | 1:F:554:LYS:HD3 | 2.13 | 0.48 |
| 1:L:540:HIS:HB3 | 1:L:543:LEU:CD1 | 2.44 | 0.48 |
| 4:U:37:CYS:HB3 | 4:U:87:PHE:O | 2.13 | 0.48 |
| 4:V:86:LEU:HD12 | 4:V:87:PHE:H | 1.79 | 0.48 |
| 1:C:562:TYR:CD2 | 1:H:568:MET:HE2 | 2.48 | 0.48 |
| 1:C:566:LEU:HD13 | 1:D:566:LEU:CD2 | 2.43 | 0.48 |
| 1:E:508:GLU:HB2 | 1:E:514:ARG:O | 2.14 | 0.48 |
| 3:P:366:TRP:O | 3:P:380:LEU:N | 2.45 | 0.48 |
| 1:E:367:CYS:N | 1:E:382:TRP:HH2 | 2.11 | 0.48 |
| 1:F:414:CYS:HB2 | 1:F:418:TRP:CD1 | 2.49 | 0.48 |
| 1:G:467:ARG:CG | 1:G:467:ARG:NH1 | 2.72 | 0.48 |
| 1:K:467:ARG:NH2 | 4:R:111:ASP:OD1 | 2.46 | 0.48 |
| 1:L:487:GLN:C | 1:L:537:VAL:HG12 | 2.37 | 0.48 |
| 3:P:243:PRO:C | 3:P:246:ALA:HB2 | 2.39 | 0.48 |
| 3:P:447:LYS:HB2 | 3:P:464:CYS:CA | 2.44 | 0.48 |
| 1:E:491:ARG:CG | 4:V:44:VAL:HG11 | 2.44 | 0.48 |
| 1:H:565:SER:HB3 | 1:K:565:SER:HB2 | 1.96 | 0.48 |
| 1:L:345:ILE:HA | 1:L:433:LEU:HD11 | 1.96 | 0.48 |
| 1:L:576:TYR:HD2 | 1:L:576:TYR:N | 2.10 | 0.48 |
| 4:R:22:GLU:HA | 4:R:117:LYS:C | 2.35 | 0.48 |
| 4:U:20:LEU:HG | 4:U:117:LYS:HB2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:U:80:GLN:OE1 | 4:U:87:PHE:HD1 | 1.95 | 0.48 |
| 1:D:514:ARG:HH21 | 1:D:514:ARG:CG | 2.23 | 0.48 |
| 1:H:514:ARG:HH12 | 4:S:65:THR:HG23 | 1.79 | 0.48 |
| 1:H:554:LYS:HZ2 | 1:H:558:LYS:HZ2 | 1.52 | 0.48 |
| 1:H:554:LYS:HZ2 | 1:H:558:LYS:NZ | 1.94 | 0.48 |
| 4:S:78:LEU:HD11 | 4:S:87:PHE:HD2 | 1.78 | 0.48 |
| 4:V:47:TYR:OH | 4:V:113:GLY:HA3 | 2.14 | 0.48 |
| 1:A:531:GLY:HA2 | 1:A:554:LYS:HB2 | 1.96 | 0.48 |
| 1:B:461:ARG:HH22 | 1:K:570:ASP:HB3 | 1.79 | 0.48 |
| 1:B:472:ILE:HG21 | 1:B:552:VAL:HG11 | 1.96 | 0.48 |
| 1:D:348:PHE:HD2 | 1:D:370:THR:HB | 1.79 | 0.48 |
| 1:K:521:LEU:C | 1:K:521:LEU:CD2 | 2.85 | 0.48 |
| 1:B:476:VAL:HG11 | 1:B:538:VAL:HG21 | 1.96 | 0.47 |
| 1:C:379:THR:HB | 1:C:429:THR:OG1 | 2.14 | 0.47 |
| 1:D:535:THR:HG22 | 1:D:551:THR:HB | 1.96 | 0.47 |
| 4:R:47:TYR:OH | 4:R:110:THR:O | 2.32 | 0.47 |
| 4:R:62:VAL:HG12 | 4:R:68:ILE:HG22 | 1.94 | 0.47 |
| 1:B:384:ARG:HB3 | 1:B:387:GLY:N | 2.29 | 0.47 |
| 1:D:384:ARG:HH11 | 1:D:390:VAL:HA | 1.79 | 0.47 |
| 1:E:457:LEU:HB2 | 1:E:473:THR:CG2 | 2.44 | 0.47 |
| 1:E:489:MET:SD | 1:E:494:PRO:N | 2.87 | 0.47 |
| 1:L:449:LEU:CA | 1:L:480:SER:HB3 | 2.44 | 0.47 |
| 3:P:120:LYS:O | 3:P:216:ASP:N | 2.47 | 0.47 |
| 3:P:286:LYS:HD3 | 3:P:286:LYS:O | 2.12 | 0.47 |
| 3:P:445:ASN:CB | 3:P:536:GLU:OE2 | 2.62 | 0.47 |
| 4:R:46:ILE:HG22 | 4:R:64:THR:HG21 | 1.95 | 0.47 |
| 4:S:105:GLY:HA3 | 4:S:114:LYS:HA | 1.95 | 0.47 |
| 1:D:359:LEU:HD21 | 1:D:485:PHE:CZ | 2.48 | 0.47 |
| 1:K:445:LYS:CE | 1:K:445:LYS:CA | 2.84 | 0.47 |
| 3:P:466:PHE:CD2 | 3:P:466:PHE:N | 2.82 | 0.47 |
| 1:B:347:VAL:HG22 | 1:B:369:VAL:HG13 | 1.95 | 0.47 |
| 1:B:363:THR:HG21 | 1:B:418:TRP:HB2 | 1.96 | 0.47 |
| 1:C:382:TRP:CH2 | 1:C:426:CYS:HB2 | 2.50 | 0.47 |
| 3:P:431:TRP:CD1 | 3:P:431:TRP:H | 2.31 | 0.47 |
| 4:V:75:ARG:HG3 | 4:V:76:VAL:HG13 | 1.97 | 0.47 |
| 1:D:493:GLN:HA | 1:D:494:PRO:HD2 | 1.45 | 0.47 |
| 1:F:524:SER:OG | 1:F:527:GLU:CD | 2.58 | 0.47 |
| 2:J:42:PRO:HG3 | 2:J:102:THR:CG2 | 2.43 | 0.47 |
| 1:K:529:ASN:HA | 1:K:554:LYS:HD3 | 1.97 | 0.47 |
| 1:K:556:THR:HG23 | 1:K:556:THR:O | 2.14 | 0.47 |
| 1:L:424:PHE:CD1 | 1:L:441:ILE:HD11 | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:452:PRO:HB3 | 1:L:479:PHE:CD1 | 2.48 | 0.47 |
| 1:L:480:SER:HB2 | 1:L:481:PRO:HD3 | 1.97 | 0.47 |
| 1:A:466:LEU:N | 1:A:466:LEU:HD13 | 2.29 | 0.47 |
| 1:E:490:GLN:HB3 | 1:E:534:TYR:HA | 1.96 | 0.47 |
| 1:F:545:ASN:CB | 1:G:358:PHE:HZ | 2.27 | 0.47 |
| 1:G:443:ARG:HA | 1:G:444:PRO:HD2 | 1.52 | 0.47 |
| 1:G:473:THR:O | 1:G:473:THR:OG1 | 2.23 | 0.47 |
| 1:H:379:THR:HG21 | 1:H:429:THR:OG1 | 2.15 | 0.47 |
| 1:K:489:MET:HE2 | 1:K:489:MET:HB2 | 1.58 | 0.47 |
| 1:K:526:GLU:HA | 1:K:529:ASN:OD1 | 2.14 | 0.47 |
| 1:L:417:ASP:O | 1:L:420:SER:OG | 2.31 | 0.47 |
| 4:S:39:LEU:HD23 | 4:S:85:ASN:C | 2.39 | 0.47 |
| 1:A:491:ARG:NH1 | 1:A:491:ARG:CG | 2.73 | 0.47 |
| 1:B:451:ARG:NH1 | 1:B:451:ARG:CB | 2.72 | 0.47 |
| 1:C:533:THR:O | 1:C:552:VAL:O | 2.33 | 0.47 |
| 1:G:468:GLU:O | 1:G:525:GLU:HB2 | 2.15 | 0.47 |
| 1:H:516:PHE:CD2 | 1:H:516:PHE:C | 2.93 | 0.47 |
| 1:K:416:ASP:OD1 | 1:K:417:ASP:N | 2.47 | 0.47 |
| 3:P:56:VAL:O | 3:P:56:VAL:HG23 | 2.14 | 0.47 |
| 3:P:445:ASN:HB2 | 3:P:536:GLU:OE2 | 2.14 | 0.47 |
| 3:P:530:GLN:NE2 | 3:P:530:GLN:C | 2.73 | 0.47 |
| 4:S:81:TYR:HB3 | 4:S:84:LYS:HB2 | 1.96 | 0.47 |
| 1:E:489:MET:O | 1:E:535:THR:CB | 2.63 | 0.47 |
| 1:H:552:VAL:HG13 | 1:H:556:THR:HG21 | 1.95 | 0.47 |
| 2:J:21:ILE:HD11 | 1:L:555:SER:CA | 2.44 | 0.47 |
| 3:P:462:VAL:HB | 3:P:509:VAL:C | 2.38 | 0.47 |
| 3:P:526:CYS:CB | 3:P:538:ALA:HB3 | 2.44 | 0.47 |
| 4:S:39:LEU:HD21 | 4:S:41:GLU:HG2 | 1.97 | 0.47 |
| 1:E:350:ILE:HB | 1:E:366:THR:HB | 1.96 | 0.47 |
| 1:E:453:ASP:OD2 | 1:E:455:TYR:OH | 2.27 | 0.47 |
| 1:F:452:PRO:HD3 | 1:F:540:HIS:HD2 | 1.79 | 0.47 |
| 1:H:364:LYS:HB3 | 1:H:410:GLU:HB3 | 1.96 | 0.47 |
| 1:K:558:LYS:O | 1:K:558:LYS:HG2 | 2.15 | 0.47 |
| 3:P:462:VAL:HG11 | 3:P:509:VAL:HG12 | 1.97 | 0.47 |
| 3:P:466:PHE:CD1 | 3:P:470:PHE:HZ | 2.31 | 0.47 |
| 1:G:413:ILE:HD13 | 1:G:424:PHE:HZ | 1.79 | 0.47 |
| 1:H:384:ARG:HD2 | 1:H:388:GLU:HB2 | 1.97 | 0.47 |
| 1:K:537:VAL:CG1 | 1:K:549:GLU:HG2 | 2.44 | 0.47 |
| 3:P:143:LYS:O | 3:P:145:LYS:HG3 | 2.14 | 0.47 |
| 4:S:105:GLY:HA2 | 4:S:115:THR:HG23 | 1.96 | 0.47 |
| 4:V:121:ASN:HD21 | 4:V:123:HIS:HB3 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:514:ARG:HH11 | 1:A:514:ARG:CG | 2.28 | 0.46 |
| 1:B:410:GLU:H | 1:B:410:GLU:HG3 | 1.47 | 0.46 |
| 1:F:546:ARG:HH11 | 1:F:546:ARG:HG3 | 1.79 | 0.46 |
| 1:G:493:GLN:HG2 | 4:U:42:MET:O | 2.15 | 0.46 |
| 1:G:521:LEU:HD21 | 1:G:534:TYR:CE2 | 2.50 | 0.46 |
| 1:H:474:CYS:HB2 | 1:H:488:TRP:CZ2 | 2.50 | 0.46 |
| 1:K:528:TRP:HH2 | 1:K:552:VAL:HG22 | 1.79 | 0.46 |
| 1:L:423:ARG:HH21 | 1:L:444:PRO:HB3 | 1.80 | 0.46 |
| 1:L:445:LYS:H | 1:L:445:LYS:HG3 | 1.48 | 0.46 |
| 3:P:412:GLN:NE2 | 3:P:412:GLN:C | 2.73 | 0.46 |
| 3:P:462:VAL:O | 3:P:509:VAL:N | 2.47 | 0.46 |
| 4:R:116:GLN:NE2 | 4:R:116:GLN:C | 2.73 | 0.46 |
| 1:C:461:ARG:NH1 | 1:C:465:ASN:CG | 2.69 | 0.46 |
| 1:E:423:ARG:HA | 1:E:442:SER:HB3 | 1.96 | 0.46 |
| 1:E:467:ARG:NH1 | 4:U:111:ASP:OD2 | 2.48 | 0.46 |
| 1:K:464:LEU:HD13 | 1:K:464:LEU:HA | 1.60 | 0.46 |
| 3:P:224:PRO:HG3 | 3:P:304:ARG:HH12 | 1.80 | 0.46 |
| 3:P:352:LEU:HD21 | 3:P:401:PRO:HG2 | 1.97 | 0.46 |
| 1:C:526:GLU:CD | 1:C:526:GLU:N | 2.73 | 0.46 |
| 1:E:468:GLU:OE2 | 4:U:45:ARG:NH1 | 2.43 | 0.46 |
| 1:F:449:LEU:HA | 1:F:481:PRO:HD2 | 1.97 | 0.46 |
| 1:L:478:GLY:O | 1:L:515:TYR:N | 2.39 | 0.46 |
| 3:P:38:CYS:HB2 | 3:P:46:CYS:HB3 | 1.52 | 0.46 |
| 4:R:45:ARG:HA | 4:R:64:THR:OG1 | 2.16 | 0.46 |
| 4:S:79:LYS:HD3 | 4:S:80:GLN:N | 2.30 | 0.46 |
| 1:B:450:HIS:C | 1:B:542:ALA:HB1 | 2.39 | 0.46 |
| 1:D:391:LYS:NZ | 1:D:394:THR:OG1 | 2.42 | 0.46 |
| 1:G:363:THR:OG1 | 1:G:413:ILE:HG13 | 2.15 | 0.46 |
| 1:K:414:CYS:SG | 1:K:415:GLU:N | 2.88 | 0.46 |
| 4:S:39:LEU:CD2 | 4:S:85:ASN:CA | 2.94 | 0.46 |
| 1:E:535:THR:HG23 | 1:E:550:ARG:O | 2.15 | 0.46 |
| 1:G:382:TRP:CG | 1:G:411:ALA:HB2 | 2.50 | 0.46 |
| 1:H:532:GLU:O | 1:H:553:ASP:HB2 | 2.14 | 0.46 |
| 3:P:365:TYR:CE1 | 3:P:379:LEU:HD13 | 2.50 | 0.46 |
| 3:P:395:LEU:CB | 3:P:410:LEU:HD12 | 2.41 | 0.46 |
| 4:R:22:GLU:CG | 4:R:119:THR:HG22 | 2.45 | 0.46 |
| 1:A:575:CYS:CB | 2:J:7:LEU:HD23 | 2.46 | 0.46 |
| 1:F:479:PHE:CD1 | 1:F:479:PHE:N | 2.84 | 0.46 |
| 1:F:506:MET:O | 1:F:516:PHE:CE2 | 2.68 | 0.46 |
| 1:G:535:THR:HG22 | 1:G:551:THR:OG1 | 2.15 | 0.46 |
| 1:H:571:THR:O | 1:H:572:ALA:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:484:VAL:HG23 | 1:K:540:HIS:CG | 2.49 | 0.46 |
| 1:L:451:ARG:HH12 | 1:L:544:PRO:HG3 | 1.80 | 0.46 |
| 4:V:36:LYS:HG2 | 4:V:86:LEU:CD1 | 2.46 | 0.46 |
| 4:V:47:TYR:HA | 4:V:63:SER:HA | 1.97 | 0.46 |
| 4:V:86:LEU:HG | 4:V:88:LEU:HD22 | 1.97 | 0.46 |
| 1:A:510:GLN:CD | 1:A:510:GLN:C | 2.84 | 0.46 |
| 1:B:570:ASP:HB2 | 1:C:571:THR:HA | 1.97 | 0.46 |
| 1:D:421:GLY:CA | 1:D:445:LYS:HZ2 | 2.10 | 0.46 |
| 1:F:413:ILE:HG13 | 1:F:414:CYS:H | 1.80 | 0.46 |
| 1:F:496:SER:OG | 1:F:499:LYS:NZ | 2.48 | 0.46 |
| 1:F:502:THR:OG1 | 1:F:519:SER:HB2 | 2.08 | 0.46 |
| 1:H:352:PRO:HD2 | 1:H:418:TRP:CH2 | 2.51 | 0.46 |
| 1:K:574:THR:OG1 | 1:K:575:CYS:N | 2.49 | 0.46 |
| 3:P:344:VAL:HG21 | 3:P:443:GLU:O | 2.16 | 0.46 |
| 1:A:390:VAL:HG13 | 1:A:391:LYS:N | 2.31 | 0.46 |
| 1:D:423:ARG:HD3 | 1:D:440:THR:HG23 | 1.98 | 0.46 |
| 1:G:372:LEU:HD11 | 1:G:433:LEU:HB2 | 1.97 | 0.46 |
| 1:H:554:LYS:CE | 1:H:558:LYS:HZ1 | 2.14 | 0.46 |
| 1:L:457:LEU:HB2 | 1:L:473:THR:OG1 | 2.15 | 0.46 |
| 3:P:351:VAL:CG1 | 3:P:435:VAL:HG11 | 2.46 | 0.46 |
| 3:P:368:LEU:HB2 | 3:P:378:PRO:HG3 | 1.89 | 0.46 |
| 3:P:450:GLY:HA2 | 3:P:462:VAL:HA | 1.97 | 0.46 |
| 4:V:28:GLU:O | 4:V:94:LEU:HB3 | 2.15 | 0.46 |
| 1:D:382:TRP:CZ3 | 1:D:424:PHE:HB3 | 2.51 | 0.46 |
| 1:E:443:ARG:HG3 | 1:E:444:PRO:HD2 | 1.97 | 0.46 |
| 1:E:481:PRO:HD2 | 1:E:540:HIS:CE1 | 2.51 | 0.46 |
| 1:E:509:PRO:HG3 | 1:F:501:VAL:HG12 | 1.97 | 0.46 |
| 1:G:443:ARG:NE | 1:G:443:ARG:C | 2.73 | 0.46 |
| 1:H:554:LYS:NZ | 1:H:558:LYS:HZ3 | 1.90 | 0.46 |
| 1:K:470:ALA:HB3 | 1:K:523:VAL:HG12 | 1.97 | 0.46 |
| 1:K:481:PRO:CG | 1:K:541:GLU:OE2 | 2.63 | 0.46 |
| 1:L:506:MET:HB3 | 1:L:507:PRO:HD2 | 1.97 | 0.46 |
| 3:P:275:PHE:HB3 | 3:P:279:ILE:HD12 | 1.98 | 0.46 |
| 4:R:35:ILE:HB | 4:R:89:VAL:HB | 1.98 | 0.46 |
| 4:S:39:LEU:HG | 4:S:41:GLU:HG2 | 1.98 | 0.46 |
| 4:V:72:TYR:HA | 4:V:75:ARG:HD3 | 1.97 | 0.46 |
| 1:D:363:THR:OG1 | 1:D:413:ILE:O | 2.30 | 0.46 |
| 1:H:486:VAL:HG11 | 1:H:519:SER:OG | 2.16 | 0.46 |
| 1:K:528:TRP:CD1 | 1:K:528:TRP:O | 2.69 | 0.46 |
| 1:L:424:PHE:O | 1:L:441:ILE:HG13 | 2.14 | 0.46 |
| 1:L:543:LEU:HA | 1:L:544:PRO:HD3 | 1.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:237:PHE:O | 3:P:291:SER:HA | 2.16 | 0.46 |
| 4:S:61:VAL:HG13 | 4:S:72:TYR:CG | 2.51 | 0.46 |
| 1:A:478:GLY:C | 1:A:514:ARG:HH12 | 2.17 | 0.45 |
| 1:A:510:GLN:CD | 1:A:510:GLN:N | 2.73 | 0.45 |
| 1:E:400:HIS:CD2 | 1:E:402:ASN:H | 2.34 | 0.45 |
| 1:F:500:TYR:CD1 | 1:F:500:TYR:O | 2.69 | 0.45 |
| 1:L:540:HIS:CE1 | 1:L:542:ALA:HB2 | 2.51 | 0.45 |
| 3:P:271:ARG:HB2 | 3:P:372:ALA:HB3 | 1.97 | 0.45 |
| 4:R:46:ILE:HG22 | 4:R:64:THR:HG22 | 1.99 | 0.45 |
| 1:A:352:PRO:HD3 | 1:A:365:LEU:HD23 | 1.97 | 0.45 |
| 1:C:555:SER:HA | 1:C:558:LYS:HD2 | 1.96 | 0.45 |
| 1:F:415:GLU:O | 1:F:416:ASP:C | 2.59 | 0.45 |
| 1:H:572:ALA:C | 1:H:574:THR:H | 2.23 | 0.45 |
| 1:K:378:VAL:HG23 | 1:K:380:ILE:HG12 | 1.97 | 0.45 |
| 1:K:568:MET:HE3 | 1:K:568:MET:HB2 | 1.62 | 0.45 |
| 1:L:382:TRP:CZ3 | 1:L:426:CYS:HB2 | 2.51 | 0.45 |
| 3:P:368:LEU:CB | 3:P:378:PRO:HG2 | 2.43 | 0.45 |
| 4:S:36:LYS:HD3 | 4:S:86:LEU:HD13 | 1.98 | 0.45 |
| 4:S:102:TYR:N | 4:S:118:VAL:O | 2.34 | 0.45 |
| 1:A:356:SER:N | 2:J:117:TYR:CZ | 2.84 | 0.45 |
| 1:A:400:HIS:HB3 | 1:A:404:THR:H | 1.82 | 0.45 |
| 1:A:476:VAL:O | 1:A:516:PHE:HA | 2.16 | 0.45 |
| 1:A:516:PHE:CD2 | 1:A:516:PHE:O | 2.69 | 0.45 |
| 1:A:565:SER:HB2 | 2:J:59:ARG:HA | 1.99 | 0.45 |
| 1:A:573:GLY:O | 1:A:574:THR:C | 2.59 | 0.45 |
| 1:B:349:ALA:HB1 | 1:B:382:TRP:CZ3 | 2.51 | 0.45 |
| 1:E:501:VAL:HG21 | 1:F:509:PRO:HD3 | 1.99 | 0.45 |
| 1:F:363:THR:HG23 | 1:F:415:GLU:HG2 | 1.97 | 0.45 |
| 1:F:477:THR:HG22 | 1:F:516:PHE:HB2 | 1.98 | 0.45 |
| 1:F:481:PRO:HG2 | 1:F:481:PRO:O | 2.16 | 0.45 |
| 1:H:418:TRP:HE3 | 1:H:443:ARG:HB2 | 1.80 | 0.45 |
| 1:L:372:LEU:HG | 1:L:407:ALA:HB3 | 1.96 | 0.45 |
| 3:P:94:LEU:HB2 | 3:P:101:LEU:HD23 | 1.99 | 0.45 |
| 4:V:48:LEU:HD13 | 4:V:89:VAL:HG11 | 1.97 | 0.45 |
| 1:E:379:THR:HB | 1:E:393:HIS:HB3 | 1.99 | 0.45 |
| 1:K:558:LYS:HZ1 | 1:L:461:ARG:HE | 1.64 | 0.45 |
| 1:L:456:LEU:HD11 | 1:L:488:TRP:CH2 | 2.52 | 0.45 |
| 1:L:493:GLN:NE2 | 1:L:494:PRO:O | 2.49 | 0.45 |
| 1:L:514:ARG:HH11 | 1:L:514:ARG:CA | 2.30 | 0.45 |
| 1:L:514:ARG:NH1 | 1:L:514:ARG:HA | 2.31 | 0.45 |
| 3:P:491:GLN:O | 3:P:507:ARG:NH1 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:500:TYR:CD2 | 1:A:500:TYR:C | 2.94 | 0.45 |
| 1:C:526:GLU:O | 1:C:530:THR:HG21 | 2.15 | 0.45 |
| 1:D:363:THR:OG1 | 1:D:363:THR:O | 2.34 | 0.45 |
| 1:E:489:MET:CE | 1:E:494:PRO:HD3 | 2.44 | 0.45 |
| 1:F:382:TRP:HB2 | 1:F:392:THR:HA | 1.98 | 0.45 |
| 1:F:438:LYS:HE2 | 1:F:438:LYS:HB2 | 1.36 | 0.45 |
| 1:H:454:VAL:CG2 | 1:H:538:VAL:HG21 | 2.47 | 0.45 |
| 4:S:47:TYR:CZ | 4:S:110:THR:HA | 2.51 | 0.45 |
| 4:V:112:ARG:CZ | 4:V:112:ARG:CB | 2.94 | 0.45 |
| 1:A:378:VAL:HG12 | 1:A:393:HIS:NE2 | 2.32 | 0.45 |
| 1:C:566:LEU:HD22 | 1:H:564:VAL:HG21 | 1.99 | 0.45 |
| 1:D:493:GLN:N | 1:D:493:GLN:CD | 2.71 | 0.45 |
| 1:F:420:SER:HB2 | 1:F:421:GLY:H | 1.50 | 0.45 |
| 1:G:365:LEU:HB2 | 1:G:411:ALA:HB3 | 1.98 | 0.45 |
| 1:G:490:GLN:NE2 | 1:G:532:GLU:OE2 | 2.30 | 0.45 |
| 1:H:383:THR:HA | 1:H:390:VAL:HG23 | 1.99 | 0.45 |
