# Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 01:29 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 5MVA |
| EMDB ID | : | EMD-3576 |
| Title | : | Structure of the thin filament at high calcium concentration |
| Authors | : | Paul, D.M.; Squire, J.M.; Morris, E.P. |
| Deposited on | : | 2017-01-16 |
| Resolution | : | 27.70 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 (i) 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 (1)) were used in the production of this report:

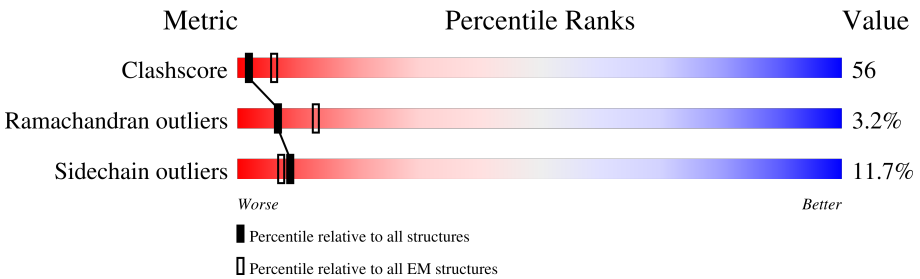
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
|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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 27.70 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 375 | 97%; 56%, 34%, 9%, • |
| 1 | B | 375 | 84%; 57%, 33%, 10%, • |
| 1 | C | 375 | 28%; 55%, 35%, 9%, • |
| 1 | D | 375 | 67%; 55%, 34%, 10%, • |
| 1 | E | 375 | 10%; 55%, 34%, 10%, • |
| 1 | F | 375 | 55%; 56%, 34%, 9%, • |
| 1 | G | 375 | 17%; 56%, 34%, 9%, • |
| 1 | H | 375 | 43%; 55%, 35%, 9%, • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | I | 375 | 34% 55% 34% 10% |
| 1 | J | 375 | 35% 55% 35% 9% |
| 1 | K | 375 | 42% 56% 34% 10% |
| 1 | L | 375 | 39% 55% 35% 9% |
| 1 | M | 375 | 43% 55% 34% 10% |
| 1 | N | 375 | 38% 55% 35% 9% |
| 1 | O | 375 | 45% 55% 34% 10% |
| 1 | P | 375 | 22% 55% 35% 9% |
| 1 | Q | 375 | 57% 56% 34% 9% |
| 1 | R | 375 | 7% 56% 34% 9% |
| 1 | S | 375 | 51% 56% 34% 9% |
| 1 | T | 375 | 20% 55% 35% 10% |
| 1 | U | 375 | 44% 56% 34% 9% |
| 1 | V | 375 | 28% 56% 34% 9% |
| 1 | W | 375 | 39% 56% 35% 9% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 68103 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 Actin, alpha skeletal muscle.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | B | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | C | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | D | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | E | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | F | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | G | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | H | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | I | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | J | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | K | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | L | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | M | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | N | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | O | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | P | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | Q | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |

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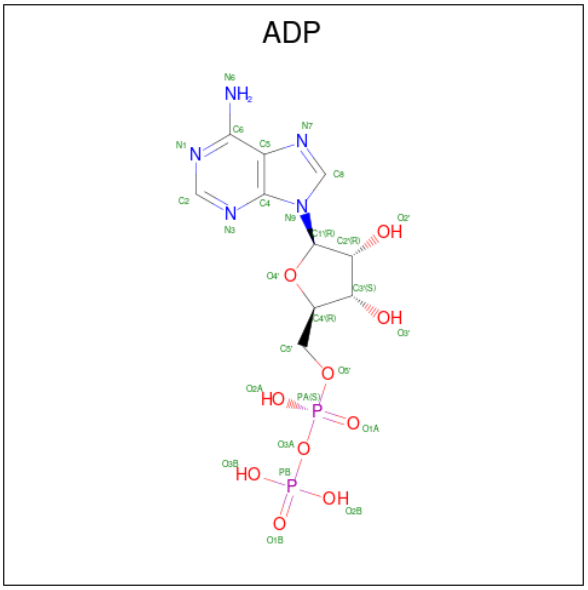
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | R | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | S | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | T | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | U | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | V | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |
| 1 | W | 375 | 2934 | 1855 | 493 | 565 | 21 | 0 | 0 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 2 | A | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | B | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | C | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | D | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | E | 1 | 27 | 10 | 5 | 10 | 2 | 0 |

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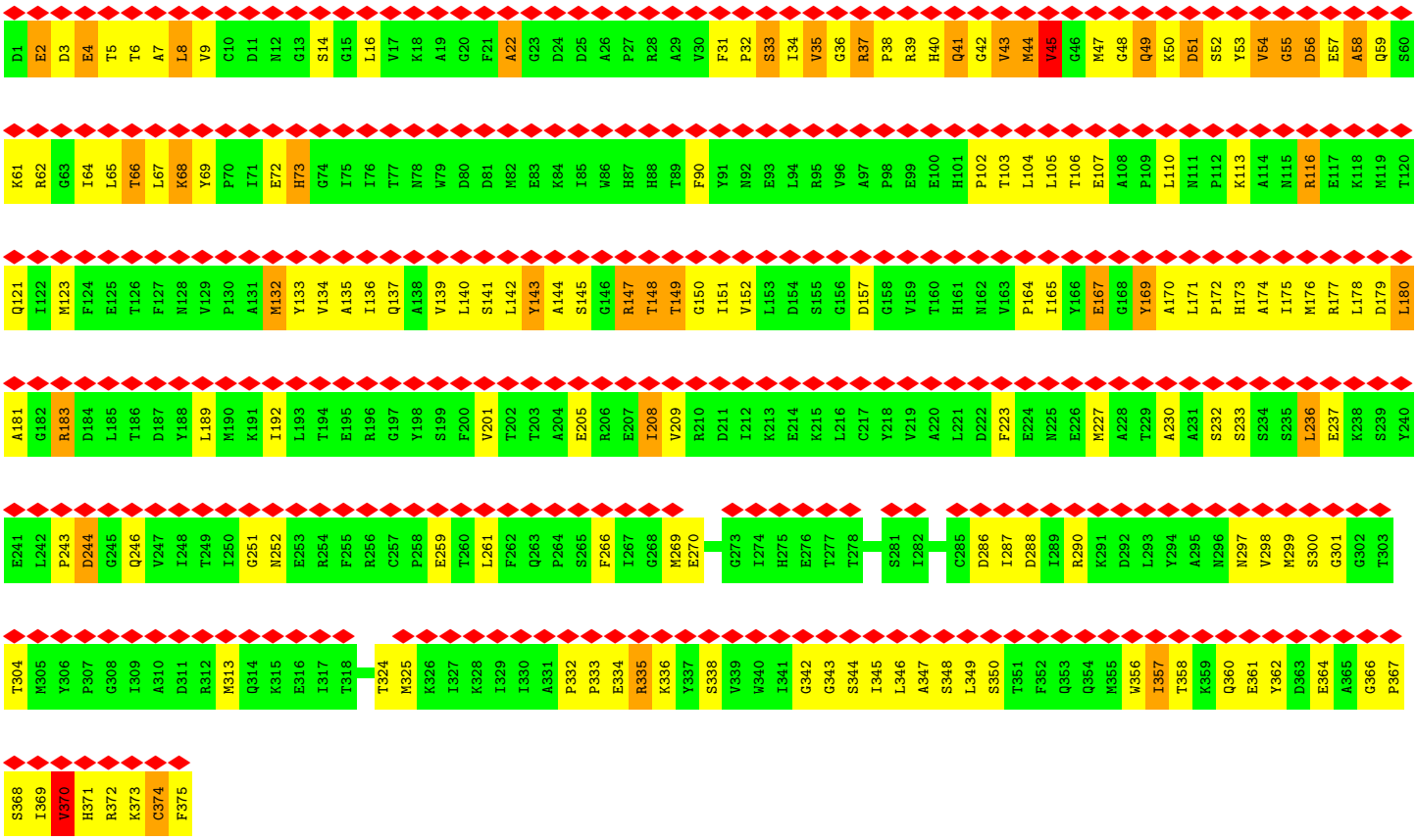
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 2 | F | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | G | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | H | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | I | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | J | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | K | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | L | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | M | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | N | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | O | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | P | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | Q | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | R | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | S | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | T | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | U | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | V | 1 | 27 | 10 | 5 | 10 | 2 | 0 |
| 2 | W | 1 | 27 | 10 | 5 | 10 | 2 | 0 |

# 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.

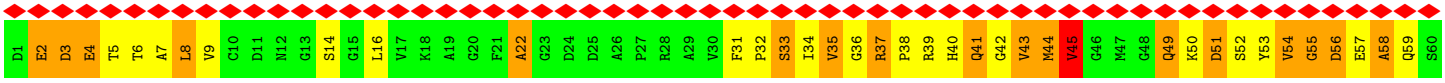
- Molecule 1: Actin, alpha skeletal muscle

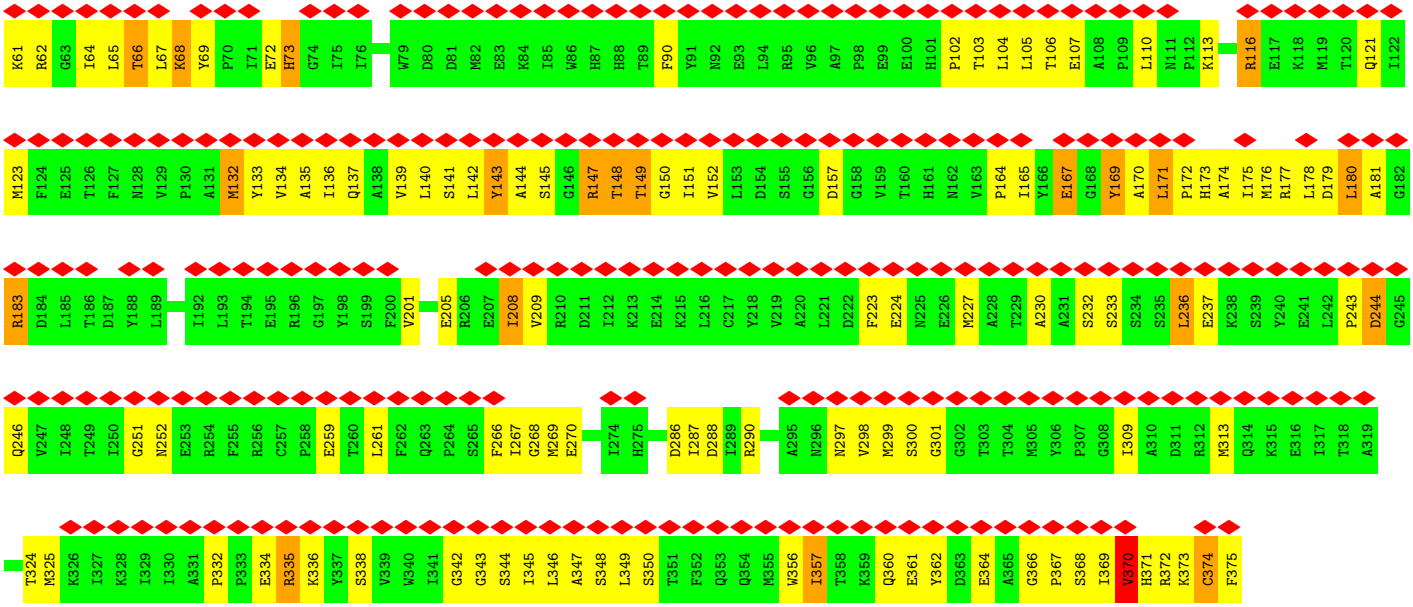
Chain A: 97%




- Molecule 1: Actin, alpha skeletal muscle

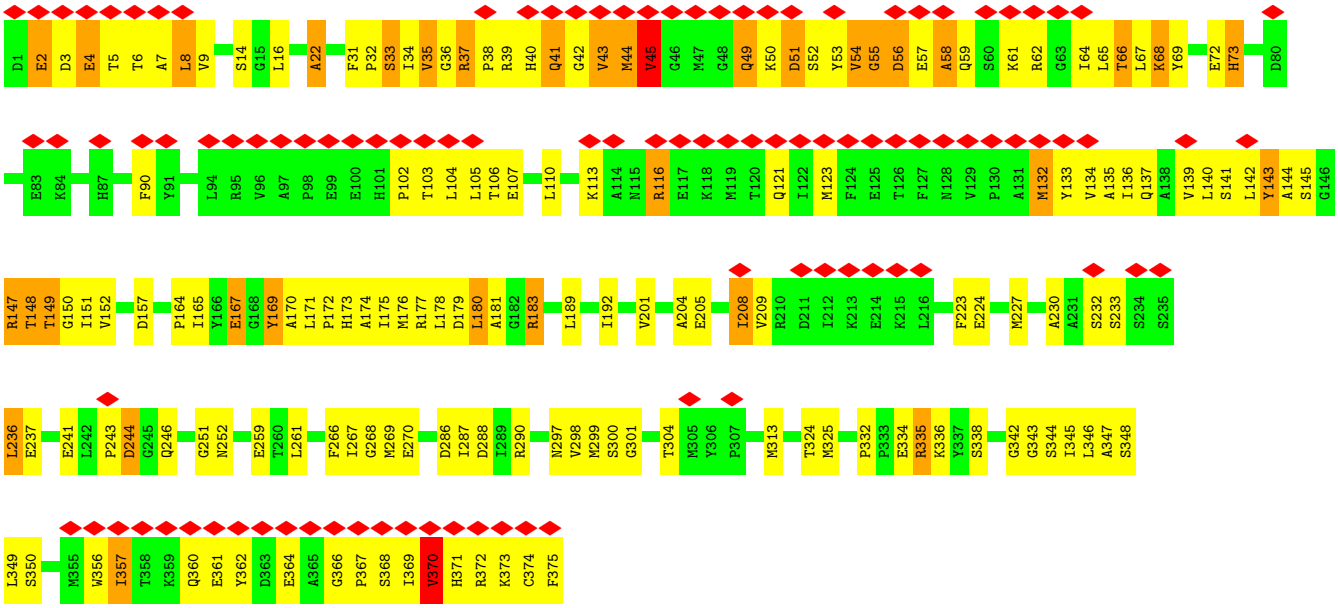
Chain B: 84%





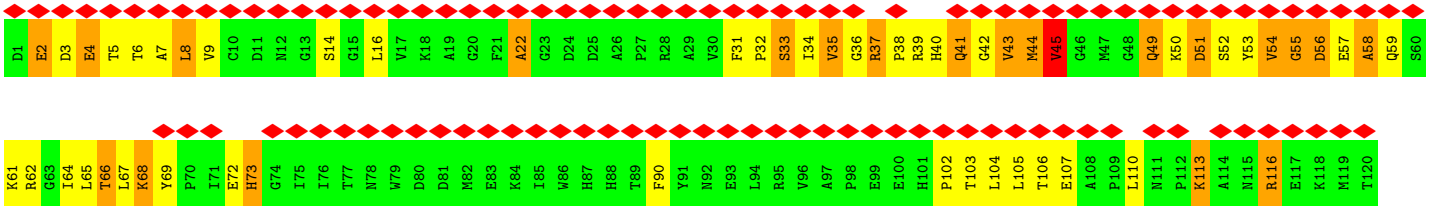

- Molecule 1: Actin, alpha skeletal muscle

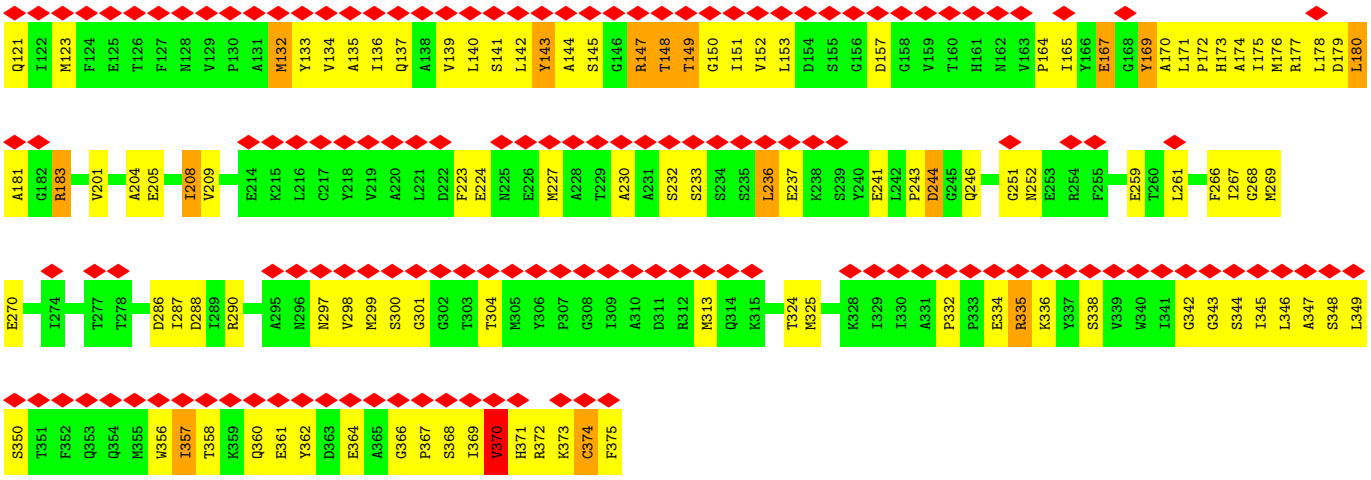
Chain C:




- Molecule 1: Actin, alpha skeletal muscle

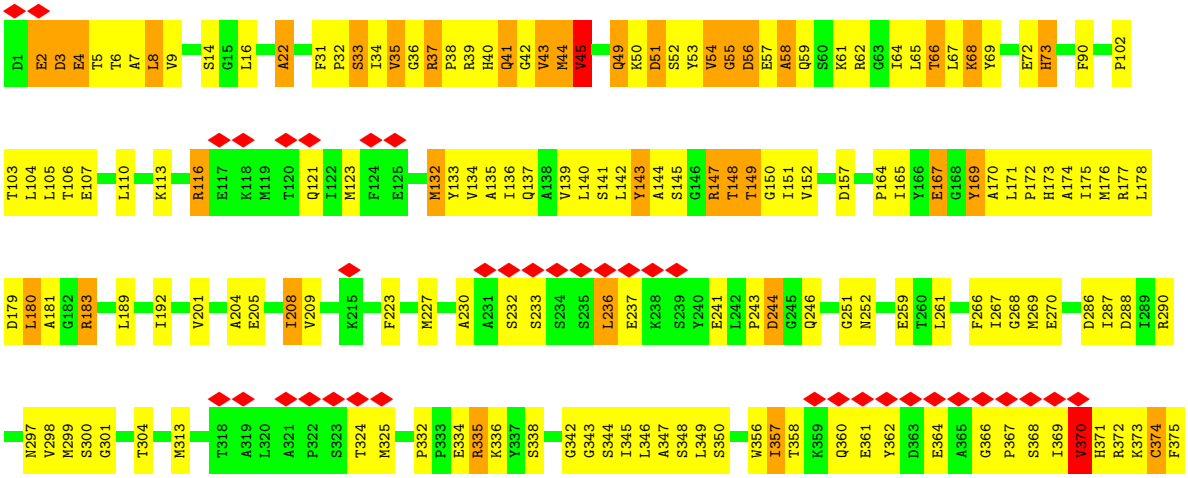
Chain D:





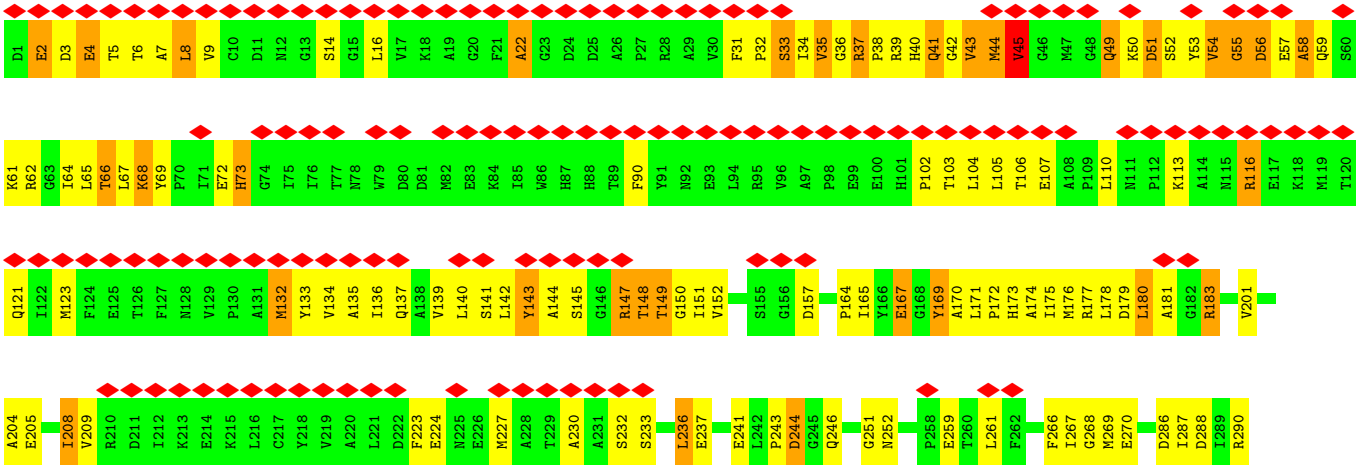

- Molecule 1: Actin, alpha skeletal muscle

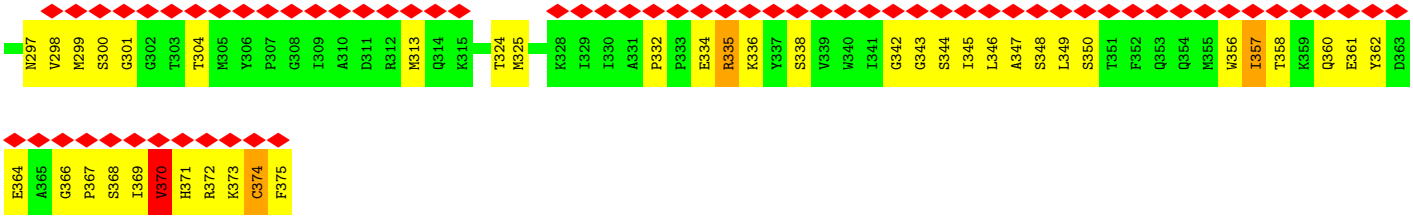
Chain E:




- Molecule 1: Actin, alpha skeletal muscle

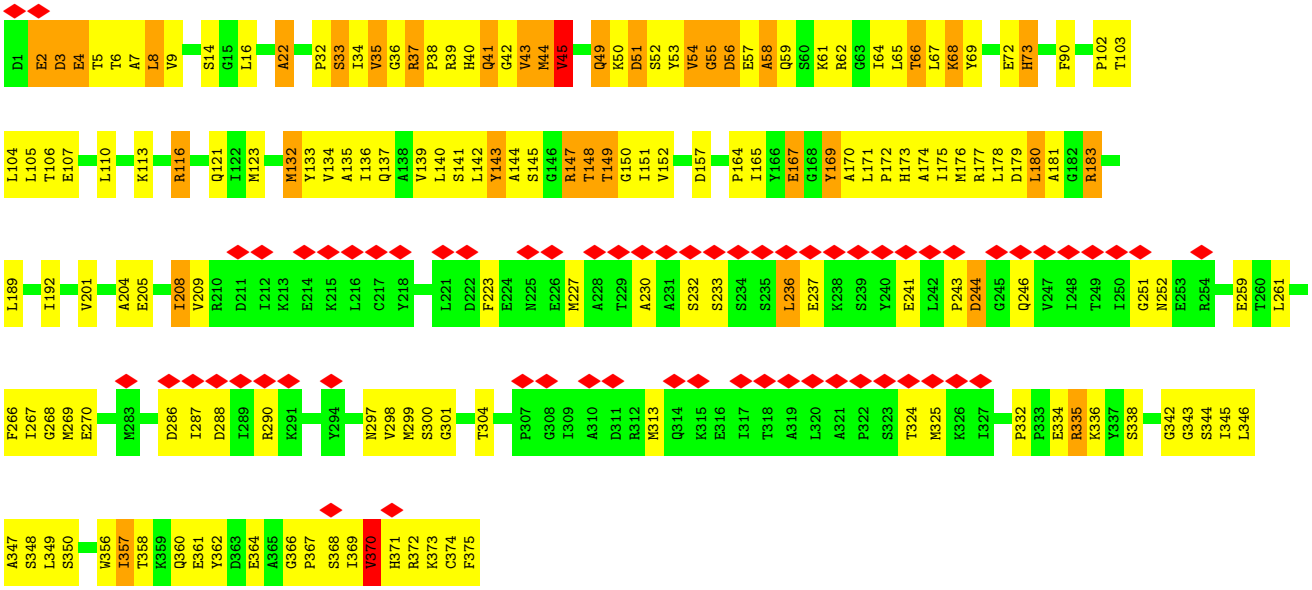
Chain F:





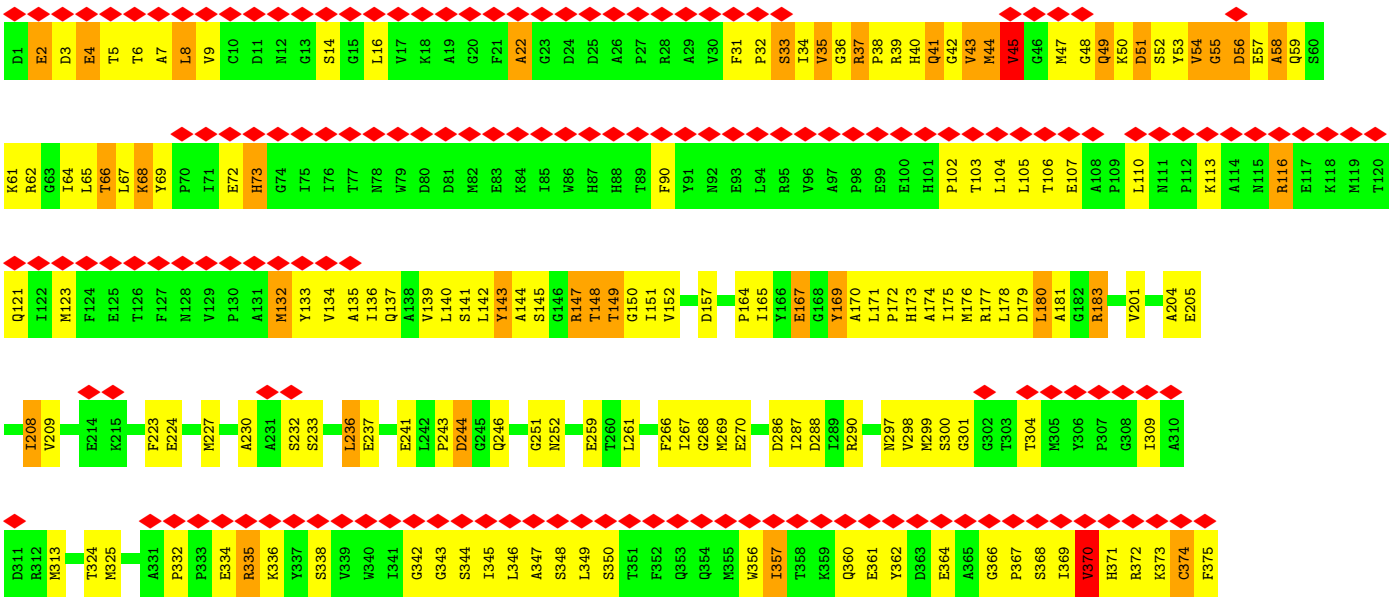

• Molecule 1: Actin, alpha skeletal muscle

Chain G: 17% 56% 34% 9%



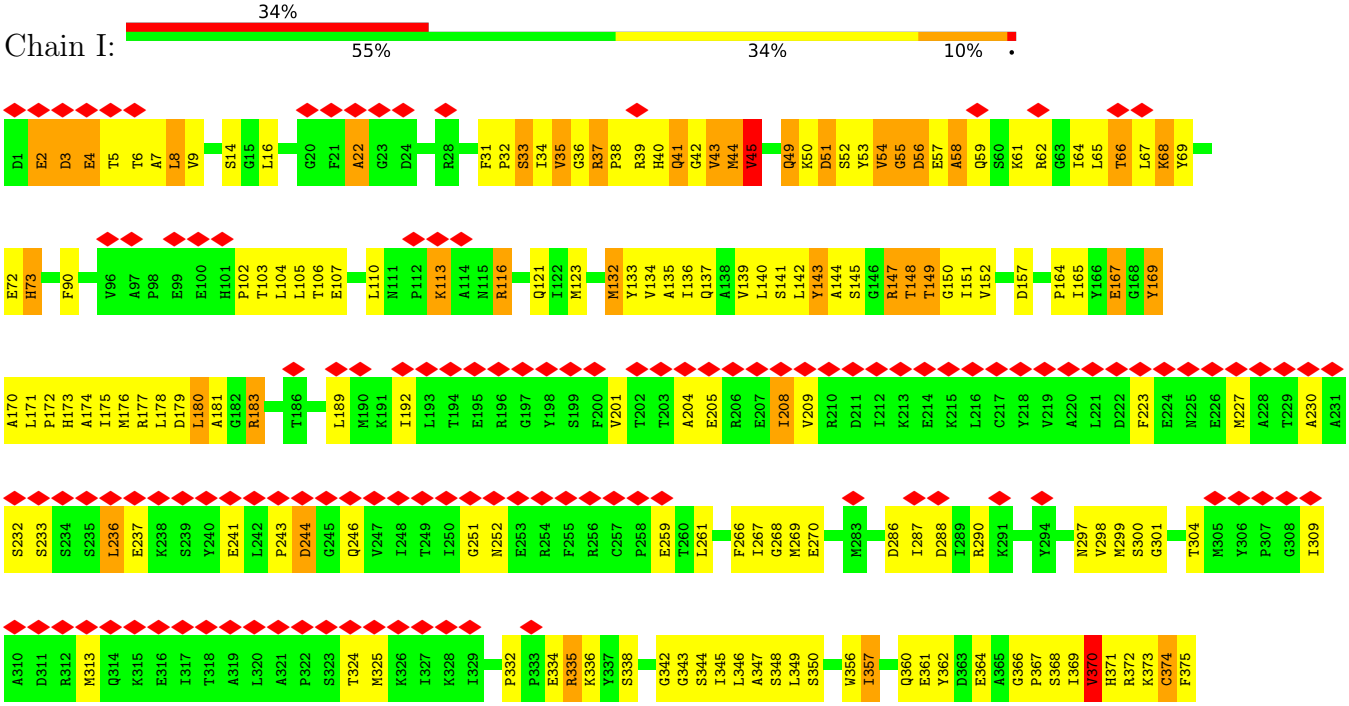

• Molecule 1: Actin, alpha skeletal muscle

Chain H: 43% 55% 35% 9%



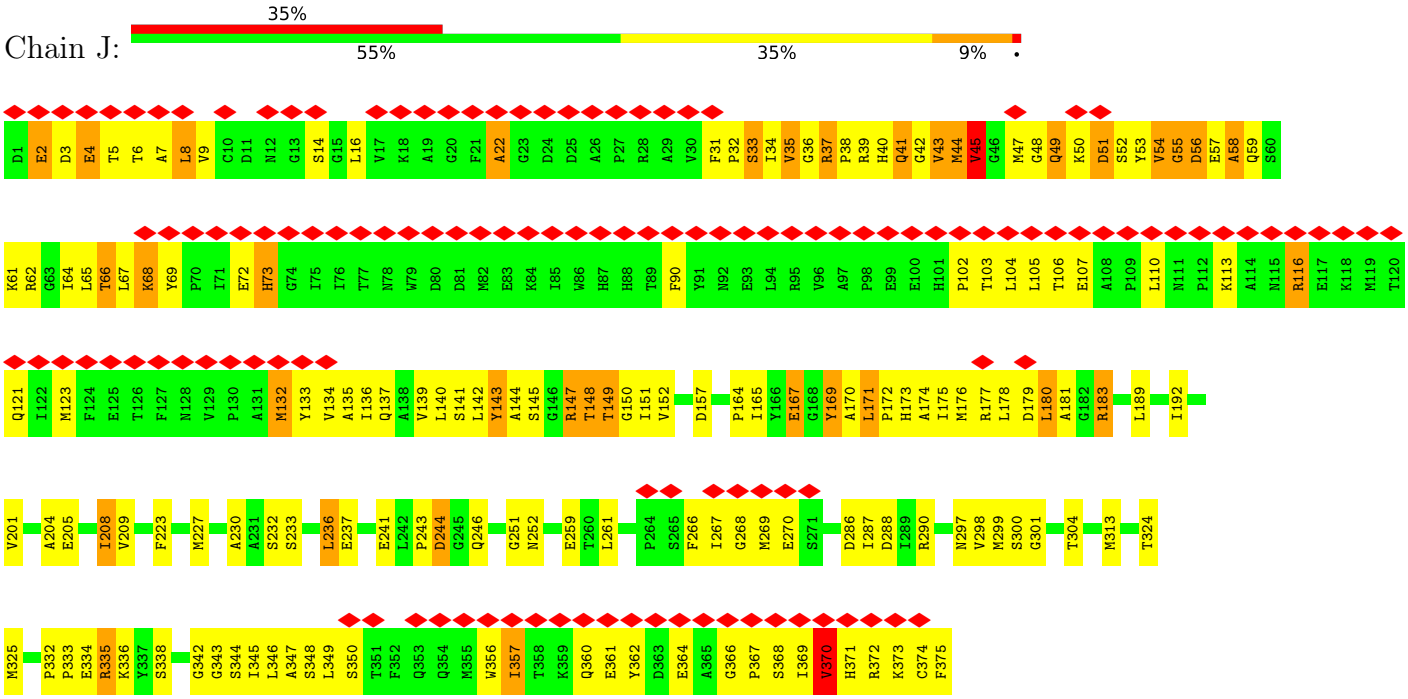
- Molecule 1: Actin, alpha skeletal muscle

Chain I:



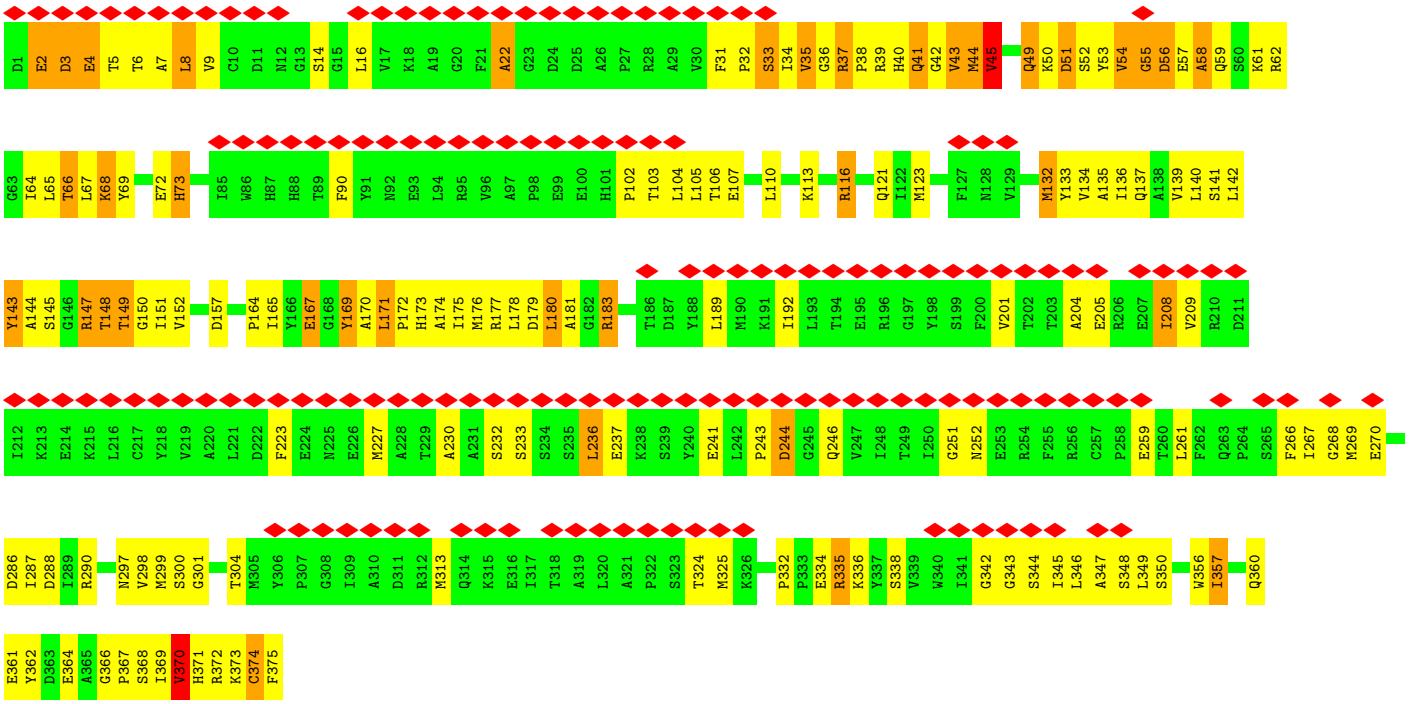

- Molecule 1: Actin, alpha skeletal muscle

Chain J:



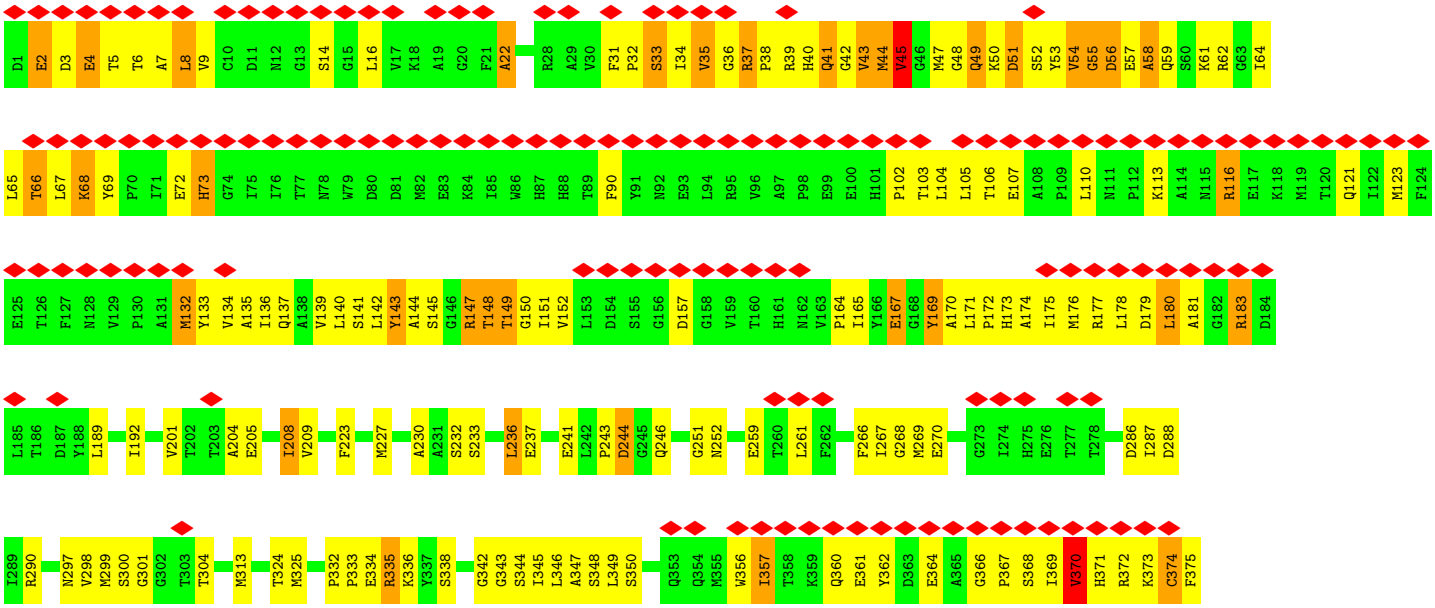

- Molecule 1: Actin, alpha skeletal muscle

Chain K:



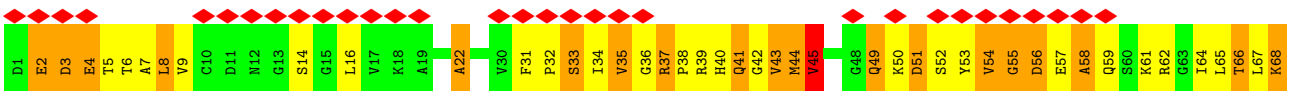

- Molecule 1: Actin, alpha skeletal muscle

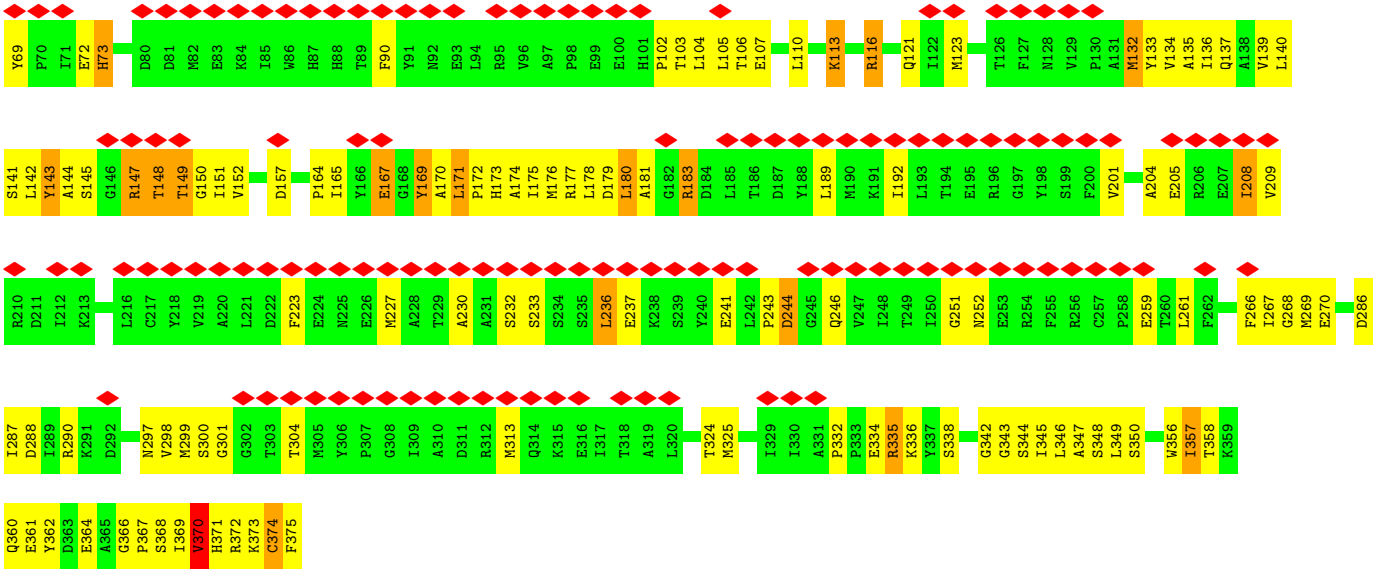
Chain L:




- Molecule 1: Actin, alpha skeletal muscle

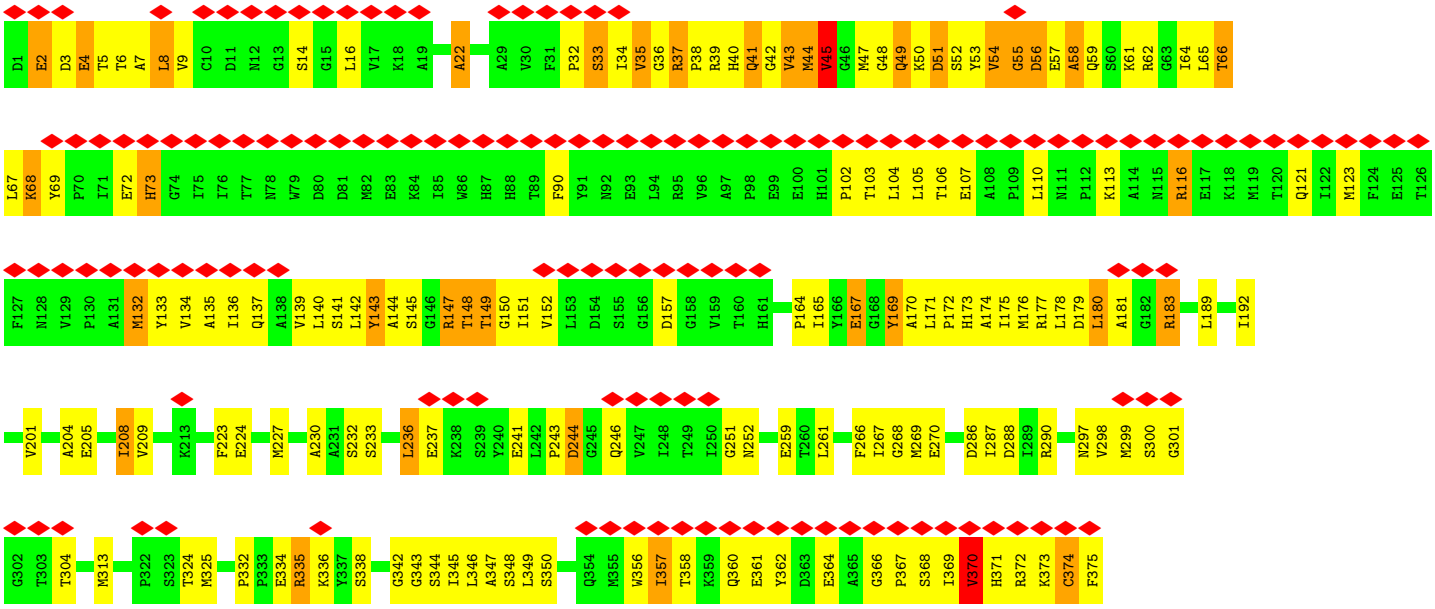
Chain M:





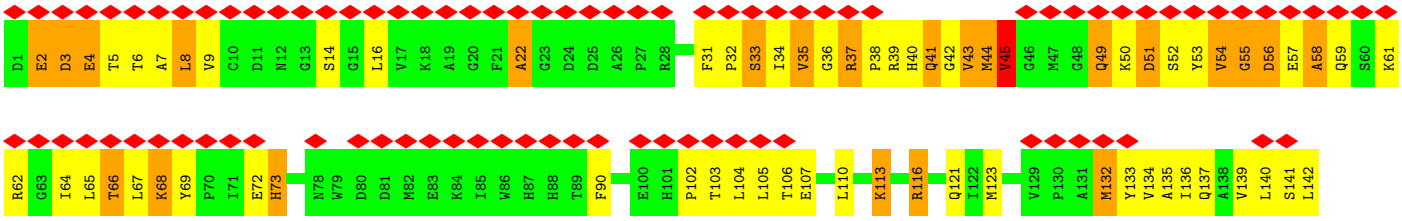

- Molecule 1: Actin, alpha skeletal muscle

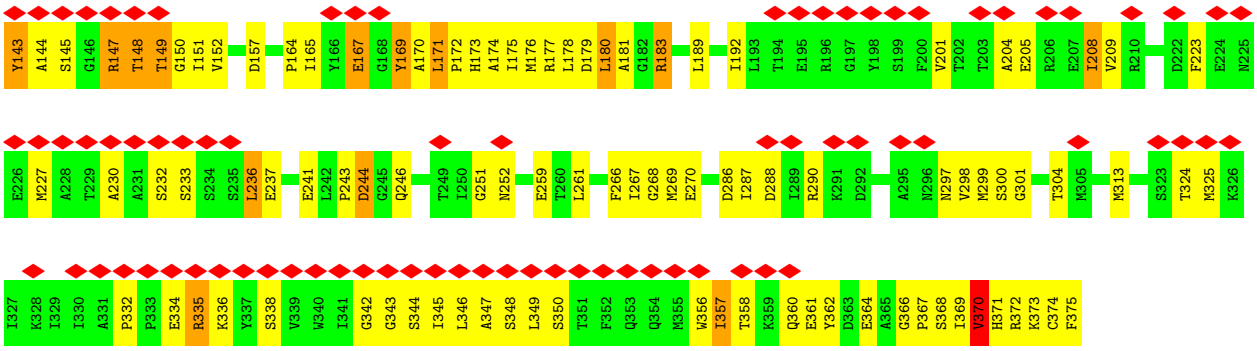
Chain N:




- Molecule 1: Actin, alpha skeletal muscle

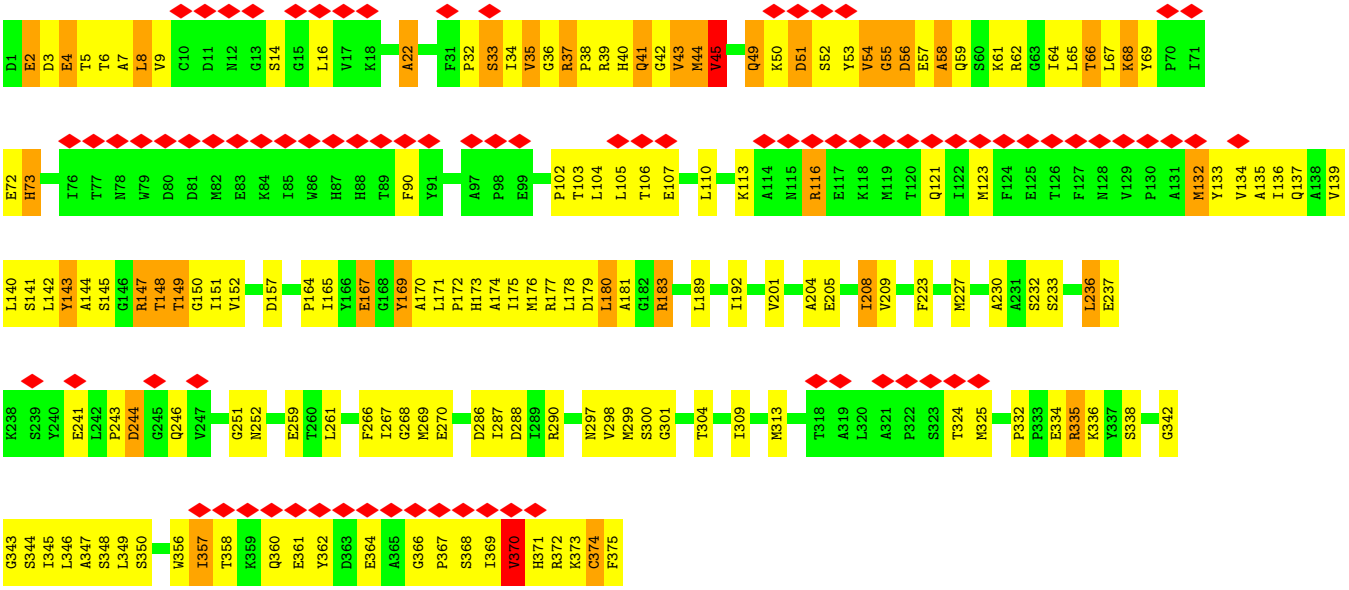
Chain O:





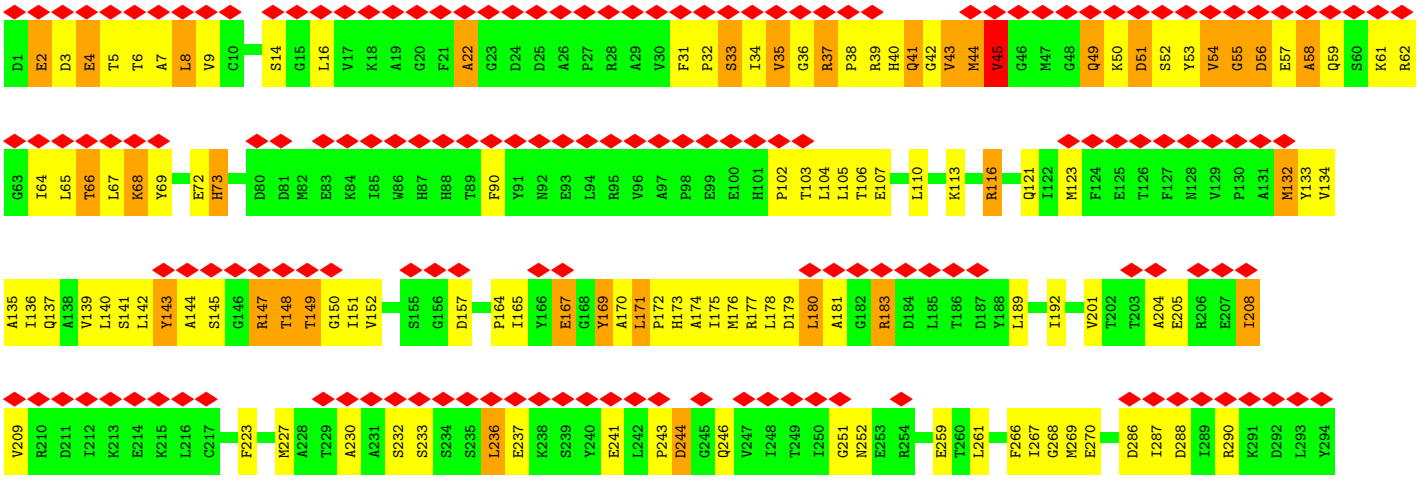

• Molecule 1: Actin, alpha skeletal muscle

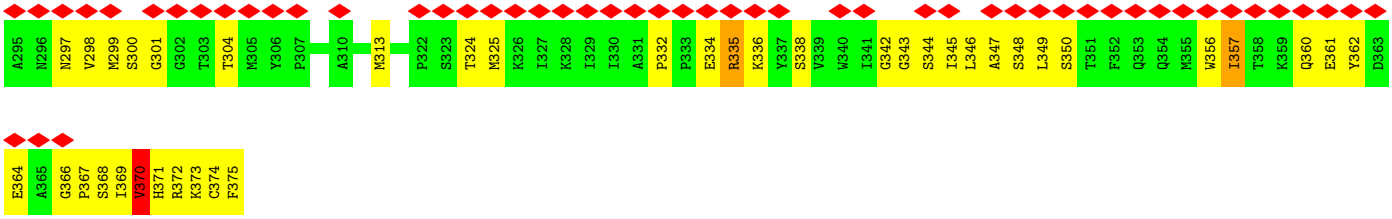
Chain P:




• Molecule 1: Actin, alpha skeletal muscle

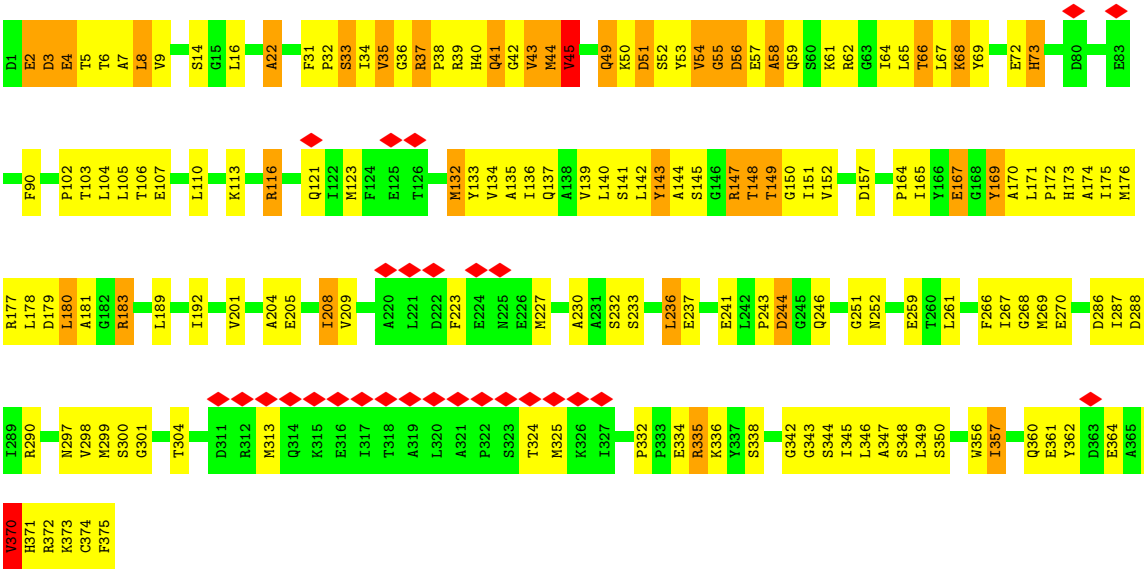
Chain Q:





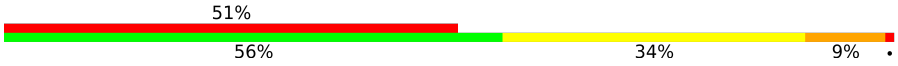

• Molecule 1: Actin, alpha skeletal muscle

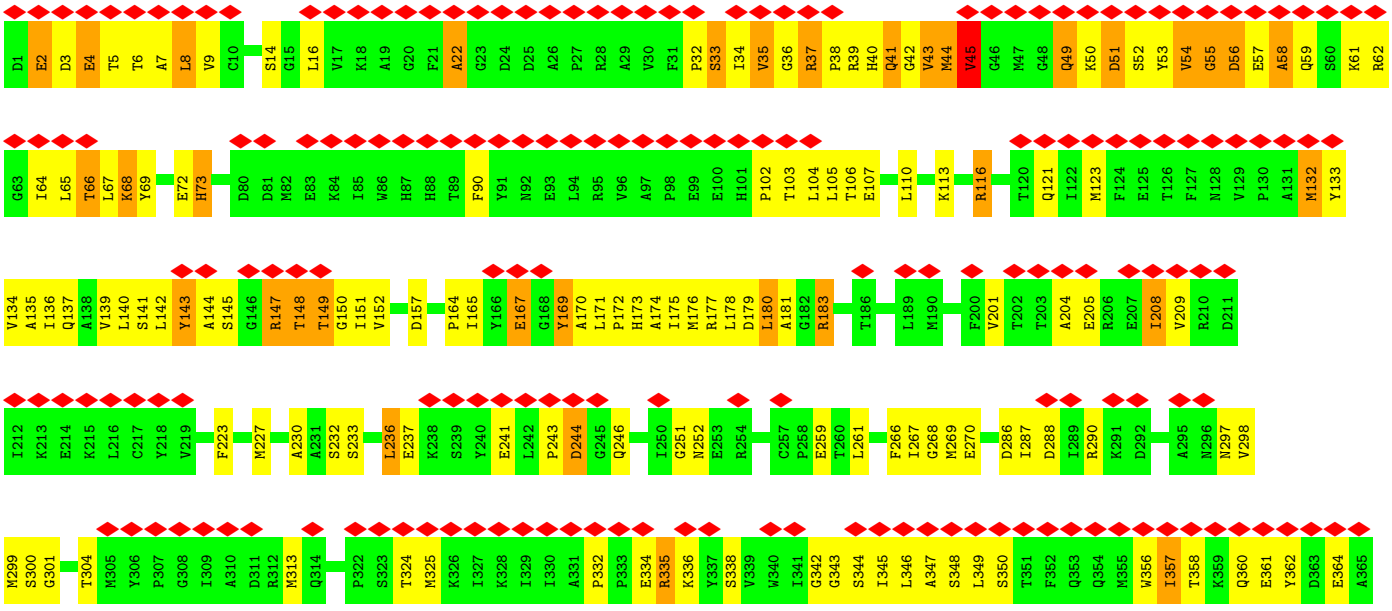
Chain R:




• Molecule 1: Actin, alpha skeletal muscle

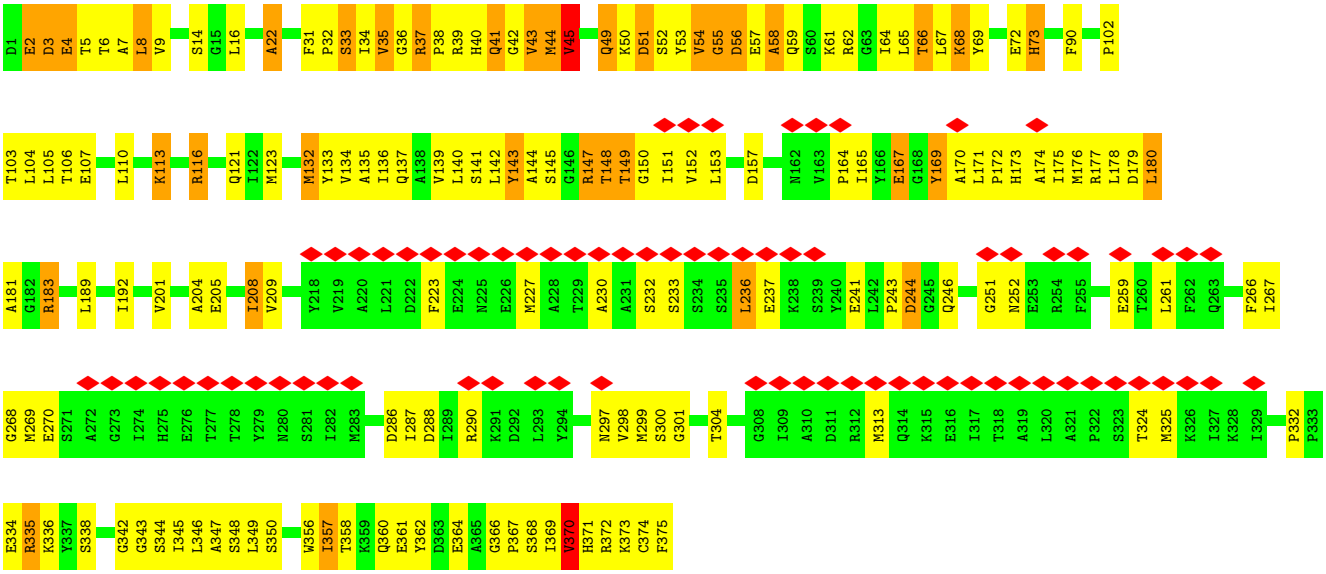
Chain S:



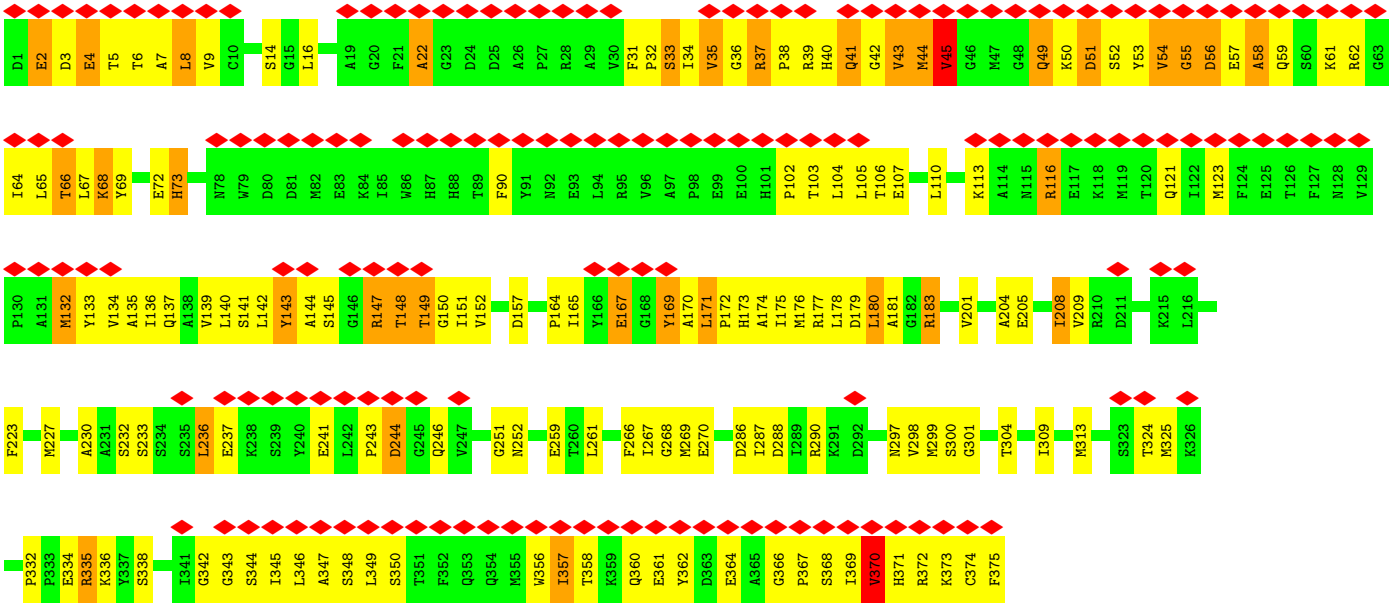
- Molecule 1: Actin, alpha skeletal muscle

Chain T:



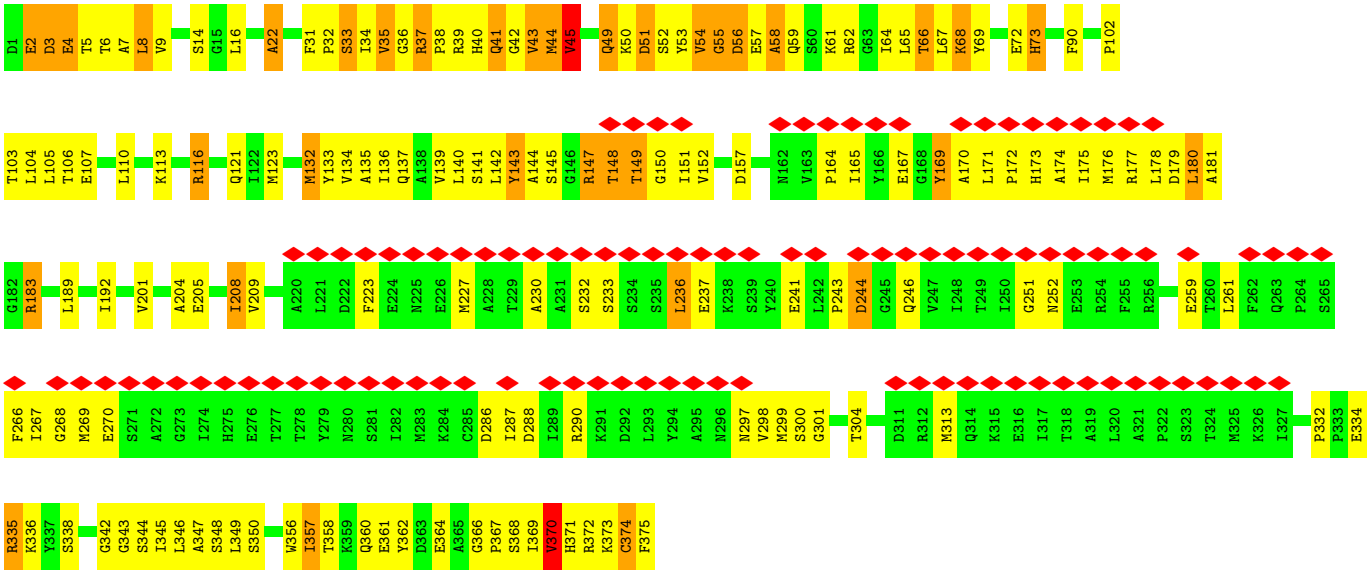

- Molecule 1: Actin, alpha skeletal muscle

Chain U:



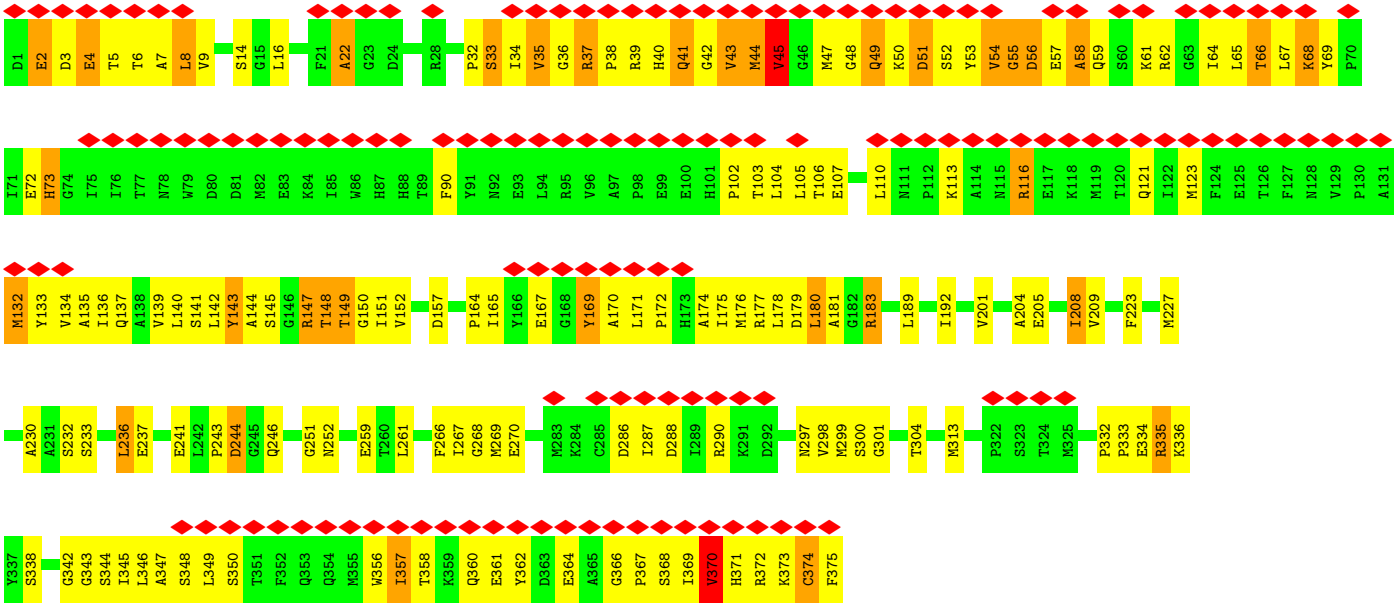

- Molecule 1: Actin, alpha skeletal muscle

Chain V:




- Molecule 1: Actin, alpha skeletal muscle

Chain W:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 1680 | Depositor |
| Resolution determination method | FSC 0.5 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI/PHILIPS CM12 | Depositor |
| Voltage (kV) | 120 | Depositor |
| Electron dose ($e^-/Å^2$) | 12 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | AGFA SCIENTA FILM | Depositor |
| Maximum map value | 24.301 | Depositor |
| Minimum map value | -12.902 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.924 | Depositor |
| Recommended contour level | 2.0 | Depositor |
| Map size (Å) | 633.6, 633.6, 633.6 | wwPDB |
| Map dimensions | 96, 96, 96 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 6.6, 6.6, 6.6 | 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: ADP, HIC

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| >5$ | RMSZ | $\#\|Z\| >5$ |
| 1 | A | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | B | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | C | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | D | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | E | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | F | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | G | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | H | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | I | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | J | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | K | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | L | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | M | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | N | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | O | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | P | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | Q | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | R | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | S | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | T | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | U | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | V | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| 1 | W | 0.66 | 0/2984 | 1.09 | 7/4040 (0.2%) |
| All | All | 0.66 | 0/68632 | 1.09 | 161/92920 (0.2%) |

There are no bond length outliers.

All (161) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 201 | VAL | O-C-N | -5.86 | 113.32 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Q | 201 | VAL | O-C-N | -5.86 | 113.33 | 122.70 |
| 1 | J | 201 | VAL | O-C-N | -5.85 | 113.35 | 122.70 |
| 1 | I | 201 | VAL | O-C-N | -5.84 | 113.35 | 122.70 |
| 1 | K | 201 | VAL | O-C-N | -5.84 | 113.36 | 122.70 |
| 1 | E | 201 | VAL | O-C-N | -5.84 | 113.36 | 122.70 |
| 1 | R | 201 | VAL | O-C-N | -5.83 | 113.37 | 122.70 |
| 1 | T | 201 | VAL | O-C-N | -5.83 | 113.37 | 122.70 |
| 1 | P | 201 | VAL | O-C-N | -5.83 | 113.38 | 122.70 |
| 1 | W | 201 | VAL | O-C-N | -5.83 | 113.38 | 122.70 |
| 1 | H | 201 | VAL | O-C-N | -5.82 | 113.39 | 122.70 |
| 1 | M | 201 | VAL | O-C-N | -5.82 | 113.39 | 122.70 |
| 1 | B | 201 | VAL | O-C-N | -5.82 | 113.39 | 122.70 |
| 1 | O | 201 | VAL | O-C-N | -5.82 | 113.39 | 122.70 |
| 1 | S | 201 | VAL | O-C-N | -5.82 | 113.39 | 122.70 |
| 1 | L | 201 | VAL | O-C-N | -5.82 | 113.40 | 122.70 |
| 1 | G | 201 | VAL | O-C-N | -5.81 | 113.40 | 122.70 |
| 1 | V | 201 | VAL | O-C-N | -5.81 | 113.40 | 122.70 |
| 1 | D | 201 | VAL | O-C-N | -5.80 | 113.41 | 122.70 |
| 1 | U | 201 | VAL | O-C-N | -5.79 | 113.44 | 122.70 |
| 1 | F | 201 | VAL | O-C-N | -5.78 | 113.45 | 122.70 |
| 1 | A | 201 | VAL | O-C-N | -5.77 | 113.46 | 122.70 |
| 1 | C | 201 | VAL | O-C-N | -5.77 | 113.47 | 122.70 |
| 1 | O | 169 | TYR | CB-CG-CD2 | -5.72 | 117.57 | 121.00 |
| 1 | V | 169 | TYR | CB-CG-CD2 | -5.71 | 117.57 | 121.00 |
| 1 | U | 169 | TYR | CB-CG-CD2 | -5.69 | 117.59 | 121.00 |
| 1 | G | 169 | TYR | CB-CG-CD2 | -5.66 | 117.61 | 121.00 |
| 1 | W | 169 | TYR | CB-CG-CD2 | -5.66 | 117.61 | 121.00 |
| 1 | K | 169 | TYR | CB-CG-CD2 | -5.65 | 117.61 | 121.00 |
| 1 | N | 169 | TYR | CB-CG-CD2 | -5.65 | 117.61 | 121.00 |
| 1 | M | 169 | TYR | CB-CG-CD2 | -5.65 | 117.61 | 121.00 |
| 1 | I | 201 | VAL | CA-C-N | 5.63 | 129.59 | 117.20 |
| 1 | J | 201 | VAL | CA-C-N | 5.63 | 129.59 | 117.20 |
| 1 | D | 201 | VAL | CA-C-N | 5.63 | 129.58 | 117.20 |
| 1 | Q | 169 | TYR | CB-CG-CD2 | -5.63 | 117.62 | 121.00 |
| 1 | A | 201 | VAL | CA-C-N | 5.62 | 129.57 | 117.20 |
| 1 | M | 201 | VAL | CA-C-N | 5.62 | 129.57 | 117.20 |
| 1 | P | 169 | TYR | CB-CG-CD2 | -5.62 | 117.63 | 121.00 |
| 1 | E | 201 | VAL | CA-C-N | 5.62 | 129.57 | 117.20 |
| 1 | E | 116 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 1 | G | 201 | VAL | CA-C-N | 5.62 | 129.56 | 117.20 |
| 1 | N | 201 | VAL | CA-C-N | 5.62 | 129.56 | 117.20 |
| 1 | B | 169 | TYR | CB-CG-CD2 | -5.62 | 117.63 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | K | 201 | VAL | CA-C-N | 5.62 | 129.56 | 117.20 |
| 1 | W | 201 | VAL | CA-C-N | 5.62 | 129.55 | 117.20 |
| 1 | Q | 201 | VAL | CA-C-N | 5.61 | 129.55 | 117.20 |
| 1 | I | 169 | TYR | CB-CG-CD2 | -5.61 | 117.63 | 121.00 |
| 1 | L | 201 | VAL | CA-C-N | 5.61 | 129.54 | 117.20 |
| 1 | O | 201 | VAL | CA-C-N | 5.61 | 129.54 | 117.20 |
| 1 | P | 201 | VAL | CA-C-N | 5.61 | 129.54 | 117.20 |
| 1 | S | 201 | VAL | CA-C-N | 5.61 | 129.54 | 117.20 |
| 1 | B | 201 | VAL | CA-C-N | 5.61 | 129.54 | 117.20 |
| 1 | D | 169 | TYR | CB-CG-CD2 | -5.61 | 117.64 | 121.00 |
| 1 | S | 169 | TYR | CB-CG-CD2 | -5.61 | 117.64 | 121.00 |
| 1 | T | 201 | VAL | CA-C-N | 5.61 | 129.53 | 117.20 |
| 1 | R | 201 | VAL | CA-C-N | 5.60 | 129.52 | 117.20 |
| 1 | F | 201 | VAL | CA-C-N | 5.60 | 129.52 | 117.20 |
| 1 | J | 169 | TYR | CB-CG-CD2 | -5.60 | 117.64 | 121.00 |
| 1 | V | 201 | VAL | CA-C-N | 5.60 | 129.52 | 117.20 |
| 1 | H | 201 | VAL | CA-C-N | 5.60 | 129.52 | 117.20 |
| 1 | C | 201 | VAL | CA-C-N | 5.60 | 129.51 | 117.20 |
| 1 | H | 169 | TYR | CB-CG-CD2 | -5.59 | 117.65 | 121.00 |
| 1 | U | 201 | VAL | CA-C-N | 5.58 | 129.49 | 117.20 |
| 1 | R | 169 | TYR | CB-CG-CD2 | -5.58 | 117.66 | 121.00 |
| 1 | L | 169 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 1 | F | 169 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 1 | T | 169 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 1 | I | 116 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | W | 116 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | U | 116 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | O | 116 | ARG | NE-CZ-NH2 | -5.55 | 117.53 | 120.30 |
| 1 | V | 116 | ARG | NE-CZ-NH2 | -5.54 | 117.53 | 120.30 |
| 1 | C | 169 | TYR | CB-CG-CD2 | -5.54 | 117.68 | 121.00 |
| 1 | R | 116 | ARG | NE-CZ-NH2 | -5.54 | 117.53 | 120.30 |
| 1 | E | 169 | TYR | CB-CG-CD2 | -5.54 | 117.68 | 121.00 |
| 1 | M | 116 | ARG | NE-CZ-NH2 | -5.53 | 117.53 | 120.30 |
| 1 | T | 116 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 1 | G | 116 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 1 | N | 116 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 1 | B | 116 | ARG | NE-CZ-NH2 | -5.51 | 117.54 | 120.30 |
| 1 | J | 116 | ARG | NE-CZ-NH2 | -5.51 | 117.54 | 120.30 |
| 1 | A | 116 | ARG | NE-CZ-NH2 | -5.51 | 117.55 | 120.30 |
| 1 | K | 116 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |
| 1 | D | 116 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |
| 1 | A | 169 | TYR | CB-CG-CD2 | -5.50 | 117.70 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | L | 116 | ARG | NE-CZ-NH2 | -5.49 | 117.55 | 120.30 |
| 1 | C | 116 | ARG | NE-CZ-NH2 | -5.48 | 117.56 | 120.30 |
| 1 | F | 116 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 1 | W | 205 | GLU | CG-CD-OE2 | -5.46 | 107.38 | 118.30 |
| 1 | C | 205 | GLU | CG-CD-OE2 | -5.45 | 107.41 | 118.30 |
| 1 | N | 205 | GLU | CG-CD-OE2 | -5.45 | 107.41 | 118.30 |
| 1 | K | 205 | GLU | CG-CD-OE2 | -5.44 | 107.41 | 118.30 |
| 1 | R | 205 | GLU | CG-CD-OE2 | -5.44 | 107.41 | 118.30 |
| 1 | S | 116 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 1 | H | 205 | GLU | CG-CD-OE2 | -5.44 | 107.42 | 118.30 |
| 1 | G | 205 | GLU | CG-CD-OE2 | -5.44 | 107.42 | 118.30 |
| 1 | T | 205 | GLU | CG-CD-OE2 | -5.44 | 107.43 | 118.30 |
| 1 | I | 205 | GLU | CG-CD-OE2 | -5.43 | 107.43 | 118.30 |
| 1 | J | 205 | GLU | CG-CD-OE2 | -5.43 | 107.43 | 118.30 |
| 1 | L | 205 | GLU | CG-CD-OE2 | -5.43 | 107.44 | 118.30 |
| 1 | Q | 116 | ARG | NE-CZ-NH2 | -5.43 | 117.58 | 120.30 |
| 1 | B | 205 | GLU | CG-CD-OE2 | -5.43 | 107.44 | 118.30 |
| 1 | O | 205 | GLU | CG-CD-OE2 | -5.43 | 107.44 | 118.30 |
| 1 | H | 116 | ARG | NE-CZ-NH2 | -5.43 | 117.59 | 120.30 |
| 1 | P | 205 | GLU | CG-CD-OE2 | -5.43 | 107.44 | 118.30 |
| 1 | S | 205 | GLU | CG-CD-OE2 | -5.43 | 107.45 | 118.30 |
| 1 | V | 205 | GLU | CG-CD-OE2 | -5.42 | 107.45 | 118.30 |
| 1 | Q | 205 | GLU | CG-CD-OE2 | -5.42 | 107.45 | 118.30 |
| 1 | M | 205 | GLU | CG-CD-OE2 | -5.42 | 107.46 | 118.30 |
| 1 | F | 205 | GLU | CG-CD-OE2 | -5.42 | 107.46 | 118.30 |
| 1 | E | 205 | GLU | CG-CD-OE2 | -5.42 | 107.47 | 118.30 |
| 1 | A | 205 | GLU | CG-CD-OE2 | -5.41 | 107.48 | 118.30 |
| 1 | U | 205 | GLU | CG-CD-OE2 | -5.41 | 107.48 | 118.30 |
| 1 | P | 116 | ARG | NE-CZ-NH2 | -5.41 | 117.60 | 120.30 |
| 1 | U | 313 | MET | CG-SD-CE | 5.40 | 108.84 | 100.20 |
| 1 | H | 313 | MET | CG-SD-CE | 5.40 | 108.84 | 100.20 |
| 1 | L | 313 | MET | CG-SD-CE | 5.40 | 108.84 | 100.20 |
| 1 | D | 205 | GLU | CG-CD-OE2 | -5.40 | 107.50 | 118.30 |
| 1 | A | 313 | MET | CG-SD-CE | 5.39 | 108.83 | 100.20 |
| 1 | J | 313 | MET | CG-SD-CE | 5.39 | 108.83 | 100.20 |
| 1 | P | 313 | MET | CG-SD-CE | 5.39 | 108.83 | 100.20 |
| 1 | O | 313 | MET | CG-SD-CE | 5.39 | 108.83 | 100.20 |
| 1 | I | 313 | MET | CG-SD-CE | 5.39 | 108.82 | 100.20 |
| 1 | T | 313 | MET | CG-SD-CE | 5.39 | 108.82 | 100.20 |
| 1 | S | 313 | MET | CG-SD-CE | 5.39 | 108.82 | 100.20 |
| 1 | B | 313 | MET | CG-SD-CE | 5.39 | 108.82 | 100.20 |
| 1 | D | 313 | MET | CG-SD-CE | 5.39 | 108.82 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | F | 313 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 1 | N | 313 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 1 | V | 313 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 1 | Q | 313 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 1 | E | 313 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 1 | R | 313 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 1 | W | 313 | MET | CG-SD-CE | 5.38 | 108.81 | 100.20 |
| 1 | M | 313 | MET | CG-SD-CE | 5.38 | 108.80 | 100.20 |
| 1 | G | 313 | MET | CG-SD-CE | 5.37 | 108.79 | 100.20 |
| 1 | K | 313 | MET | CG-SD-CE | 5.36 | 108.78 | 100.20 |
| 1 | C | 313 | MET | CG-SD-CE | 5.36 | 108.77 | 100.20 |
| 1 | J | 22 | ALA | C-N-CA | -5.15 | 111.48 | 122.30 |
| 1 | Q | 22 | ALA | C-N-CA | -5.15 | 111.49 | 122.30 |
| 1 | M | 22 | ALA | C-N-CA | -5.15 | 111.49 | 122.30 |
| 1 | C | 22 | ALA | C-N-CA | -5.15 | 111.49 | 122.30 |
| 1 | A | 22 | ALA | C-N-CA | -5.14 | 111.50 | 122.30 |
| 1 | W | 22 | ALA | C-N-CA | -5.14 | 111.51 | 122.30 |
| 1 | E | 22 | ALA | C-N-CA | -5.14 | 111.51 | 122.30 |
| 1 | F | 22 | ALA | C-N-CA | -5.14 | 111.51 | 122.30 |
| 1 | P | 22 | ALA | C-N-CA | -5.14 | 111.51 | 122.30 |
| 1 | I | 22 | ALA | C-N-CA | -5.13 | 111.52 | 122.30 |
| 1 | H | 22 | ALA | C-N-CA | -5.13 | 111.53 | 122.30 |
| 1 | K | 22 | ALA | C-N-CA | -5.13 | 111.53 | 122.30 |
| 1 | B | 22 | ALA | C-N-CA | -5.13 | 111.53 | 122.30 |
| 1 | V | 22 | ALA | C-N-CA | -5.13 | 111.53 | 122.30 |
| 1 | D | 22 | ALA | C-N-CA | -5.12 | 111.54 | 122.30 |
| 1 | N | 22 | ALA | C-N-CA | -5.12 | 111.54 | 122.30 |
| 1 | S | 22 | ALA | C-N-CA | -5.12 | 111.54 | 122.30 |
| 1 | G | 22 | ALA | C-N-CA | -5.12 | 111.54 | 122.30 |
| 1 | L | 22 | ALA | C-N-CA | -5.12 | 111.54 | 122.30 |
| 1 | O | 22 | ALA | C-N-CA | -5.12 | 111.55 | 122.30 |
| 1 | U | 22 | ALA | C-N-CA | -5.12 | 111.55 | 122.30 |
| 1 | T | 22 | ALA | C-N-CA | -5.12 | 111.55 | 122.30 |
| 1 | R | 22 | ALA | C-N-CA | -5.12 | 111.56 | 122.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2934 | 0 | 2895 | 334 | 0 |
| 1 | B | 2934 | 0 | 2895 | 336 | 0 |
| 1 | C | 2934 | 0 | 2895 | 374 | 0 |
| 1 | D | 2934 | 0 | 2895 | 378 | 0 |
| 1 | E | 2934 | 0 | 2895 | 380 | 0 |
| 1 | F | 2934 | 0 | 2895 | 377 | 0 |
| 1 | G | 2934 | 0 | 2895 | 375 | 0 |
| 1 | H | 2934 | 0 | 2895 | 375 | 0 |
| 1 | I | 2934 | 0 | 2895 | 369 | 0 |
| 1 | J | 2934 | 0 | 2895 | 377 | 0 |
| 1 | K | 2934 | 0 | 2895 | 372 | 0 |
| 1 | L | 2934 | 0 | 2895 | 369 | 0 |
| 1 | M | 2934 | 0 | 2895 | 370 | 0 |
| 1 | N | 2934 | 0 | 2895 | 377 | 0 |
| 1 | O | 2934 | 0 | 2895 | 376 | 0 |
| 1 | P | 2934 | 0 | 2895 | 372 | 0 |
| 1 | Q | 2934 | 0 | 2895 | 375 | 0 |
| 1 | R | 2934 | 0 | 2895 | 370 | 0 |
| 1 | S | 2934 | 0 | 2895 | 371 | 0 |
| 1 | T | 2934 | 0 | 2895 | 374 | 0 |
| 1 | U | 2934 | 0 | 2895 | 375 | 0 |
| 1 | V | 2934 | 0 | 2895 | 337 | 0 |
| 1 | W | 2934 | 0 | 2895 | 333 | 0 |
| 2 | A | 27 | 0 | 12 | 4 | 0 |
| 2 | B | 27 | 0 | 12 | 5 | 0 |
| 2 | C | 27 | 0 | 12 | 4 | 0 |
| 2 | D | 27 | 0 | 12 | 5 | 0 |
| 2 | E | 27 | 0 | 12 | 4 | 0 |
| 2 | F | 27 | 0 | 12 | 4 | 0 |
| 2 | G | 27 | 0 | 12 | 4 | 0 |
| 2 | H | 27 | 0 | 12 | 4 | 0 |
| 2 | I | 27 | 0 | 12 | 4 | 0 |
| 2 | J | 27 | 0 | 12 | 4 | 0 |
| 2 | K | 27 | 0 | 12 | 5 | 0 |
| 2 | L | 27 | 0 | 12 | 4 | 0 |
| 2 | M | 27 | 0 | 12 | 4 | 0 |
| 2 | N | 27 | 0 | 12 | 4 | 0 |
| 2 | O | 27 | 0 | 12 | 4 | 0 |
| 2 | P | 27 | 0 | 12 | 4 | 0 |
| 2 | Q | 27 | 0 | 12 | 4 | 0 |
| 2 | R | 27 | 0 | 12 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | S | 27 | 0 | 12 | 4 | 0 |
| 2 | T | 27 | 0 | 12 | 4 | 0 |
| 2 | U | 27 | 0 | 12 | 4 | 0 |
| 2 | V | 27 | 0 | 12 | 4 | 0 |
| 2 | W | 27 | 0 | 12 | 4 | 0 |
| All | All | 68103 | 0 | 66861 | 7549 | 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 56.