| 1:K:516:PHE:CE2 | 1:L:520:ILE:HD11 | 2.46 | 0.45 |
| 3:P:136:PHE:O | 3:P:136:PHE:CD2 | 2.70 | 0.45 |
| 3:P:413:LEU:H | 3:P:413:LEU:CD2 | 2.07 | 0.45 |
| 1:A:485:PHE:CD2 | 1:A:485:PHE:O | 2.70 | 0.45 |
| 1:A:510:GLN:H | 1:A:510:GLN:HE21 | 1.63 | 0.45 |
| 1:B:528:TRP:O | 1:B:528:TRP:CG | 2.69 | 0.45 |
| 1:F:365:LEU:HD23 | 1:F:365:LEU:HA | 1.84 | 0.45 |
| 1:G:481:PRO:HD2 | 1:G:540:HIS:HE1 | 1.81 | 0.45 |
| 1:K:485:PHE:O | 1:K:485:PHE:CD1 | 2.70 | 0.45 |
| 1:L:372:LEU:HB2 | 1:L:405:PHE:O | 2.17 | 0.45 |
| 3:P:272:ALA:HA | 3:P:273:PRO:HD3 | 1.57 | 0.45 |
| 3:P:382:ASP:OD1 | 3:P:386:TRP:N | 2.48 | 0.45 |
| 1:B:345:ILE:HG22 | 1:B:372:LEU:HD13 | 1.98 | 0.45 |
| 1:B:365:LEU:HB3 | 1:B:382:TRP:NE1 | 2.31 | 0.45 |
| 1:D:416:ASP:OD2 | 1:D:417:ASP:N | 2.50 | 0.45 |
| 1:F:449:LEU:CA | 1:F:480:SER:CB | 2.93 | 0.45 |
| 1:F:523:VAL:HG11 | 1:F:534:TYR:OH | 2.16 | 0.45 |
| 1:F:543:LEU:CD2 | 1:F:548:THR:CG2 | 2.94 | 0.45 |
| 1:K:468:GLU:HA | 4:R:67:PHE:CE2 | 2.51 | 0.45 |
| 3:P:290:PHE:CD1 | 3:P:290:PHE:O | 2.69 | 0.45 |
| 1:A:545:ASN:C | 1:A:547:VAL:H | 2.24 | 0.45 |
| 1:C:525:GLU:N | 1:C:525:GLU:CD | 2.72 | 0.45 |
| 1:D:495:LEU:HD22 | 1:D:495:LEU:HA | 1.70 | 0.45 |
| 1:H:560:THR:CB | 1:K:560:THR:O | 2.65 | 0.45 |
| 3:P:448:VAL:HG23 | 3:P:463:PRO:HG3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:35:ILE:O | 4:R:88:LEU:HA | 2.17 | 0.45 |
| 1:A:500:TYR:HA | 1:A:520:ILE:O | 2.17 | 0.45 |
| 1:E:384:ARG:HD3 | 1:E:388:GLU:HB3 | 1.99 | 0.45 |
| 1:E:543:LEU:HD13 | 1:E:548:THR:OG1 | 2.15 | 0.45 |
| 1:F:536:CYS:O | 1:F:549:GLU:HB2 | 2.17 | 0.45 |
| 1:K:485:PHE:O | 1:K:485:PHE:CG | 2.69 | 0.45 |
| 3:P:99:ARG:HA | 3:P:99:ARG:HD3 | 1.58 | 0.45 |
| 3:P:173:ILE:HD13 | 3:P:189:ILE:HB | 1.99 | 0.45 |
| 3:P:243:PRO:O | 3:P:246:ALA:N | 2.50 | 0.45 |
| 3:P:345:ALA:CA | 3:P:413:LEU:CD1 | 2.74 | 0.45 |
| 4:V:36:LYS:HG2 | 4:V:86:LEU:HD11 | 1.98 | 0.45 |
| 1:B:404:THR:O | 1:B:405:PHE:C | 2.59 | 0.44 |
| 1:B:500:TYR:HA | 1:B:520:ILE:O | 2.17 | 0.44 |
| 1:C:384:ARG:HG3 | 1:C:385:GLN:N | 2.32 | 0.44 |
| 1:C:568:MET:CE | 1:K:564:VAL:HG21 | 2.47 | 0.44 |
| 1:G:372:LEU:HD21 | 1:G:433:LEU:HD12 | 1.97 | 0.44 |
| 1:G:480:SER:OG | 1:G:481:PRO:HD3 | 2.16 | 0.44 |
| 3:P:127:GLY:HA2 | 3:P:191:GLN:HA | 1.99 | 0.44 |
| 3:P:149:LYS:HG2 | 3:P:200:TYR:CE1 | 2.52 | 0.44 |
| 3:P:526:CYS:HB3 | 3:P:538:ALA:CB | 2.45 | 0.44 |
| 1:B:451:ARG:HB2 | 1:B:451:ARG:CZ | 2.45 | 0.44 |
| 1:B:528:TRP:O | 1:B:528:TRP:CD2 | 2.70 | 0.44 |
| 1:C:509:PRO:HG2 | 1:D:522:THR:HG21 | 1.98 | 0.44 |
| 1:F:471:THR:CG2 | 1:F:522:THR:HG23 | 2.47 | 0.44 |
| 1:G:363:THR:OG1 | 1:G:414:CYS:O | 2.29 | 0.44 |
| 2:J:117:TYR:CG | 2:J:117:TYR:O | 2.69 | 0.44 |
| 3:P:149:LYS:HD2 | 3:P:151:ILE:HG21 | 1.99 | 0.44 |
| 3:P:310:HIS:O | 3:P:310:HIS:CG | 2.70 | 0.44 |
| 4:U:47:TYR:CE2 | 4:U:110:THR:HG23 | 2.53 | 0.44 |
| 1:A:514:ARG:CD | 1:A:514:ARG:N | 2.78 | 0.44 |
| 1:B:461:ARG:NE | 1:L:570:ASP:OD2 | 2.51 | 0.44 |
| 1:D:423:ARG:HH11 | 1:D:425:THR:HB | 1.83 | 0.44 |
| 1:E:540:HIS:CD2 | 1:E:542:ALA:H | 2.34 | 0.44 |
| 1:G:500:TYR:CD1 | 1:G:500:TYR:C | 2.95 | 0.44 |
| 1:K:476:VAL:HG12 | 1:K:479:PHE:CD1 | 2.53 | 0.44 |
| 3:P:439:ILE:CD1 | 3:P:439:ILE:H | 2.22 | 0.44 |
| 3:P:480:TRP:C | 3:P:480:TRP:CD2 | 2.93 | 0.44 |
| 4:V:104:CYS:HB2 | 4:V:116:GLN:HB3 | 1.98 | 0.44 |
| 1:A:372:LEU:HD21 | 1:A:405:PHE:HD2 | 1.83 | 0.44 |
| 1:A:386:ASN:OD1 | 1:A:388:GLU:HG2 | 2.17 | 0.44 |
| 1:D:452:PRO:HG3 | 1:D:479:PHE:HB3 | 1.97 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:417:ASP:HB3 | 1:E:424:PHE:CZ | 2.52 | 0.44 |
| 1:F:456:LEU:HD13 | 1:F:550:ARG:HB2 | 1.99 | 0.44 |
| 1:H:367:CYS:HB2 | 1:H:380:ILE:HG13 | 1.99 | 0.44 |
| 1:K:345:ILE:HG22 | 1:K:372:LEU:HD21 | 1.98 | 0.44 |
| 1:K:428:VAL:HG12 | 1:K:430:HIS:HB2 | 2.00 | 0.44 |
| 1:L:511:ALA:O | 1:L:514:ARG:HG3 | 2.16 | 0.44 |
| 3:P:31:ARG:HD2 | 3:P:70:PRO:HB3 | 1.98 | 0.44 |
| 3:P:287:ASP:HB2 | 3:P:288:GLY:H | 1.47 | 0.44 |
| 3:P:368:LEU:CB | 3:P:378:PRO:HD2 | 2.43 | 0.44 |
| 3:P:411:ASN:HD22 | 3:P:537:THR:HG21 | 1.83 | 0.44 |
| 3:P:414:THR:OG1 | 3:P:417:ASP:CG | 2.56 | 0.44 |
| 3:P:418:ALA:N | 3:P:439:ILE:HD11 | 2.31 | 0.44 |
| 4:S:99:SER:HB2 | 4:S:120:LEU:HB3 | 1.98 | 0.44 |
| 4:U:22:GLU:HB2 | 4:U:119:THR:CA | 2.47 | 0.44 |
| 1:C:454:VAL:CG1 | 1:C:474:CYS:SG | 3.05 | 0.44 |
| 1:C:459:PRO:HG3 | 1:C:470:ALA:HB1 | 2.00 | 0.44 |
| 1:D:350:ILE:HB | 1:D:366:THR:OG1 | 2.17 | 0.44 |
| 1:E:391:LYS:HG3 | 1:E:412:SER:H | 1.82 | 0.44 |
| 1:G:347:VAL:HG22 | 1:G:369:VAL:HG13 | 1.99 | 0.44 |
| 1:H:575:CYS:HB2 | 1:K:575:CYS:HB3 | 1.61 | 0.44 |
| 3:P:471:SER:HA | 3:P:475:LYS:NZ | 2.22 | 0.44 |
| 1:B:421:GLY:H | 1:B:443:ARG:NH2 | 2.11 | 0.44 |
| 1:C:371:ASP:N | 1:C:404:THR:HG23 | 2.29 | 0.44 |
| 1:C:447:VAL:HG11 | 1:C:481:PRO:HB3 | 1.99 | 0.44 |
| 1:F:491:ARG:HE | 1:F:491:ARG:HB2 | 1.58 | 0.44 |
| 1:K:493:GLN:HG3 | 4:S:44:VAL:HG22 | 2.00 | 0.44 |
| 3:P:526:CYS:C | 3:P:538:ALA:HB3 | 2.42 | 0.44 |
| 1:B:393:HIS:CG | 1:B:409:GLY:HA3 | 2.53 | 0.44 |
| 1:F:501:VAL:O | 1:F:501:VAL:HG22 | 2.17 | 0.44 |
| 4:S:28:GLU:O | 4:S:94:LEU:HG | 2.18 | 0.44 |
| 4:V:112:ARG:NH1 | 4:V:112:ARG:HB2 | 2.33 | 0.44 |
| 1:C:346:ARG:HH21 | 1:C:348:PHE:HB2 | 1.82 | 0.44 |
| 1:D:447:VAL:O | 1:D:447:VAL:HG22 | 2.18 | 0.44 |
| 1:E:511:ALA:HB1 | 1:E:514:ARG:CG | 2.39 | 0.44 |
| 1:E:541:GLU:C | 1:E:543:LEU:H | 2.25 | 0.44 |
| 1:F:365:LEU:HG | 1:F:413:ILE:HG21 | 2.00 | 0.44 |
| 1:H:562:TYR:H | 1:H:562:TYR:HD2 | 1.64 | 0.44 |
| 1:K:462:GLU:HB3 | 1:L:455:TYR:HE1 | 1.83 | 0.44 |
| 4:V:41:GLU:OE1 | 4:V:82:PRO:HB3 | 2.18 | 0.44 |
| 1:A:390:VAL:O | 1:A:391:LYS:HD2 | 2.18 | 0.44 |
| 1:B:426:CYS:O | 1:B:438:LYS:HA | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:545:ASN:ND2 | 1:B:545:ASN:C | 2.75 | 0.44 |
| 1:F:385:GLN:HG2 | 1:F:422:GLU:HB2 | 1.99 | 0.44 |
| 1:B:352:PRO:HG2 | 1:B:418:TRP:CZ2 | 2.53 | 0.43 |
| 1:D:345:ILE:HB | 1:D:372:LEU:HD13 | 2.00 | 0.43 |
| 1:E:530:THR:HG1 | 1:E:531:GLY:H | 1.66 | 0.43 |
| 1:H:558:LYS:HA | 1:H:559:PRO:HD3 | 1.79 | 0.43 |
| 1:K:385:GLN:HE21 | 1:K:423:ARG:H | 1.66 | 0.43 |
| 3:P:47:ILE:HG13 | 3:P:47:ILE:O | 2.17 | 0.43 |
| 4:R:36:LYS:O | 4:R:116:GLN:HG3 | 2.18 | 0.43 |
| 4:R:46:ILE:N | 4:R:64:THR:CG2 | 2.57 | 0.43 |
| 4:S:96:GLU:CD | 4:S:96:GLU:C | 2.86 | 0.43 |
| 1:A:418:TRP:CD1 | 1:A:443:ARG:HE | 2.36 | 0.43 |
| 1:B:478:GLY:O | 1:B:514:ARG:HG2 | 2.14 | 0.43 |
| 1:B:481:PRO:CD | 1:B:540:HIS:NE2 | 2.72 | 0.43 |
| 1:E:382:TRP:CD2 | 1:E:411:ALA:HB2 | 2.53 | 0.43 |
| 1:F:364:LYS:HB3 | 1:F:364:LYS:HE3 | 1.80 | 0.43 |
| 3:P:151:ILE:HD12 | 3:P:152:GLY:N | 2.32 | 0.43 |
| 4:S:19:ILE:HG22 | 4:S:21:PRO:HD3 | 2.00 | 0.43 |
| 4:S:37:CYS:HA | 4:S:116:GLN:CD | 2.32 | 0.43 |
| 4:V:49:CYS:HB3 | 4:V:103:ALA:HB3 | 2.00 | 0.43 |
| 1:A:514:ARG:NH1 | 1:A:514:ARG:CG | 2.77 | 0.43 |
| 1:B:396:ILE:H | 1:B:396:ILE:HG13 | 1.38 | 0.43 |
| 1:F:424:PHE:O | 1:F:440:THR:HA | 2.18 | 0.43 |
| 1:G:450:HIS:ND1 | 1:G:450:HIS:N | 2.66 | 0.43 |
| 1:K:374:THR:HA | 1:K:405:PHE:HB2 | 1.99 | 0.43 |
| 1:K:380:ILE:CG2 | 1:K:409:GLY:HA2 | 2.49 | 0.43 |
| 1:G:516:PHE:CZ | 1:H:520:ILE:HD12 | 2.54 | 0.43 |
| 3:P:149:LYS:H | 3:P:155:PRO:HB3 | 1.84 | 0.43 |
| 4:R:50:ARG:HG2 | 4:R:50:ARG:HH11 | 1.82 | 0.43 |
| 1:A:352:PRO:HD2 | 1:A:418:TRP:CH2 | 2.53 | 0.43 |
| 1:A:499:LYS:HB3 | 1:A:521:LEU:HD12 | 2.01 | 0.43 |
| 1:C:466:LEU:HD13 | 1:C:468:GLU:CD | 2.43 | 0.43 |
| 1:C:508:GLU:CB | 1:C:509:PRO:CD | 2.90 | 0.43 |
| 1:E:354:PHE:HD1 | 1:E:357:ILE:HD11 | 1.84 | 0.43 |
| 1:F:390:VAL:HB | 1:F:391:LYS:H | 1.72 | 0.43 |
| 1:F:402:ASN:HD22 | 1:F:402:ASN:HA | 1.49 | 0.43 |
| 1:F:450:HIS:HE2 | 1:F:514:ARG:NH1 | 1.99 | 0.43 |
| 1:H:457:LEU:HB2 | 1:H:473:THR:OG1 | 2.19 | 0.43 |
| 1:K:490:GLN:OE1 | 1:K:491:ARG:N | 2.51 | 0.43 |
| 1:L:569:SER:HB3 | 1:L:572:ALA:HB2 | 1.99 | 0.43 |
| 3:P:345:ALA:O | 3:P:413:LEU:CD1 | 2.46 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:456:LEU:HD12 | 1:A:550:ARG:O | 2.15 | 0.43 |
| 1:B:443:ARG:CG | 1:B:443:ARG:NH1 | 2.73 | 0.43 |
| 1:E:534:TYR:CD2 | 1:E:534:TYR:N | 2.85 | 0.43 |
| 1:L:430:HIS:CE1 | 1:L:432:ASP:CB | 3.01 | 0.43 |
| 3:P:477:TRP:CD1 | 3:P:526:CYS:HB2 | 2.52 | 0.43 |
| 1:A:374:THR:HG22 | 1:A:405:PHE:HB2 | 2.01 | 0.43 |
| 1:A:467:ARG:HE | 1:A:467:ARG:HB2 | 1.38 | 0.43 |
| 1:B:400:HIS:CE1 | 1:B:404:THR:HG22 | 2.53 | 0.43 |
| 1:D:451:ARG:HH12 | 1:D:544:PRO:HD3 | 1.83 | 0.43 |
| 6:H:601:NAG:C6 | 6:K:601:NAG:H61 | 2.37 | 0.43 |
| 2:J:32:ILE:HG23 | 1:L:560:THR:HB | 2.00 | 0.43 |
| 2:J:46:ARG:HD2 | 2:J:54:SER:O | 2.19 | 0.43 |
| 1:K:405:PHE:CE2 | 1:K:407:ALA:HB2 | 2.53 | 0.43 |
| 1:L:450:HIS:CA | 1:L:480:SER:HB2 | 2.40 | 0.43 |
| 3:P:253:CYS:SG | 3:P:315:LEU:CB | 2.99 | 0.43 |
| 1:B:384:ARG:HG2 | 1:B:386:ASN:H | 1.83 | 0.43 |
| 1:B:454:VAL:HG22 | 1:B:454:VAL:O | 2.18 | 0.43 |
| 1:B:496:SER:CB | 1:B:497:PRO:HD2 | 2.42 | 0.43 |
| 1:B:541:GLU:C | 1:B:543:LEU:H | 2.27 | 0.43 |
| 1:B:549:GLU:O | 1:B:550:ARG:NH1 | 2.42 | 0.43 |
| 1:D:380:ILE:HD12 | 1:D:393:HIS:CG | 2.54 | 0.43 |
| 1:D:384:ARG:HD3 | 1:D:390:VAL:HG22 | 2.01 | 0.43 |
| 1:F:447:VAL:HG21 | 1:F:481:PRO:HB3 | 2.01 | 0.43 |
| 1:G:353:SER:O | 1:G:357:ILE:HG12 | 2.18 | 0.43 |
| 2:J:29:ASN:HD21 | 1:L:464:LEU:C | 2.26 | 0.43 |
| 3:P:148:TYR:HB3 | 3:P:155:PRO:HB3 | 2.01 | 0.43 |
| 3:P:150:GLN:OE1 | 3:P:201:LEU:HD23 | 2.18 | 0.43 |
| 3:P:466:PHE:CE2 | 3:P:475:LYS:HB3 | 2.53 | 0.43 |
| 1:B:418:TRP:HE3 | 1:B:419:ASN:HB2 | 1.83 | 0.43 |
| 1:B:552:VAL:HG23 | 1:B:556:THR:HG21 | 2.00 | 0.43 |
| 1:C:450:HIS:ND1 | 1:C:450:HIS:N | 2.67 | 0.43 |
| 1:D:485:PHE:HB3 | 1:D:539:ALA:HB3 | 2.00 | 0.43 |
| 1:F:382:TRP:HZ3 | 1:F:424:PHE:O | 2.02 | 0.43 |
| 1:F:535:THR:CG2 | 1:F:551:THR:HG21 | 2.30 | 0.43 |
| 1:H:520:ILE:HG21 | 1:H:520:ILE:HD13 | 1.59 | 0.43 |
| 3:P:128:ARG:HD3 | 3:P:128:ARG:HA | 1.77 | 0.43 |
| 3:P:410:LEU:HD12 | 3:P:410:LEU:HA | 1.88 | 0.43 |
| 3:P:480:TRP:O | 3:P:480:TRP:CE3 | 2.72 | 0.43 |
| 1:A:526:GLU:O | 1:A:530:THR:N | 2.52 | 0.43 |
| 1:B:456:LEU:C | 1:B:456:LEU:HD12 | 2.43 | 0.43 |
| 1:C:451:ARG:O | 1:C:451:ARG:HG3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:400:HIS:CG | 1:E:401:PRO:HD2 | 2.54 | 0.43 |
| 1:F:529:ASN:OD1 | 1:F:530:THR:N | 2.52 | 0.43 |
| 1:G:347:VAL:HG22 | 1:G:369:VAL:HA | 2.00 | 0.43 |
| 1:G:443:ARG:C | 1:G:443:ARG:HE | 2.18 | 0.43 |
| 1:K:455:TYR:CZ | 1:L:463:GLN:HB3 | 2.54 | 0.43 |
| 3:P:298:ARG:NH2 | 3:P:300:GLU:OE2 | 2.52 | 0.43 |
| 4:R:52:MET:CE | 4:R:69:LYS:NZ | 2.81 | 0.43 |
| 1:A:571:THR:HG21 | 1:B:568:MET:HE3 | 2.00 | 0.42 |
| 1:B:530:THR:O | 1:B:530:THR:CG2 | 2.67 | 0.42 |
| 1:E:526:GLU:HG2 | 1:E:527:GLU:OE1 | 2.19 | 0.42 |
| 1:F:355:ALA:HA | 1:F:485:PHE:HB2 | 2.00 | 0.42 |
| 1:K:450:HIS:CE1 | 1:K:514:ARG:NH1 | 2.87 | 0.42 |
| 1:L:550:ARG:HD3 | 1:L:550:ARG:HA | 1.61 | 0.42 |
| 3:P:290:PHE:H | 3:P:290:PHE:HD1 | 1.66 | 0.42 |
| 4:R:46:ILE:CG2 | 4:R:64:THR:CG2 | 2.96 | 0.42 |
| 1:A:496:SER:O | 1:A:496:SER:OG | 2.28 | 0.42 |
| 1:C:466:LEU:CD2 | 4:V:45:ARG:NH2 | 2.82 | 0.42 |
| 1:E:395:ASN:HB3 | 1:E:408:VAL:HB | 2.00 | 0.42 |
| 1:F:376:ASP:O | 1:F:377:SER:C | 2.62 | 0.42 |
| 1:F:543:LEU:HD21 | 1:F:548:THR:HG21 | 1.99 | 0.42 |
| 1:H:448:ALA:HB3 | 1:H:480:SER:OG | 2.19 | 0.42 |
| 1:H:529:ASN:C | 1:H:531:GLY:N | 2.73 | 0.42 |
| 2:J:21:ILE:HG13 | 1:L:555:SER:CB | 2.48 | 0.42 |
| 1:K:429:THR:HA | 1:K:436:PRO:HB3 | 2.01 | 0.42 |
| 1:K:475:LEU:O | 1:K:475:LEU:HG | 2.19 | 0.42 |
| 1:K:554:LYS:HB3 | 1:K:554:LYS:HE3 | 1.81 | 0.42 |
| 4:S:39:LEU:HD22 | 4:S:85:ASN:C | 2.40 | 0.42 |
| 4:U:28:GLU:HG3 | 4:U:30:GLY:H | 1.84 | 0.42 |
| 1:B:452:PRO:HG2 | 1:B:452:PRO:O | 2.19 | 0.42 |
| 1:B:478:GLY:HA2 | 1:B:514:ARG:HG2 | 2.00 | 0.42 |
| 1:E:457:LEU:HB2 | 1:E:473:THR:HG23 | 2.02 | 0.42 |
| 3:P:334:ILE:HG23 | 3:P:431:TRP:CE3 | 2.54 | 0.42 |
| 1:B:414:CYS:SG | 1:B:415:GLU:N | 2.92 | 0.42 |
| 1:C:347:VAL:HG22 | 1:C:369:VAL:HG23 | 2.01 | 0.42 |
| 1:E:474:CYS:HB2 | 1:E:488:TRP:CZ2 | 2.54 | 0.42 |
| 1:E:543:LEU:HD23 | 1:E:543:LEU:HA | 1.61 | 0.42 |
| 1:F:449:LEU:H | 1:F:449:LEU:CD2 | 2.30 | 0.42 |
| 1:H:445:LYS:HE2 | 1:H:445:LYS:HB3 | 1.56 | 0.42 |
| 1:H:481:PRO:HD2 | 1:H:540:HIS:CE1 | 2.55 | 0.42 |
| 4:R:48:LEU:HD22 | 4:R:89:VAL:HG21 | 2.01 | 0.42 |
| 1:A:520:ILE:HD12 | 1:B:516:PHE:CE2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:418:TRP:HB3 | 1:B:419:ASN:H | 1.48 | 0.42 |
| 1:B:540:HIS:O | 1:B:543:LEU:HB2 | 2.19 | 0.42 |
| 1:C:459:PRO:HD2 | 1:C:528:TRP:CZ2 | 2.54 | 0.42 |
| 1:D:508:GLU:HB3 | 1:D:514:ARG:O | 2.19 | 0.42 |
| 1:G:413:ILE:HD13 | 1:G:424:PHE:CZ | 2.54 | 0.42 |
| 1:G:561:LEU:HA | 1:G:561:LEU:HD23 | 1.76 | 0.42 |
| 2:J:107:LYS:HB3 | 2:J:107:LYS:HE3 | 1.54 | 0.42 |
| 1:K:479:PHE:CD2 | 1:K:482:ALA:HA | 2.55 | 0.42 |
| 1:L:476:VAL:O | 1:L:516:PHE:HA | 2.20 | 0.42 |
| 3:P:357:ARG:HG2 | 3:P:404:GLY:HA3 | 2.01 | 0.42 |
| 3:P:447:LYS:HD3 | 3:P:447:LYS:HA | 1.37 | 0.42 |
| 4:S:19:ILE:HG22 | 4:S:21:PRO:CD | 2.49 | 0.42 |
| 4:S:39:LEU:HD23 | 4:S:85:ASN:CA | 2.49 | 0.42 |
| 1:A:375:TYR:HD2 | 1:A:430:HIS:CE1 | 2.38 | 0.42 |
| 1:A:375:TYR:HB2 | 1:A:430:HIS:NE2 | 2.35 | 0.42 |
| 1:A:511:ALA:HA | 1:A:512:PRO:HD2 | 1.59 | 0.42 |
| 1:A:532:GLU:O | 1:A:553:ASP:CB | 2.67 | 0.42 |
| 1:B:466:LEU:O | 3:P:34:ARG:NH1 | 2.51 | 0.42 |
| 1:C:400:HIS:CG | 1:C:401:PRO:HD2 | 2.54 | 0.42 |
| 1:D:423:ARG:HA | 1:D:442:SER:HB2 | 2.02 | 0.42 |
| 1:D:429:THR:OG1 | 1:D:433:LEU:O | 2.38 | 0.42 |
| 1:F:449:LEU:N | 1:F:481:PRO:HD3 | 2.34 | 0.42 |
| 1:F:506:MET:O | 1:F:516:PHE:CD2 | 2.73 | 0.42 |
| 1:H:415:GLU:O | 1:H:418:TRP:HB2 | 2.20 | 0.42 |
| 1:H:558:LYS:HB2 | 1:K:559:PRO:HG2 | 2.00 | 0.42 |
| 1:K:518:HIS:CE1 | 1:L:518:HIS:CG | 3.08 | 0.42 |
| 3:P:345:ALA:C | 3:P:413:LEU:CB | 2.71 | 0.42 |
| 3:P:377:CYS:O | 3:P:377:CYS:SG | 2.78 | 0.42 |
| 3:P:395:LEU:CD1 | 3:P:410:LEU:HD12 | 2.35 | 0.42 |
| 1:D:513:GLY:C | 1:D:514:ARG:HD3 | 2.45 | 0.42 |
| 1:E:493:GLN:NE2 | 4:V:42:MET:HE3 | 2.35 | 0.42 |
| 1:E:527:GLU:C | 1:E:530:THR:HG1 | 2.21 | 0.42 |
| 1:K:464:LEU:CD1 | 1:K:525:GLU:CG | 2.97 | 0.42 |
| 1:L:474:CYS:HB2 | 1:L:488:TRP:CZ2 | 2.55 | 0.42 |
| 3:P:264:VAL:HG22 | 3:P:275:PHE:CE2 | 2.49 | 0.42 |
| 3:P:471:SER:HB2 | 3:P:475:LYS:HZ3 | 1.83 | 0.42 |
| 4:R:111:ASP:O | 4:R:114:LYS:HE2 | 2.15 | 0.42 |
| 4:U:61:VAL:HG12 | 4:U:69:LYS:HD2 | 2.02 | 0.42 |
| 1:B:479:PHE:CD1 | 1:B:479:PHE:N | 2.86 | 0.42 |
| 1:B:543:LEU:HA | 1:B:543:LEU:HD23 | 1.40 | 0.42 |
| 1:E:370:THR:HG22 | 1:E:371:ASP:N | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:384:ARG:HE | 1:H:390:VAL:CG2 | 2.31 | 0.42 |
| 1:H:566:LEU:O | 1:H:567:VAL:C | 2.63 | 0.42 |
| 1:K:405:PHE:HE2 | 1:K:407:ALA:HB2 | 1.85 | 0.42 |
| 1:K:476:VAL:O | 1:K:479:PHE:HE1 | 2.02 | 0.42 |
| 1:L:400:HIS:HE1 | 1:L:405:PHE:HA | 1.82 | 0.42 |
| 1:L:445:LYS:HB2 | 1:L:445:LYS:HE2 | 1.70 | 0.42 |
| 3:P:317:GLU:CD | 3:P:317:GLU:H | 2.25 | 0.42 |
| 3:P:526:CYS:CA | 3:P:538:ALA:HB3 | 2.50 | 0.42 |
| 4:U:37:CYS:CB | 4:U:87:PHE:O | 2.68 | 0.42 |
| 4:V:52:MET:HE3 | 4:V:54:GLY:H | 1.84 | 0.42 |
| 1:B:376:ASP:HB2 | 1:B:377:SER:H | 1.61 | 0.42 |
| 1:B:568:MET:HB3 | 1:C:568:MET:HG2 | 2.02 | 0.42 |
| 1:C:466:LEU:HD23 | 4:V:45:ARG:NH2 | 2.34 | 0.42 |
| 1:E:515:TYR:CD1 | 1:E:515:TYR:N | 2.83 | 0.42 |
| 1:F:461:ARG:HD3 | 1:F:461:ARG:HA | 1.79 | 0.42 |
| 1:K:400:HIS:HB3 | 1:K:404:THR:O | 2.20 | 0.42 |
| 4:V:86:LEU:HD12 | 4:V:87:PHE:N | 2.35 | 0.42 |
| 1:A:484:VAL:O | 1:A:484:VAL:HG13 | 2.16 | 0.42 |
| 1:A:486:VAL:HG22 | 1:A:538:VAL:HG12 | 2.02 | 0.42 |
| 1:A:496:SER:HA | 1:A:497:PRO:HD3 | 1.75 | 0.42 |
| 1:A:543:LEU:HD23 | 1:A:544:PRO:HD2 | 2.02 | 0.42 |
| 1:B:500:TYR:CD1 | 1:B:500:TYR:N | 2.86 | 0.42 |
| 1:F:523:VAL:HB | 1:F:524:SER:H | 1.41 | 0.42 |
| 1:H:423:ARG:HH11 | 1:H:425:THR:HB | 1.85 | 0.42 |
| 1:L:372:LEU:HD23 | 1:L:407:ALA:H | 1.85 | 0.42 |
| 1:B:445:LYS:CA | 1:B:445:LYS:NZ | 2.82 | 0.41 |
| 1:C:454:VAL:CG2 | 1:C:538:VAL:CG2 | 2.98 | 0.41 |
| 1:D:489:MET:HB2 | 1:D:489:MET:HE2 | 1.83 | 0.41 |
| 1:F:536:CYS:O | 1:F:549:GLU:HA | 2.20 | 0.41 |
| 1:H:427:THR:OG1 | 1:H:436:PRO:HB3 | 2.20 | 0.41 |
| 1:K:369:VAL:O | 1:K:406:SER:HA | 2.21 | 0.41 |
| 3:P:148:TYR:CE2 | 3:P:203:GLN:HG2 | 2.55 | 0.41 |
| 4:S:49:CYS:HB2 | 4:S:103:ALA:HB3 | 2.01 | 0.41 |
| 4:U:104:CYS:O | 4:U:115:THR:N | 2.33 | 0.41 |
| 1:A:382:TRP:CD1 | 1:A:411:ALA:HB2 | 2.54 | 0.41 |
| 1:G:365:LEU:HG | 1:G:424:PHE:CD2 | 2.55 | 0.41 |
| 1:H:568:MET:HB3 | 1:H:568:MET:HE3 | 1.50 | 0.41 |
| 4:U:81:TYR:OH | 4:U:88:LEU:HD12 | 2.20 | 0.41 |
| 4:V:75:ARG:O | 4:V:92:THR:N | 2.53 | 0.41 |
| 1:A:379:THR:H | 1:A:429:THR:HB | 1.84 | 0.41 |
| 1:A:495:LEU:CD1 | 1:A:521:LEU:HD11 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:384:ARG:HG3 | 1:B:424:PHE:CZ | 2.55 | 0.41 |
| 1:B:525:GLU:O | 1:B:525:GLU:CG | 2.68 | 0.41 |
| 1:C:423:ARG:HE | 1:C:442:SER:CB | 2.33 | 0.41 |
| 1:C:462:GLU:O | 1:C:465:ASN:HB2 | 2.20 | 0.41 |
| 1:C:467:ARG:N | 1:C:467:ARG:CD | 2.72 | 0.41 |
| 1:G:489:MET:SD | 1:G:537:VAL:HG21 | 2.60 | 0.41 |
| 4:V:33:VAL:HG22 | 4:V:91:VAL:HB | 2.01 | 0.41 |
| 1:B:483:ASP:O | 1:B:540:HIS:HD2 | 2.03 | 0.41 |
| 1:D:533:THR:HA | 1:D:552:VAL:O | 2.21 | 0.41 |
| 1:E:370:THR:HG22 | 1:E:371:ASP:H | 1.86 | 0.41 |
| 1:E:467:ARG:O | 4:U:60:THR:HB | 2.20 | 0.41 |
| 1:E:481:PRO:HD2 | 1:E:540:HIS:NE2 | 2.35 | 0.41 |
| 1:E:532:GLU:HB3 | 1:E:534:TYR:CE2 | 2.56 | 0.41 |
| 1:G:439:GLN:HG3 | 1:G:441:ILE:HG23 | 2.01 | 0.41 |
| 2:J:104:ASP:HB3 | 2:J:107:LYS:HB2 | 2.03 | 0.41 |
| 1:L:354:PHE:CG | 1:L:541:GLU:HB3 | 2.55 | 0.41 |
| 1:L:400:HIS:CD2 | 1:L:402:ASN:HB2 | 2.55 | 0.41 |
| 1:L:528:TRP:CH2 | 1:L:554:LYS:HA | 2.55 | 0.41 |
| 1:L:556:THR:O | 1:L:556:THR:CG2 | 2.69 | 0.41 |
| 3:P:25:PRO:HB3 | 3:P:329:ASN:HD21 | 1.86 | 0.41 |
| 3:P:479:LYS:CE | 3:P:524:TYR:HE1 | 2.34 | 0.41 |
| 4:S:39:LEU:CD2 | 4:S:41:GLU:HG2 | 2.51 | 0.41 |
| 1:C:466:LEU:CD2 | 1:C:466:LEU:O | 2.69 | 0.41 |
| 1:E:421:GLY:N | 1:E:445:LYS:HE2 | 2.35 | 0.41 |
| 1:F:449:LEU:CA | 1:F:481:PRO:HD3 | 2.44 | 0.41 |
| 1:F:546:ARG:NH1 | 1:F:546:ARG:HG2 | 2.35 | 0.41 |
| 1:G:432:ASP:OD1 | 1:G:433:LEU:N | 2.53 | 0.41 |
| 1:K:558:LYS:HA | 1:K:559:PRO:HD3 | 1.87 | 0.41 |
| 1:L:348:PHE:HB3 | 1:L:368:LEU:HB2 | 2.02 | 0.41 |
| 1:L:393:HIS:ND1 | 1:L:396:ILE:HD13 | 2.36 | 0.41 |
| 3:P:315:LEU:CG | 3:P:315:LEU:O | 2.69 | 0.41 |
| 3:P:388:LYS:HD2 | 3:P:388:LYS:HA | 1.61 | 0.41 |
| 3:P:446:LEU:C | 3:P:446:LEU:CD1 | 2.93 | 0.41 |
| 4:R:48:LEU:HD22 | 4:R:89:VAL:HG11 | 2.02 | 0.41 |
| 1:A:490:GLN:HB2 | 1:A:534:TYR:HE1 | 1.85 | 0.41 |
| 1:C:397:SER:H | 1:C:408:VAL:HG22 | 1.85 | 0.41 |
| 1:C:509:PRO:HG2 | 1:D:522:THR:CG2 | 2.50 | 0.41 |
| 1:D:514:ARG:N | 1:D:514:ARG:CD | 2.77 | 0.41 |
| 1:F:348:PHE:N | 1:F:369:VAL:HG13 | 2.29 | 0.41 |
| 1:F:484:VAL:O | 1:F:484:VAL:HG13 | 2.18 | 0.41 |
| 1:H:352:PRO:HD2 | 1:H:418:TRP:HH2 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:450:HIS:HB3 | 1:K:514:ARG:NH2 | 2.36 | 0.41 |
| 1:L:488:TRP:CE2 | 1:L:536:CYS:HB2 | 2.55 | 0.41 |
| 1:L:532:GLU:O | 1:L:534:TYR:CE2 | 2.74 | 0.41 |
| 3:P:131:THR:HG22 | 3:P:188:VAL:N | 2.36 | 0.41 |
| 3:P:295:THR:CG2 | 3:P:432:ARG:HB2 | 2.49 | 0.41 |
| 3:P:340:VAL:HG11 | 3:P:436:GLU:OE1 | 2.20 | 0.41 |
| 4:U:109:ASN:HD22 | 4:U:112:ARG:NH2 | 2.19 | 0.41 |
| 1:A:525:GLU:O | 1:A:529:ASN:N | 2.54 | 0.41 |
| 1:B:495:LEU:HA | 1:B:495:LEU:HD23 | 1.60 | 0.41 |
| 1:D:449:LEU:H | 1:D:449:LEU:HG | 1.44 | 0.41 |
| 1:D:539:ALA:HA | 1:D:546:ARG:O | 2.20 | 0.41 |
| 1:E:450:HIS:HB3 | 1:E:514:ARG:HH21 | 1.85 | 0.41 |
| 1:F:368:LEU:HD12 | 1:F:408:VAL:HA | 2.03 | 0.41 |
| 1:F:545:ASN:ND2 | 1:F:545:ASN:H | 2.19 | 0.41 |
| 1:H:489:MET:SD | 1:H:537:VAL:HG11 | 2.61 | 0.41 |
| 1:K:509:PRO:O | 1:L:498:GLU:OE2 | 2.39 | 0.41 |
| 1:L:362:SER:OG | 1:L:363:THR:N | 2.53 | 0.41 |
| 1:L:485:PHE:CE2 | 1:L:487:GLN:HB2 | 2.56 | 0.41 |
| 3:P:148:TYR:HB3 | 3:P:155:PRO:CG | 2.51 | 0.41 |
| 3:P:245:VAL:CG2 | 3:P:309:ALA:HB3 | 2.51 | 0.41 |
| 3:P:466:PHE:CD2 | 3:P:507:ARG:HG2 | 2.55 | 0.41 |
| 1:A:548:THR:OG1 | 1:A:549:GLU:N | 2.54 | 0.41 |
| 1:B:545:ASN:HD21 | 1:C:547:VAL:HG21 | 1.85 | 0.41 |
| 1:C:400:HIS:HD2 | 1:C:402:ASN:CG | 2.29 | 0.41 |
| 1:C:400:HIS:ND1 | 1:C:401:PRO:HD2 | 2.35 | 0.41 |
| 1:D:367:CYS:SG | 1:D:382:TRP:NE1 | 2.93 | 0.41 |
| 1:F:481:PRO:O | 1:F:540:HIS:HE1 | 2.04 | 0.41 |
| 1:G:455:TYR:CZ | 1:H:463:GLN:HG3 | 2.56 | 0.41 |
| 1:L:354:PHE:HD2 | 1:L:546:ARG:NH2 | 2.16 | 0.41 |
| 3:P:25:PRO:HA | 3:P:26:PRO:HD3 | 1.89 | 0.41 |
| 1:A:454:VAL:HG21 | 1:A:538:VAL:HG21 | 2.02 | 0.41 |
| 1:C:564:VAL:H | 1:C:564:VAL:HG23 | 1.56 | 0.41 |
| 1:D:536:CYS:O | 1:D:536:CYS:SG | 2.78 | 0.41 |
| 1:G:365:LEU:HD11 | 1:G:418:TRP:CZ3 | 2.55 | 0.41 |
| 1:H:496:SER:HB3 | 1:H:499:LYS:HZ3 | 1.85 | 0.41 |
| 1:K:463:GLN:HA | 1:L:455:TYR:OH | 2.21 | 0.41 |
| 1:K:564:VAL:H | 1:K:564:VAL:HG23 | 1.59 | 0.41 |
| 1:L:454:VAL:HG13 | 1:L:550:ARG:HB2 | 2.02 | 0.41 |
| 1:L:459:PRO:HD3 | 1:L:472:ILE:HG12 | 2.02 | 0.41 |
| 3:P:140:ASN:ND2 | 3:P:143:LYS:HB2 | 2.35 | 0.41 |
| 3:P:239:CYS:HB2 | 3:P:290:PHE:HE1 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:462:VAL:CG1 | 3:P:509:VAL:HB | 2.51 | 0.41 |
| 3:P:480:TRP:HH2 | 3:P:482:ASN:HB3 | 1.82 | 0.41 |
| 4:R:24:LYS:HD3 | 4:R:119:THR:HG23 | 2.03 | 0.41 |
| 4:R:45:ARG:HD3 | 4:R:108:MET:HE2 | 2.03 | 0.41 |
| 4:V:22:GLU:HB2 | 4:V:119:THR:H | 1.85 | 0.41 |
| 1:B:456:LEU:HG | 1:B:552:VAL:HB | 2.02 | 0.41 |
| 1:C:532:GLU:OE2 | 1:C:532:GLU:HA | 2.21 | 0.41 |
| 1:D:369:VAL:HG13 | 1:D:405:PHE:CD2 | 2.56 | 0.41 |
| 1:F:381:SER:O | 1:F:426:CYS:HA | 2.21 | 0.41 |
| 1:K:352:PRO:HG2 | 1:K:363:THR:HG23 | 2.02 | 0.41 |
| 1:K:430:HIS:HD2 | 1:K:433:LEU:H | 1.69 | 0.41 |
| 1:K:526:GLU:C | 1:K:526:GLU:CD | 2.89 | 0.41 |
| 1:L:511:ALA:HB1 | 1:L:514:ARG:NE | 2.36 | 0.41 |
| 3:P:340:VAL:HG12 | 3:P:436:GLU:CA | 2.51 | 0.41 |
| 4:V:69:LYS:O | 4:V:73:LYS:HG2 | 2.21 | 0.41 |
| 4:V:112:ARG:HB2 | 4:V:112:ARG:HH11 | 1.85 | 0.41 |
| 1:A:502:THR:CB | 1:A:519:SER:HB2 | 2.33 | 0.40 |
| 1:C:354:PHE:HD1 | 1:C:357:ILE:HD12 | 1.85 | 0.40 |
| 1:C:428:VAL:O | 1:C:436:PRO:HA | 2.21 | 0.40 |
| 1:D:382:TRP:HZ3 | 1:D:424:PHE:HB3 | 1.86 | 0.40 |
| 1:D:415:GLU:O | 1:D:419:ASN:ND2 | 2.34 | 0.40 |
| 1:F:476:VAL:O | 1:F:516:PHE:HA | 2.21 | 0.40 |
| 1:F:523:VAL:HG12 | 1:F:534:TYR:OH | 2.21 | 0.40 |
| 1:H:508:GLU:HB3 | 1:H:511:ALA:HB3 | 2.03 | 0.40 |
| 1:L:367:CYS:O | 1:L:369:VAL:HG23 | 2.21 | 0.40 |
| 3:P:172:ARG:HD2 | 3:P:190:ASN:O | 2.21 | 0.40 |
| 4:V:58:CYS:SG | 4:V:110:THR:HG22 | 2.61 | 0.40 |
| 1:A:441:ILE:HD12 | 1:A:441:ILE:HA | 1.90 | 0.40 |
| 1:B:456:LEU:HD11 | 1:B:472:ILE:HG22 | 2.03 | 0.40 |
| 1:B:510:GLN:OE1 | 1:B:510:GLN:CA | 2.69 | 0.40 |
| 1:F:438:LYS:H | 1:F:438:LYS:HG3 | 1.72 | 0.40 |
| 1:F:523:VAL:HG11 | 1:F:534:TYR:CE2 | 2.56 | 0.40 |
| 1:H:408:VAL:HG13 | 1:H:408:VAL:O | 2.21 | 0.40 |
| 1:K:506:MET:HB2 | 1:K:516:PHE:HE1 | 1.85 | 0.40 |
| 4:R:52:MET:HE3 | 4:R:69:LYS:HZ2 | 1.86 | 0.40 |
| 1:A:390:VAL:HG13 | 1:A:391:LYS:H | 1.86 | 0.40 |
| 1:A:452:PRO:HG3 | 1:A:479:PHE:HB3 | 2.02 | 0.40 |
| 1:A:545:ASN:O | 1:A:547:VAL:N | 2.52 | 0.40 |
| 1:E:543:LEU:HA | 1:E:544:PRO:HD3 | 1.84 | 0.40 |
| 3:P:11:ASN:HA | 3:P:108:GLU:O | 2.21 | 0.40 |
| 3:P:317:GLU:N | 3:P:317:GLU:CD | 2.78 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:20:LEU:HD23 | 4:R:117:LYS:HG2 | 1.92 | 0.40 |
| 4:R:95:THR:C | 4:R:97:SER:N | 2.80 | 0.40 |
| 4:V:46:ILE:H | 4:V:64:THR:HG1 | 1.63 | 0.40 |
| 1:C:510:GLN:OE1 | 1:C:510:GLN:CA | 2.70 | 0.40 |
| 1:F:476:VAL:HG12 | 1:F:479:PHE:CE1 | 2.56 | 0.40 |
| 1:H:349:ALA:HA | 1:H:366:THR:O | 2.22 | 0.40 |
| 1:H:567:VAL:HG21 | 1:H:576:TYR:OH | 2.21 | 0.40 |
| 1:K:385:GLN:NE2 | 1:K:423:ARG:H | 2.20 | 0.40 |
| 3:P:354:PRO:HA | 3:P:405:THR:HB | 2.03 | 0.40 |
| 3:P:471:SER:CB | 3:P:475:LYS:HZ3 | 2.29 | 0.40 |
| 4:S:93:GLN:OE1 | 4:S:93:GLN:CA | 2.70 | 0.40 |
| 5:I:2:NAG:O3 | 5:I:2:NAG:C7 | 2.70 | 0.40 |
| 1:B:481:PRO:O | 1:B:481:PRO:CG | 2.69 | 0.40 |
| 1:B:498:GLU:O | 1:B:498:GLU:CG | 2.69 | 0.40 |
| 1:B:546:ARG:HE | 1:B:546:ARG:HB2 | 1.47 | 0.40 |
| 1:C:464:LEU:O | 1:C:466:LEU:N | 2.55 | 0.40 |
| 1:D:365:LEU:HD23 | 1:D:365:LEU:H | 1.86 | 0.40 |
| 1:D:367:CYS:SG | 1:D:393:HIS:HE1 | 2.45 | 0.40 |
| 1:D:499:LYS:HB3 | 1:D:499:LYS:HE2 | 1.71 | 0.40 |
| 1:E:364:LYS:HD3 | 1:E:411:ALA:O | 2.21 | 0.40 |
| 1:G:363:THR:OG1 | 1:G:413:ILE:O | 2.40 | 0.40 |
| 1:H:363:THR:O | 1:H:412:SER:HA | 2.22 | 0.40 |
| 1:H:369:VAL:HG12 | 1:H:372:LEU:HD23 | 2.02 | 0.40 |
| 3:P:25:PRO:HB3 | 3:P:329:ASN:ND2 | 2.36 | 0.40 |
| 3:P:377:CYS:HA | 3:P:378:PRO:HD3 | 1.97 | 0.40 |
| 3:P:447:LYS:H | 3:P:465:HIS:CA | 2.31 | 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 | 229/232 (99%) | 195 (85%) | 24 (10%) | 10 (4%) | 2 14 |
| 1 | B | 226/232 (97%) | 192 (85%) | 27 (12%) | 7 (3%) | 3 20 |
| 1 | C | 225/232 (97%) | 188 (84%) | 26 (12%) | 11 (5%) | 2 12 |
| 1 | D | 222/232 (96%) | 204 (92%) | 16 (7%) | 2 (1%) | 14 47 |
| 1 | E | 222/232 (96%) | 198 (89%) | 19 (9%) | 5 (2%) | 5 27 |
| 1 | F | 222/232 (96%) | 185 (83%) | 23 (10%) | 14 (6%) | 1 8 |
| 1 | G | 222/232 (96%) | 205 (92%) | 15 (7%) | 2 (1%) | 14 47 |
| 1 | H | 230/232 (99%) | 202 (88%) | 19 (8%) | 9 (4%) | 2 16 |
| 1 | K | 230/232 (99%) | 202 (88%) | 19 (8%) | 9 (4%) | 2 16 |
| 1 | L | 230/232 (99%) | 193 (84%) | 29 (13%) | 8 (4%) | 3 18 |
| 2 | J | 102/136 (75%) | 92 (90%) | 8 (8%) | 2 (2%) | 6 29 |
| 3 | P | 481/541 (89%) | 408 (85%) | 54 (11%) | 19 (4%) | 2 15 |
| 4 | R | 99/107 (92%) | 80 (81%) | 17 (17%) | 2 (2%) | 6 29 |
| 4 | S | 101/107 (94%) | 88 (87%) | 11 (11%) | 2 (2%) | 6 29 |
| 4 | U | 99/107 (92%) | 88 (89%) | 8 (8%) | 3 (3%) | 3 21 |
| 4 | V | 104/107 (97%) | 97 (93%) | 6 (6%) | 1 (1%) | 13 45 |
| All | All | 3244/3425 (95%) | 2817 (87%) | 321 (10%) | 106 (3%) | 5 18 |