All (7549) 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:R:59:GLN:O | 1:R:62:ARG:HG3 | 1.43 | 1.19 |
| 1:T:59:GLN:O | 1:T:62:ARG:HG3 | 1.43 | 1.19 |
| 1:W:59:GLN:O | 1:W:62:ARG:HG3 | 1.43 | 1.19 |
| 1:A:59:GLN:O | 1:A:62:ARG:HG3 | 1.43 | 1.19 |
| 1:H:59:GLN:O | 1:H:62:ARG:HG3 | 1.43 | 1.18 |
| 1:K:59:GLN:O | 1:K:62:ARG:HG3 | 1.43 | 1.18 |
| 1:F:59:GLN:O | 1:F:62:ARG:HG3 | 1.43 | 1.18 |
| 1:C:59:GLN:O | 1:C:62:ARG:HG3 | 1.43 | 1.18 |
| 1:L:59:GLN:O | 1:L:62:ARG:HG3 | 1.43 | 1.18 |
| 1:M:59:GLN:O | 1:M:62:ARG:HG3 | 1.43 | 1.18 |
| 1:P:59:GLN:O | 1:P:62:ARG:HG3 | 1.43 | 1.18 |
| 1:I:59:GLN:O | 1:I:62:ARG:HG3 | 1.43 | 1.18 |
| 1:J:59:GLN:O | 1:J:62:ARG:HG3 | 1.43 | 1.18 |
| 1:V:59:GLN:O | 1:V:62:ARG:HG3 | 1.43 | 1.18 |
| 1:Q:290:ARG:HD2 | 1:S:244:ASP:HB2 | 1.21 | 1.17 |
| 1:M:43:VAL:HG13 | 1:M:44:MET:N | 1.54 | 1.17 |
| 1:O:290:ARG:HD2 | 1:Q:244:ASP:HB2 | 1.21 | 1.17 |
| 1:D:59:GLN:O | 1:D:62:ARG:HG3 | 1.43 | 1.17 |
| 1:O:59:GLN:O | 1:O:62:ARG:HG3 | 1.43 | 1.17 |
| 1:S:290:ARG:HD2 | 1:U:244:ASP:HB2 | 1.21 | 1.17 |
| 1:U:59:GLN:O | 1:U:62:ARG:HG3 | 1.43 | 1.16 |
| 1:N:59:GLN:O | 1:N:62:ARG:HG3 | 1.43 | 1.16 |
| 1:E:59:GLN:O | 1:E:62:ARG:HG3 | 1.43 | 1.16 |
| 1:G:59:GLN:O | 1:G:62:ARG:HG3 | 1.43 | 1.16 |
| 1:J:290:ARG:HD2 | 1:L:244:ASP:HB2 | 1.21 | 1.16 |
| 1:K:43:VAL:HG13 | 1:K:44:MET:N | 1.54 | 1.16 |
| 1:L:290:ARG:HD2 | 1:N:244:ASP:HB2 | 1.21 | 1.16 |
| 1:B:59:GLN:O | 1:B:62:ARG:HG3 | 1.43 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:59:GLN:O | 1:Q:62:ARG:HG3 | 1.43 | 1.15 |
| 1:U:290:ARG:HD2 | 1:W:244:ASP:HB2 | 1.21 | 1.15 |
| 1:M:290:ARG:HD2 | 1:O:244:ASP:HB2 | 1.21 | 1.15 |
| 1:S:59:GLN:O | 1:S:62:ARG:HG3 | 1.43 | 1.15 |
| 1:K:361:GLU:HB3 | 1:K:369:ILE:HD13 | 1.19 | 1.15 |
| 1:H:290:ARG:HD2 | 1:J:244:ASP:HB2 | 1.21 | 1.15 |
| 1:D:361:GLU:HB3 | 1:D:369:ILE:HD13 | 1.20 | 1.15 |
| 1:D:43:VAL:HG13 | 1:D:44:MET:N | 1.54 | 1.14 |
| 1:I:43:VAL:HG13 | 1:I:44:MET:N | 1.54 | 1.14 |
| 1:O:361:GLU:HB3 | 1:O:369:ILE:HD13 | 1.19 | 1.14 |
| 1:N:290:ARG:HD2 | 1:P:244:ASP:HB2 | 1.21 | 1.14 |
| 1:Q:361:GLU:HB3 | 1:Q:369:ILE:HD13 | 1.19 | 1.14 |
| 1:L:43:VAL:HG13 | 1:L:44:MET:N | 1.54 | 1.14 |
| 1:F:290:ARG:HD2 | 1:H:244:ASP:HB2 | 1.22 | 1.13 |
| 1:R:34:ILE:HB | 1:R:54:VAL:HG11 | 1.30 | 1.13 |
| 1:F:357:ILE:HG12 | 1:F:370:VAL:HG23 | 1.13 | 1.13 |
| 1:N:43:VAL:HG13 | 1:N:44:MET:N | 1.54 | 1.13 |
| 1:U:357:ILE:HG12 | 1:U:370:VAL:HG23 | 1.13 | 1.13 |
| 1:J:43:VAL:HG13 | 1:J:44:MET:N | 1.54 | 1.13 |
| 1:E:34:ILE:HB | 1:E:54:VAL:HG11 | 1.30 | 1.13 |
| 1:K:357:ILE:HG12 | 1:K:370:VAL:HG23 | 1.13 | 1.13 |
| 1:O:357:ILE:HG12 | 1:O:370:VAL:HG23 | 1.13 | 1.13 |
| 1:A:34:ILE:HB | 1:A:54:VAL:HG11 | 1.30 | 1.13 |
| 1:G:34:ILE:HB | 1:G:54:VAL:HG11 | 1.30 | 1.13 |
| 1:J:357:ILE:HG12 | 1:J:370:VAL:HG23 | 1.13 | 1.12 |
| 1:N:34:ILE:HB | 1:N:54:VAL:HG11 | 1.30 | 1.13 |
| 1:Q:357:ILE:HG12 | 1:Q:370:VAL:HG23 | 1.13 | 1.12 |
| 1:T:34:ILE:HB | 1:T:54:VAL:HG11 | 1.30 | 1.12 |
| 1:K:290:ARG:HD2 | 1:M:244:ASP:HB2 | 1.21 | 1.12 |
| 1:L:34:ILE:HB | 1:L:54:VAL:HG11 | 1.29 | 1.12 |
| 1:P:43:VAL:HG13 | 1:P:44:MET:N | 1.54 | 1.12 |
| 1:V:357:ILE:HG12 | 1:V:370:VAL:HG23 | 1.13 | 1.12 |
| 1:V:361:GLU:HB3 | 1:V:369:ILE:HD13 | 1.19 | 1.12 |
| 1:P:290:ARG:HD2 | 1:R:244:ASP:HB2 | 1.22 | 1.12 |
| 1:A:43:VAL:HG13 | 1:A:44:MET:N | 1.54 | 1.12 |
| 1:A:361:GLU:HB3 | 1:A:369:ILE:HD13 | 1.19 | 1.12 |
| 1:B:43:VAL:HG13 | 1:B:44:MET:N | 1.54 | 1.12 |
| 1:B:357:ILE:HG12 | 1:B:370:VAL:HG23 | 1.13 | 1.12 |
| 1:D:290:ARG:HD2 | 1:F:244:ASP:HB2 | 1.21 | 1.12 |
| 1:D:357:ILE:HG12 | 1:D:370:VAL:HG23 | 1.13 | 1.12 |
| 1:H:357:ILE:HG12 | 1:H:370:VAL:HG23 | 1.13 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:361:GLU:HB3 | 1:M:369:ILE:HD13 | 1.19 | 1.12 |
| 1:P:34:ILE:HB | 1:P:54:VAL:HG11 | 1.30 | 1.12 |
| 1:H:43:VAL:HG13 | 1:H:44:MET:N | 1.54 | 1.12 |
| 1:I:357:ILE:HG12 | 1:I:370:VAL:HG23 | 1.13 | 1.12 |
| 1:M:357:ILE:HG12 | 1:M:370:VAL:HG23 | 1.13 | 1.12 |
| 1:S:357:ILE:HG12 | 1:S:370:VAL:HG23 | 1.13 | 1.12 |
| 1:U:361:GLU:HB3 | 1:U:369:ILE:HD13 | 1.19 | 1.12 |
| 1:G:357:ILE:HG12 | 1:G:370:VAL:HG23 | 1.13 | 1.11 |
| 1:P:361:GLU:HB3 | 1:P:369:ILE:HD13 | 1.19 | 1.11 |
| 1:W:43:VAL:HG13 | 1:W:44:MET:N | 1.54 | 1.11 |
| 1:W:357:ILE:HG12 | 1:W:370:VAL:HG23 | 1.13 | 1.11 |
| 1:C:34:ILE:HB | 1:C:54:VAL:HG11 | 1.30 | 1.11 |
| 1:F:361:GLU:HB3 | 1:F:369:ILE:HD13 | 1.19 | 1.11 |
| 1:T:357:ILE:HG12 | 1:T:370:VAL:HG23 | 1.13 | 1.11 |
| 1:L:357:ILE:HG12 | 1:L:370:VAL:HG23 | 1.13 | 1.11 |
| 1:G:361:GLU:HB3 | 1:G:369:ILE:HD13 | 1.19 | 1.11 |
| 1:N:357:ILE:HG12 | 1:N:370:VAL:HG23 | 1.13 | 1.11 |
| 1:N:361:GLU:HB3 | 1:N:369:ILE:HD13 | 1.19 | 1.11 |
| 1:C:43:VAL:HG13 | 1:C:44:MET:N | 1.54 | 1.10 |
| 1:C:357:ILE:HG12 | 1:C:370:VAL:HG23 | 1.13 | 1.10 |
| 1:R:43:VAL:HG13 | 1:R:44:MET:N | 1.54 | 1.10 |
| 1:R:357:ILE:HG12 | 1:R:370:VAL:HG23 | 1.13 | 1.10 |
| 1:D:180:LEU:HD21 | 1:D:261:LEU:HD23 | 1.34 | 1.10 |
| 1:I:34:ILE:HB | 1:I:54:VAL:HG11 | 1.29 | 1.10 |
| 1:L:361:GLU:HB3 | 1:L:369:ILE:HD13 | 1.19 | 1.10 |
| 1:Q:180:LEU:HD21 | 1:Q:261:LEU:HD23 | 1.34 | 1.10 |
| 1:R:290:ARG:HD2 | 1:T:244:ASP:HB2 | 1.21 | 1.10 |
| 1:U:43:VAL:HG13 | 1:U:44:MET:N | 1.54 | 1.10 |
| 1:B:361:GLU:HB3 | 1:B:369:ILE:HD13 | 1.19 | 1.10 |
| 1:E:180:LEU:HD21 | 1:E:261:LEU:HD23 | 1.34 | 1.10 |
| 1:I:180:LEU:HD21 | 1:I:261:LEU:HD23 | 1.34 | 1.10 |
| 1:I:290:ARG:HD2 | 1:K:244:ASP:HB2 | 1.21 | 1.10 |
| 1:V:180:LEU:HD21 | 1:V:261:LEU:HD23 | 1.34 | 1.10 |
| 1:A:290:ARG:HD2 | 1:C:244:ASP:HB2 | 1.22 | 1.10 |
| 1:B:290:ARG:HD2 | 1:D:244:ASP:HB2 | 1.22 | 1.10 |
| 1:C:361:GLU:HB3 | 1:C:369:ILE:HD13 | 1.19 | 1.10 |
| 1:E:357:ILE:HG12 | 1:E:370:VAL:HG23 | 1.13 | 1.10 |
| 1:S:361:GLU:HB3 | 1:S:369:ILE:HD13 | 1.19 | 1.10 |
| 1:B:180:LEU:HD21 | 1:B:261:LEU:HD23 | 1.34 | 1.10 |
| 1:F:43:VAL:HG13 | 1:F:44:MET:N | 1.54 | 1.10 |
| 1:O:180:LEU:HD21 | 1:O:261:LEU:HD23 | 1.33 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:180:LEU:HD21 | 1:U:261:LEU:HD23 | 1.34 | 1.10 |
| 1:V:34:ILE:HB | 1:V:54:VAL:HG11 | 1.30 | 1.10 |
| 1:W:34:ILE:HB | 1:W:54:VAL:HG11 | 1.30 | 1.10 |
| 1:A:357:ILE:HG12 | 1:A:370:VAL:HG23 | 1.13 | 1.09 |
| 1:B:208:ILE:HD11 | 1:B:243:PRO:HD2 | 1.34 | 1.09 |
| 1:J:34:ILE:HB | 1:J:54:VAL:HG11 | 1.30 | 1.09 |
| 1:K:180:LEU:HD21 | 1:K:261:LEU:HD23 | 1.34 | 1.09 |
| 1:S:208:ILE:HD11 | 1:S:243:PRO:HD2 | 1.34 | 1.09 |
| 1:C:180:LEU:HD21 | 1:C:261:LEU:HD23 | 1.34 | 1.09 |
| 1:E:361:GLU:HB3 | 1:E:369:ILE:HD13 | 1.19 | 1.09 |
| 1:J:361:GLU:HB3 | 1:J:369:ILE:HD13 | 1.20 | 1.09 |
| 1:P:180:LEU:HD21 | 1:P:261:LEU:HD23 | 1.34 | 1.09 |
| 1:P:208:ILE:HD11 | 1:P:243:PRO:HD2 | 1.34 | 1.09 |
| 1:R:180:LEU:HD21 | 1:R:261:LEU:HD23 | 1.34 | 1.09 |
| 1:A:43:VAL:HG13 | 1:A:44:MET:H | 0.92 | 1.09 |
| 1:H:180:LEU:HD21 | 1:H:261:LEU:HD23 | 1.34 | 1.09 |
| 1:J:180:LEU:HD21 | 1:J:261:LEU:HD23 | 1.34 | 1.09 |
| 1:J:208:ILE:HD11 | 1:J:243:PRO:HD2 | 1.34 | 1.09 |
| 1:W:180:LEU:HD21 | 1:W:261:LEU:HD23 | 1.34 | 1.09 |
| 1:H:208:ILE:HD11 | 1:H:243:PRO:HD2 | 1.34 | 1.09 |
| 1:M:208:ILE:HD11 | 1:M:243:PRO:HD2 | 1.34 | 1.09 |
| 1:N:208:ILE:HD11 | 1:N:243:PRO:HD2 | 1.34 | 1.09 |
| 1:R:361:GLU:HB3 | 1:R:369:ILE:HD13 | 1.19 | 1.09 |
| 1:S:43:VAL:HG13 | 1:S:44:MET:N | 1.54 | 1.09 |
| 1:S:180:LEU:HD21 | 1:S:261:LEU:HD23 | 1.34 | 1.09 |
| 1:C:208:ILE:HD11 | 1:C:243:PRO:HD2 | 1.34 | 1.09 |
| 1:D:208:ILE:HD11 | 1:D:243:PRO:HD2 | 1.34 | 1.09 |
| 1:F:180:LEU:HD21 | 1:F:261:LEU:HD23 | 1.34 | 1.09 |
| 1:G:180:LEU:HD21 | 1:G:261:LEU:HD23 | 1.34 | 1.09 |
| 1:J:43:VAL:HG13 | 1:J:44:MET:H | 0.92 | 1.09 |
| 1:K:34:ILE:HB | 1:K:54:VAL:HG11 | 1.30 | 1.09 |
| 1:O:208:ILE:HD11 | 1:O:243:PRO:HD2 | 1.34 | 1.09 |
| 1:P:357:ILE:HG12 | 1:P:370:VAL:HG23 | 1.13 | 1.09 |
| 1:R:43:VAL:HG13 | 1:R:44:MET:H | 0.92 | 1.09 |
| 1:T:43:VAL:HG13 | 1:T:44:MET:H | 0.92 | 1.09 |
| 1:T:180:LEU:HD21 | 1:T:261:LEU:HD23 | 1.34 | 1.09 |
| 1:T:290:ARG:HD2 | 1:V:244:ASP:HB2 | 1.21 | 1.09 |
| 1:L:43:VAL:HG13 | 1:L:44:MET:H | 0.92 | 1.08 |
| 1:T:43:VAL:HG13 | 1:T:44:MET:N | 1.54 | 1.08 |
| 1:T:208:ILE:HD11 | 1:T:243:PRO:HD2 | 1.34 | 1.08 |
| 1:E:208:ILE:HD11 | 1:E:243:PRO:HD2 | 1.34 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:361:GLU:HB3 | 1:H:369:ILE:HD13 | 1.19 | 1.08 |
| 1:I:208:ILE:HD11 | 1:I:243:PRO:HD2 | 1.34 | 1.08 |
| 1:U:43:VAL:HG13 | 1:U:44:MET:H | 0.92 | 1.08 |
| 1:E:43:VAL:HG13 | 1:E:44:MET:N | 1.54 | 1.08 |
| 1:E:290:ARG:HD2 | 1:G:244:ASP:HB2 | 1.21 | 1.08 |
| 1:G:290:ARG:HD2 | 1:I:244:ASP:HB2 | 1.21 | 1.08 |
| 1:I:43:VAL:HG13 | 1:I:44:MET:H | 0.92 | 1.08 |
| 1:U:208:ILE:HD11 | 1:U:243:PRO:HD2 | 1.34 | 1.08 |
| 1:H:35:VAL:HG12 | 1:H:68:LYS:HB2 | 1.36 | 1.08 |
| 1:L:180:LEU:HD21 | 1:L:261:LEU:HD23 | 1.34 | 1.08 |
| 1:N:180:LEU:HD21 | 1:N:261:LEU:HD23 | 1.34 | 1.08 |
| 1:O:35:VAL:HG12 | 1:O:68:LYS:HB2 | 1.36 | 1.08 |
| 1:B:34:ILE:HB | 1:B:54:VAL:HG11 | 1.30 | 1.08 |
| 1:C:43:VAL:HG13 | 1:C:44:MET:H | 0.92 | 1.08 |
| 1:D:34:ILE:HB | 1:D:54:VAL:HG11 | 1.30 | 1.08 |
| 1:M:180:LEU:HD21 | 1:M:261:LEU:HD23 | 1.34 | 1.08 |
| 1:S:35:VAL:HG12 | 1:S:68:LYS:HB2 | 1.36 | 1.08 |
| 1:W:361:GLU:HB3 | 1:W:369:ILE:HD13 | 1.19 | 1.08 |
| 1:D:35:VAL:HG12 | 1:D:68:LYS:HB2 | 1.36 | 1.07 |
| 1:H:34:ILE:HB | 1:H:54:VAL:HG11 | 1.30 | 1.07 |
| 1:I:361:GLU:HB3 | 1:I:369:ILE:HD13 | 1.19 | 1.07 |
| 1:T:361:GLU:HB3 | 1:T:369:ILE:HD13 | 1.19 | 1.07 |
| 1:A:180:LEU:HD21 | 1:A:261:LEU:HD23 | 1.34 | 1.07 |
| 1:Q:43:VAL:HG13 | 1:Q:44:MET:N | 1.54 | 1.07 |
| 1:S:43:VAL:HG13 | 1:S:44:MET:H | 0.92 | 1.07 |
| 1:K:43:VAL:HG13 | 1:K:44:MET:H | 0.92 | 1.07 |
| 1:M:34:ILE:HB | 1:M:54:VAL:HG11 | 1.30 | 1.07 |
| 1:U:34:ILE:HB | 1:U:54:VAL:HG11 | 1.30 | 1.07 |
| 1:W:43:VAL:HG13 | 1:W:44:MET:H | 0.92 | 1.07 |
| 1:G:43:VAL:HG13 | 1:G:44:MET:H | 0.92 | 1.07 |
| 1:I:35:VAL:HG12 | 1:I:68:LYS:HB2 | 1.36 | 1.07 |
| 1:B:43:VAL:HG13 | 1:B:44:MET:H | 0.92 | 1.07 |
| 1:C:290:ARG:HD2 | 1:E:244:ASP:HB2 | 1.21 | 1.07 |
| 1:F:34:ILE:HB | 1:F:54:VAL:HG11 | 1.30 | 1.07 |
| 1:G:43:VAL:HG13 | 1:G:44:MET:N | 1.54 | 1.07 |
| 1:K:35:VAL:HG12 | 1:K:68:LYS:HB2 | 1.36 | 1.07 |
| 1:H:43:VAL:HG13 | 1:H:44:MET:H | 0.92 | 1.06 |
| 1:S:34:ILE:HB | 1:S:54:VAL:HG11 | 1.30 | 1.06 |
| 1:V:43:VAL:HG13 | 1:V:44:MET:N | 1.54 | 1.06 |
| 1:V:43:VAL:HG13 | 1:V:44:MET:H | 0.92 | 1.06 |
| 1:N:35:VAL:HG12 | 1:N:68:LYS:HB2 | 1.36 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:43:VAL:HG13 | 1:N:44:MET:H | 0.92 | 1.06 |
| 1:O:43:VAL:HG13 | 1:O:44:MET:N | 1.54 | 1.06 |
| 1:P:43:VAL:HG13 | 1:P:44:MET:H | 0.92 | 1.06 |
| 1:A:208:ILE:HD11 | 1:A:243:PRO:HD2 | 1.34 | 1.06 |
| 1:B:35:VAL:HG12 | 1:B:68:LYS:HB2 | 1.36 | 1.06 |
| 1:T:35:VAL:HG12 | 1:T:68:LYS:HB2 | 1.36 | 1.06 |
| 1:U:35:VAL:HG12 | 1:U:68:LYS:HB2 | 1.36 | 1.06 |
| 1:D:43:VAL:HG13 | 1:D:44:MET:H | 0.92 | 1.06 |
| 1:Q:208:ILE:HD11 | 1:Q:243:PRO:HD2 | 1.34 | 1.06 |
| 1:V:35:VAL:HG12 | 1:V:68:LYS:HB2 | 1.36 | 1.06 |
| 1:W:35:VAL:HG12 | 1:W:68:LYS:HB2 | 1.36 | 1.06 |
| 1:C:35:VAL:HG12 | 1:C:68:LYS:HB2 | 1.36 | 1.05 |
| 1:J:35:VAL:HG12 | 1:J:68:LYS:HB2 | 1.36 | 1.05 |
| 1:L:208:ILE:HD11 | 1:L:243:PRO:HD2 | 1.34 | 1.05 |
| 1:Q:43:VAL:HG13 | 1:Q:44:MET:H | 0.92 | 1.05 |
| 1:V:208:ILE:HD11 | 1:V:243:PRO:HD2 | 1.34 | 1.05 |
| 1:A:34:ILE:HB | 1:A:54:VAL:CG1 | 1.87 | 1.05 |
| 1:C:34:ILE:HB | 1:C:54:VAL:CG1 | 1.87 | 1.05 |
| 1:J:37:ARG:HG3 | 1:J:38:PRO:HD2 | 1.37 | 1.05 |
| 1:L:35:VAL:HG12 | 1:L:68:LYS:HB2 | 1.36 | 1.05 |
| 1:M:43:VAL:HG13 | 1:M:44:MET:H | 0.92 | 1.05 |
| 1:O:34:ILE:HB | 1:O:54:VAL:HG11 | 1.30 | 1.05 |
| 1:Q:34:ILE:HB | 1:Q:54:VAL:HG11 | 1.30 | 1.05 |
| 1:R:34:ILE:HB | 1:R:54:VAL:CG1 | 1.87 | 1.05 |
| 1:T:34:ILE:HB | 1:T:54:VAL:CG1 | 1.87 | 1.05 |
| 1:W:34:ILE:HB | 1:W:54:VAL:CG1 | 1.87 | 1.05 |
| 1:F:208:ILE:HD11 | 1:F:243:PRO:HD2 | 1.34 | 1.05 |
| 1:L:37:ARG:HG3 | 1:L:38:PRO:HD2 | 1.37 | 1.05 |
| 1:V:34:ILE:HB | 1:V:54:VAL:CG1 | 1.87 | 1.05 |
| 1:E:34:ILE:HB | 1:E:54:VAL:CG1 | 1.87 | 1.05 |
| 1:G:208:ILE:HD11 | 1:G:243:PRO:HD2 | 1.34 | 1.05 |
| 1:L:45:VAL:HG22 | 1:L:45:VAL:O | 1.57 | 1.05 |
| 1:M:35:VAL:HG12 | 1:M:68:LYS:HB2 | 1.36 | 1.05 |
| 1:P:34:ILE:HB | 1:P:54:VAL:CG1 | 1.87 | 1.05 |
| 1:W:37:ARG:HG3 | 1:W:38:PRO:HD2 | 1.37 | 1.05 |
| 1:E:35:VAL:HG12 | 1:E:68:LYS:HB2 | 1.36 | 1.04 |
| 1:E:43:VAL:HG13 | 1:E:44:MET:H | 0.92 | 1.04 |
| 1:T:34:ILE:HG21 | 1:T:67:LEU:HD22 | 1.40 | 1.04 |
| 1:U:34:ILE:HB | 1:U:54:VAL:CG1 | 1.87 | 1.04 |
| 1:G:34:ILE:HG21 | 1:G:67:LEU:HD22 | 1.40 | 1.04 |
| 1:H:45:VAL:O | 1:H:45:VAL:HG22 | 1.57 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:34:ILE:HG21 | 1:K:67:LEU:HD22 | 1.40 | 1.04 |
| 1:K:208:ILE:HD11 | 1:K:243:PRO:HD2 | 1.34 | 1.04 |
| 1:B:34:ILE:HG21 | 1:B:67:LEU:HD22 | 1.40 | 1.04 |
| 1:E:34:ILE:HG21 | 1:E:67:LEU:HD22 | 1.40 | 1.04 |
| 1:G:34:ILE:HB | 1:G:54:VAL:CG1 | 1.87 | 1.04 |
| 1:H:37:ARG:HG3 | 1:H:38:PRO:HD2 | 1.37 | 1.04 |
| 1:R:208:ILE:HD11 | 1:R:243:PRO:HD2 | 1.34 | 1.04 |