All (106) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 546 | ARG |
| 1 | A | 554 | LYS |
| 1 | B | 415 | GLU |
| 1 | B | 418 | TRP |
| 1 | B | 480 | SER |
| 1 | C | 482 | ALA |
| 1 | E | 494 | PRO |
| 1 | E | 533 | THR |
| 1 | E | 546 | ARG |
| 1 | F | 444 | PRO |
| 1 | F | 480 | SER |
| 1 | F | 546 | ARG |
| 1 | G | 444 | PRO |
| 1 | H | 442 | SER |
| 1 | H | 569 | SER |
| 1 | H | 574 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 447 | VAL |
| 1 | K | 492 | GLY |
| 1 | K | 511 | ALA |
| 1 | K | 512 | PRO |
| 1 | K | 541 | GLU |
| 1 | L | 441 | ILE |
| 1 | L | 443 | ARG |
| 1 | L | 481 | PRO |
| 3 | P | 101 | LEU |
| 3 | P | 259 | GLU |
| 3 | P | 261 | CYS |
| 3 | P | 262 | ASP |
| 3 | P | 311 | SER |
| 3 | P | 379 | LEU |
| 3 | P | 399 | GLU |
| 3 | P | 413 | LEU |
| 3 | P | 448 | VAL |
| 4 | R | 66 | ASN |
| 4 | S | 53 | ALA |
| 4 | S | 98 | ASP |
| 4 | U | 96 | GLU |
| 1 | A | 446 | GLY |
| 1 | B | 405 | PHE |
| 1 | B | 410 | GLU |
| 1 | B | 497 | PRO |
| 1 | C | 531 | GLY |
| 1 | E | 534 | TYR |
| 1 | F | 390 | VAL |
| 1 | F | 419 | ASN |
| 1 | F | 421 | GLY |
| 1 | F | 449 | LEU |
| 1 | F | 507 | PRO |
| 1 | F | 523 | VAL |
| 1 | G | 478 | GLY |
| 1 | H | 531 | GLY |
| 1 | H | 564 | VAL |
| 2 | J | 64 | LEU |
| 1 | L | 478 | GLY |
| 1 | L | 534 | TYR |
| 3 | P | 310 | HIS |
| 3 | P | 403 | ASN |
| 3 | P | 416 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 491 | ARG |
| 1 | A | 512 | PRO |
| 1 | C | 448 | ALA |
| 1 | C | 509 | PRO |
| 1 | C | 510 | GLN |
| 1 | C | 512 | PRO |
| 1 | D | 497 | PRO |
| 1 | F | 415 | GLU |
| 1 | H | 444 | PRO |
| 1 | H | 449 | LEU |
| 1 | H | 559 | PRO |
| 2 | J | 120 | GLU |
| 1 | K | 572 | ALA |
| 1 | L | 444 | PRO |
| 1 | L | 447 | VAL |
| 3 | P | 155 | PRO |
| 3 | P | 378 | PRO |
| 3 | P | 473 | TYR |
| 4 | U | 98 | ASP |
| 1 | A | 497 | PRO |
| 1 | A | 573 | GLY |
| 1 | C | 481 | PRO |
| 1 | C | 523 | VAL |
| 1 | C | 557 | GLY |
| 1 | D | 447 | VAL |
| 1 | E | 509 | PRO |
| 1 | F | 377 | SER |
| 1 | F | 544 | PRO |
| 1 | H | 560 | THR |
| 1 | K | 519 | SER |
| 1 | K | 544 | PRO |
| 1 | L | 483 | ASP |
| 3 | P | 57 | SER |
| 3 | P | 287 | ASP |
| 4 | R | 96 | GLU |
| 4 | V | 113 | GLY |
| 1 | C | 466 | LEU |
| 1 | C | 558 | LYS |
| 3 | P | 157 | LEU |
| 1 | A | 501 | VAL |
| 1 | F | 559 | PRO |
| 4 | U | 42 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 444 | PRO |
| 1 | A | 531 | GLY |
| 1 | B | 413 | ILE |
| 1 | F | 413 | ILE |
| 3 | P | 288 | GLY |
| 1 | A | 481 | 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 | 205/206 (100%) | 183 (89%) | 22 (11%) | 5 22 |
| 1 | B | 203/206 (98%) | 155 (76%) | 48 (24%) | 0 2 |
| 1 | C | 203/206 (98%) | 181 (89%) | 22 (11%) | 5 21 |
| 1 | D | 200/206 (97%) | 195 (98%) | 5 (2%) | 42 68 |
| 1 | E | 200/206 (97%) | 193 (96%) | 7 (4%) | 31 60 |
| 1 | F | 200/206 (97%) | 151 (76%) | 49 (24%) | 0 2 |
| 1 | G | 200/206 (97%) | 188 (94%) | 12 (6%) | 16 44 |
| 1 | H | 206/206 (100%) | 187 (91%) | 19 (9%) | 7 27 |
| 1 | K | 206/206 (100%) | 176 (85%) | 30 (15%) | 2 12 |
| 1 | L | 206/206 (100%) | 183 (89%) | 23 (11%) | 5 20 |
| 2 | J | 100/128 (78%) | 92 (92%) | 8 (8%) | 10 34 |
| 3 | P | 423/461 (92%) | 365 (86%) | 58 (14%) | 3 13 |
| 4 | R | 86/92 (94%) | 76 (88%) | 10 (12%) | 4 19 |
| 4 | S | 88/92 (96%) | 75 (85%) | 13 (15%) | 2 11 |
| 4 | U | 86/92 (94%) | 78 (91%) | 8 (9%) | 7 27 |
| 4 | V | 91/92 (99%) | 89 (98%) | 2 (2%) | 47 71 |
| All | All | 2903/3017 (96%) | 2567 (88%) | 336 (12%) | 7 19 |