| 1:S:34:ILE:HB | 1:S:54:VAL:CG1 | 1.87 | 1.04 |
| 1:V:37:ARG:HG3 | 1:V:38:PRO:HD2 | 1.37 | 1.04 |
| 1:W:208:ILE:HD11 | 1:W:243:PRO:HD2 | 1.34 | 1.04 |
| 1:A:37:ARG:HG3 | 1:A:38:PRO:HD2 | 1.37 | 1.04 |
| 1:B:34:ILE:HB | 1:B:54:VAL:CG1 | 1.87 | 1.04 |
| 1:F:34:ILE:HB | 1:F:54:VAL:CG1 | 1.87 | 1.04 |
| 1:F:43:VAL:HG13 | 1:F:44:MET:H | 0.92 | 1.04 |
| 1:H:34:ILE:HB | 1:H:54:VAL:CG1 | 1.87 | 1.04 |
| 1:J:34:ILE:HB | 1:J:54:VAL:CG1 | 1.87 | 1.04 |
| 1:M:34:ILE:HG21 | 1:M:67:LEU:HD22 | 1.40 | 1.04 |
| 1:N:34:ILE:HB | 1:N:54:VAL:CG1 | 1.87 | 1.04 |
| 1:A:35:VAL:HG12 | 1:A:68:LYS:HB2 | 1.36 | 1.04 |
| 1:D:34:ILE:HB | 1:D:54:VAL:CG1 | 1.87 | 1.04 |
| 1:D:34:ILE:HG21 | 1:D:67:LEU:HD22 | 1.40 | 1.04 |
| 1:D:45:VAL:HG22 | 1:D:45:VAL:O | 1.57 | 1.04 |
| 1:P:34:ILE:HG21 | 1:P:67:LEU:HD22 | 1.40 | 1.04 |
| 1:P:45:VAL:O | 1:P:45:VAL:HG22 | 1.57 | 1.04 |
| 1:Q:34:ILE:HG21 | 1:Q:67:LEU:HD22 | 1.40 | 1.04 |
| 1:R:34:ILE:HG21 | 1:R:67:LEU:HD22 | 1.40 | 1.04 |
| 1:V:34:ILE:HG21 | 1:V:67:LEU:HD22 | 1.40 | 1.04 |
| 1:C:45:VAL:O | 1:C:45:VAL:HG22 | 1.57 | 1.03 |
| 1:F:35:VAL:HG12 | 1:F:68:LYS:HB2 | 1.36 | 1.03 |
| 1:L:34:ILE:HB | 1:L:54:VAL:CG1 | 1.87 | 1.03 |
| 1:M:37:ARG:HG3 | 1:M:38:PRO:HD2 | 1.37 | 1.03 |
| 1:N:37:ARG:HG3 | 1:N:38:PRO:HD2 | 1.37 | 1.03 |
| 1:P:35:VAL:HG12 | 1:P:68:LYS:HB2 | 1.36 | 1.03 |
| 1:U:45:VAL:O | 1:U:45:VAL:HG22 | 1.57 | 1.03 |
| 1:B:37:ARG:HG3 | 1:B:38:PRO:HD2 | 1.37 | 1.03 |
| 1:C:37:ARG:HG3 | 1:C:38:PRO:HD2 | 1.37 | 1.03 |
| 1:I:34:ILE:HB | 1:I:54:VAL:CG1 | 1.87 | 1.03 |
| 1:K:37:ARG:HG3 | 1:K:38:PRO:HD2 | 1.37 | 1.03 |
| 1:N:34:ILE:HG21 | 1:N:67:LEU:HD22 | 1.40 | 1.03 |
| 1:O:34:ILE:HG21 | 1:O:67:LEU:HD22 | 1.40 | 1.03 |
| 1:O:37:ARG:HG3 | 1:O:38:PRO:HD2 | 1.37 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:34:ILE:HB | 1:Q:54:VAL:CG1 | 1.87 | 1.03 |
| 1:Q:35:VAL:HG12 | 1:Q:68:LYS:HB2 | 1.36 | 1.03 |
| 1:A:34:ILE:HG21 | 1:A:67:LEU:HD22 | 1.40 | 1.03 |
| 1:I:34:ILE:HG21 | 1:I:67:LEU:HD22 | 1.40 | 1.03 |
| 1:S:34:ILE:HG21 | 1:S:67:LEU:HD22 | 1.40 | 1.03 |
| 1:T:37:ARG:HG3 | 1:T:38:PRO:HD2 | 1.37 | 1.03 |
| 1:U:37:ARG:HG3 | 1:U:38:PRO:HD2 | 1.37 | 1.03 |
| 1:M:34:ILE:HB | 1:M:54:VAL:CG1 | 1.87 | 1.03 |
| 1:O:34:ILE:HB | 1:O:54:VAL:CG1 | 1.87 | 1.03 |
| 1:P:37:ARG:HG3 | 1:P:38:PRO:HD2 | 1.37 | 1.03 |
| 1:Q:45:VAL:HG22 | 1:Q:45:VAL:O | 1.57 | 1.03 |
| 1:R:35:VAL:HG12 | 1:R:68:LYS:HB2 | 1.36 | 1.03 |
| 1:C:34:ILE:HG21 | 1:C:67:LEU:HD22 | 1.40 | 1.03 |
| 1:K:34:ILE:HB | 1:K:54:VAL:CG1 | 1.87 | 1.03 |
| 1:O:43:VAL:HG13 | 1:O:44:MET:H | 0.92 | 1.03 |
| 1:Q:37:ARG:HG3 | 1:Q:38:PRO:HD2 | 1.37 | 1.03 |
| 1:F:34:ILE:HG21 | 1:F:67:LEU:HD22 | 1.40 | 1.02 |
| 1:G:35:VAL:HG12 | 1:G:68:LYS:HB2 | 1.36 | 1.02 |
| 1:L:34:ILE:HG21 | 1:L:67:LEU:HD22 | 1.40 | 1.02 |
| 1:F:37:ARG:HG3 | 1:F:38:PRO:HD2 | 1.37 | 1.02 |
| 1:I:37:ARG:HG3 | 1:I:38:PRO:HD2 | 1.37 | 1.02 |
| 1:R:37:ARG:HG3 | 1:R:38:PRO:HD2 | 1.37 | 1.02 |
| 1:S:45:VAL:O | 1:S:45:VAL:HG22 | 1.57 | 1.02 |
| 1:U:34:ILE:HG21 | 1:U:67:LEU:HD22 | 1.40 | 1.02 |
| 1:W:45:VAL:O | 1:W:45:VAL:HG22 | 1.57 | 1.02 |
| 1:S:37:ARG:HG3 | 1:S:38:PRO:HD2 | 1.37 | 1.02 |
| 1:E:37:ARG:HG3 | 1:E:38:PRO:HD2 | 1.37 | 1.02 |
| 1:J:34:ILE:HG21 | 1:J:67:LEU:HD22 | 1.40 | 1.01 |
| 1:D:37:ARG:HG3 | 1:D:38:PRO:HD2 | 1.37 | 1.01 |
| 1:W:34:ILE:HG21 | 1:W:67:LEU:HD22 | 1.40 | 1.01 |
| 1:A:45:VAL:HG22 | 1:A:45:VAL:O | 1.57 | 1.01 |
| 1:G:45:VAL:O | 1:G:45:VAL:HG22 | 1.57 | 1.01 |
| 1:M:45:VAL:O | 1:M:45:VAL:HG22 | 1.57 | 1.01 |
| 1:H:34:ILE:HG21 | 1:H:67:LEU:HD22 | 1.40 | 1.01 |
| 1:T:45:VAL:HG22 | 1:T:45:VAL:O | 1.57 | 1.01 |
| 1:F:45:VAL:HG22 | 1:F:45:VAL:O | 1.57 | 1.01 |
| 1:G:37:ARG:HG3 | 1:G:38:PRO:HD2 | 1.37 | 1.00 |
| 1:R:208:ILE:HD11 | 1:R:243:PRO:CD | 1.92 | 1.00 |
| 1:B:208:ILE:HD11 | 1:B:243:PRO:CD | 1.92 | 1.00 |
| 1:J:45:VAL:O | 1:J:45:VAL:HG22 | 1.57 | 1.00 |
| 1:R:43:VAL:CG1 | 1:R:44:MET:H | 1.74 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:8:LEU:HD12 | 1:S:90:PHE:HE1 | 1.27 | 1.00 |
| 1:T:208:ILE:HD11 | 1:T:243:PRO:CD | 1.92 | 1.00 |
| 1:D:208:ILE:HD11 | 1:D:243:PRO:CD | 1.92 | 1.00 |
| 1:G:43:VAL:CG1 | 1:G:44:MET:H | 1.74 | 1.00 |
| 1:I:8:LEU:HD12 | 1:I:90:PHE:HE1 | 1.27 | 1.00 |
| 1:P:208:ILE:HD11 | 1:P:243:PRO:CD | 1.92 | 1.00 |
| 1:U:208:ILE:HD11 | 1:U:243:PRO:CD | 1.92 | 1.00 |
| 1:W:208:ILE:HD11 | 1:W:243:PRO:CD | 1.92 | 1.00 |
| 1:I:208:ILE:HD11 | 1:I:243:PRO:CD | 1.92 | 1.00 |
| 1:K:208:ILE:HD11 | 1:K:243:PRO:CD | 1.92 | 1.00 |
| 1:O:8:LEU:HD12 | 1:O:90:PHE:HE1 | 1.27 | 1.00 |
| 1:D:8:LEU:HD12 | 1:D:90:PHE:HE1 | 1.27 | 1.00 |
| 1:H:8:LEU:HD12 | 1:H:90:PHE:HE1 | 1.27 | 1.00 |
| 1:U:43:VAL:CG1 | 1:U:44:MET:H | 1.74 | 1.00 |
| 1:W:43:VAL:CG1 | 1:W:44:MET:H | 1.74 | 1.00 |
| 1:A:208:ILE:HD11 | 1:A:243:PRO:CD | 1.92 | 1.00 |
| 1:F:208:ILE:HD11 | 1:F:243:PRO:CD | 1.92 | 1.00 |
| 1:M:208:ILE:HD11 | 1:M:243:PRO:CD | 1.92 | 1.00 |
| 1:S:208:ILE:HD11 | 1:S:243:PRO:CD | 1.92 | 1.00 |
| 1:T:8:LEU:HD12 | 1:T:90:PHE:HE1 | 1.27 | 1.00 |
| 1:E:8:LEU:HD12 | 1:E:90:PHE:HE1 | 1.27 | 1.00 |
| 1:P:43:VAL:CG1 | 1:P:44:MET:H | 1.74 | 1.00 |
| 1:B:8:LEU:HD12 | 1:B:90:PHE:HE1 | 1.27 | 0.99 |
| 1:G:208:ILE:HD11 | 1:G:243:PRO:CD | 1.92 | 0.99 |
| 1:N:45:VAL:HG22 | 1:N:45:VAL:O | 1.57 | 0.99 |
| 1:N:208:ILE:HD11 | 1:N:243:PRO:CD | 1.92 | 0.99 |
| 1:V:45:VAL:HG22 | 1:V:45:VAL:O | 1.57 | 0.99 |
| 1:V:208:ILE:HD11 | 1:V:243:PRO:CD | 1.92 | 0.99 |
| 1:N:8:LEU:HD12 | 1:N:90:PHE:HE1 | 1.27 | 0.99 |
| 1:M:8:LEU:HD12 | 1:M:90:PHE:HE1 | 1.27 | 0.99 |
| 1:P:8:LEU:HD12 | 1:P:90:PHE:HE1 | 1.27 | 0.99 |
| 1:C:208:ILE:HD11 | 1:C:243:PRO:CD | 1.92 | 0.99 |
| 1:S:43:VAL:CG1 | 1:S:44:MET:H | 1.74 | 0.99 |
| 1:W:8:LEU:HD12 | 1:W:90:PHE:HE1 | 1.27 | 0.99 |
| 1:H:208:ILE:HD11 | 1:H:243:PRO:CD | 1.92 | 0.99 |
| 1:E:43:VAL:CG1 | 1:E:44:MET:H | 1.74 | 0.99 |
| 1:L:8:LEU:HD12 | 1:L:90:PHE:HE1 | 1.27 | 0.99 |
| 1:L:208:ILE:HD11 | 1:L:243:PRO:CD | 1.92 | 0.99 |
| 1:N:43:VAL:CG1 | 1:N:44:MET:H | 1.74 | 0.99 |
| 1:O:208:ILE:HD11 | 1:O:243:PRO:CD | 1.92 | 0.99 |
| 1:A:43:VAL:CG1 | 1:A:44:MET:H | 1.74 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:208:ILE:HD11 | 1:Q:243:PRO:CD | 1.92 | 0.99 |
| 1:E:208:ILE:HD11 | 1:E:243:PRO:CD | 1.92 | 0.99 |
| 1:V:8:LEU:HD12 | 1:V:90:PHE:HE1 | 1.27 | 0.99 |
| 1:A:8:LEU:HD12 | 1:A:90:PHE:HE1 | 1.27 | 0.99 |
| 1:I:45:VAL:HG22 | 1:I:45:VAL:O | 1.57 | 0.98 |
| 1:J:208:ILE:HD11 | 1:J:243:PRO:CD | 1.92 | 0.98 |
| 1:L:43:VAL:CG1 | 1:L:44:MET:H | 1.74 | 0.98 |
| 1:Q:43:VAL:CG1 | 1:Q:44:MET:H | 1.74 | 0.98 |
| 1:R:45:VAL:O | 1:R:45:VAL:HG22 | 1.57 | 0.98 |
| 1:K:8:LEU:HD12 | 1:K:90:PHE:HE1 | 1.27 | 0.98 |
| 1:K:45:VAL:O | 1:K:45:VAL:HG22 | 1.57 | 0.98 |
| 1:F:8:LEU:HD12 | 1:F:90:PHE:HE1 | 1.27 | 0.98 |
| 1:C:43:VAL:CG1 | 1:C:44:MET:H | 1.74 | 0.97 |
| 1:J:43:VAL:CG1 | 1:J:44:MET:H | 1.74 | 0.97 |
| 1:O:45:VAL:O | 1:O:45:VAL:HG22 | 1.57 | 0.97 |
| 1:U:8:LEU:HD12 | 1:U:90:PHE:HE1 | 1.27 | 0.97 |
| 1:O:43:VAL:CG1 | 1:O:44:MET:H | 1.74 | 0.97 |
| 1:B:45:VAL:O | 1:B:45:VAL:HG22 | 1.57 | 0.97 |
| 1:E:45:VAL:O | 1:E:45:VAL:HG22 | 1.57 | 0.97 |
| 1:G:8:LEU:HD12 | 1:G:90:PHE:HE1 | 1.27 | 0.97 |
| 1:R:8:LEU:HD12 | 1:R:90:PHE:HE1 | 1.27 | 0.97 |
| 1:V:43:VAL:CG1 | 1:V:44:MET:H | 1.74 | 0.97 |
| 1:Q:8:LEU:HD12 | 1:Q:90:PHE:HE1 | 1.27 | 0.97 |
| 1:C:8:LEU:HD12 | 1:C:90:PHE:HE1 | 1.27 | 0.96 |
| 1:H:43:VAL:CG1 | 1:H:44:MET:H | 1.74 | 0.96 |
| 1:N:300:SER:HA | 1:N:335:ARG:CG | 1.96 | 0.96 |
| 1:U:300:SER:HA | 1:U:335:ARG:CG | 1.96 | 0.96 |
| 1:E:300:SER:HA | 1:E:335:ARG:CG | 1.96 | 0.96 |
| 1:J:300:SER:HA | 1:J:335:ARG:CG | 1.96 | 0.96 |
| 1:C:300:SER:HA | 1:C:335:ARG:CG | 1.96 | 0.96 |
| 1:T:300:SER:HA | 1:T:335:ARG:CG | 1.96 | 0.96 |
| 1:M:43:VAL:CG1 | 1:M:44:MET:H | 1.74 | 0.95 |
| 1:P:300:SER:HA | 1:P:335:ARG:CG | 1.96 | 0.95 |
| 1:J:8:LEU:HD12 | 1:J:90:PHE:HE1 | 1.27 | 0.95 |
| 1:F:43:VAL:CG1 | 1:F:44:MET:H | 1.74 | 0.95 |
| 1:F:300:SER:HA | 1:F:335:ARG:CG | 1.96 | 0.95 |
| 1:H:300:SER:HA | 1:H:335:ARG:CG | 1.96 | 0.95 |
| 1:A:300:SER:HA | 1:A:335:ARG:CG | 1.96 | 0.95 |
| 1:L:300:SER:HA | 1:L:335:ARG:CG | 1.96 | 0.95 |
| 1:Q:300:SER:HA | 1:Q:335:ARG:CG | 1.96 | 0.95 |
| 1:O:300:SER:HA | 1:O:335:ARG:CG | 1.96 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:300:SER:HA | 1:W:335:ARG:CG | 1.96 | 0.95 |
| 1:T:43:VAL:CG1 | 1:T:44:MET:H | 1.74 | 0.95 |
| 1:V:39:ARG:HE | 1:V:66:THR:HB | 1.32 | 0.95 |
| 1:S:300:SER:HA | 1:S:335:ARG:CG | 1.96 | 0.94 |
| 1:R:300:SER:HA | 1:R:335:ARG:CG | 1.96 | 0.94 |
| 1:T:39:ARG:HE | 1:T:66:THR:HB | 1.32 | 0.94 |
| 1:I:300:SER:HA | 1:I:335:ARG:CG | 1.96 | 0.94 |
| 1:M:300:SER:HA | 1:M:335:ARG:CG | 1.96 | 0.94 |
| 1:B:300:SER:HA | 1:B:335:ARG:CG | 1.96 | 0.94 |
| 1:G:300:SER:HA | 1:G:335:ARG:CG | 1.96 | 0.94 |
| 1:H:43:VAL:CG1 | 1:H:44:MET:N | 2.30 | 0.94 |
| 1:K:300:SER:HA | 1:K:335:ARG:CG | 1.96 | 0.94 |
| 1:N:133:TYR:CZ | 1:N:375:PHE:HB2 | 2.03 | 0.94 |
| 1:L:133:TYR:CZ | 1:L:375:PHE:HB2 | 2.03 | 0.94 |
| 1:C:133:TYR:CZ | 1:C:375:PHE:HB2 | 2.03 | 0.94 |
| 1:D:300:SER:HA | 1:D:335:ARG:CG | 1.96 | 0.94 |
| 1:N:43:VAL:CG1 | 1:N:44:MET:N | 2.30 | 0.94 |
| 1:P:133:TYR:CZ | 1:P:375:PHE:HB2 | 2.03 | 0.94 |
| 1:A:39:ARG:HE | 1:A:66:THR:HB | 1.32 | 0.94 |
| 1:B:133:TYR:CZ | 1:B:375:PHE:HB2 | 2.03 | 0.94 |
| 1:C:39:ARG:HE | 1:C:66:THR:HB | 1.32 | 0.94 |
| 1:K:39:ARG:HE | 1:K:66:THR:HB | 1.32 | 0.94 |
| 1:K:43:VAL:CG1 | 1:K:44:MET:H | 1.74 | 0.94 |
| 1:R:39:ARG:HE | 1:R:66:THR:HB | 1.32 | 0.94 |
| 1:V:300:SER:HA | 1:V:335:ARG:CG | 1.96 | 0.94 |
| 1:D:43:VAL:CG1 | 1:D:44:MET:H | 1.74 | 0.94 |
| 1:M:39:ARG:HE | 1:M:66:THR:HB | 1.32 | 0.94 |
| 1:E:133:TYR:CZ | 1:E:375:PHE:HB2 | 2.03 | 0.93 |
| 1:W:43:VAL:CG1 | 1:W:44:MET:N | 2.30 | 0.93 |
| 1:W:133:TYR:CZ | 1:W:375:PHE:HB2 | 2.03 | 0.93 |
| 1:A:133:TYR:CZ | 1:A:375:PHE:HB2 | 2.03 | 0.93 |
| 1:G:133:TYR:CZ | 1:G:375:PHE:HB2 | 2.03 | 0.93 |
| 1:R:133:TYR:CZ | 1:R:375:PHE:HB2 | 2.03 | 0.93 |
| 1:D:133:TYR:CZ | 1:D:375:PHE:HB2 | 2.03 | 0.93 |
| 1:U:133:TYR:CZ | 1:U:375:PHE:HB2 | 2.03 | 0.93 |
| 1:E:39:ARG:HE | 1:E:66:THR:HB | 1.32 | 0.93 |
| 1:K:133:TYR:CZ | 1:K:375:PHE:HB2 | 2.03 | 0.93 |
| 1:Q:133:TYR:CZ | 1:Q:375:PHE:HB2 | 2.03 | 0.93 |
| 1:S:133:TYR:CZ | 1:S:375:PHE:HB2 | 2.03 | 0.93 |
| 1:C:43:VAL:CG1 | 1:C:44:MET:N | 2.30 | 0.93 |
| 1:I:39:ARG:HE | 1:I:66:THR:HB | 1.32 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:133:TYR:CZ | 1:J:375:PHE:HB2 | 2.03 | 0.93 |
| 1:I:133:TYR:CZ | 1:I:375:PHE:HB2 | 2.03 | 0.93 |
| 1:Q:34:ILE:CB | 1:Q:54:VAL:HG11 | 1.99 | 0.93 |
| 1:S:39:ARG:HE | 1:S:66:THR:HB | 1.32 | 0.93 |
| 1:U:39:ARG:HE | 1:U:66:THR:HB | 1.32 | 0.93 |
| 1:M:133:TYR:CZ | 1:M:375:PHE:HB2 | 2.03 | 0.93 |
| 1:O:39:ARG:HE | 1:O:66:THR:HB | 1.32 | 0.93 |
| 1:G:39:ARG:HE | 1:G:66:THR:HB | 1.32 | 0.92 |
| 1:S:34:ILE:CB | 1:S:54:VAL:HG11 | 1.99 | 0.92 |
| 1:D:357:ILE:CG1 | 1:D:370:VAL:HG23 | 2.00 | 0.92 |
| 1:O:34:ILE:CB | 1:O:54:VAL:HG11 | 1.99 | 0.92 |
| 1:O:133:TYR:CZ | 1:O:375:PHE:HB2 | 2.03 | 0.92 |
| 1:R:43:VAL:CG1 | 1:R:44:MET:N | 2.30 | 0.92 |
| 1:F:43:VAL:CG1 | 1:F:44:MET:N | 2.30 | 0.92 |
| 1:F:133:TYR:CZ | 1:F:375:PHE:HB2 | 2.03 | 0.92 |
| 1:B:34:ILE:CB | 1:B:54:VAL:HG11 | 1.99 | 0.92 |
| 1:O:357:ILE:CG1 | 1:O:370:VAL:HG23 | 2.00 | 0.92 |
| 1:T:133:TYR:CZ | 1:T:375:PHE:HB2 | 2.03 | 0.92 |
| 1:W:39:ARG:HE | 1:W:66:THR:HB | 1.32 | 0.92 |
| 1:H:39:ARG:HE | 1:H:66:THR:HB | 1.32 | 0.92 |
| 1:J:39:ARG:HE | 1:J:66:THR:HB | 1.32 | 0.92 |
| 1:U:34:ILE:CB | 1:U:54:VAL:HG11 | 1.99 | 0.92 |
| 1:U:357:ILE:CG1 | 1:U:370:VAL:HG23 | 2.00 | 0.92 |
| 1:V:34:ILE:CB | 1:V:54:VAL:HG11 | 1.99 | 0.92 |
| 1:V:133:TYR:CZ | 1:V:375:PHE:HB2 | 2.03 | 0.92 |
| 1:H:133:TYR:CZ | 1:H:375:PHE:HB2 | 2.03 | 0.92 |
| 1:M:34:ILE:CB | 1:M:54:VAL:HG11 | 1.99 | 0.92 |
| 1:P:39:ARG:HE | 1:P:66:THR:HB | 1.32 | 0.92 |
| 1:A:300:SER:HA | 1:A:335:ARG:HG3 | 1.51 | 0.92 |
| 1:B:43:VAL:CG1 | 1:B:44:MET:H | 1.74 | 0.92 |
| 1:J:34:ILE:CB | 1:J:54:VAL:HG11 | 1.99 | 0.92 |
| 1:L:43:VAL:CG1 | 1:L:44:MET:N | 2.30 | 0.92 |
| 1:C:34:ILE:CB | 1:C:54:VAL:HG11 | 1.99 | 0.91 |
| 1:D:39:ARG:HE | 1:D:66:THR:HB | 1.32 | 0.91 |
| 1:H:34:ILE:CB | 1:H:54:VAL:HG11 | 1.99 | 0.91 |
| 1:M:357:ILE:CG1 | 1:M:370:VAL:HG23 | 2.00 | 0.91 |
| 1:Q:39:ARG:HE | 1:Q:66:THR:HB | 1.32 | 0.91 |
| 1:B:357:ILE:CG1 | 1:B:370:VAL:HG23 | 2.00 | 0.91 |
| 1:D:34:ILE:CB | 1:D:54:VAL:HG11 | 1.99 | 0.91 |
| 1:A:34:ILE:CB | 1:A:54:VAL:HG11 | 1.99 | 0.91 |
| 1:C:357:ILE:CG1 | 1:C:370:VAL:HG23 | 2.00 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:39:ARG:HE | 1:F:66:THR:HB | 1.31 | 0.91 |
| 1:G:34:ILE:CB | 1:G:54:VAL:HG11 | 1.99 | 0.91 |
| 1:I:34:ILE:CB | 1:I:54:VAL:HG11 | 1.99 | 0.91 |
| 1:I:43:VAL:CG1 | 1:I:44:MET:H | 1.74 | 0.91 |
| 1:L:39:ARG:HE | 1:L:66:THR:HB | 1.32 | 0.91 |
| 1:B:39:ARG:HE | 1:B:66:THR:HB | 1.32 | 0.91 |
| 1:C:300:SER:HA | 1:C:335:ARG:HG3 | 1.51 | 0.91 |
| 1:L:34:ILE:CB | 1:L:54:VAL:HG11 | 1.99 | 0.91 |
| 1:S:357:ILE:CG1 | 1:S:370:VAL:HG23 | 2.00 | 0.91 |