All (336) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 445 | LYS |
| 1 | A | 447 | VAL |
| 1 | A | 466 | LEU |
| 1 | A | 467 | ARG |
| 1 | A | 477 | THR |
| 1 | A | 490 | GLN |
| 1 | A | 502 | THR |
| 1 | A | 508 | GLU |
| 1 | A | 510 | GLN |
| 1 | A | 514 | ARG |
| 1 | A | 518 | HIS |
| 1 | A | 519 | SER |
| 1 | A | 532 | GLU |
| 1 | A | 543 | LEU |
| 1 | A | 545 | ASN |
| 1 | A | 549 | GLU |
| 1 | A | 554 | LYS |
| 1 | A | 556 | THR |
| 1 | A | 566 | LEU |
| 1 | A | 568 | MET |
| 1 | A | 571 | THR |
| 1 | A | 574 | THR |
| 1 | B | 366 | THR |
| 1 | B | 368 | LEU |
| 1 | B | 371 | ASP |
| 1 | B | 374 | THR |
| 1 | B | 375 | TYR |
| 1 | B | 376 | ASP |
| 1 | B | 378 | VAL |
| 1 | B | 380 | ILE |
| 1 | B | 391 | LYS |
| 1 | B | 392 | THR |
| 1 | B | 393 | HIS |
| 1 | B | 394 | THR |
| 1 | B | 395 | ASN |
| 1 | B | 396 | ILE |
| 1 | B | 398 | GLU |
| 1 | B | 400 | HIS |
| 1 | B | 402 | ASN |
| 1 | B | 408 | VAL |
| 1 | B | 410 | GLU |
| 1 | B | 412 | SER |
| 1 | B | 413 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 420 | SER |
| 1 | B | 423 | ARG |
| 1 | B | 424 | PHE |
| 1 | B | 427 | THR |
| 1 | B | 429 | THR |
| 1 | B | 431 | THR |
| 1 | B | 433 | LEU |
| 1 | B | 437 | LEU |
| 1 | B | 440 | THR |
| 1 | B | 441 | ILE |
| 1 | B | 442 | SER |
| 1 | B | 443 | ARG |
| 1 | B | 445 | LYS |
| 1 | B | 449 | LEU |
| 1 | B | 451 | ARG |
| 1 | B | 454 | VAL |
| 1 | B | 456 | LEU |
| 1 | B | 462 | GLU |
| 1 | B | 480 | SER |
| 1 | B | 498 | GLU |
| 1 | B | 499 | LYS |
| 1 | B | 526 | GLU |
| 1 | B | 529 | ASN |
| 1 | B | 530 | THR |
| 1 | B | 532 | GLU |
| 1 | B | 535 | THR |
| 1 | B | 546 | ARG |
| 1 | C | 445 | LYS |
| 1 | C | 450 | HIS |
| 1 | C | 451 | ARG |
| 1 | C | 453 | ASP |
| 1 | C | 456 | LEU |
| 1 | C | 457 | LEU |
| 1 | C | 466 | LEU |
| 1 | C | 468 | GLU |
| 1 | C | 480 | SER |
| 1 | C | 494 | PRO |
| 1 | C | 510 | GLN |
| 1 | C | 514 | ARG |
| 1 | C | 525 | GLU |
| 1 | C | 526 | GLU |
| 1 | C | 527 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 530 | THR |
| 1 | C | 533 | THR |
| 1 | C | 554 | LYS |
| 1 | C | 564 | VAL |
| 1 | C | 565 | SER |
| 1 | C | 566 | LEU |
| 1 | C | 567 | VAL |
| 1 | D | 495 | LEU |
| 1 | D | 499 | LYS |
| 1 | D | 514 | ARG |
| 1 | D | 536 | CYS |
| 1 | D | 537 | VAL |
| 1 | E | 445 | LYS |
| 1 | E | 493 | GLN |
| 1 | E | 514 | ARG |
| 1 | E | 532 | GLU |
| 1 | E | 535 | THR |
| 1 | E | 538 | VAL |
| 1 | E | 545 | ASN |
| 1 | F | 363 | THR |
| 1 | F | 368 | LEU |
| 1 | F | 374 | THR |
| 1 | F | 376 | ASP |
| 1 | F | 377 | SER |
| 1 | F | 378 | VAL |
| 1 | F | 379 | THR |
| 1 | F | 380 | ILE |
| 1 | F | 383 | THR |
| 1 | F | 390 | VAL |
| 1 | F | 391 | LYS |
| 1 | F | 396 | ILE |
| 1 | F | 402 | ASN |
| 1 | F | 405 | PHE |
| 1 | F | 406 | SER |
| 1 | F | 408 | VAL |
| 1 | F | 410 | GLU |
| 1 | F | 412 | SER |
| 1 | F | 414 | CYS |
| 1 | F | 416 | ASP |
| 1 | F | 420 | SER |
| 1 | F | 422 | GLU |
| 1 | F | 423 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 425 | THR |
| 1 | F | 429 | THR |
| 1 | F | 432 | ASP |
| 1 | F | 437 | LEU |
| 1 | F | 438 | LYS |
| 1 | F | 439 | GLN |
| 1 | F | 440 | THR |
| 1 | F | 441 | ILE |
| 1 | F | 443 | ARG |
| 1 | F | 445 | LYS |
| 1 | F | 479 | PHE |
| 1 | F | 501 | VAL |
| 1 | F | 502 | THR |
| 1 | F | 506 | MET |
| 1 | F | 520 | ILE |
| 1 | F | 521 | LEU |
| 1 | F | 523 | VAL |
| 1 | F | 543 | LEU |
| 1 | F | 544 | PRO |
| 1 | F | 545 | ASN |
| 1 | F | 546 | ARG |
| 1 | F | 548 | THR |
| 1 | F | 550 | ARG |
| 1 | F | 554 | LYS |
| 1 | F | 556 | THR |
| 1 | F | 561 | LEU |
| 1 | G | 345 | ILE |
| 1 | G | 443 | ARG |
| 1 | G | 445 | LYS |
| 1 | G | 447 | VAL |
| 1 | G | 449 | LEU |
| 1 | G | 466 | LEU |
| 1 | G | 473 | THR |
| 1 | G | 475 | LEU |
| 1 | G | 477 | THR |
| 1 | G | 516 | PHE |
| 1 | G | 564 | VAL |
| 1 | G | 567 | VAL |
| 1 | H | 442 | SER |
| 1 | H | 443 | ARG |
| 1 | H | 444 | PRO |
| 1 | H | 445 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 449 | LEU |
| 1 | H | 486 | VAL |
| 1 | H | 519 | SER |
| 1 | H | 532 | GLU |
| 1 | H | 533 | THR |
| 1 | H | 535 | THR |
| 1 | H | 536 | CYS |
| 1 | H | 537 | VAL |
| 1 | H | 556 | THR |
| 1 | H | 558 | LYS |
| 1 | H | 561 | LEU |
| 1 | H | 563 | ASN |
| 1 | H | 566 | LEU |
| 1 | H | 568 | MET |
| 1 | H | 574 | THR |
| 2 | J | 23 | ARG |
| 2 | J | 26 | GLU |
| 2 | J | 30 | GLU |
| 2 | J | 34 | GLU |
| 2 | J | 35 | ARG |
| 2 | J | 107 | LYS |
| 2 | J | 116 | VAL |
| 2 | J | 117 | TYR |
| 1 | K | 445 | LYS |
| 1 | K | 447 | VAL |
| 1 | K | 449 | LEU |
| 1 | K | 462 | GLU |
| 1 | K | 464 | LEU |
| 1 | K | 474 | CYS |
| 1 | K | 475 | LEU |
| 1 | K | 477 | THR |
| 1 | K | 484 | VAL |
| 1 | K | 489 | MET |
| 1 | K | 490 | GLN |
| 1 | K | 491 | ARG |
| 1 | K | 508 | GLU |
| 1 | K | 514 | ARG |
| 1 | K | 516 | PHE |
| 1 | K | 520 | ILE |
| 1 | K | 521 | LEU |
| 1 | K | 524 | SER |
| 1 | K | 526 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 530 | THR |
| 1 | K | 533 | THR |
| 1 | K | 535 | THR |
| 1 | K | 543 | LEU |
| 1 | K | 545 | ASN |
| 1 | K | 556 | THR |
| 1 | K | 558 | LYS |
| 1 | K | 561 | LEU |
| 1 | K | 565 | SER |
| 1 | K | 568 | MET |
| 1 | K | 574 | THR |
| 1 | L | 441 | ILE |
| 1 | L | 443 | ARG |
| 1 | L | 445 | LYS |
| 1 | L | 449 | LEU |
| 1 | L | 450 | HIS |
| 1 | L | 479 | PHE |
| 1 | L | 480 | SER |
| 1 | L | 514 | ARG |
| 1 | L | 534 | TYR |
| 1 | L | 535 | THR |
| 1 | L | 536 | CYS |
| 1 | L | 543 | LEU |
| 1 | L | 545 | ASN |
| 1 | L | 547 | VAL |
| 1 | L | 548 | THR |
| 1 | L | 551 | THR |
| 1 | L | 552 | VAL |
| 1 | L | 556 | THR |
| 1 | L | 558 | LYS |
| 1 | L | 566 | LEU |
| 1 | L | 567 | VAL |
| 1 | L | 574 | THR |
| 1 | L | 575 | CYS |
| 3 | P | 10 | VAL |
| 3 | P | 43 | ARG |
| 3 | P | 60 | TYR |
| 3 | P | 99 | ARG |
| 3 | P | 131 | THR |
| 3 | P | 132 | ILE |
| 3 | P | 151 | ILE |
| 3 | P | 245 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | P | 247 | ASN |
| 3 | P | 257 | SER |
| 3 | P | 259 | GLU |
| 3 | P | 260 | ASN |
| 3 | P | 275 | PHE |
| 3 | P | 287 | ASP |
| 3 | P | 290 | PHE |
| 3 | P | 314 | GLN |
| 3 | P | 315 | LEU |
| 3 | P | 316 | GLN |
| 3 | P | 317 | GLU |
| 3 | P | 340 | VAL |
| 3 | P | 342 | LYS |
| 3 | P | 344 | VAL |
| 3 | P | 349 | VAL |
| 3 | P | 358 | LYS |
| 3 | P | 361 | LYS |
| 3 | P | 379 | LEU |
| 3 | P | 387 | VAL |
| 3 | P | 388 | LYS |
| 3 | P | 390 | GLN |
| 3 | P | 392 | GLU |
| 3 | P | 398 | LEU |
| 3 | P | 399 | GLU |
| 3 | P | 400 | GLU |
| 3 | P | 403 | ASN |
| 3 | P | 405 | THR |
| 3 | P | 409 | ILE |
| 3 | P | 412 | GLN |
| 3 | P | 413 | LEU |
| 3 | P | 414 | THR |
| 3 | P | 430 | LEU |
| 3 | P | 431 | TRP |
| 3 | P | 432 | ARG |
| 3 | P | 439 | ILE |
| 3 | P | 446 | LEU |
| 3 | P | 447 | LYS |
| 3 | P | 462 | VAL |
| 3 | P | 464 | CYS |
| 3 | P | 466 | PHE |
| 3 | P | 469 | LYS |
| 3 | P | 470 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | P | 473 | TYR |
| 3 | P | 475 | LYS |
| 3 | P | 478 | CYS |
| 3 | P | 533 | PHE |
| 3 | P | 536 | GLU |
| 3 | P | 537 | THR |
| 3 | P | 540 | VAL |
| 3 | P | 541 | TYR |
| 4 | R | 20 | LEU |
| 4 | R | 24 | LYS |
| 4 | R | 55 | SER |
| 4 | R | 65 | THR |
| 4 | R | 93 | GLN |
| 4 | R | 94 | LEU |
| 4 | R | 95 | THR |
| 4 | R | 96 | GLU |
| 4 | R | 115 | THR |
| 4 | R | 116 | GLN |
| 4 | S | 39 | LEU |
| 4 | S | 42 | MET |
| 4 | S | 71 | GLU |
| 4 | S | 72 | TYR |
| 4 | S | 73 | LYS |
| 4 | S | 92 | THR |
| 4 | S | 93 | GLN |
| 4 | S | 94 | LEU |
| 4 | S | 96 | GLU |
| 4 | S | 115 | THR |
| 4 | S | 116 | GLN |
| 4 | S | 117 | LYS |
| 4 | S | 118 | VAL |
| 4 | U | 23 | VAL |
| 4 | U | 24 | LYS |
| 4 | U | 25 | VAL |
| 4 | U | 26 | GLU |
| 4 | U | 41 | GLU |
| 4 | U | 44 | VAL |
| 4 | U | 117 | LYS |
| 4 | U | 119 | THR |
| 4 | V | 96 | GLU |
| 4 | V | 114 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 510 | GLN |
| 1 | A | 540 | HIS |
| 1 | B | 385 | GLN |
| 1 | B | 393 | HIS |
| 1 | B | 400 | HIS |
| 1 | B | 450 | HIS |
| 1 | B | 529 | ASN |
| 1 | B | 545 | ASN |
| 1 | C | 400 | HIS |
| 1 | C | 465 | ASN |
| 1 | D | 393 | HIS |
| 1 | E | 400 | HIS |
| 1 | E | 493 | GLN |
| 1 | E | 529 | ASN |
| 1 | F | 402 | ASN |
| 1 | F | 439 | GLN |
| 1 | F | 540 | HIS |
| 1 | F | 545 | ASN |
| 1 | G | 563 | ASN |
| 1 | H | 419 | ASN |
| 1 | H | 430 | HIS |
| 1 | H | 439 | GLN |
| 1 | K | 430 | HIS |
| 1 | K | 487 | GLN |
| 1 | K | 545 | ASN |
| 1 | K | 563 | ASN |
| 1 | L | 430 | HIS |
| 1 | L | 463 | GLN |
| 1 | L | 490 | GLN |
| 1 | L | 545 | ASN |
| 3 | P | 40 | GLN |
| 3 | P | 199 | GLN |
| 3 | P | 260 | ASN |
| 3 | P | 310 | HIS |
| 3 | P | 314 | GLN |
| 3 | P | 322 | GLN |
| 3 | P | 390 | GLN |
| 3 | P | 403 | ASN |
| 3 | P | 411 | ASN |
| 3 | P | 412 | GLN |
| 3 | P | 481 | ASN |
| 3 | P | 530 | GLN |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | P | 532 | HIS |
| 4 | R | 93 | GLN |
| 4 | R | 116 | GLN |
| 4 | U | 109 | ASN |
| 4 | V | 66 | ASN |
| 4 | V | 121 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