| 1:E:34:ILE:CB | 1:E:54:VAL:HG11 | 1.99 | 0.91 |
| 1:U:43:VAL:CG1 | 1:U:44:MET:N | 2.30 | 0.91 |
| 1:F:34:ILE:CB | 1:F:54:VAL:HG11 | 1.99 | 0.91 |
| 1:A:357:ILE:CG1 | 1:A:370:VAL:HG23 | 2.00 | 0.91 |
| 1:E:357:ILE:CG1 | 1:E:370:VAL:HG23 | 2.00 | 0.91 |
| 1:B:300:SER:HA | 1:B:335:ARG:HG3 | 1.51 | 0.91 |
| 1:N:39:ARG:HE | 1:N:66:THR:HB | 1.32 | 0.91 |
| 1:T:34:ILE:CB | 1:T:54:VAL:HG11 | 1.99 | 0.91 |
| 1:T:357:ILE:CG1 | 1:T:370:VAL:HG23 | 2.00 | 0.91 |
| 1:H:357:ILE:CG1 | 1:H:370:VAL:HG23 | 2.00 | 0.91 |
| 1:N:357:ILE:CG1 | 1:N:370:VAL:HG23 | 2.00 | 0.91 |
| 1:T:300:SER:HA | 1:T:335:ARG:HG3 | 1.51 | 0.91 |
| 1:W:34:ILE:CB | 1:W:54:VAL:HG11 | 1.99 | 0.91 |
| 1:D:300:SER:HA | 1:D:335:ARG:HG3 | 1.51 | 0.91 |
| 1:K:34:ILE:CB | 1:K:54:VAL:HG11 | 1.99 | 0.91 |
| 1:N:34:ILE:CB | 1:N:54:VAL:HG11 | 1.99 | 0.91 |
| 1:V:300:SER:HA | 1:V:335:ARG:HG3 | 1.51 | 0.91 |
| 1:E:290:ARG:HD2 | 1:G:244:ASP:CB | 2.01 | 0.90 |
| 1:E:300:SER:HA | 1:E:335:ARG:HG3 | 1.51 | 0.90 |
| 1:L:357:ILE:CG1 | 1:L:370:VAL:HG23 | 2.00 | 0.90 |
| 1:M:300:SER:HA | 1:M:335:ARG:HG3 | 1.51 | 0.90 |
| 1:P:290:ARG:HD2 | 1:R:244:ASP:CB | 2.02 | 0.90 |
| 1:R:34:ILE:CB | 1:R:54:VAL:HG11 | 1.99 | 0.90 |
| 1:R:300:SER:HA | 1:R:335:ARG:HG3 | 1.51 | 0.90 |
| 1:V:357:ILE:CG1 | 1:V:370:VAL:HG23 | 2.00 | 0.90 |
| 1:K:290:ARG:HD2 | 1:M:244:ASP:CB | 2.02 | 0.90 |
| 1:M:290:ARG:HD2 | 1:O:244:ASP:CB | 2.01 | 0.90 |
| 1:O:300:SER:HA | 1:O:335:ARG:HG3 | 1.51 | 0.90 |
| 1:Q:300:SER:HA | 1:Q:335:ARG:HG3 | 1.51 | 0.90 |
| 1:R:357:ILE:CG1 | 1:R:370:VAL:HG23 | 2.00 | 0.90 |
| 1:G:290:ARG:HD2 | 1:I:244:ASP:CB | 2.01 | 0.90 |
| 1:P:34:ILE:CB | 1:P:54:VAL:HG11 | 1.99 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:300:SER:HA | 1:P:335:ARG:HG3 | 1.51 | 0.90 |
| 1:Q:290:ARG:HD2 | 1:S:244:ASP:CB | 2.02 | 0.90 |
| 1:A:290:ARG:HD2 | 1:C:244:ASP:CB | 2.02 | 0.90 |
| 1:G:43:VAL:CG1 | 1:G:44:MET:N | 2.30 | 0.90 |
| 1:J:290:ARG:HD2 | 1:L:244:ASP:CB | 2.02 | 0.90 |
| 1:P:357:ILE:CG1 | 1:P:370:VAL:HG23 | 2.00 | 0.90 |
| 1:B:290:ARG:HD2 | 1:D:244:ASP:CB | 2.02 | 0.90 |
| 1:F:290:ARG:HD2 | 1:H:244:ASP:CB | 2.02 | 0.90 |
| 1:L:290:ARG:HD2 | 1:N:244:ASP:CB | 2.01 | 0.90 |
| 1:R:290:ARG:HD2 | 1:T:244:ASP:CB | 2.01 | 0.90 |
| 1:S:300:SER:HA | 1:S:335:ARG:HG3 | 1.51 | 0.90 |
| 1:T:104:LEU:HB2 | 1:T:356:TRP:CH2 | 2.07 | 0.90 |
| 1:H:73:HIC:HA | 1:H:183:ARG:HH12 | 1.36 | 0.90 |
| 1:H:104:LEU:HB2 | 1:H:356:TRP:CH2 | 2.07 | 0.90 |
| 1:R:104:LEU:HB2 | 1:R:356:TRP:CH2 | 2.07 | 0.90 |
| 1:F:104:LEU:HB2 | 1:F:356:TRP:CH2 | 2.07 | 0.90 |
| 1:F:300:SER:HA | 1:F:335:ARG:HG3 | 1.51 | 0.90 |
| 1:N:104:LEU:HB2 | 1:N:356:TRP:CH2 | 2.07 | 0.90 |
| 1:N:300:SER:HA | 1:N:335:ARG:HG3 | 1.51 | 0.90 |
| 1:P:104:LEU:HB2 | 1:P:356:TRP:CH2 | 2.07 | 0.90 |
| 1:W:300:SER:HA | 1:W:335:ARG:HG3 | 1.51 | 0.90 |
| 1:D:104:LEU:HB2 | 1:D:356:TRP:CH2 | 2.07 | 0.90 |
| 1:F:34:ILE:HG21 | 1:F:67:LEU:CD2 | 2.02 | 0.90 |
| 1:F:73:HIC:HA | 1:F:183:ARG:HH12 | 1.36 | 0.90 |
| 1:G:357:ILE:CG1 | 1:G:370:VAL:HG23 | 2.00 | 0.90 |
| 1:J:357:ILE:CG1 | 1:J:370:VAL:HG23 | 2.00 | 0.90 |
| 1:M:43:VAL:CG1 | 1:M:44:MET:N | 2.30 | 0.90 |
| 1:U:34:ILE:HG21 | 1:U:67:LEU:CD2 | 2.02 | 0.90 |
| 1:U:290:ARG:HD2 | 1:W:244:ASP:CB | 2.02 | 0.90 |
| 1:V:104:LEU:HB2 | 1:V:356:TRP:CH2 | 2.07 | 0.90 |
| 1:A:104:LEU:HB2 | 1:A:356:TRP:CH2 | 2.07 | 0.90 |
| 1:B:104:LEU:HB2 | 1:B:356:TRP:CH2 | 2.07 | 0.90 |
| 1:H:300:SER:HA | 1:H:335:ARG:HG3 | 1.51 | 0.90 |
| 1:J:104:LEU:HB2 | 1:J:356:TRP:CH2 | 2.07 | 0.90 |
| 1:L:34:ILE:HG21 | 1:L:67:LEU:CD2 | 2.02 | 0.90 |
| 1:N:290:ARG:HD2 | 1:P:244:ASP:CB | 2.01 | 0.90 |
| 1:A:43:VAL:CG1 | 1:A:44:MET:N | 2.30 | 0.89 |
| 1:C:290:ARG:HD2 | 1:E:244:ASP:CB | 2.01 | 0.89 |
| 1:J:73:HIC:HA | 1:J:183:ARG:HH12 | 1.36 | 0.89 |
| 1:L:104:LEU:HB2 | 1:L:356:TRP:CH2 | 2.07 | 0.89 |
| 1:O:34:ILE:HG21 | 1:O:67:LEU:CD2 | 2.02 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:73:HIC:HA | 1:Q:183:ARG:HH12 | 1.36 | 0.89 |
| 1:W:104:LEU:HB2 | 1:W:356:TRP:CH2 | 2.07 | 0.89 |
| 1:I:357:ILE:CG1 | 1:I:370:VAL:HG23 | 2.00 | 0.89 |
| 1:J:300:SER:HA | 1:J:335:ARG:HG3 | 1.51 | 0.89 |
| 1:K:300:SER:HA | 1:K:335:ARG:HG3 | 1.51 | 0.89 |
| 1:N:34:ILE:HG21 | 1:N:67:LEU:CD2 | 2.02 | 0.89 |
| 1:S:73:HIC:HA | 1:S:183:ARG:HH12 | 1.36 | 0.89 |
| 1:S:236:LEU:HD13 | 1:S:251:GLY:CA | 2.02 | 0.89 |
| 1:T:290:ARG:HD2 | 1:V:244:ASP:CB | 2.01 | 0.89 |
| 1:C:104:LEU:HB2 | 1:C:356:TRP:CH2 | 2.07 | 0.89 |
| 1:L:300:SER:HA | 1:L:335:ARG:HG3 | 1.51 | 0.89 |
| 1:O:236:LEU:HD13 | 1:O:251:GLY:CA | 2.02 | 0.89 |
| 1:Q:236:LEU:HD13 | 1:Q:251:GLY:CA | 2.03 | 0.89 |
| 1:U:104:LEU:HB2 | 1:U:356:TRP:CH2 | 2.07 | 0.89 |
| 1:W:236:LEU:HD13 | 1:W:251:GLY:CA | 2.02 | 0.89 |
| 1:G:300:SER:HA | 1:G:335:ARG:HG3 | 1.51 | 0.89 |
| 1:H:34:ILE:HG21 | 1:H:67:LEU:CD2 | 2.02 | 0.89 |
| 1:K:357:ILE:CG1 | 1:K:370:VAL:HG23 | 2.00 | 0.89 |
| 1:S:290:ARG:HD2 | 1:U:244:ASP:CB | 2.01 | 0.89 |
| 1:U:236:LEU:HD13 | 1:U:251:GLY:CA | 2.02 | 0.89 |
| 1:W:34:ILE:HG21 | 1:W:67:LEU:CD2 | 2.02 | 0.89 |
| 1:A:236:LEU:HD13 | 1:A:251:GLY:CA | 2.03 | 0.89 |
| 1:D:290:ARG:HD2 | 1:F:244:ASP:CB | 2.01 | 0.89 |
| 1:V:73:HIC:HA | 1:V:183:ARG:HH12 | 1.36 | 0.89 |
| 1:W:357:ILE:CG1 | 1:W:370:VAL:HG23 | 2.00 | 0.89 |
| 1:D:43:VAL:CG1 | 1:D:44:MET:N | 2.30 | 0.89 |
| 1:E:34:ILE:HG21 | 1:E:67:LEU:CD2 | 2.02 | 0.89 |
| 1:E:104:LEU:HB2 | 1:E:356:TRP:CH2 | 2.07 | 0.89 |
| 1:H:8:LEU:HD12 | 1:H:90:PHE:CE1 | 2.08 | 0.89 |
| 1:K:104:LEU:HB2 | 1:K:356:TRP:CH2 | 2.07 | 0.89 |
| 1:O:73:HIC:HA | 1:O:183:ARG:HH12 | 1.36 | 0.89 |
| 1:O:290:ARG:HD2 | 1:Q:244:ASP:CB | 2.01 | 0.89 |
| 1:Q:34:ILE:HG21 | 1:Q:67:LEU:CD2 | 2.02 | 0.89 |
| 1:Q:357:ILE:CG1 | 1:Q:370:VAL:HG23 | 2.00 | 0.89 |
| 1:R:8:LEU:HD12 | 1:R:90:PHE:CE1 | 2.08 | 0.89 |
| 1:R:236:LEU:HD13 | 1:R:251:GLY:CA | 2.02 | 0.89 |
| 1:S:104:LEU:HB2 | 1:S:356:TRP:CH2 | 2.07 | 0.89 |
| 1:T:236:LEU:HD13 | 1:T:251:GLY:CA | 2.03 | 0.89 |
| 1:A:8:LEU:HD12 | 1:A:90:PHE:CE1 | 2.08 | 0.89 |
| 1:B:34:ILE:HG21 | 1:B:67:LEU:CD2 | 2.02 | 0.89 |
| 1:G:8:LEU:HD12 | 1:G:90:PHE:CE1 | 2.08 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:290:ARG:HD2 | 1:K:244:ASP:CB | 2.02 | 0.89 |
| 1:K:236:LEU:HD13 | 1:K:251:GLY:CA | 2.02 | 0.89 |
| 1:S:8:LEU:HD12 | 1:S:90:PHE:CE1 | 2.08 | 0.89 |
| 1:C:34:ILE:HG21 | 1:C:67:LEU:CD2 | 2.02 | 0.89 |
| 1:M:34:ILE:HG21 | 1:M:67:LEU:CD2 | 2.02 | 0.89 |
| 1:M:104:LEU:HB2 | 1:M:356:TRP:CH2 | 2.07 | 0.89 |
| 1:Q:104:LEU:HB2 | 1:Q:356:TRP:CH2 | 2.07 | 0.89 |
| 1:T:73:HIC:HA | 1:T:183:ARG:HH12 | 1.36 | 0.89 |
| 1:V:43:VAL:CG1 | 1:V:44:MET:N | 2.30 | 0.89 |
| 1:C:236:LEU:HD13 | 1:C:251:GLY:CA | 2.02 | 0.89 |
| 1:G:104:LEU:HB2 | 1:G:356:TRP:CH2 | 2.07 | 0.89 |
| 1:H:290:ARG:HD2 | 1:J:244:ASP:CB | 2.01 | 0.89 |
| 1:L:8:LEU:HD12 | 1:L:90:PHE:CE1 | 2.08 | 0.89 |
| 1:M:236:LEU:HD13 | 1:M:251:GLY:CA | 2.03 | 0.89 |
| 1:P:43:VAL:CG1 | 1:P:44:MET:N | 2.30 | 0.89 |
| 1:S:34:ILE:HG21 | 1:S:67:LEU:CD2 | 2.02 | 0.89 |
| 1:T:34:ILE:HG21 | 1:T:67:LEU:CD2 | 2.02 | 0.89 |
| 1:V:236:LEU:HD13 | 1:V:251:GLY:CA | 2.02 | 0.89 |
| 1:W:8:LEU:HD12 | 1:W:90:PHE:CE1 | 2.08 | 0.89 |
| 1:D:73:HIC:HA | 1:D:183:ARG:HH12 | 1.36 | 0.89 |
| 1:G:34:ILE:HG21 | 1:G:67:LEU:CD2 | 2.02 | 0.89 |
| 1:I:236:LEU:HD13 | 1:I:251:GLY:CA | 2.03 | 0.89 |
| 1:N:8:LEU:HD12 | 1:N:90:PHE:CE1 | 2.08 | 0.89 |
| 1:O:104:LEU:HB2 | 1:O:356:TRP:CH2 | 2.07 | 0.89 |
| 1:V:34:ILE:HG21 | 1:V:67:LEU:CD2 | 2.02 | 0.89 |
| 1:B:8:LEU:HD12 | 1:B:90:PHE:CE1 | 2.08 | 0.88 |
| 1:D:34:ILE:HG21 | 1:D:67:LEU:CD2 | 2.02 | 0.88 |
| 1:D:236:LEU:HD13 | 1:D:251:GLY:CA | 2.02 | 0.88 |
| 1:I:300:SER:HA | 1:I:335:ARG:HG3 | 1.51 | 0.88 |
| 1:J:34:ILE:HG21 | 1:J:67:LEU:CD2 | 2.02 | 0.88 |
| 1:M:8:LEU:HD12 | 1:M:90:PHE:CE1 | 2.08 | 0.88 |
| 1:D:8:LEU:HD12 | 1:D:90:PHE:CE1 | 2.08 | 0.88 |
| 1:E:8:LEU:HD12 | 1:E:90:PHE:CE1 | 2.08 | 0.88 |
| 1:F:236:LEU:HD13 | 1:F:251:GLY:CA | 2.02 | 0.88 |
| 1:F:357:ILE:CG1 | 1:F:370:VAL:HG23 | 2.00 | 0.88 |
| 1:I:104:LEU:HB2 | 1:I:356:TRP:CH2 | 2.07 | 0.88 |
| 1:P:236:LEU:HD13 | 1:P:251:GLY:CA | 2.02 | 0.88 |
| 1:C:8:LEU:HD12 | 1:C:90:PHE:CE1 | 2.08 | 0.88 |
| 1:C:73:HIC:HA | 1:C:183:ARG:HH12 | 1.36 | 0.88 |
| 1:P:8:LEU:HD12 | 1:P:90:PHE:CE1 | 2.08 | 0.88 |
| 1:R:34:ILE:HG21 | 1:R:67:LEU:CD2 | 2.02 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:73:HIC:HA | 1:U:183:ARG:HH12 | 1.36 | 0.88 |
| 1:U:300:SER:HA | 1:U:335:ARG:HG3 | 1.51 | 0.88 |
| 1:E:73:HIC:HA | 1:E:183:ARG:HH12 | 1.36 | 0.88 |
| 1:U:8:LEU:HD12 | 1:U:90:PHE:CE1 | 2.08 | 0.88 |
| 1:V:8:LEU:HD12 | 1:V:90:PHE:CE1 | 2.08 | 0.88 |
| 1:J:43:VAL:CG1 | 1:J:44:MET:N | 2.30 | 0.88 |
| 1:L:73:HIC:HA | 1:L:183:ARG:HH12 | 1.36 | 0.88 |
| 1:A:34:ILE:HG21 | 1:A:67:LEU:CD2 | 2.02 | 0.88 |
| 1:B:236:LEU:HD13 | 1:B:251:GLY:CA | 2.02 | 0.88 |
| 1:F:8:LEU:HD12 | 1:F:90:PHE:CE1 | 2.08 | 0.88 |
| 1:H:236:LEU:HD13 | 1:H:251:GLY:CA | 2.03 | 0.88 |
| 1:A:73:HIC:HA | 1:A:183:ARG:HH12 | 1.36 | 0.88 |
| 1:E:236:LEU:HD13 | 1:E:251:GLY:CA | 2.02 | 0.88 |
| 1:G:236:LEU:HD13 | 1:G:251:GLY:CA | 2.03 | 0.88 |
| 1:J:8:LEU:HD12 | 1:J:90:PHE:CE1 | 2.08 | 0.88 |
| 1:K:8:LEU:HD12 | 1:K:90:PHE:CE1 | 2.08 | 0.88 |
| 1:O:8:LEU:HD12 | 1:O:90:PHE:CE1 | 2.08 | 0.88 |
| 1:I:34:ILE:HG21 | 1:I:67:LEU:CD2 | 2.02 | 0.88 |
| 1:M:73:HIC:HA | 1:M:183:ARG:HH12 | 1.36 | 0.88 |
| 1:P:34:ILE:HG21 | 1:P:67:LEU:CD2 | 2.02 | 0.88 |
| 1:Q:8:LEU:HD12 | 1:Q:90:PHE:CE1 | 2.08 | 0.88 |
| 1:T:8:LEU:HD12 | 1:T:90:PHE:CE1 | 2.08 | 0.88 |
| 1:G:73:HIC:HA | 1:G:183:ARG:HH12 | 1.36 | 0.88 |
| 1:R:73:HIC:HA | 1:R:183:ARG:HH12 | 1.36 | 0.88 |
| 1:K:34:ILE:HG21 | 1:K:67:LEU:CD2 | 2.02 | 0.87 |
| 1:S:43:VAL:CG1 | 1:S:44:MET:N | 2.30 | 0.87 |
| 1:I:8:LEU:HD12 | 1:I:90:PHE:CE1 | 2.08 | 0.87 |
| 1:N:236:LEU:HD13 | 1:N:251:GLY:CA | 2.02 | 0.87 |
| 1:J:236:LEU:HD13 | 1:J:251:GLY:CA | 2.03 | 0.87 |
| 1:B:73:HIC:HA | 1:B:183:ARG:HH12 | 1.36 | 0.87 |
| 1:L:236:LEU:HD13 | 1:L:251:GLY:CA | 2.03 | 0.87 |
| 1:K:73:HIC:HA | 1:K:183:ARG:HH12 | 1.36 | 0.87 |
| 1:W:73:HIC:HA | 1:W:183:ARG:HH12 | 1.36 | 0.87 |
| 1:I:73:HIC:HA | 1:I:183:ARG:HH12 | 1.36 | 0.86 |
| 1:K:43:VAL:CG1 | 1:K:44:MET:N | 2.30 | 0.86 |
| 1:N:73:HIC:HA | 1:N:183:ARG:HH12 | 1.36 | 0.86 |
| 1:J:134:VAL:O | 1:J:375:PHE:HB3 | 1.76 | 0.86 |
| 1:L:134:VAL:O | 1:L:375:PHE:HB3 | 1.76 | 0.86 |
| 1:N:134:VAL:O | 1:N:375:PHE:HB3 | 1.76 | 0.86 |
| 1:W:134:VAL:O | 1:W:375:PHE:HB3 | 1.76 | 0.86 |
| 1:A:134:VAL:O | 1:A:375:PHE:HB3 | 1.76 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:43:VAL:CG1 | 1:E:44:MET:N | 2.30 | 0.86 |
| 1:C:134:VAL:O | 1:C:375:PHE:HB3 | 1.76 | 0.85 |
| 1:P:134:VAL:O | 1:P:375:PHE:HB3 | 1.76 | 0.85 |
| 1:H:134:VAL:O | 1:H:375:PHE:HB3 | 1.76 | 0.85 |
| 1:P:73:HIC:HA | 1:P:183:ARG:HH12 | 1.36 | 0.85 |
| 1:B:361:GLU:CB | 1:B:369:ILE:HD13 | 2.06 | 0.85 |
| 1:K:361:GLU:CB | 1:K:369:ILE:HD13 | 2.06 | 0.85 |
| 1:V:361:GLU:CB | 1:V:369:ILE:HD13 | 2.06 | 0.85 |
| 1:U:134:VAL:O | 1:U:375:PHE:HB3 | 1.76 | 0.85 |
| 1:R:134:VAL:O | 1:R:375:PHE:HB3 | 1.76 | 0.85 |
| 1:E:134:VAL:O | 1:E:375:PHE:HB3 | 1.76 | 0.85 |
| 1:F:134:VAL:O | 1:F:375:PHE:HB3 | 1.76 | 0.85 |
| 1:S:134:VAL:O | 1:S:375:PHE:HB3 | 1.76 | 0.85 |
| 1:W:361:GLU:CB | 1:W:369:ILE:HD13 | 2.06 | 0.85 |
| 1:H:236:LEU:HD13 | 1:H:251:GLY:HA3 | 1.58 | 0.85 |
| 1:T:134:VAL:O | 1:T:375:PHE:HB3 | 1.76 | 0.85 |
| 1:T:361:GLU:CB | 1:T:369:ILE:HD13 | 2.06 | 0.85 |
| 1:G:134:VAL:O | 1:G:375:PHE:HB3 | 1.76 | 0.85 |
| 1:U:236:LEU:HD13 | 1:U:251:GLY:HA3 | 1.58 | 0.85 |
| 1:U:361:GLU:CB | 1:U:369:ILE:HD13 | 2.06 | 0.85 |
| 1:B:43:VAL:CG1 | 1:B:44:MET:N | 2.30 | 0.85 |
| 1:D:134:VAL:O | 1:D:375:PHE:HB3 | 1.76 | 0.85 |
| 1:F:236:LEU:HD13 | 1:F:251:GLY:HA3 | 1.58 | 0.84 |
| 1:L:236:LEU:HD13 | 1:L:251:GLY:HA3 | 1.58 | 0.84 |
| 1:Q:134:VAL:O | 1:Q:375:PHE:HB3 | 1.76 | 0.84 |
| 1:I:361:GLU:CB | 1:I:369:ILE:HD13 | 2.06 | 0.84 |
| 1:V:134:VAL:O | 1:V:375:PHE:HB3 | 1.76 | 0.84 |
| 1:B:134:VAL:O | 1:B:375:PHE:HB3 | 1.76 | 0.84 |
| 1:I:134:VAL:O | 1:I:375:PHE:HB3 | 1.76 | 0.84 |
| 1:M:8:LEU:CD1 | 1:M:90:PHE:HE1 | 1.90 | 0.84 |
| 1:N:236:LEU:HD13 | 1:N:251:GLY:HA3 | 1.58 | 0.84 |
| 1:O:43:VAL:CG1 | 1:O:44:MET:N | 2.30 | 0.84 |
| 1:T:43:VAL:CG1 | 1:T:44:MET:N | 2.30 | 0.84 |
| 1:J:236:LEU:HD13 | 1:J:251:GLY:HA3 | 1.58 | 0.84 |
| 1:K:8:LEU:CD1 | 1:K:90:PHE:HE1 | 1.90 | 0.84 |
| 1:O:134:VAL:O | 1:O:375:PHE:HB3 | 1.76 | 0.84 |
| 1:R:361:GLU:CB | 1:R:369:ILE:HD13 | 2.06 | 0.84 |
| 1:V:236:LEU:HD13 | 1:V:251:GLY:HA3 | 1.58 | 0.84 |
| 1:W:236:LEU:HD13 | 1:W:251:GLY:HA3 | 1.58 | 0.84 |
| 1:A:236:LEU:HD13 | 1:A:251:GLY:HA3 | 1.58 | 0.84 |
| 1:K:134:VAL:O | 1:K:375:PHE:HB3 | 1.76 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:287:ILE:HD11 | 1:N:208:ILE:HD13 | 1.60 | 0.84 |
| 1:M:134:VAL:O | 1:M:375:PHE:HB3 | 1.76 | 0.84 |
| 1:N:8:LEU:CD1 | 1:N:90:PHE:HE1 | 1.90 | 0.84 |
| 1:S:236:LEU:HD13 | 1:S:251:GLY:HA3 | 1.58 | 0.84 |
| 1:S:361:GLU:CB | 1:S:369:ILE:HD13 | 2.06 | 0.84 |