2 monosaccharides 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 | NAG | I | 1 | 2,5 | 14,14,15 | 3.15 | 2 (14%) | 17,19,21 | 2.98 | 7 (41%) |
| 5 | NAG | I | 2 | 5 | 14,14,15 | 1.09 | 0 | 17,19,21 | 3.30 | 7 (41%) |

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 | NAG | I | 1 | 2,5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 2 | 5 | - | 3/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | I | 1 | NAG | C1-C2 | 10.08 | 1.67 | 1.52 |
| 5 | I | 1 | NAG | O5-C1 | -4.51 | 1.36 | 1.43 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | I | 2 | NAG | C2-N2-C7 | -9.79 | 108.97 | 122.90 |
| 5 | I | 1 | NAG | O5-C5-C6 | -6.42 | 97.13 | 107.20 |
| 5 | I | 1 | NAG | C1-O5-C5 | 5.30 | 119.37 | 112.19 |
| 5 | I | 2 | NAG | C1-O5-C5 | 5.11 | 119.11 | 112.19 |
| 5 | I | 1 | NAG | C4-C3-C2 | -4.59 | 104.29 | 111.02 |
| 5 | I | 2 | NAG | C3-C4-C5 | -4.37 | 102.44 | 110.24 |
| 5 | I | 2 | NAG | C4-C3-C2 | -4.22 | 104.84 | 111.02 |
| 5 | I | 1 | NAG | O4-C4-C3 | -3.46 | 102.35 | 110.35 |
| 5 | I | 1 | NAG | O5-C1-C2 | -3.22 | 106.20 | 111.29 |
| 5 | I | 1 | NAG | C1-C2-N2 | 3.10 | 115.78 | 110.49 |
| 5 | I | 1 | NAG | O3-C3-C2 | -2.80 | 103.68 | 109.47 |
| 5 | I | 2 | NAG | O3-C3-C2 | -2.21 | 104.88 | 109.47 |
| 5 | I | 2 | NAG | O5-C1-C2 | 2.17 | 114.72 | 111.29 |
| 5 | I | 2 | NAG | C1-C2-N2 | 2.03 | 113.95 | 110.49 |

There are no chirality outliers.

All (7) torsion outliers are listed below:

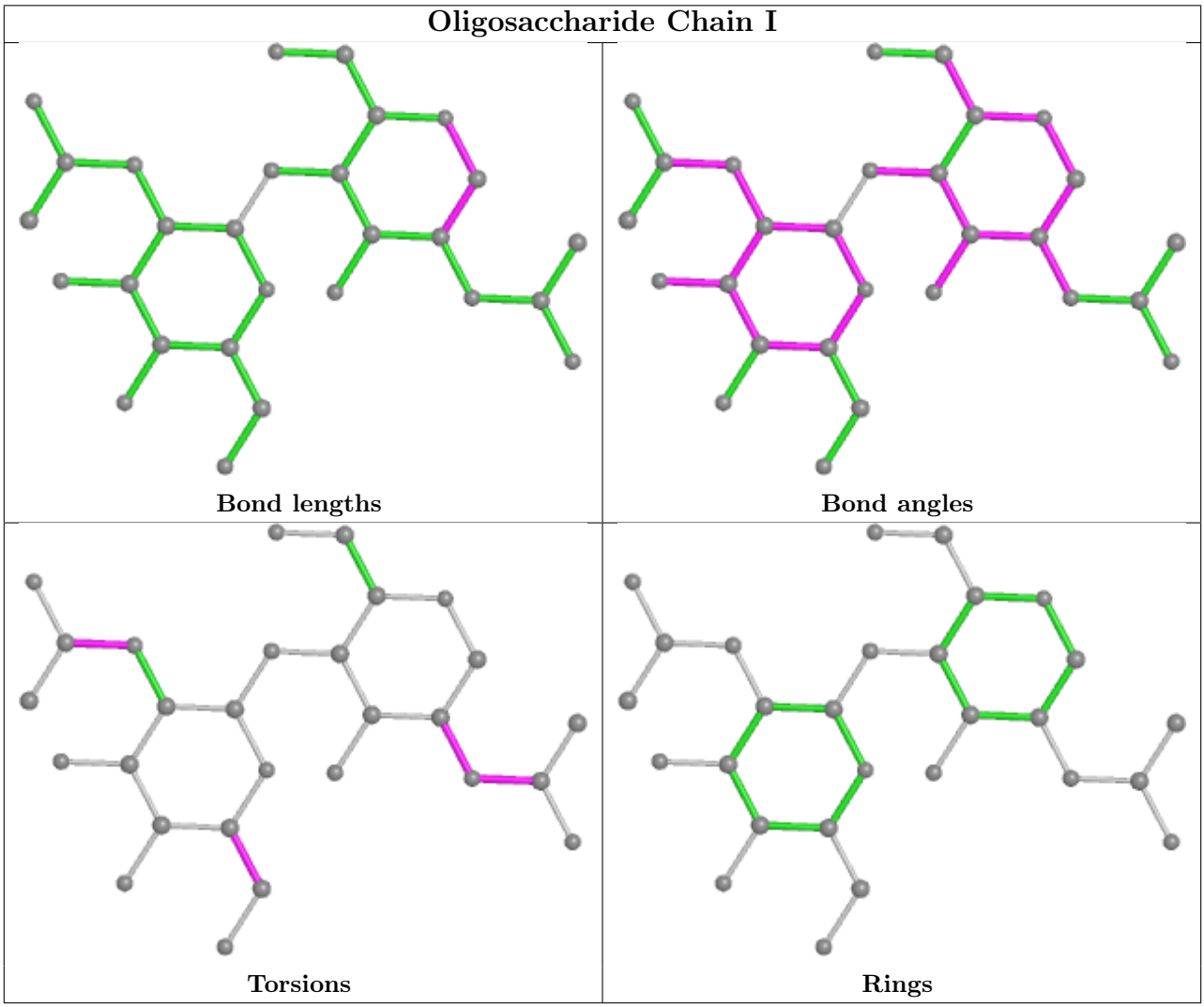
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | I | 1 | NAG | C8-C7-N2-C2 |
| 5 | I | 1 | NAG | O7-C7-N2-C2 |
| 5 | I | 2 | NAG | C8-C7-N2-C2 |
| 5 | I | 2 | NAG | O7-C7-N2-C2 |
| 5 | I | 2 | NAG | O5-C5-C6-O6 |
| 5 | I | 1 | NAG | C3-C2-N2-C7 |
| 5 | I | 1 | NAG | C1-C2-N2-C7 |

There are no ring outliers.

2 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | I | 1 | NAG | 3 | 0 |
| 5 | I | 2 | NAG | 3 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.




## 5.6 Ligand geometry (i)

10 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 | $\#\|Z\| > 2$ |
| 6 | NAG | E | 601 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.42 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 6 | NAG | G | 601 | - | 15,15,15 | 0.46 | 0 | 21,21,21 | 1.55 | 2 (9%) |
| 6 | NAG | L | 601 | 1 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.51 | 0 |
| 6 | NAG | B | 601 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.41 | 0 |
| 6 | NAG | F | 601 | 1 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.48 | 0 |
| 6 | NAG | A | 601 | 1 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.35 | 0 |
| 6 | NAG | C | 601 | - | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.41 | 0 |
| 6 | NAG | H | 601 | 1 | 14,14,15 | 2.59 | 4 (28%) | 17,19,21 | 3.75 | 7 (41%) |
| 6 | NAG | K | 601 | - | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.33 | 0 |
| 6 | NAG | D | 601 | 1 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.42 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 6 | NAG | E | 601 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | G | 601 | - | - | 4/6/26/26 | 0/1/1/1 |
| 6 | NAG | L | 601 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 601 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | F | 601 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | A | 601 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 601 | - | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | H | 601 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | K | 601 | - | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 601 | 1 | - | 2/6/23/26 | 0/1/1/1 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | H | 601 | NAG | C1-C2 | 7.75 | 1.63 | 1.52 |
| 6 | H | 601 | NAG | C2-N2 | -4.09 | 1.39 | 1.46 |
| 6 | H | 601 | NAG | C3-C2 | -2.14 | 1.48 | 1.52 |
| 6 | H | 601 | NAG | O5-C1 | -2.11 | 1.40 | 1.43 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 601 | NAG | C1-C2-N2 | -9.97 | 93.46 | 110.49 |
| 6 | H | 601 | NAG | C4-C3-C2 | -8.07 | 99.20 | 111.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | H | 601 | NAG | O5-C1-C2 | -5.85 | 102.05 | 111.29 |
| 6 | G | 601 | NAG | O5-C1-C2 | 4.53 | 114.07 | 109.52 |
| 6 | H | 601 | NAG | C3-C4-C5 | -3.39 | 104.20 | 110.24 |
| 6 | G | 601 | NAG | C1-O5-C5 | 3.33 | 119.94 | 113.66 |
| 6 | H | 601 | NAG | C2-N2-C7 | -3.17 | 118.39 | 122.90 |
| 6 | H | 601 | NAG | O4-C4-C5 | 2.41 | 115.28 | 109.30 |
| 6 | H | 601 | NAG | O3-C3-C2 | 2.31 | 114.24 | 109.47 |

There are no chirality outliers.

All (25) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | G | 601 | NAG | C8-C7-N2-C2 |
| 6 | G | 601 | NAG | O7-C7-N2-C2 |
| 6 | H | 601 | NAG | C8-C7-N2-C2 |
| 6 | H | 601 | NAG | O7-C7-N2-C2 |
| 6 | C | 601 | NAG | C4-C5-C6-O6 |
| 6 | H | 601 | NAG | C4-C5-C6-O6 |
| 6 | D | 601 | NAG | O5-C5-C6-O6 |
| 6 | D | 601 | NAG | C4-C5-C6-O6 |
| 6 | K | 601 | NAG | C4-C5-C6-O6 |
| 6 | C | 601 | NAG | O5-C5-C6-O6 |
| 6 | L | 601 | NAG | O5-C5-C6-O6 |
| 6 | K | 601 | NAG | O5-C5-C6-O6 |
| 6 | B | 601 | NAG | O5-C5-C6-O6 |
| 6 | G | 601 | NAG | C4-C5-C6-O6 |
| 6 | C | 601 | NAG | C8-C7-N2-C2 |
| 6 | C | 601 | NAG | O7-C7-N2-C2 |
| 6 | K | 601 | NAG | C8-C7-N2-C2 |
| 6 | K | 601 | NAG | O7-C7-N2-C2 |
| 6 | B | 601 | NAG | C4-C5-C6-O6 |
| 6 | E | 601 | NAG | O5-C5-C6-O6 |
| 6 | G | 601 | NAG | O5-C5-C6-O6 |
| 6 | H | 601 | NAG | O5-C5-C6-O6 |
| 6 | F | 601 | NAG | O5-C5-C6-O6 |
| 6 | L | 601 | NAG | C4-C5-C6-O6 |
| 6 | E | 601 | NAG | C4-C5-C6-O6 |

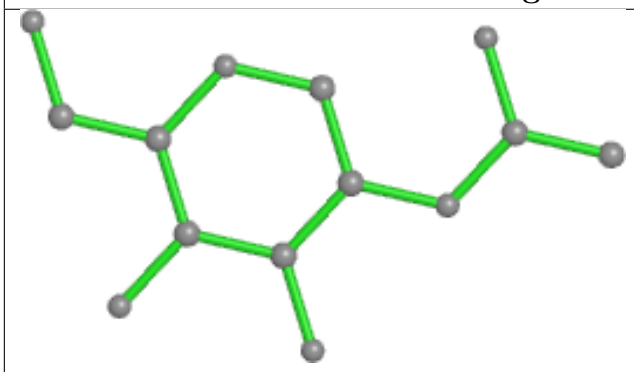
There are no ring outliers.

7 monomers are involved in 10 short contacts:

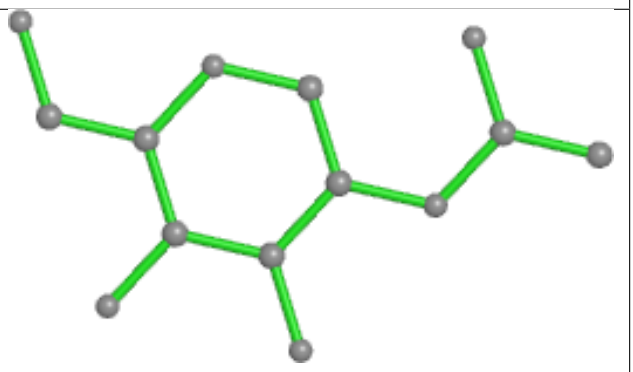
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 6 | E | 601 | NAG | 1 | 0 |
| 6 | B | 601 | NAG | 1 | 0 |
| 6 | F | 601 | NAG | 1 | 0 |
| 6 | A | 601 | NAG | 1 | 0 |
| 6 | C | 601 | NAG | 2 | 0 |
| 6 | H | 601 | NAG | 3 | 0 |
| 6 | K | 601 | NAG | 4 | 0 |

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.