| 1:B:8:LEU:CD1 | 1:B:90:PHE:HE1 | 1.90 | 0.84 |
| 1:K:236:LEU:HD13 | 1:K:251:GLY:HA3 | 1.58 | 0.84 |
| 1:T:236:LEU:HD13 | 1:T:251:GLY:HA3 | 1.58 | 0.84 |
| 1:W:8:LEU:CD1 | 1:W:90:PHE:HE1 | 1.90 | 0.84 |
| 1:A:361:GLU:CB | 1:A:369:ILE:HD13 | 2.06 | 0.84 |
| 1:F:287:ILE:HD11 | 1:H:208:ILE:HD13 | 1.60 | 0.84 |
| 1:M:236:LEU:HD13 | 1:M:251:GLY:HA3 | 1.58 | 0.84 |
| 1:U:287:ILE:HD11 | 1:W:208:ILE:HD13 | 1.60 | 0.84 |
| 1:V:8:LEU:CD1 | 1:V:90:PHE:HE1 | 1.90 | 0.84 |
| 1:H:287:ILE:HD11 | 1:J:208:ILE:HD13 | 1.60 | 0.84 |
| 1:C:361:GLU:CB | 1:C:369:ILE:HD13 | 2.06 | 0.84 |
| 1:D:8:LEU:CD1 | 1:D:90:PHE:HE1 | 1.90 | 0.84 |
| 1:E:361:GLU:CB | 1:E:369:ILE:HD13 | 2.06 | 0.84 |
| 1:L:8:LEU:CD1 | 1:L:90:PHE:HE1 | 1.90 | 0.84 |
| 1:P:8:LEU:CD1 | 1:P:90:PHE:HE1 | 1.90 | 0.84 |
| 1:J:361:GLU:CB | 1:J:369:ILE:HD13 | 2.06 | 0.84 |
| 1:N:287:ILE:HD11 | 1:P:208:ILE:HD13 | 1.60 | 0.84 |
| 1:P:361:GLU:CB | 1:P:369:ILE:HD13 | 2.06 | 0.84 |
| 1:O:8:LEU:CD1 | 1:O:90:PHE:HE1 | 1.90 | 0.83 |
| 1:S:287:ILE:HD11 | 1:U:208:ILE:HD13 | 1.60 | 0.83 |
| 1:T:8:LEU:CD1 | 1:T:90:PHE:HE1 | 1.90 | 0.83 |
| 1:U:8:LEU:CD1 | 1:U:90:PHE:HE1 | 1.90 | 0.83 |
| 1:I:8:LEU:CD1 | 1:I:90:PHE:HE1 | 1.90 | 0.83 |
| 1:J:287:ILE:HD11 | 1:L:208:ILE:HD13 | 1.60 | 0.83 |
| 1:O:287:ILE:HD11 | 1:Q:208:ILE:HD13 | 1.60 | 0.83 |
| 1:B:287:ILE:HD11 | 1:D:208:ILE:HD13 | 1.60 | 0.83 |
| 1:C:287:ILE:HD11 | 1:E:208:ILE:HD13 | 1.60 | 0.83 |
| 1:E:236:LEU:HD13 | 1:E:251:GLY:HA3 | 1.58 | 0.83 |
| 1:G:361:GLU:CB | 1:G:369:ILE:HD13 | 2.06 | 0.83 |
| 1:N:361:GLU:CB | 1:N:369:ILE:HD13 | 2.06 | 0.83 |
| 1:Q:287:ILE:HD11 | 1:S:208:ILE:HD13 | 1.60 | 0.83 |
| 1:D:236:LEU:HD13 | 1:D:251:GLY:HA3 | 1.58 | 0.83 |
| 1:R:236:LEU:HD13 | 1:R:251:GLY:HA3 | 1.58 | 0.83 |
| 1:D:287:ILE:HD11 | 1:F:208:ILE:HD13 | 1.60 | 0.83 |
| 1:E:8:LEU:CD1 | 1:E:90:PHE:HE1 | 1.90 | 0.83 |
| 1:L:361:GLU:CB | 1:L:369:ILE:HD13 | 2.06 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:236:LEU:HD13 | 1:O:251:GLY:HA3 | 1.58 | 0.83 |
| 1:P:236:LEU:HD13 | 1:P:251:GLY:HA3 | 1.58 | 0.83 |
| 1:C:8:LEU:CD1 | 1:C:90:PHE:HE1 | 1.90 | 0.83 |
| 1:E:287:ILE:HD11 | 1:G:208:ILE:HD13 | 1.60 | 0.83 |
| 1:P:287:ILE:HD11 | 1:R:208:ILE:HD13 | 1.60 | 0.83 |
| 1:R:8:LEU:CD1 | 1:R:90:PHE:HE1 | 1.90 | 0.83 |
| 1:R:287:ILE:HD11 | 1:T:208:ILE:HD13 | 1.60 | 0.83 |
| 1:A:287:ILE:HD11 | 1:C:208:ILE:HD13 | 1.60 | 0.83 |
| 1:C:236:LEU:HD13 | 1:C:251:GLY:HA3 | 1.58 | 0.83 |
| 1:I:236:LEU:HD13 | 1:I:251:GLY:HA3 | 1.58 | 0.83 |
| 1:J:8:LEU:CD1 | 1:J:90:PHE:HE1 | 1.90 | 0.83 |
| 1:Q:43:VAL:CG1 | 1:Q:44:MET:N | 2.30 | 0.83 |
| 1:M:287:ILE:HD11 | 1:O:208:ILE:HD13 | 1.60 | 0.83 |
| 1:Q:361:GLU:CB | 1:Q:369:ILE:HD13 | 2.06 | 0.83 |
| 1:F:8:LEU:CD1 | 1:F:90:PHE:HE1 | 1.90 | 0.83 |
| 1:G:8:LEU:CD1 | 1:G:90:PHE:HE1 | 1.90 | 0.83 |
| 1:Q:236:LEU:HD13 | 1:Q:251:GLY:HA3 | 1.58 | 0.83 |
| 1:A:8:LEU:CD1 | 1:A:90:PHE:HE1 | 1.90 | 0.83 |
| 1:B:236:LEU:HD13 | 1:B:251:GLY:HA3 | 1.58 | 0.83 |
| 1:S:8:LEU:CD1 | 1:S:90:PHE:HE1 | 1.90 | 0.82 |
| 1:T:287:ILE:HD11 | 1:V:208:ILE:HD13 | 1.60 | 0.82 |
| 1:G:287:ILE:HD11 | 1:I:208:ILE:HD13 | 1.60 | 0.82 |
| 1:H:8:LEU:CD1 | 1:H:90:PHE:HE1 | 1.90 | 0.82 |
| 1:Q:35:VAL:N | 1:Q:54:VAL:HG21 | 1.95 | 0.82 |
| 1:E:35:VAL:N | 1:E:54:VAL:HG21 | 1.95 | 0.82 |
| 1:G:35:VAL:N | 1:G:54:VAL:HG21 | 1.95 | 0.82 |
| 1:Q:8:LEU:CD1 | 1:Q:90:PHE:HE1 | 1.90 | 0.82 |
| 1:R:35:VAL:N | 1:R:54:VAL:HG21 | 1.95 | 0.82 |
| 1:F:35:VAL:N | 1:F:54:VAL:HG21 | 1.95 | 0.82 |
| 1:K:287:ILE:HD11 | 1:M:208:ILE:HD13 | 1.60 | 0.82 |
| 1:C:35:VAL:N | 1:C:54:VAL:HG21 | 1.95 | 0.82 |
| 1:D:35:VAL:N | 1:D:54:VAL:HG21 | 1.95 | 0.82 |
| 1:H:361:GLU:CB | 1:H:369:ILE:HD13 | 2.06 | 0.82 |
| 1:A:35:VAL:N | 1:A:54:VAL:HG21 | 1.95 | 0.82 |
| 1:I:35:VAL:N | 1:I:54:VAL:HG21 | 1.95 | 0.82 |
| 1:I:287:ILE:HD11 | 1:K:208:ILE:HD13 | 1.60 | 0.82 |
| 1:K:35:VAL:N | 1:K:54:VAL:HG21 | 1.95 | 0.82 |
| 1:M:35:VAL:N | 1:M:54:VAL:HG21 | 1.95 | 0.82 |
| 1:B:35:VAL:N | 1:B:54:VAL:HG21 | 1.95 | 0.82 |
| 1:H:140:LEU:O | 1:H:342:GLY:HA3 | 1.80 | 0.82 |
| 1:J:140:LEU:O | 1:J:342:GLY:HA3 | 1.80 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:35:VAL:N | 1:W:54:VAL:HG21 | 1.95 | 0.82 |
| 1:F:140:LEU:O | 1:F:342:GLY:HA3 | 1.80 | 0.82 |
| 1:G:236:LEU:HD13 | 1:G:251:GLY:HA3 | 1.58 | 0.82 |
| 1:L:35:VAL:N | 1:L:54:VAL:HG21 | 1.95 | 0.82 |
| 1:V:35:VAL:N | 1:V:54:VAL:HG21 | 1.95 | 0.82 |
| 1:K:169:TYR:CZ | 1:M:40:HIS:HB3 | 2.15 | 0.81 |
| 1:U:35:VAL:N | 1:U:54:VAL:HG21 | 1.95 | 0.81 |
| 1:L:140:LEU:O | 1:L:342:GLY:HA3 | 1.80 | 0.81 |
| 1:O:35:VAL:N | 1:O:54:VAL:HG21 | 1.95 | 0.81 |
| 1:S:35:VAL:N | 1:S:54:VAL:HG21 | 1.95 | 0.81 |
| 1:T:35:VAL:N | 1:T:54:VAL:HG21 | 1.95 | 0.81 |
| 1:A:169:TYR:CZ | 1:C:40:HIS:HB3 | 2.15 | 0.81 |
| 1:B:140:LEU:O | 1:B:342:GLY:HA3 | 1.80 | 0.81 |
| 1:B:169:TYR:CZ | 1:D:40:HIS:HB3 | 2.15 | 0.81 |
| 1:C:362:TYR:HE1 | 1:C:367:PRO:HB3 | 1.46 | 0.81 |
| 1:D:140:LEU:O | 1:D:342:GLY:HA3 | 1.80 | 0.81 |
| 1:E:140:LEU:O | 1:E:342:GLY:HA3 | 1.80 | 0.81 |
| 1:H:35:VAL:N | 1:H:54:VAL:HG21 | 1.95 | 0.81 |
| 1:I:169:TYR:CZ | 1:K:40:HIS:HB3 | 2.16 | 0.81 |
| 1:J:362:TYR:HE1 | 1:J:367:PRO:HB3 | 1.46 | 0.81 |
| 1:M:169:TYR:CZ | 1:O:40:HIS:HB3 | 2.16 | 0.81 |
| 1:N:35:VAL:N | 1:N:54:VAL:HG21 | 1.95 | 0.81 |
| 1:N:140:LEU:O | 1:N:342:GLY:HA3 | 1.80 | 0.81 |
| 1:T:169:TYR:CZ | 1:V:40:HIS:HB3 | 2.15 | 0.81 |
| 1:V:362:TYR:HE1 | 1:V:367:PRO:HB3 | 1.46 | 0.81 |
| 1:C:140:LEU:O | 1:C:342:GLY:HA3 | 1.80 | 0.81 |
| 1:J:35:VAL:N | 1:J:54:VAL:HG21 | 1.95 | 0.81 |
| 1:L:362:TYR:HE1 | 1:L:367:PRO:HB3 | 1.46 | 0.81 |
| 1:M:362:TYR:HE1 | 1:M:367:PRO:HB3 | 1.46 | 0.81 |
| 1:P:140:LEU:O | 1:P:342:GLY:HA3 | 1.80 | 0.81 |
| 1:R:169:TYR:CZ | 1:T:40:HIS:HB3 | 2.16 | 0.81 |
| 1:A:362:TYR:HE1 | 1:A:367:PRO:HB3 | 1.46 | 0.81 |
| 1:C:169:TYR:CZ | 1:E:40:HIS:HB3 | 2.15 | 0.81 |
| 1:D:169:TYR:CZ | 1:F:40:HIS:HB3 | 2.15 | 0.81 |
| 1:O:361:GLU:CB | 1:O:369:ILE:HD13 | 2.06 | 0.81 |
| 1:E:362:TYR:HE1 | 1:E:367:PRO:HB3 | 1.46 | 0.81 |
| 1:I:140:LEU:O | 1:I:342:GLY:HA3 | 1.80 | 0.81 |
| 1:K:140:LEU:O | 1:K:342:GLY:HA3 | 1.80 | 0.81 |
| 1:O:169:TYR:CZ | 1:Q:40:HIS:HB3 | 2.15 | 0.81 |
| 1:U:143:TYR:HD1 | 1:U:143:TYR:O | 1.64 | 0.81 |
| 1:G:143:TYR:HD1 | 1:G:143:TYR:O | 1.64 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:143:TYR:HD1 | 1:J:143:TYR:O | 1.64 | 0.81 |
| 1:N:362:TYR:HE1 | 1:N:367:PRO:HB3 | 1.46 | 0.81 |
| 1:P:35:VAL:N | 1:P:54:VAL:HG21 | 1.95 | 0.81 |
| 1:T:140:LEU:O | 1:T:342:GLY:HA3 | 1.80 | 0.81 |
| 1:T:362:TYR:HE1 | 1:T:367:PRO:HB3 | 1.46 | 0.81 |
| 1:V:140:LEU:O | 1:V:342:GLY:HA3 | 1.80 | 0.81 |
| 1:H:362:TYR:HE1 | 1:H:367:PRO:HB3 | 1.46 | 0.81 |
| 1:K:362:TYR:HE1 | 1:K:367:PRO:HB3 | 1.46 | 0.81 |
| 1:R:140:LEU:O | 1:R:342:GLY:HA3 | 1.80 | 0.81 |
| 1:V:143:TYR:O | 1:V:143:TYR:HD1 | 1.64 | 0.81 |
| 1:D:143:TYR:O | 1:D:143:TYR:HD1 | 1.64 | 0.81 |
| 1:F:169:TYR:CZ | 1:H:40:HIS:HB3 | 2.16 | 0.81 |
| 1:F:361:GLU:CB | 1:F:369:ILE:HD13 | 2.06 | 0.81 |
| 1:G:140:LEU:O | 1:G:342:GLY:HA3 | 1.80 | 0.81 |
| 1:G:169:TYR:CZ | 1:I:40:HIS:HB3 | 2.15 | 0.81 |
| 1:I:362:TYR:HE1 | 1:I:367:PRO:HB3 | 1.46 | 0.81 |
| 1:O:362:TYR:HE1 | 1:O:367:PRO:HB3 | 1.46 | 0.81 |
| 1:E:143:TYR:HD1 | 1:E:143:TYR:O | 1.64 | 0.81 |
| 1:F:143:TYR:O | 1:F:143:TYR:HD1 | 1.64 | 0.81 |
| 1:L:169:TYR:CZ | 1:N:40:HIS:HB3 | 2.16 | 0.81 |
| 1:N:169:TYR:CZ | 1:P:40:HIS:HB3 | 2.16 | 0.81 |
| 1:W:362:TYR:HE1 | 1:W:367:PRO:HB3 | 1.46 | 0.81 |
| 1:B:362:TYR:HE1 | 1:B:367:PRO:HB3 | 1.46 | 0.80 |
| 1:C:357:ILE:HG12 | 1:C:370:VAL:CG2 | 2.07 | 0.80 |
| 1:H:169:TYR:CZ | 1:J:40:HIS:HB3 | 2.15 | 0.80 |
| 1:J:169:TYR:CZ | 1:L:40:HIS:HB3 | 2.15 | 0.80 |
| 1:M:140:LEU:O | 1:M:342:GLY:HA3 | 1.80 | 0.80 |
| 1:Q:143:TYR:O | 1:Q:143:TYR:HD1 | 1.64 | 0.80 |
| 1:U:362:TYR:HE1 | 1:U:367:PRO:HB3 | 1.46 | 0.80 |
| 1:D:362:TYR:HE1 | 1:D:367:PRO:HB3 | 1.46 | 0.80 |
| 1:F:362:TYR:HE1 | 1:F:367:PRO:HB3 | 1.46 | 0.80 |
| 1:Q:169:TYR:CZ | 1:S:40:HIS:HB3 | 2.16 | 0.80 |
| 1:E:169:TYR:CZ | 1:G:40:HIS:HB3 | 2.15 | 0.80 |
| 1:E:357:ILE:HG12 | 1:E:370:VAL:CG2 | 2.07 | 0.80 |
| 1:N:357:ILE:HG12 | 1:N:370:VAL:CG2 | 2.07 | 0.80 |
| 1:P:143:TYR:O | 1:P:143:TYR:HD1 | 1.64 | 0.80 |
| 1:P:357:ILE:HG12 | 1:P:370:VAL:CG2 | 2.07 | 0.80 |
| 1:R:32:PRO:HG2 | 1:R:55:GLY:O | 1.82 | 0.80 |
| 1:G:32:PRO:HG2 | 1:G:55:GLY:O | 1.82 | 0.80 |
| 1:O:143:TYR:O | 1:O:143:TYR:HD1 | 1.64 | 0.80 |
| 1:P:169:TYR:CZ | 1:R:40:HIS:HB3 | 2.15 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:32:PRO:HG2 | 1:C:55:GLY:O | 1.82 | 0.80 |
| 1:N:143:TYR:O | 1:N:143:TYR:HD1 | 1.64 | 0.80 |
| 1:O:140:LEU:O | 1:O:342:GLY:HA3 | 1.80 | 0.80 |
| 1:Q:362:TYR:HE1 | 1:Q:367:PRO:HB3 | 1.46 | 0.80 |
| 1:A:32:PRO:HG2 | 1:A:55:GLY:O | 1.82 | 0.80 |
| 1:A:357:ILE:HG12 | 1:A:370:VAL:CG2 | 2.07 | 0.80 |
| 1:G:39:ARG:HE | 1:G:66:THR:CB | 1.95 | 0.80 |
| 1:H:143:TYR:O | 1:H:143:TYR:HD1 | 1.64 | 0.80 |
| 1:I:43:VAL:CG1 | 1:I:44:MET:N | 2.30 | 0.80 |
| 1:J:58:ALA:HB1 | 1:J:65:LEU:HD22 | 1.64 | 0.80 |
| 1:L:58:ALA:HB1 | 1:L:65:LEU:HD22 | 1.64 | 0.80 |
| 1:P:39:ARG:HE | 1:P:66:THR:CB | 1.95 | 0.80 |
| 1:S:169:TYR:CZ | 1:U:40:HIS:HB3 | 2.15 | 0.80 |
| 1:U:32:PRO:HG2 | 1:U:55:GLY:O | 1.82 | 0.80 |
| 1:A:58:ALA:HB1 | 1:A:65:LEU:HD22 | 1.64 | 0.80 |
| 1:E:39:ARG:HE | 1:E:66:THR:CB | 1.95 | 0.80 |
| 1:G:362:TYR:HE1 | 1:G:367:PRO:HB3 | 1.46 | 0.80 |
| 1:I:32:PRO:HG2 | 1:I:55:GLY:O | 1.82 | 0.80 |
| 1:I:45:VAL:O | 1:I:45:VAL:CG2 | 2.30 | 0.80 |
| 1:P:362:TYR:HE1 | 1:P:367:PRO:HB3 | 1.46 | 0.80 |
| 1:Q:32:PRO:HG2 | 1:Q:55:GLY:O | 1.82 | 0.80 |
| 1:R:45:VAL:O | 1:R:45:VAL:CG2 | 2.30 | 0.80 |
| 1:S:32:PRO:HG2 | 1:S:55:GLY:O | 1.82 | 0.80 |
| 1:C:143:TYR:O | 1:C:143:TYR:HD1 | 1.64 | 0.80 |
| 1:E:45:VAL:O | 1:E:45:VAL:CG2 | 2.30 | 0.80 |
| 1:K:143:TYR:O | 1:K:143:TYR:HD1 | 1.64 | 0.80 |
| 1:L:32:PRO:HG2 | 1:L:55:GLY:O | 1.82 | 0.80 |
| 1:L:45:VAL:O | 1:L:45:VAL:CG2 | 2.30 | 0.80 |
| 1:R:39:ARG:HE | 1:R:66:THR:CB | 1.95 | 0.80 |
| 1:U:58:ALA:HB1 | 1:U:65:LEU:HD22 | 1.64 | 0.80 |
| 1:U:140:LEU:O | 1:U:342:GLY:HA3 | 1.80 | 0.80 |
| 1:M:143:TYR:HD1 | 1:M:143:TYR:O | 1.64 | 0.80 |
| 1:N:58:ALA:HB1 | 1:N:65:LEU:HD22 | 1.64 | 0.80 |
| 1:P:58:ALA:HB1 | 1:P:65:LEU:HD22 | 1.64 | 0.80 |
| 1:Q:140:LEU:O | 1:Q:342:GLY:HA3 | 1.80 | 0.80 |
| 1:R:362:TYR:HE1 | 1:R:367:PRO:HB3 | 1.46 | 0.80 |
| 1:S:362:TYR:HE1 | 1:S:367:PRO:HB3 | 1.46 | 0.80 |
| 1:U:45:VAL:O | 1:U:45:VAL:CG2 | 2.30 | 0.80 |
| 1:U:169:TYR:CZ | 1:W:40:HIS:HB3 | 2.16 | 0.80 |
| 1:V:45:VAL:O | 1:V:45:VAL:CG2 | 2.30 | 0.80 |
| 1:W:58:ALA:HB1 | 1:W:65:LEU:HD22 | 1.64 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:140:LEU:O | 1:A:342:GLY:HA3 | 1.80 | 0.79 |
| 1:C:45:VAL:O | 1:C:45:VAL:CG2 | 2.30 | 0.79 |
| 1:H:45:VAL:O | 1:H:45:VAL:CG2 | 2.30 | 0.79 |
| 1:L:357:ILE:HG12 | 1:L:370:VAL:CG2 | 2.07 | 0.79 |
| 1:S:143:TYR:O | 1:S:143:TYR:HD1 | 1.64 | 0.79 |
| 1:V:32:PRO:HG2 | 1:V:55:GLY:O | 1.82 | 0.79 |
| 1:V:39:ARG:HE | 1:V:66:THR:CB | 1.95 | 0.79 |
| 1:W:32:PRO:HG2 | 1:W:55:GLY:O | 1.82 | 0.79 |
| 1:W:143:TYR:O | 1:W:143:TYR:HD1 | 1.64 | 0.79 |
| 1:D:336:LYS:HE2 | 2:D:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:F:58:ALA:HB1 | 1:F:65:LEU:HD22 | 1.64 | 0.79 |
| 1:M:8:LEU:CD1 | 1:M:90:PHE:CE1 | 2.66 | 0.79 |
| 1:N:39:ARG:HE | 1:N:66:THR:CB | 1.95 | 0.79 |
| 1:O:32:PRO:HG2 | 1:O:55:GLY:O | 1.82 | 0.79 |
| 1:F:45:VAL:O | 1:F:45:VAL:CG2 | 2.30 | 0.79 |
| 1:F:336:LYS:HE2 | 2:F:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:I:336:LYS:HE2 | 2:I:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:K:8:LEU:CD1 | 1:K:90:PHE:CE1 | 2.66 | 0.79 |
| 1:S:140:LEU:O | 1:S:342:GLY:HA3 | 1.80 | 0.79 |
| 1:T:32:PRO:HG2 | 1:T:55:GLY:O | 1.82 | 0.79 |
| 1:W:140:LEU:O | 1:W:342:GLY:HA3 | 1.80 | 0.79 |
| 1:H:58:ALA:HB1 | 1:H:65:LEU:HD22 | 1.64 | 0.79 |
| 1:I:39:ARG:HE | 1:I:66:THR:CB | 1.95 | 0.79 |
| 1:K:336:LYS:HE2 | 2:K:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:M:32:PRO:HG2 | 1:M:55:GLY:O | 1.82 | 0.79 |
| 1:M:39:ARG:HE | 1:M:66:THR:CB | 1.95 | 0.79 |
| 1:O:39:ARG:HE | 1:O:66:THR:CB | 1.95 | 0.79 |
| 1:T:143:TYR:O | 1:T:143:TYR:HD1 | 1.64 | 0.79 |
| 1:T:357:ILE:HG12 | 1:T:370:VAL:CG2 | 2.07 | 0.79 |
| 1:A:39:ARG:HE | 1:A:66:THR:CB | 1.95 | 0.79 |
| 1:B:336:LYS:HE2 | 2:B:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:D:54:VAL:HA | 1:D:58:ALA:HB2 | 1.65 | 0.79 |
| 1:G:336:LYS:HE2 | 2:G:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:G:357:ILE:HG12 | 1:G:370:VAL:CG2 | 2.07 | 0.79 |
| 1:H:39:ARG:HE | 1:H:66:THR:CB | 1.95 | 0.79 |
| 1:P:32:PRO:HG2 | 1:P:55:GLY:O | 1.82 | 0.79 |
| 1:P:45:VAL:O | 1:P:45:VAL:CG2 | 2.30 | 0.79 |
| 1:R:357:ILE:HG12 | 1:R:370:VAL:CG2 | 2.07 | 0.79 |
| 1:V:8:LEU:CD1 | 1:V:90:PHE:CE1 | 2.66 | 0.79 |
| 1:B:143:TYR:HD1 | 1:B:143:TYR:O | 1.64 | 0.79 |
| 1:E:58:ALA:HB1 | 1:E:65:LEU:HD22 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:39:ARG:HE | 1:F:66:THR:CB | 1.95 | 0.79 |