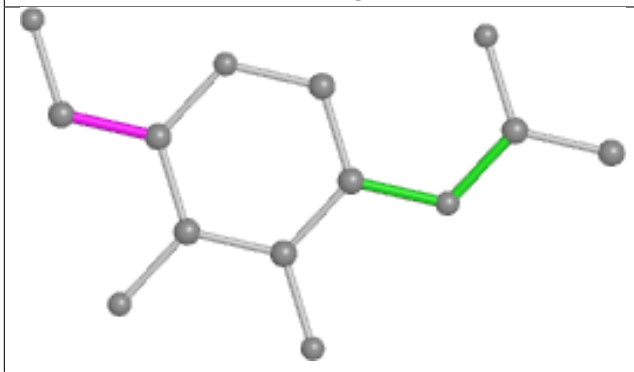
**Ligand NAG E 601**



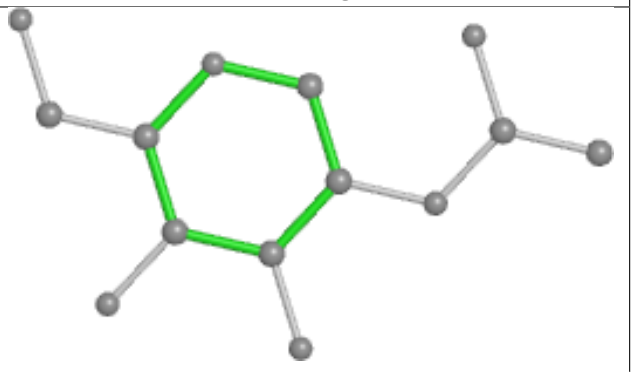
**Bond lengths**



**Bond angles**

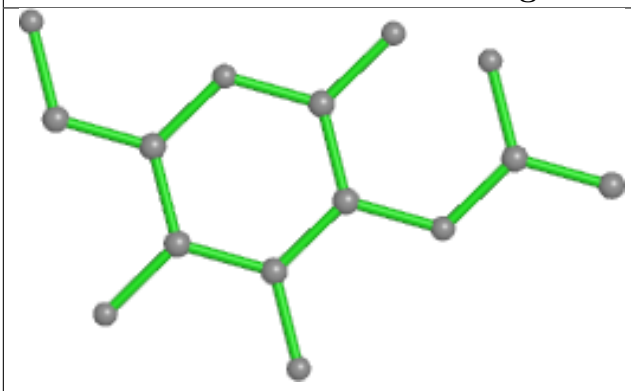


**Torsions**

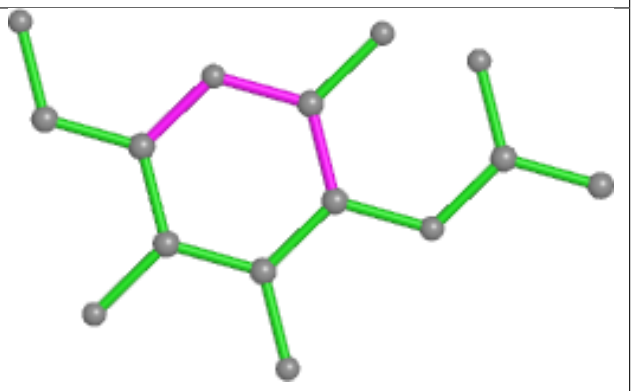


**Rings**

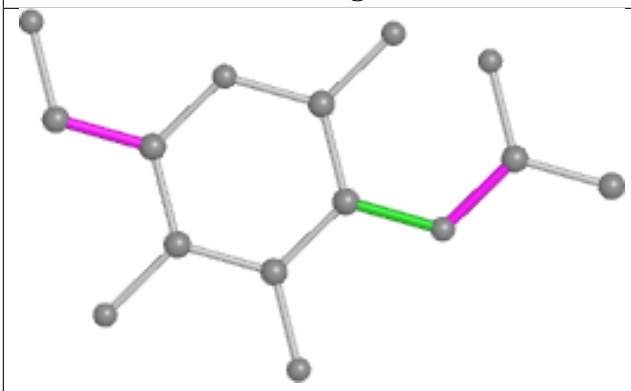
**Ligand NAG G 601**



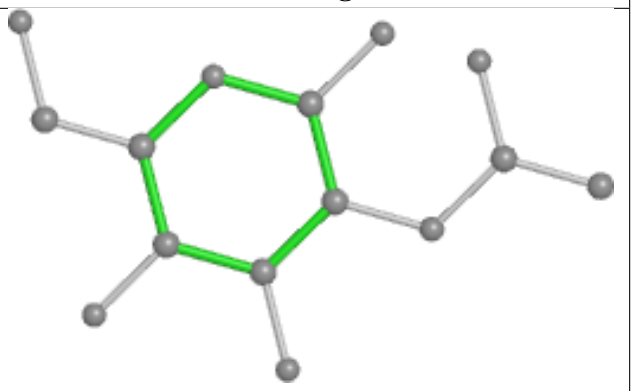
Bond lengths



Bond angles

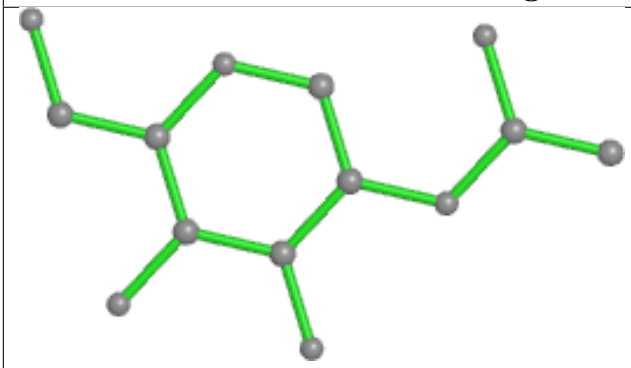


Torsions

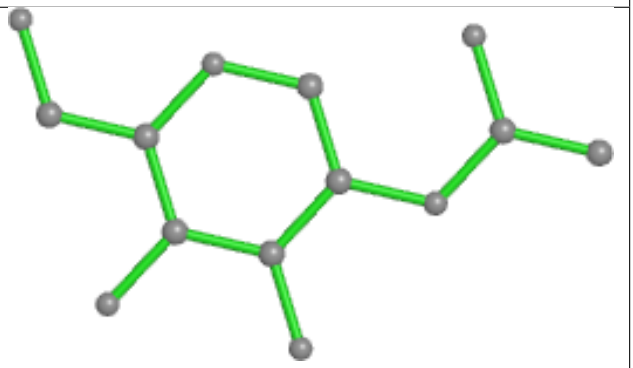


Rings

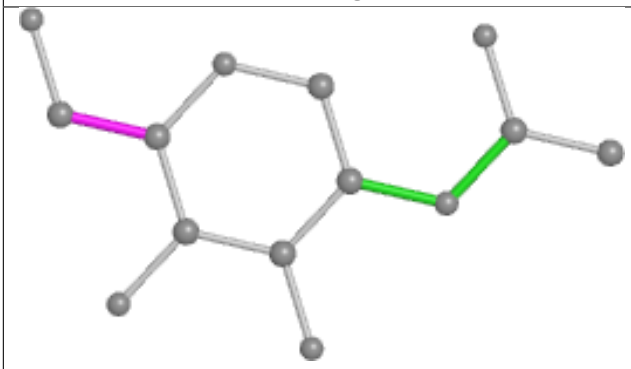
**Ligand NAG L 601**



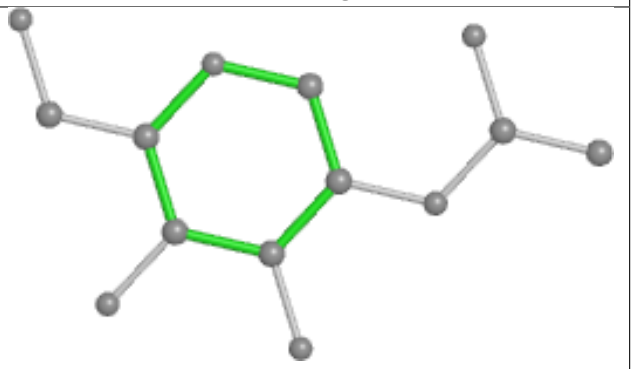
Bond lengths



Bond angles

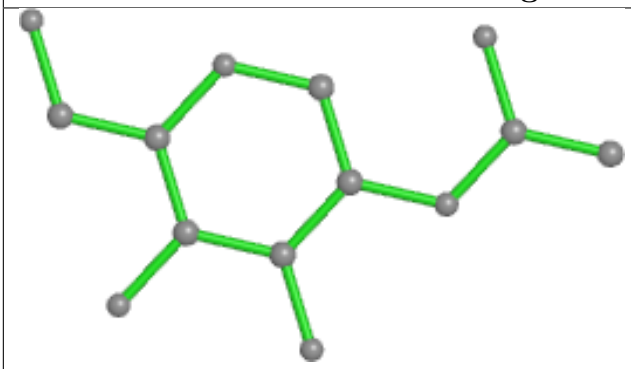


Torsions

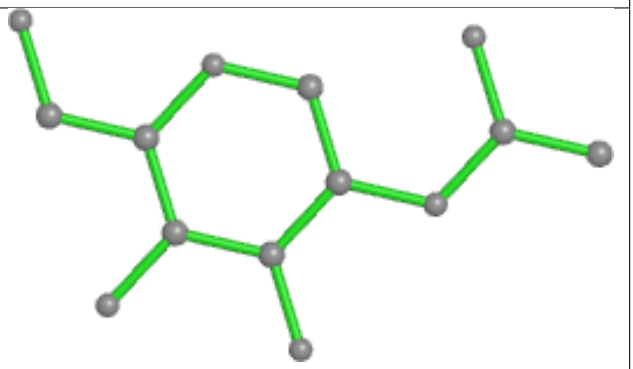


Rings

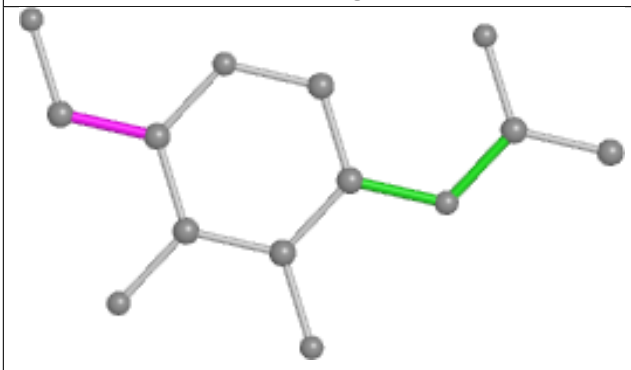
## Ligand NAG B 601



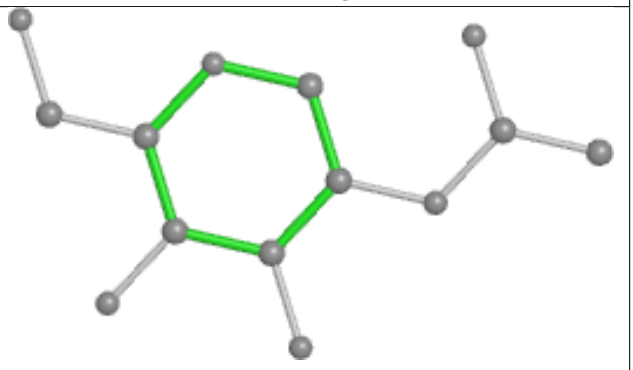
Bond lengths



Bond angles

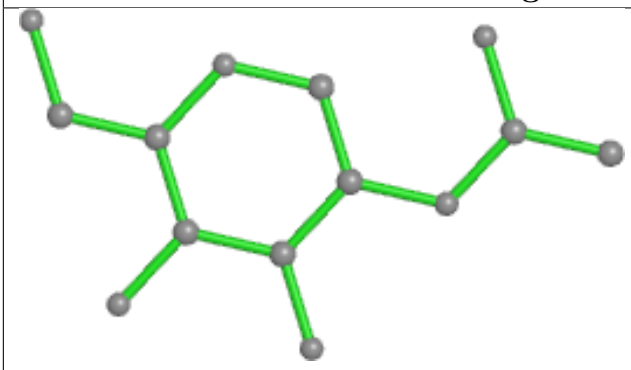


Torsions

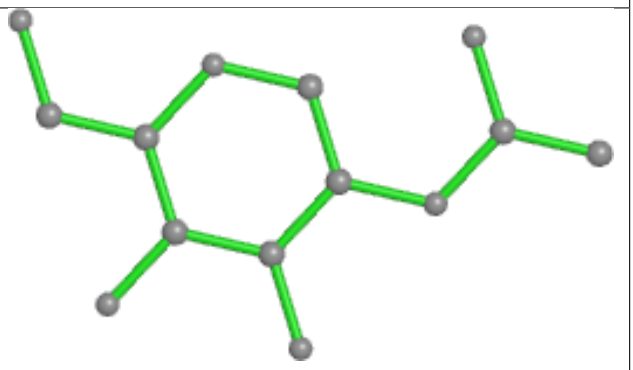


Rings

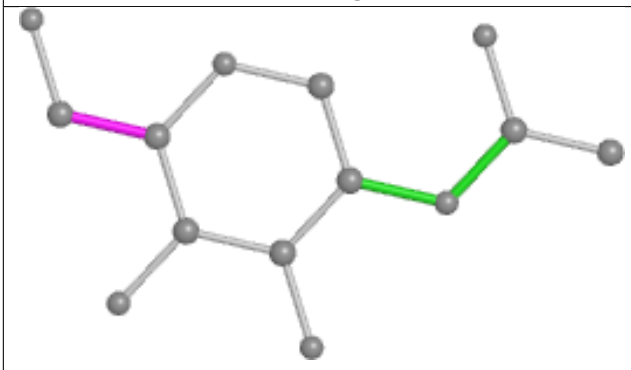
## Ligand NAG F 601



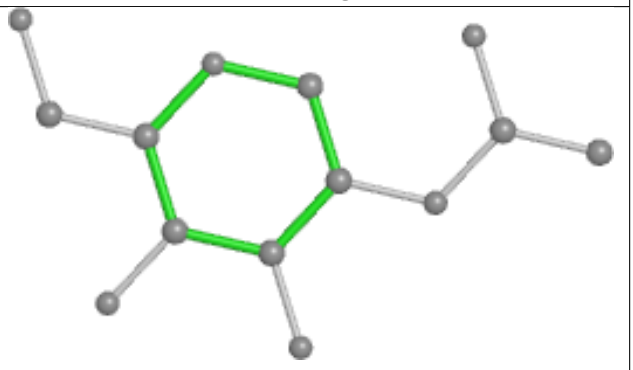
Bond lengths



Bond angles

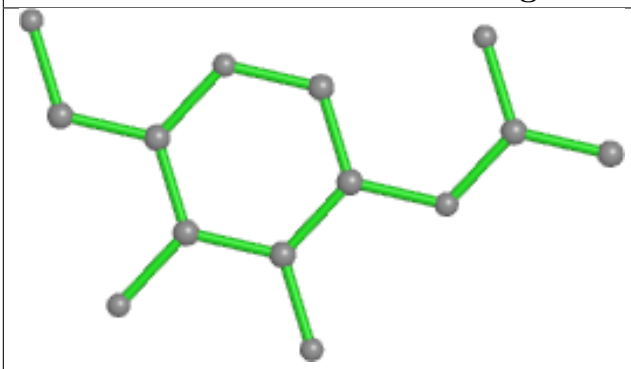


Torsions

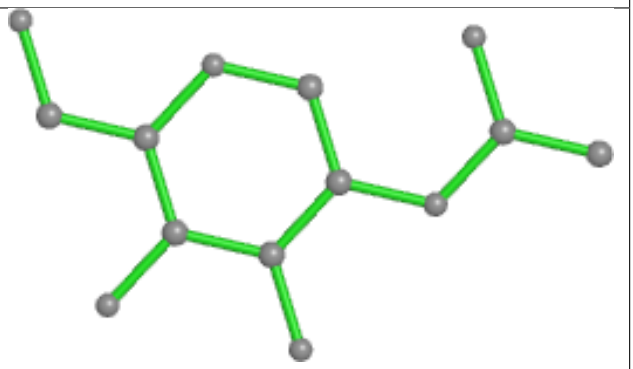


Rings

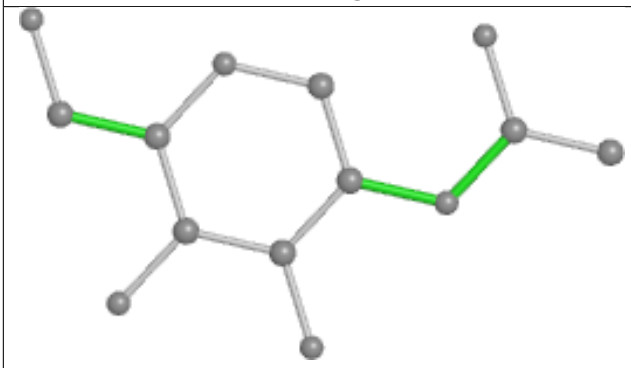
**Ligand NAG A 601**



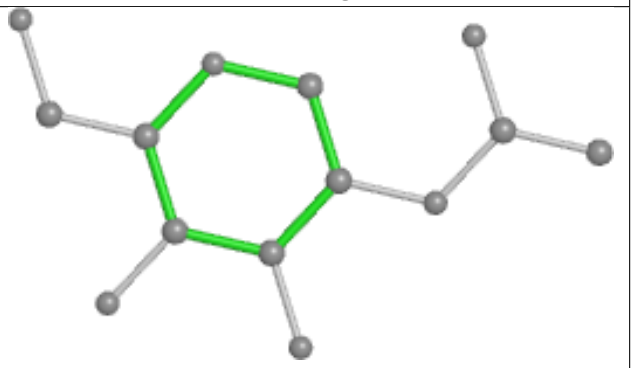
Bond lengths



Bond angles

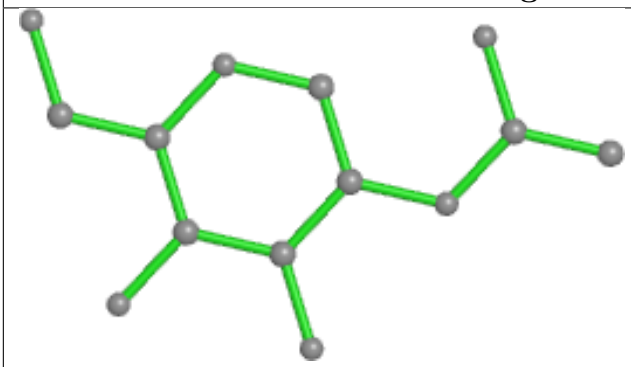


Torsions

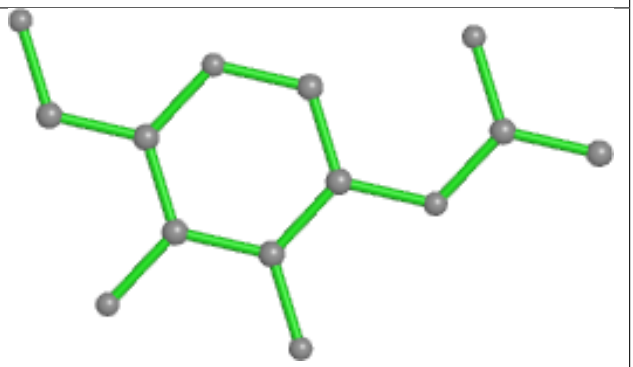


Rings

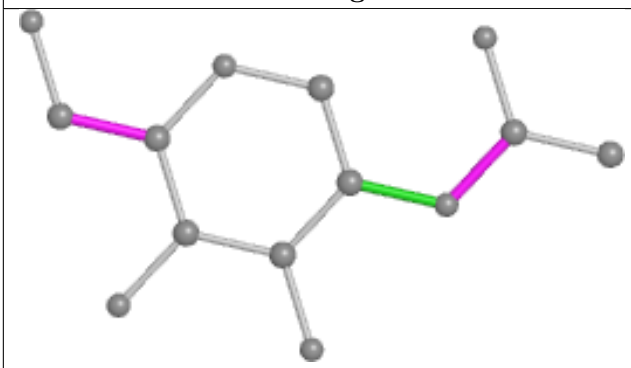
**Ligand NAG C 601**



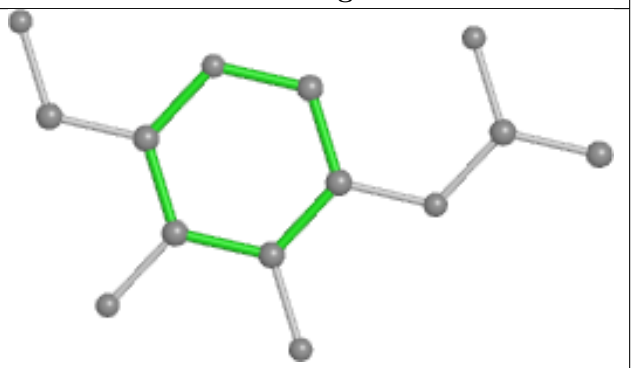
Bond lengths



Bond angles

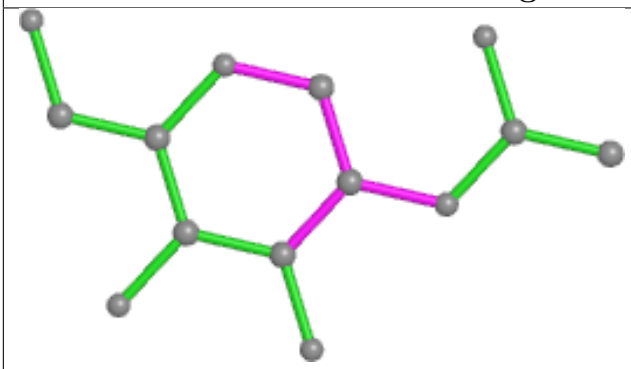


Torsions

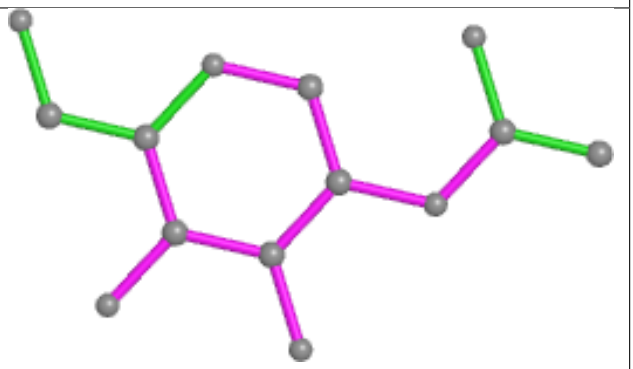


Rings

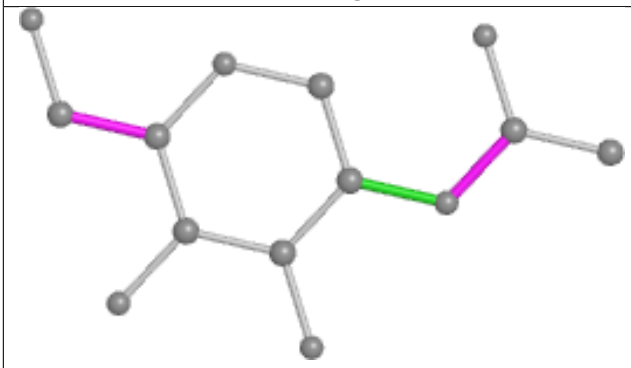
**Ligand NAG H 601**



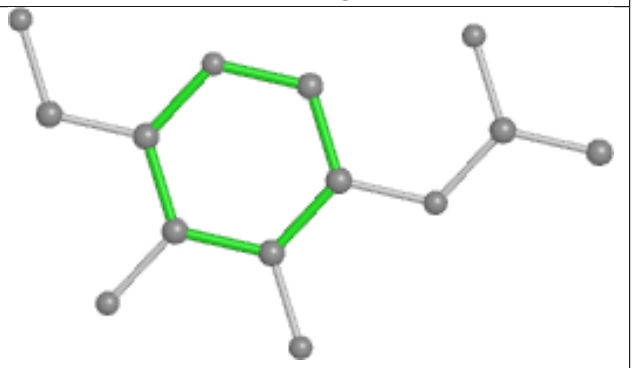
Bond lengths



Bond angles

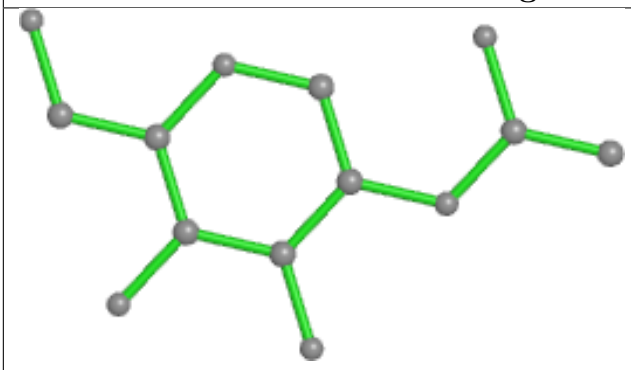


Torsions

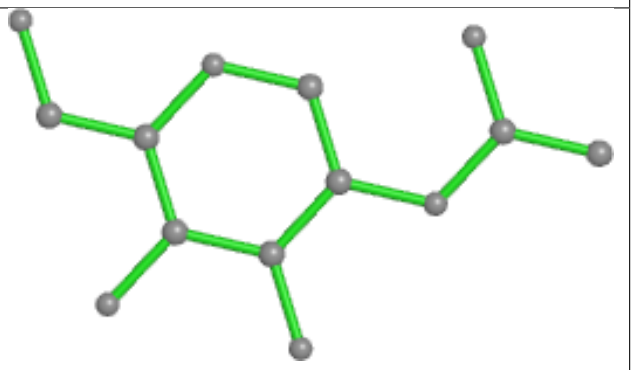


Rings

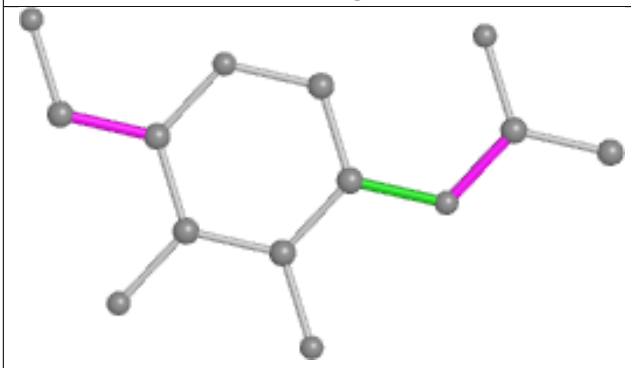
**Ligand NAG K 601**



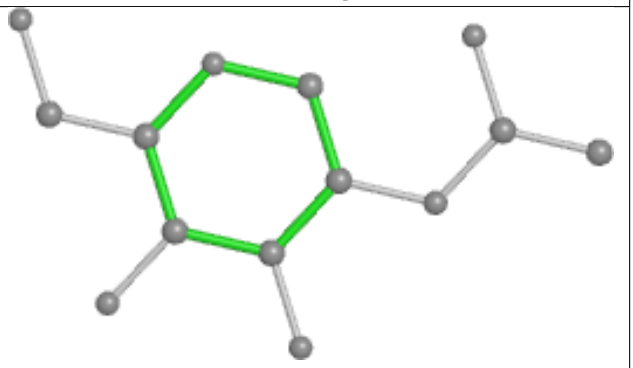
Bond lengths



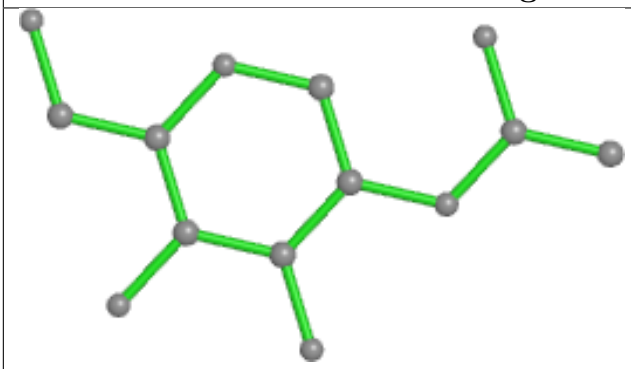
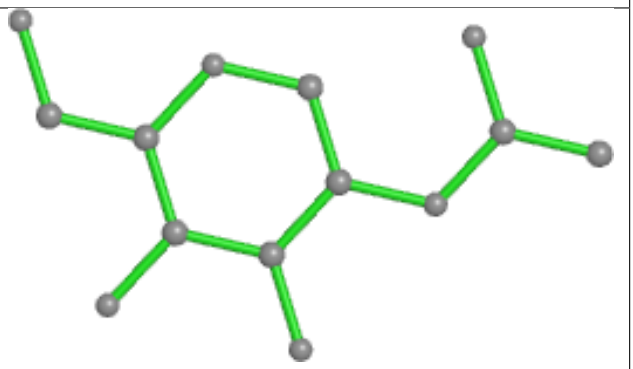
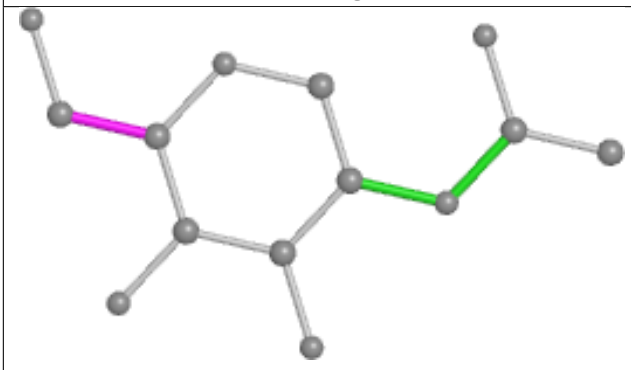
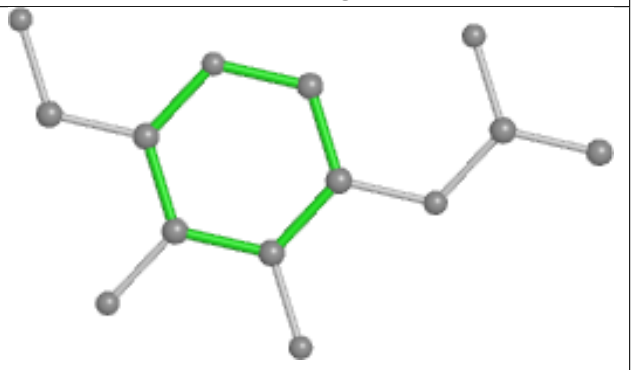
Bond angles



Torsions



Rings

| Ligand NAG D 601 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

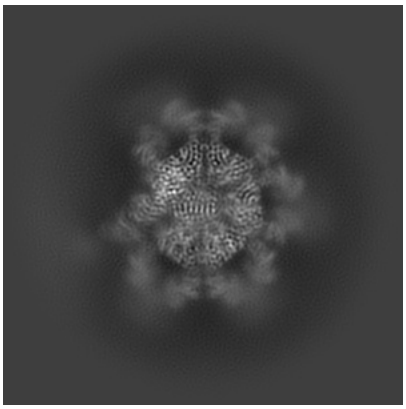
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34074. These allow visual inspection of the internal detail of the map and identification of artifacts.

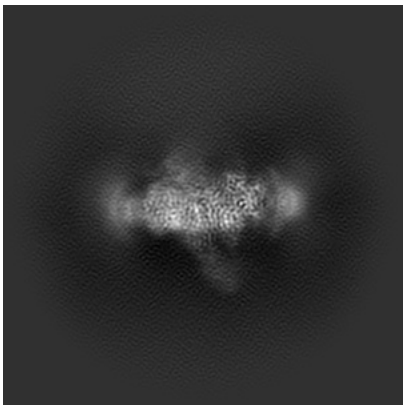
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

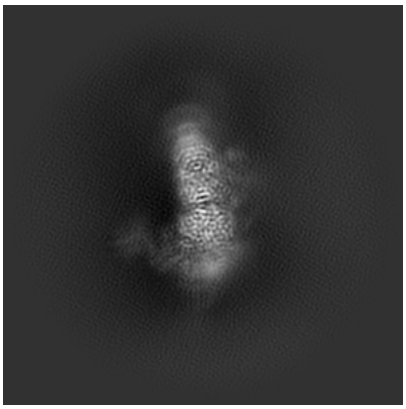
### 6.1.1 Primary map



X

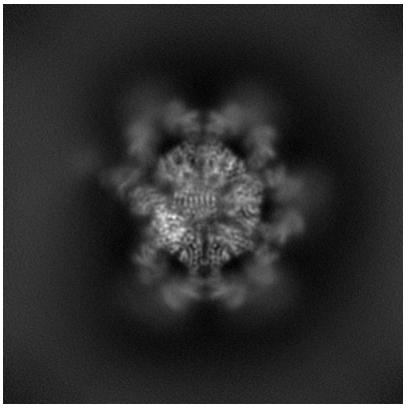


Y

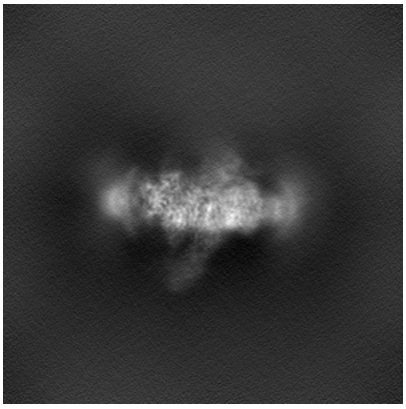


Z

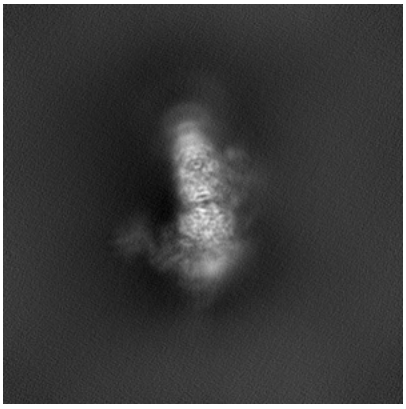
### 6.1.2 Raw map



X



Y

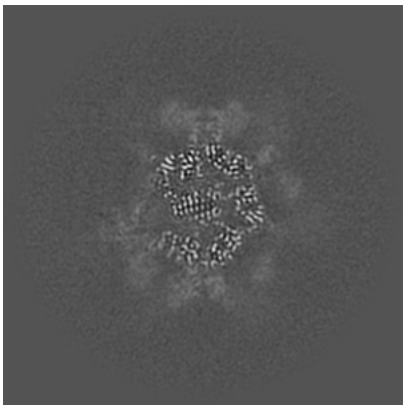


Z

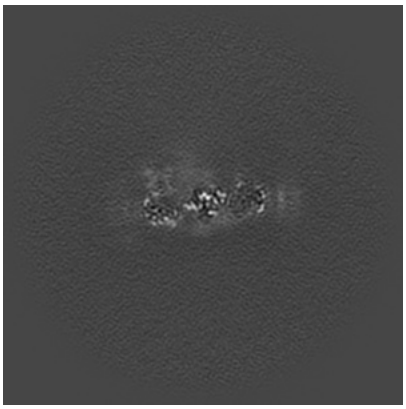
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

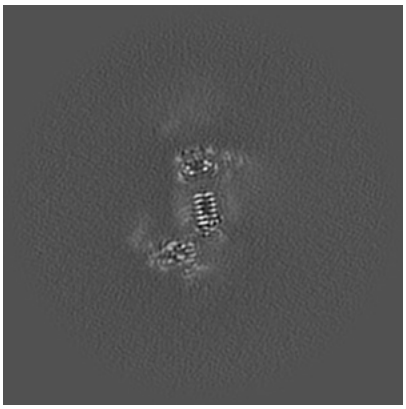
### 6.2.1 Primary map



X Index: 160

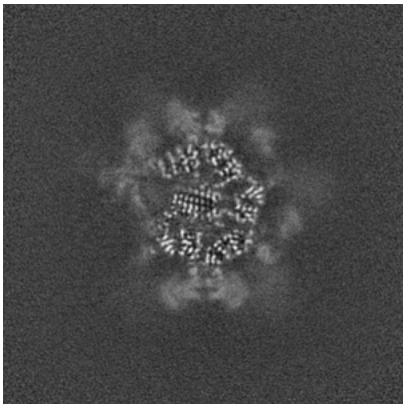


Y Index: 160

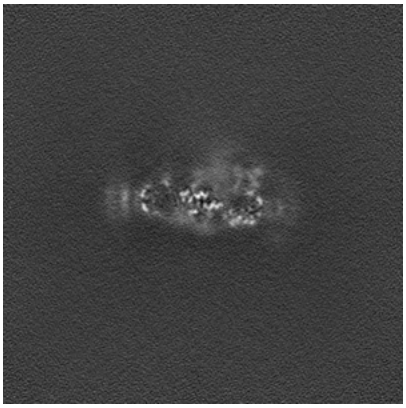


Z Index: 160

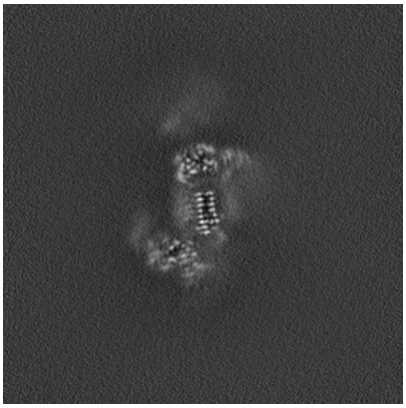
### 6.2.2 Raw map



X Index: 160



Y Index: 160

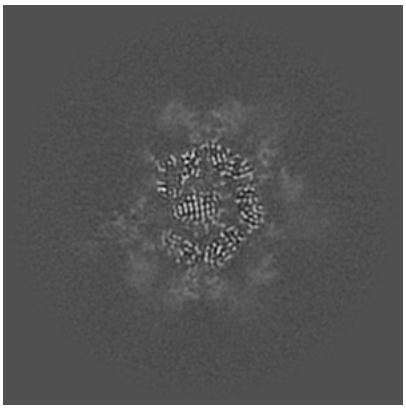


Z Index: 160

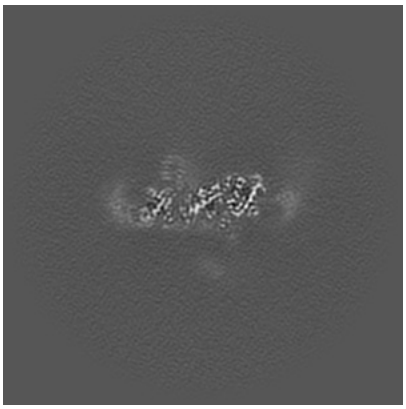
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

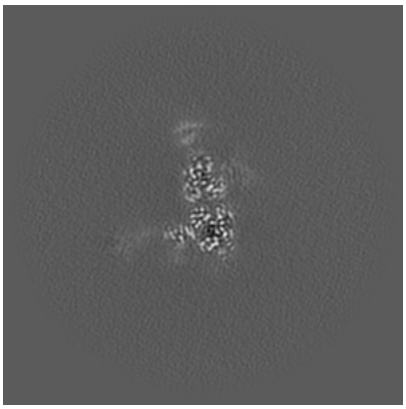
### 6.3.1 Primary map



X Index: 158

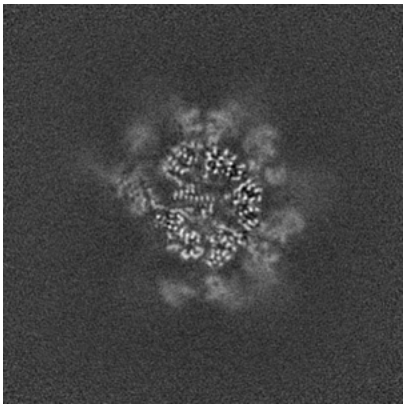


Y Index: 146

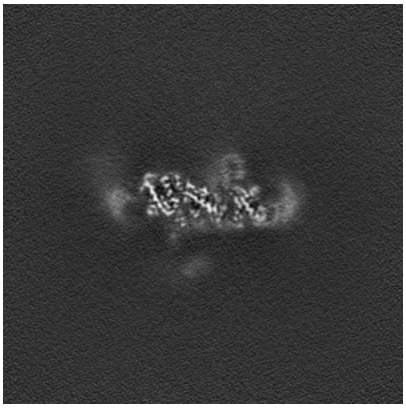


Z Index: 187

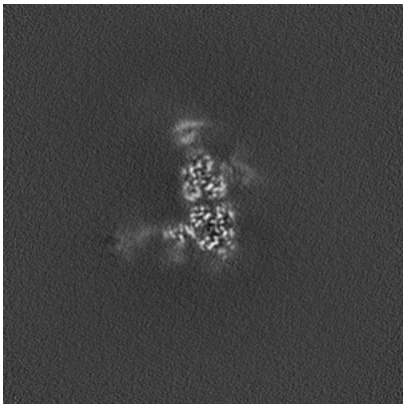
### 6.3.2 Raw map



X Index: 153



Y Index: 146

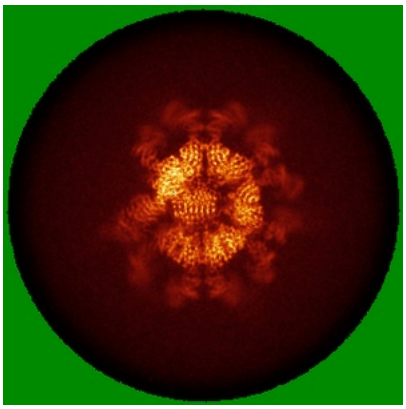


Z Index: 132

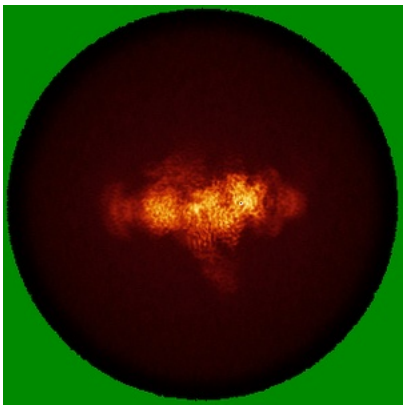
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

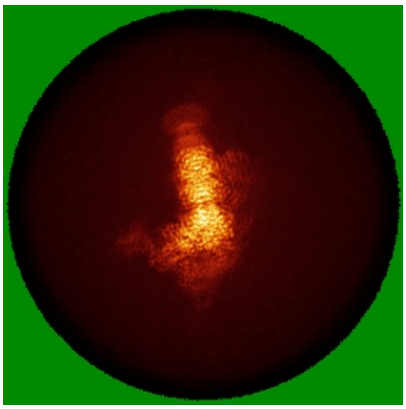
### 6.4.1 Primary map



X

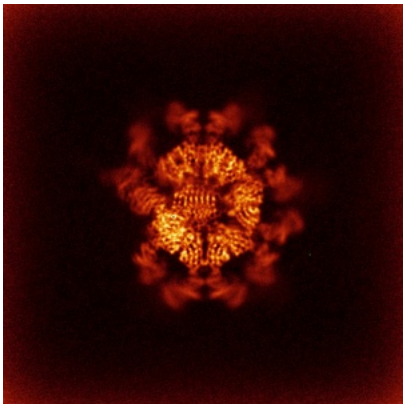


Y

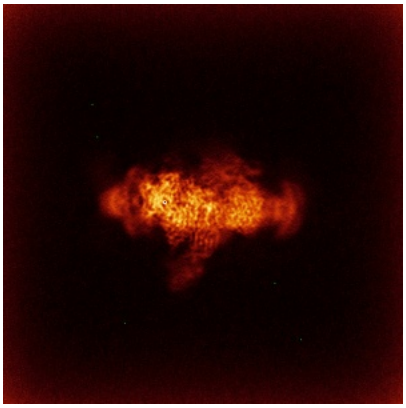


Z

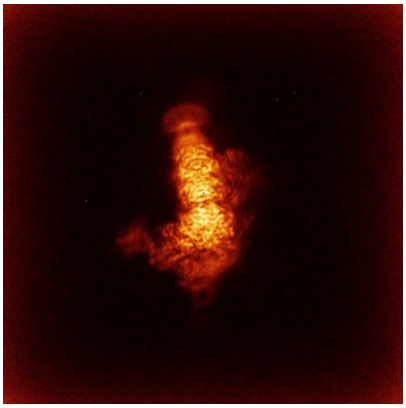
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

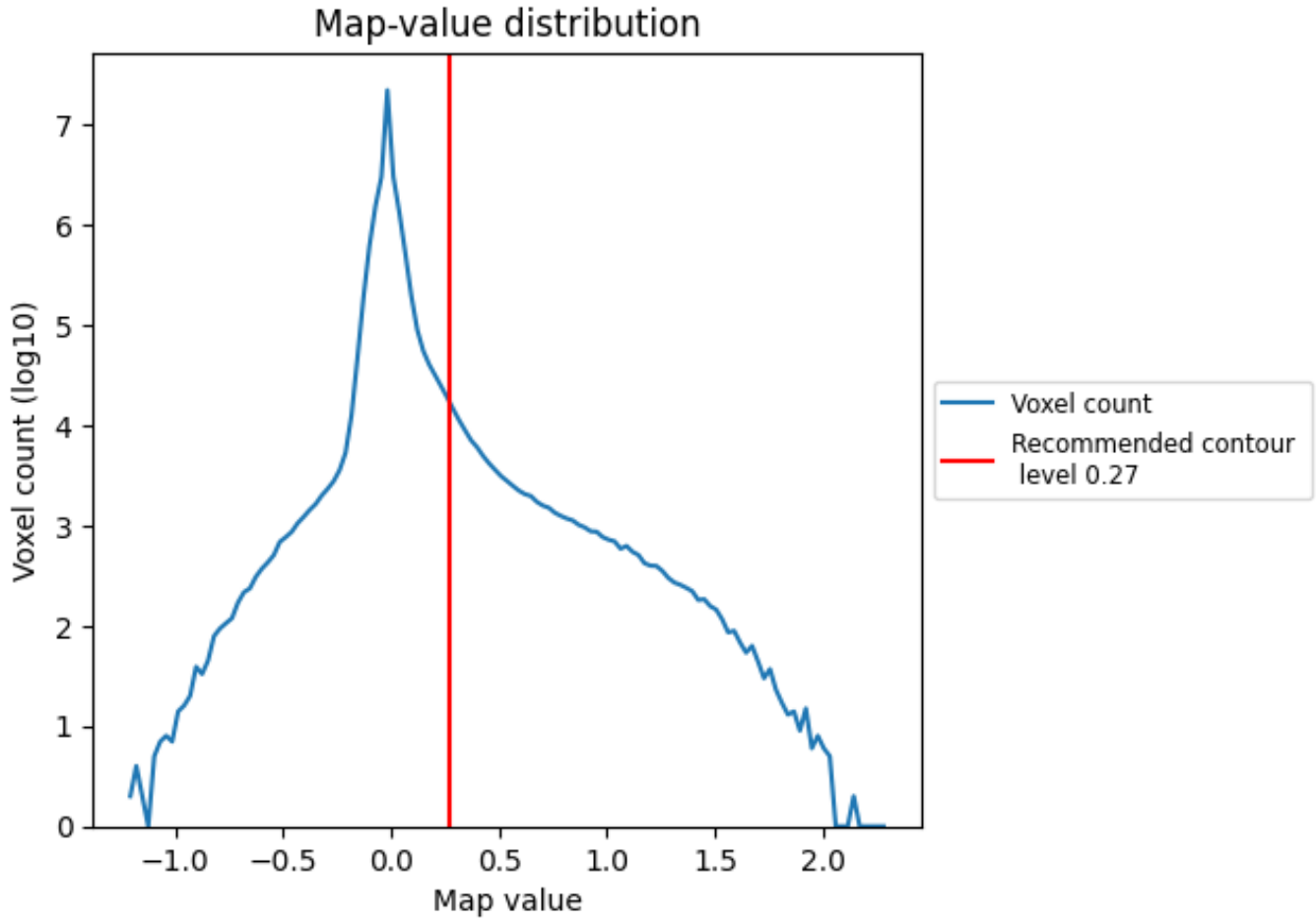
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

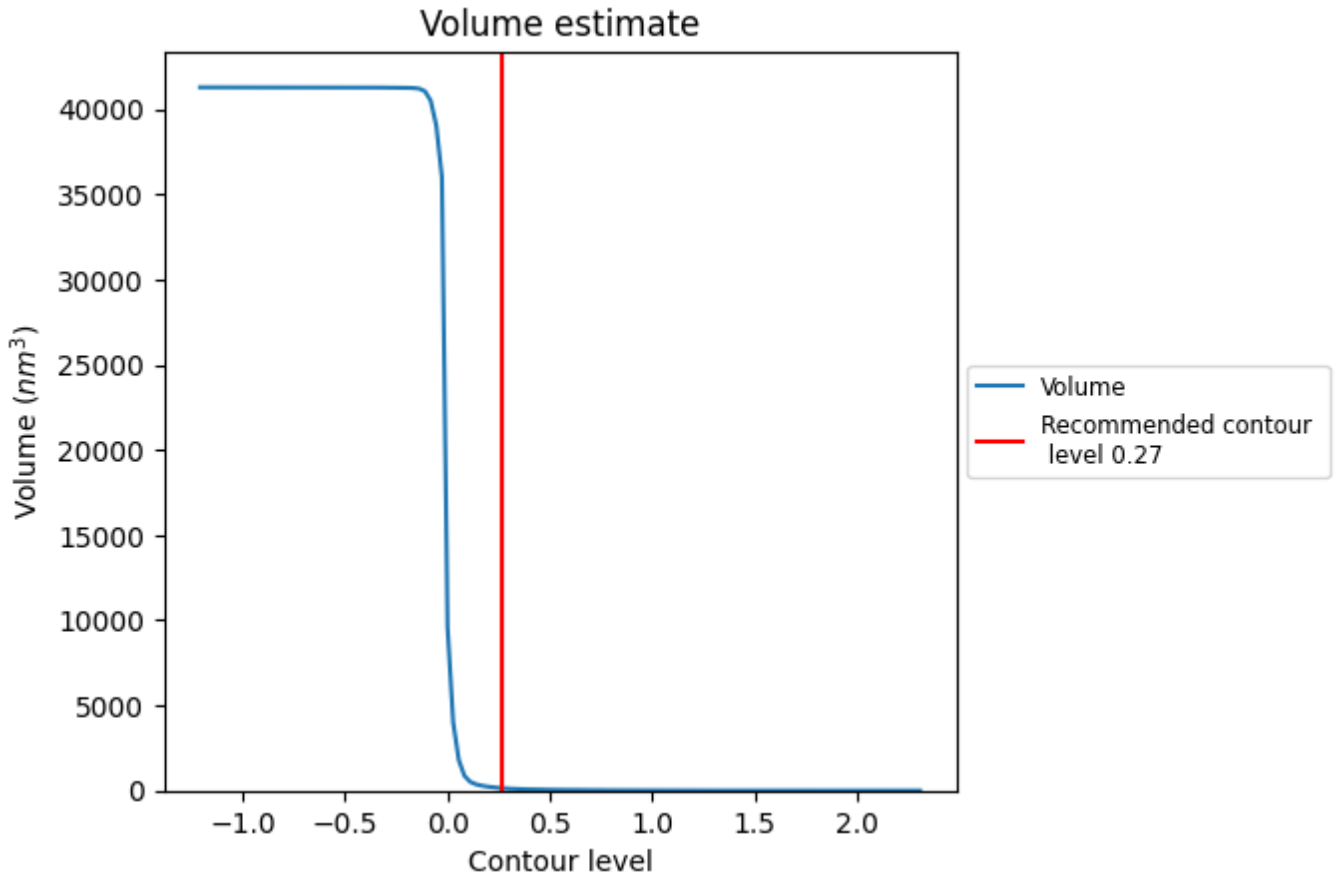
This section contains the results of statistical analysis of the map.

## 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.

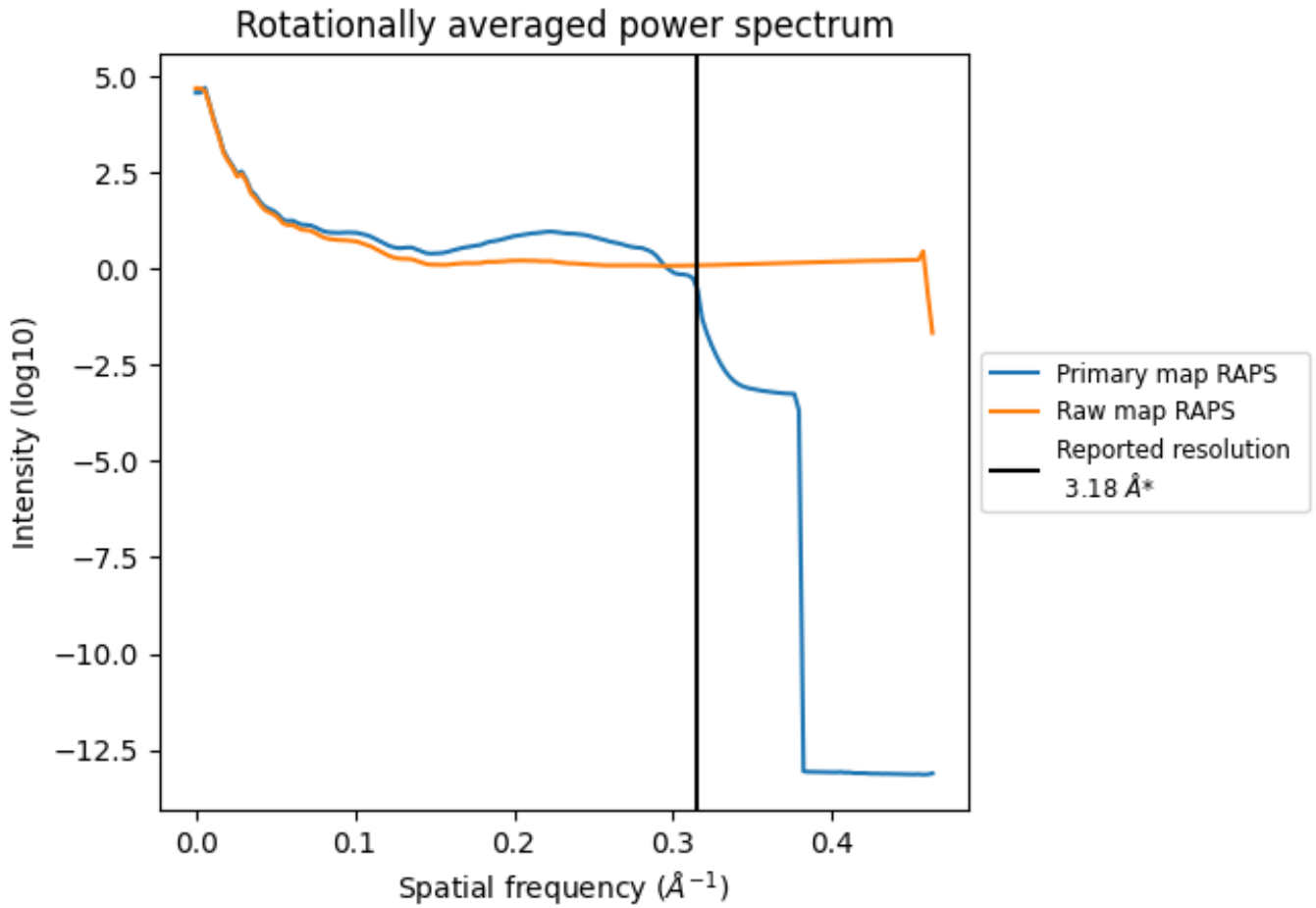
## 7.2 Volume estimate




The volume at the recommended contour level is 137 $nm^3$; this corresponds to an approximate mass of 124 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 (i)

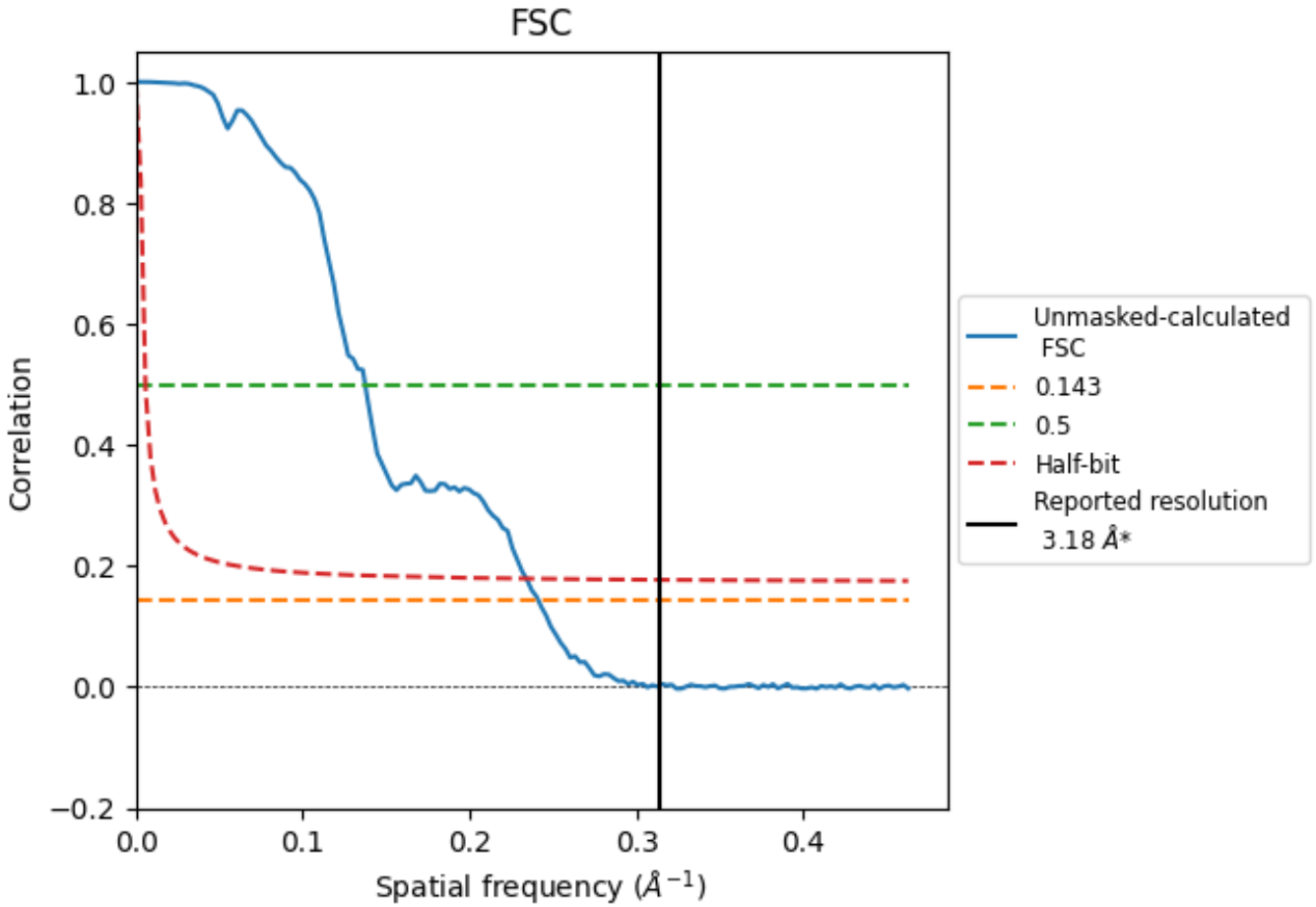



*Reported resolution corresponds to spatial frequency of 0.314 $Å^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.314 Å$^{-1}$

## 8.2 Resolution estimates (i)

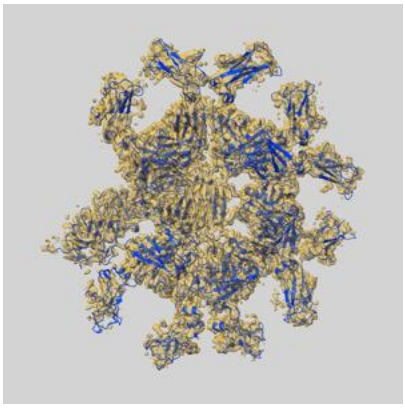
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.18 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 4.15 | 7.28 | 4.27 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.18 by more than 10 %

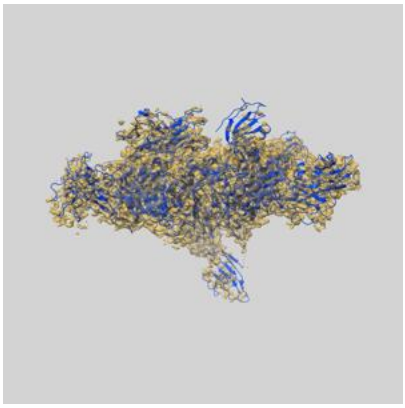
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34074 and PDB model 7YSG. Per-residue inclusion information can be found in section 3 on page 7.

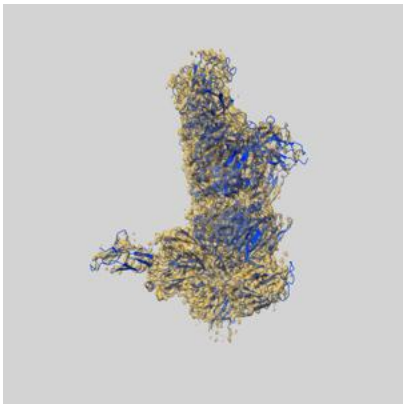
## 9.1 Map-model overlay



X



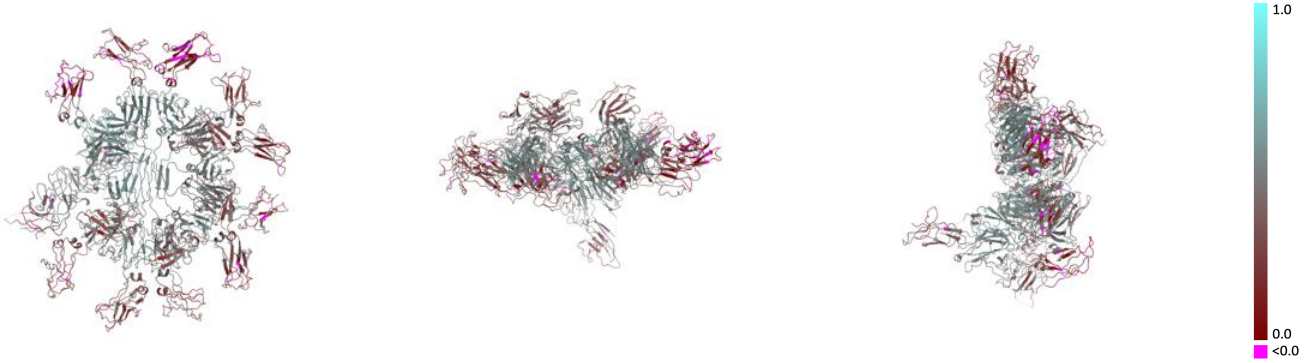
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.27 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.

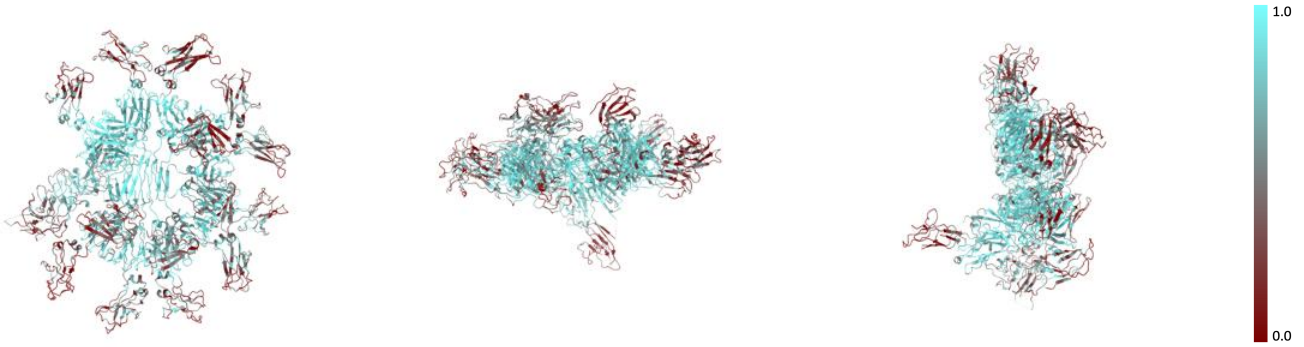
## 9.2 Q-score mapped to coordinate model (i)




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.

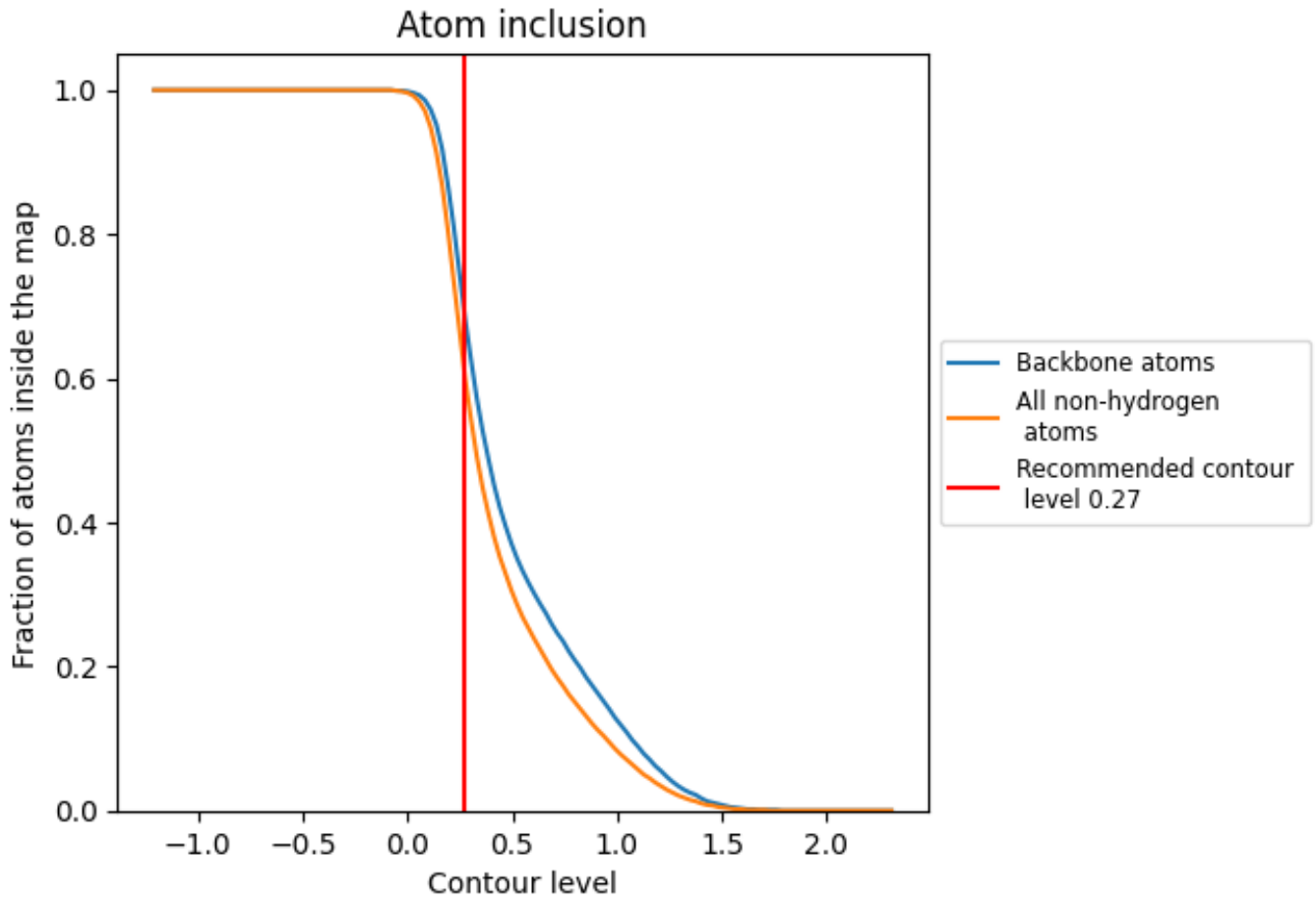
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.27).

## 9.4 Atom inclusion (i)




At the recommended contour level, 70% of all backbone atoms, 61% 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 (0.27) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6130 | 0.4170 |
| A | 0.7060 | 0.4120 |
| B | 0.6740 | 0.4140 |
| C | 0.6330 | 0.3630 |
| D | 0.6710 | 0.4220 |
| E | 0.6530 | 0.4120 |
| F | 0.6720 | 0.4230 |
| G | 0.6590 | 0.4200 |
| H | 0.6520 | 0.4220 |
| I | 0.8570 | 0.5310 |
| J | 0.8730 | 0.5460 |
| K | 0.6670 | 0.4280 |
| L | 0.5250 | 0.3900 |
| P | 0.5720 | 0.4370 |
| R | 0.3350 | 0.3800 |
| S | 0.4800 | 0.4030 |
| U | 0.4590 | 0.4160 |
| V | 0.2330 | 0.3610 |