| 1:H:336:LYS:HE2 | 2:H:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:Q:54:VAL:HA | 1:Q:58:ALA:HB2 | 1.65 | 0.79 |
| 1:S:45:VAL:O | 1:S:45:VAL:CG2 | 2.30 | 0.79 |
| 1:T:8:LEU:CD1 | 1:T:90:PHE:CE1 | 2.66 | 0.79 |
| 1:B:8:LEU:CD1 | 1:B:90:PHE:CE1 | 2.66 | 0.79 |
| 1:C:39:ARG:HE | 1:C:66:THR:CB | 1.95 | 0.79 |
| 1:D:8:LEU:CD1 | 1:D:90:PHE:CE1 | 2.66 | 0.79 |
| 1:I:143:TYR:O | 1:I:143:TYR:HD1 | 1.64 | 0.79 |
| 1:J:54:VAL:HA | 1:J:58:ALA:HB2 | 1.65 | 0.79 |
| 1:L:54:VAL:HA | 1:L:58:ALA:HB2 | 1.65 | 0.79 |
| 1:N:32:PRO:HG2 | 1:N:55:GLY:O | 1.82 | 0.79 |
| 1:N:45:VAL:O | 1:N:45:VAL:CG2 | 2.30 | 0.79 |
| 1:R:143:TYR:HD1 | 1:R:143:TYR:O | 1.64 | 0.79 |
| 1:S:54:VAL:HA | 1:S:58:ALA:HB2 | 1.65 | 0.79 |
| 1:S:58:ALA:HB1 | 1:S:65:LEU:HD22 | 1.64 | 0.79 |
| 1:J:45:VAL:O | 1:J:45:VAL:CG2 | 2.30 | 0.79 |
| 1:J:332:PRO:HG2 | 1:J:335:ARG:CZ | 2.13 | 0.79 |
| 1:K:45:VAL:O | 1:K:45:VAL:CG2 | 2.30 | 0.79 |
| 1:L:143:TYR:O | 1:L:143:TYR:HD1 | 1.64 | 0.79 |
| 1:M:361:GLU:CB | 1:M:369:ILE:HD13 | 2.06 | 0.79 |
| 1:B:32:PRO:HG2 | 1:B:55:GLY:O | 1.82 | 0.79 |
| 1:B:54:VAL:HA | 1:B:58:ALA:HB2 | 1.65 | 0.79 |
| 1:C:58:ALA:HB1 | 1:C:65:LEU:HD22 | 1.64 | 0.79 |
| 1:D:32:PRO:HG2 | 1:D:55:GLY:O | 1.82 | 0.79 |
| 1:E:8:LEU:CD1 | 1:E:90:PHE:CE1 | 2.66 | 0.79 |
| 1:E:336:LYS:HE2 | 2:E:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:F:54:VAL:HA | 1:F:58:ALA:HB2 | 1.65 | 0.79 |
| 1:G:8:LEU:CD1 | 1:G:90:PHE:CE1 | 2.66 | 0.79 |
| 1:H:332:PRO:HG2 | 1:H:335:ARG:CZ | 2.13 | 0.79 |
| 1:J:39:ARG:HE | 1:J:66:THR:CB | 1.95 | 0.79 |
| 1:L:332:PRO:HG2 | 1:L:335:ARG:CZ | 2.13 | 0.79 |
| 1:O:54:VAL:HA | 1:O:58:ALA:HB2 | 1.65 | 0.79 |
| 1:Q:39:ARG:HE | 1:Q:66:THR:CB | 1.95 | 0.79 |
| 1:U:54:VAL:HA | 1:U:58:ALA:HB2 | 1.65 | 0.79 |
| 1:W:39:ARG:HE | 1:W:66:THR:CB | 1.95 | 0.79 |
| 1:D:39:ARG:HE | 1:D:66:THR:CB | 1.95 | 0.79 |
| 1:H:54:VAL:HA | 1:H:58:ALA:HB2 | 1.65 | 0.79 |
| 1:M:336:LYS:HE2 | 2:M:401:ADP:H5'2 | 1.65 | 0.79 |
| 1:V:357:ILE:HG12 | 1:V:370:VAL:CG2 | 2.07 | 0.79 |
| 1:W:8:LEU:CD1 | 1:W:90:PHE:CE1 | 2.66 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:8:LEU:CD1 | 1:A:90:PHE:CE1 | 2.66 | 0.78 |
| 1:A:143:TYR:O | 1:A:143:TYR:HD1 | 1.64 | 0.78 |
| 1:Q:58:ALA:HB1 | 1:Q:65:LEU:HD22 | 1.64 | 0.78 |
| 1:R:58:ALA:HB1 | 1:R:65:LEU:HD22 | 1.64 | 0.78 |
| 1:S:8:LEU:CD1 | 1:S:90:PHE:CE1 | 2.66 | 0.78 |
| 1:W:54:VAL:HA | 1:W:58:ALA:HB2 | 1.65 | 0.78 |
| 1:D:361:GLU:CB | 1:D:369:ILE:HD13 | 2.06 | 0.78 |
| 1:E:32:PRO:HG2 | 1:E:55:GLY:O | 1.82 | 0.78 |
| 1:F:332:PRO:HG2 | 1:F:335:ARG:CZ | 2.13 | 0.78 |
| 1:K:39:ARG:HE | 1:K:66:THR:CB | 1.95 | 0.78 |
| 1:T:39:ARG:HE | 1:T:66:THR:CB | 1.95 | 0.78 |
| 1:W:45:VAL:O | 1:W:45:VAL:CG2 | 2.30 | 0.78 |
| 1:W:332:PRO:HG2 | 1:W:335:ARG:CZ | 2.13 | 0.78 |
| 1:F:32:PRO:HG2 | 1:F:55:GLY:O | 1.82 | 0.78 |
| 1:G:45:VAL:O | 1:G:45:VAL:CG2 | 2.30 | 0.78 |
| 1:I:8:LEU:CD1 | 1:I:90:PHE:CE1 | 2.66 | 0.78 |
| 1:I:332:PRO:HG2 | 1:I:335:ARG:CZ | 2.13 | 0.78 |
| 1:K:332:PRO:HG2 | 1:K:335:ARG:CZ | 2.13 | 0.78 |
| 1:Q:8:LEU:CD1 | 1:Q:90:PHE:CE1 | 2.66 | 0.78 |
| 1:S:39:ARG:HE | 1:S:66:THR:CB | 1.95 | 0.78 |
| 1:T:58:ALA:HB1 | 1:T:65:LEU:HD22 | 1.64 | 0.78 |
| 1:W:357:ILE:HG12 | 1:W:370:VAL:CG2 | 2.07 | 0.78 |
| 1:C:236:LEU:HD12 | 1:C:237:GLU:N | 1.99 | 0.78 |
| 1:C:336:LYS:HE2 | 2:C:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:D:58:ALA:HB1 | 1:D:65:LEU:HD22 | 1.64 | 0.78 |
| 1:J:336:LYS:HE2 | 2:J:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:L:39:ARG:HE | 1:L:66:THR:CB | 1.95 | 0.78 |
| 1:O:45:VAL:O | 1:O:45:VAL:CG2 | 2.30 | 0.78 |
| 1:A:332:PRO:HG2 | 1:A:335:ARG:CZ | 2.13 | 0.78 |
| 1:J:8:LEU:CD1 | 1:J:90:PHE:CE1 | 2.66 | 0.78 |
| 1:J:357:ILE:HG12 | 1:J:370:VAL:CG2 | 2.07 | 0.78 |
| 1:L:236:LEU:HD12 | 1:L:237:GLU:N | 1.99 | 0.78 |
| 1:N:54:VAL:HA | 1:N:58:ALA:HB2 | 1.65 | 0.78 |
| 1:N:332:PRO:HG2 | 1:N:335:ARG:CZ | 2.13 | 0.78 |
| 1:T:332:PRO:HG2 | 1:T:335:ARG:CZ | 2.13 | 0.78 |
| 1:U:8:LEU:CD1 | 1:U:90:PHE:CE1 | 2.66 | 0.78 |
| 1:A:54:VAL:HA | 1:A:58:ALA:HB2 | 1.65 | 0.78 |
| 1:B:39:ARG:HE | 1:B:66:THR:CB | 1.95 | 0.78 |
| 1:C:8:LEU:CD1 | 1:C:90:PHE:CE1 | 2.66 | 0.78 |
| 1:G:332:PRO:HG2 | 1:G:335:ARG:CZ | 2.13 | 0.78 |
| 1:H:8:LEU:CD1 | 1:H:90:PHE:CE1 | 2.66 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:32:PRO:HG2 | 1:H:55:GLY:O | 1.82 | 0.78 |
| 1:J:32:PRO:HG2 | 1:J:55:GLY:O | 1.82 | 0.78 |
| 1:K:32:PRO:HG2 | 1:K:55:GLY:O | 1.82 | 0.78 |
| 1:M:332:PRO:HG2 | 1:M:335:ARG:CZ | 2.13 | 0.78 |
| 1:U:332:PRO:HG2 | 1:U:335:ARG:CZ | 2.13 | 0.78 |
| 1:U:336:LYS:HE2 | 2:U:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:V:332:PRO:HG2 | 1:V:335:ARG:CZ | 2.13 | 0.78 |
| 1:W:336:LYS:HE2 | 2:W:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:B:58:ALA:HB1 | 1:B:65:LEU:HD22 | 1.64 | 0.78 |
| 1:D:332:PRO:HG2 | 1:D:335:ARG:CZ | 2.13 | 0.78 |
| 1:O:336:LYS:HE2 | 2:O:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:Q:236:LEU:HD12 | 1:Q:237:GLU:N | 1.99 | 0.78 |
| 1:A:336:LYS:HE2 | 2:A:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:G:58:ALA:HB1 | 1:G:65:LEU:HD22 | 1.64 | 0.78 |
| 1:L:8:LEU:CD1 | 1:L:90:PHE:CE1 | 2.66 | 0.78 |
| 1:M:54:VAL:HA | 1:M:58:ALA:HB2 | 1.65 | 0.78 |
| 1:O:236:LEU:HD12 | 1:O:237:GLU:N | 1.99 | 0.78 |
| 1:R:236:LEU:HD12 | 1:R:237:GLU:N | 1.99 | 0.78 |
| 1:S:332:PRO:HG2 | 1:S:335:ARG:CZ | 2.13 | 0.78 |
| 1:T:45:VAL:O | 1:T:45:VAL:CG2 | 2.30 | 0.78 |
| 1:V:336:LYS:HE2 | 2:V:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:C:54:VAL:HA | 1:C:58:ALA:HB2 | 1.65 | 0.78 |
| 1:F:8:LEU:CD1 | 1:F:90:PHE:CE1 | 2.66 | 0.78 |
| 1:I:58:ALA:HB1 | 1:I:65:LEU:HD22 | 1.64 | 0.78 |
| 1:K:54:VAL:HA | 1:K:58:ALA:HB2 | 1.65 | 0.78 |
| 1:K:58:ALA:HB1 | 1:K:65:LEU:HD22 | 1.64 | 0.78 |
| 1:P:8:LEU:CD1 | 1:P:90:PHE:CE1 | 2.66 | 0.78 |
| 1:S:236:LEU:HD12 | 1:S:237:GLU:N | 1.99 | 0.78 |
| 1:I:173:HIS:CE1 | 1:J:268:GLY:HA3 | 2.19 | 0.78 |
| 1:K:173:HIS:CE1 | 1:L:268:GLY:HA3 | 2.19 | 0.78 |
| 1:L:336:LYS:HE2 | 2:L:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:R:332:PRO:HG2 | 1:R:335:ARG:CZ | 2.13 | 0.78 |
| 1:S:336:LYS:HE2 | 2:S:401:ADP:H5'2 | 1.65 | 0.78 |
| 1:A:173:HIS:CE1 | 1:B:268:GLY:HA3 | 2.20 | 0.77 |
| 1:G:173:HIS:CE1 | 1:H:268:GLY:HA3 | 2.19 | 0.77 |
| 1:O:8:LEU:CD1 | 1:O:90:PHE:CE1 | 2.66 | 0.77 |
| 1:O:58:ALA:HB1 | 1:O:65:LEU:HD22 | 1.64 | 0.77 |
| 1:P:332:PRO:HG2 | 1:P:335:ARG:CZ | 2.13 | 0.77 |
| 1:U:39:ARG:HE | 1:U:66:THR:CB | 1.95 | 0.77 |
| 1:A:45:VAL:O | 1:A:45:VAL:CG2 | 2.30 | 0.77 |
| 1:I:357:ILE:HG12 | 1:I:370:VAL:CG2 | 2.07 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:58:ALA:HB1 | 1:M:65:LEU:HD22 | 1.64 | 0.77 |
| 1:N:8:LEU:CD1 | 1:N:90:PHE:CE1 | 2.66 | 0.77 |
| 1:N:236:LEU:HD12 | 1:N:237:GLU:N | 1.99 | 0.77 |
| 1:O:332:PRO:HG2 | 1:O:335:ARG:CZ | 2.13 | 0.77 |
| 1:R:8:LEU:CD1 | 1:R:90:PHE:CE1 | 2.66 | 0.77 |
| 1:T:236:LEU:HD12 | 1:T:237:GLU:N | 1.99 | 0.77 |
| 1:V:58:ALA:HB1 | 1:V:65:LEU:HD22 | 1.64 | 0.77 |
| 1:A:35:VAL:HG22 | 1:A:52:SER:HB2 | 1.66 | 0.77 |
| 1:A:39:ARG:NE | 1:A:66:THR:HA | 2.00 | 0.77 |
| 1:B:236:LEU:HD12 | 1:B:237:GLU:N | 1.99 | 0.77 |
| 1:C:173:HIS:CE1 | 1:D:268:GLY:HA3 | 2.20 | 0.77 |
| 1:C:332:PRO:HG2 | 1:C:335:ARG:CZ | 2.13 | 0.77 |
| 1:E:173:HIS:CE1 | 1:F:268:GLY:HA3 | 2.19 | 0.77 |
| 1:E:236:LEU:HD12 | 1:E:237:GLU:N | 1.99 | 0.77 |
| 1:R:54:VAL:HA | 1:R:58:ALA:HB2 | 1.65 | 0.77 |
| 1:E:54:VAL:HA | 1:E:58:ALA:HB2 | 1.65 | 0.77 |
| 1:G:287:ILE:CD1 | 1:I:208:ILE:HD13 | 2.15 | 0.77 |
| 1:L:173:HIS:CE1 | 1:M:268:GLY:HA3 | 2.19 | 0.77 |
| 1:M:287:ILE:CD1 | 1:O:208:ILE:HD13 | 2.15 | 0.77 |
| 1:N:336:LYS:HE2 | 2:N:401:ADP:H5'2 | 1.65 | 0.77 |
| 1:Q:332:PRO:HG2 | 1:Q:335:ARG:CZ | 2.13 | 0.77 |
| 1:V:236:LEU:HD12 | 1:V:237:GLU:N | 1.99 | 0.77 |
| 1:A:236:LEU:HD12 | 1:A:237:GLU:N | 1.99 | 0.77 |
| 1:D:287:ILE:CD1 | 1:F:208:ILE:HD13 | 2.15 | 0.77 |
| 1:E:332:PRO:HG2 | 1:E:335:ARG:CZ | 2.13 | 0.77 |
| 1:I:54:VAL:HA | 1:I:58:ALA:HB2 | 1.65 | 0.77 |
| 1:K:287:ILE:CD1 | 1:M:208:ILE:HD13 | 2.15 | 0.77 |
| 1:L:35:VAL:HG22 | 1:L:52:SER:HB2 | 1.66 | 0.77 |
| 1:M:236:LEU:HD12 | 1:M:237:GLU:N | 1.99 | 0.77 |
| 1:P:54:VAL:HA | 1:P:58:ALA:HB2 | 1.65 | 0.77 |
| 1:R:36:GLY:O | 1:R:52:SER:HA | 1.85 | 0.77 |
| 1:S:287:ILE:CD1 | 1:U:208:ILE:HD13 | 2.15 | 0.77 |
| 1:J:39:ARG:NE | 1:J:66:THR:HA | 2.00 | 0.77 |
| 1:J:173:HIS:CE1 | 1:K:268:GLY:HA3 | 2.19 | 0.77 |
| 1:N:287:ILE:CD1 | 1:P:208:ILE:HD13 | 2.15 | 0.77 |
| 1:S:173:HIS:CE1 | 1:T:268:GLY:HA3 | 2.19 | 0.77 |
| 1:T:36:GLY:O | 1:T:52:SER:HA | 1.85 | 0.77 |
| 1:T:54:VAL:HA | 1:T:58:ALA:HB2 | 1.65 | 0.77 |
| 1:U:173:HIS:CE1 | 1:V:268:GLY:HA3 | 2.20 | 0.77 |
| 1:V:173:HIS:CE1 | 1:W:268:GLY:HA3 | 2.19 | 0.77 |
| 1:A:34:ILE:C | 1:A:54:VAL:HG21 | 2.05 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:45:VAL:O | 1:D:45:VAL:CG2 | 2.30 | 0.77 |
| 1:F:287:ILE:CD1 | 1:H:208:ILE:HD13 | 2.15 | 0.77 |
| 1:N:173:HIS:CE1 | 1:O:268:GLY:HA3 | 2.20 | 0.77 |
| 1:P:36:GLY:O | 1:P:52:SER:HA | 1.85 | 0.77 |
| 1:P:236:LEU:HD12 | 1:P:237:GLU:N | 1.99 | 0.77 |
| 1:P:287:ILE:CD1 | 1:R:208:ILE:HD13 | 2.15 | 0.77 |
| 1:P:336:LYS:HE2 | 2:P:401:ADP:H5'2 | 1.65 | 0.77 |
| 1:Q:336:LYS:HE2 | 2:Q:401:ADP:H5'2 | 1.65 | 0.77 |
| 1:R:39:ARG:NE | 1:R:66:THR:HA | 2.00 | 0.77 |
| 1:U:287:ILE:CD1 | 1:W:208:ILE:HD13 | 2.15 | 0.77 |
| 1:U:357:ILE:HG12 | 1:U:370:VAL:CG2 | 2.07 | 0.77 |
| 1:W:236:LEU:HD12 | 1:W:237:GLU:N | 1.99 | 0.77 |
| 1:B:173:HIS:CE1 | 1:C:268:GLY:HA3 | 2.19 | 0.77 |
| 1:C:39:ARG:NE | 1:C:66:THR:HA | 2.00 | 0.77 |
| 1:E:287:ILE:CD1 | 1:G:208:ILE:HD13 | 2.15 | 0.77 |
| 1:H:173:HIS:CE1 | 1:I:268:GLY:HA3 | 2.20 | 0.77 |
| 1:J:34:ILE:C | 1:J:54:VAL:HG21 | 2.05 | 0.77 |
| 1:K:34:ILE:C | 1:K:54:VAL:HG21 | 2.06 | 0.77 |
| 1:R:336:LYS:HE2 | 2:R:401:ADP:H5'2 | 1.65 | 0.77 |
| 1:T:173:HIS:CE1 | 1:U:268:GLY:HA3 | 2.20 | 0.77 |
| 1:T:287:ILE:CD1 | 1:V:208:ILE:HD13 | 2.15 | 0.77 |
| 1:T:336:LYS:HE2 | 2:T:401:ADP:H5'2 | 1.65 | 0.77 |
| 1:U:236:LEU:HD12 | 1:U:237:GLU:N | 1.99 | 0.77 |
| 1:V:36:GLY:O | 1:V:52:SER:HA | 1.85 | 0.77 |
| 1:V:54:VAL:HA | 1:V:58:ALA:HB2 | 1.65 | 0.77 |
| 1:B:34:ILE:C | 1:B:54:VAL:HG21 | 2.06 | 0.77 |
| 1:B:332:PRO:HG2 | 1:B:335:ARG:CZ | 2.13 | 0.77 |
| 1:C:37:ARG:HG3 | 1:C:38:PRO:CD | 2.15 | 0.77 |
| 1:E:34:ILE:C | 1:E:54:VAL:HG21 | 2.06 | 0.77 |
| 1:H:236:LEU:HD12 | 1:H:237:GLU:N | 1.99 | 0.77 |
| 1:M:173:HIS:CE1 | 1:N:268:GLY:HA3 | 2.19 | 0.77 |
| 1:N:34:ILE:C | 1:N:54:VAL:HG21 | 2.06 | 0.77 |
| 1:P:173:HIS:CE1 | 1:Q:268:GLY:HA3 | 2.19 | 0.77 |
| 1:A:54:VAL:HG12 | 1:A:55:GLY:N | 2.00 | 0.77 |
| 1:A:287:ILE:CD1 | 1:C:208:ILE:HD13 | 2.15 | 0.77 |
| 1:H:36:GLY:O | 1:H:52:SER:HA | 1.85 | 0.77 |
| 1:J:236:LEU:HD12 | 1:J:237:GLU:N | 1.99 | 0.77 |
| 1:L:287:ILE:CD1 | 1:N:208:ILE:HD13 | 2.15 | 0.77 |
| 1:N:36:GLY:O | 1:N:52:SER:HA | 1.85 | 0.77 |
| 1:P:35:VAL:HG22 | 1:P:52:SER:HB2 | 1.67 | 0.77 |
| 1:Q:36:GLY:O | 1:Q:52:SER:HA | 1.85 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:34:ILE:C | 1:R:54:VAL:HG21 | 2.05 | 0.77 |
| 1:R:173:HIS:CE1 | 1:S:268:GLY:HA3 | 2.19 | 0.77 |
| 1:B:36:GLY:O | 1:B:52:SER:HA | 1.85 | 0.76 |
| 1:D:37:ARG:HG3 | 1:D:38:PRO:CD | 2.15 | 0.76 |
| 1:D:236:LEU:HD12 | 1:D:237:GLU:N | 1.99 | 0.76 |
| 1:F:37:ARG:HG3 | 1:F:38:PRO:CD | 2.15 | 0.76 |
| 1:I:236:LEU:HD12 | 1:I:237:GLU:N | 1.99 | 0.76 |
| 1:N:35:VAL:HG22 | 1:N:52:SER:HB2 | 1.66 | 0.76 |
| 1:O:34:ILE:C | 1:O:54:VAL:HG21 | 2.06 | 0.76 |
| 1:P:39:ARG:NE | 1:P:66:THR:HA | 2.00 | 0.76 |
| 1:P:54:VAL:HG12 | 1:P:55:GLY:N | 2.01 | 0.76 |
| 1:Q:34:ILE:C | 1:Q:54:VAL:HG21 | 2.06 | 0.76 |
| 1:W:34:ILE:C | 1:W:54:VAL:HG21 | 2.05 | 0.76 |
| 1:A:37:ARG:HG3 | 1:A:38:PRO:CD | 2.15 | 0.76 |
| 1:E:35:VAL:HG22 | 1:E:52:SER:HB2 | 1.67 | 0.76 |
| 1:E:54:VAL:HG12 | 1:E:55:GLY:N | 2.01 | 0.76 |
| 1:F:34:ILE:C | 1:F:54:VAL:HG21 | 2.06 | 0.76 |
| 1:F:173:HIS:CE1 | 1:G:268:GLY:HA3 | 2.19 | 0.76 |
| 1:F:236:LEU:HD12 | 1:F:237:GLU:N | 1.99 | 0.76 |
| 1:G:54:VAL:HA | 1:G:58:ALA:HB2 | 1.65 | 0.76 |
| 1:G:236:LEU:HD12 | 1:G:237:GLU:N | 1.99 | 0.76 |
| 1:H:37:ARG:HG3 | 1:H:38:PRO:CD | 2.15 | 0.76 |
| 1:L:39:ARG:NE | 1:L:66:THR:HA | 2.00 | 0.76 |
| 1:O:287:ILE:CD1 | 1:Q:208:ILE:HD13 | 2.15 | 0.76 |
| 1:S:36:GLY:O | 1:S:52:SER:HA | 1.85 | 0.76 |
| 1:U:34:ILE:C | 1:U:54:VAL:HG21 | 2.05 | 0.76 |
| 1:U:35:VAL:HG22 | 1:U:52:SER:HB2 | 1.67 | 0.76 |
| 1:W:36:GLY:O | 1:W:52:SER:HA | 1.85 | 0.76 |
| 1:B:287:ILE:CD1 | 1:D:208:ILE:HD13 | 2.15 | 0.76 |
| 1:G:34:ILE:C | 1:G:54:VAL:HG21 | 2.05 | 0.76 |
| 1:K:357:ILE:HG12 | 1:K:370:VAL:CG2 | 2.07 | 0.76 |
| 1:L:54:VAL:HG12 | 1:L:55:GLY:N | 2.01 | 0.76 |
| 1:O:173:HIS:CE1 | 1:P:268:GLY:HA3 | 2.19 | 0.76 |
| 1:Q:287:ILE:CD1 | 1:S:208:ILE:HD13 | 2.15 | 0.76 |
| 1:T:34:ILE:C | 1:T:54:VAL:HG21 | 2.06 | 0.76 |
| 1:B:37:ARG:HG3 | 1:B:38:PRO:CD | 2.15 | 0.76 |
| 1:D:173:HIS:CE1 | 1:E:268:GLY:HA3 | 2.20 | 0.76 |
| 1:F:36:GLY:O | 1:F:52:SER:HA | 1.85 | 0.76 |
| 1:H:35:VAL:HG22 | 1:H:52:SER:HB2 | 1.66 | 0.76 |
| 1:H:357:ILE:HG12 | 1:H:370:VAL:CG2 | 2.07 | 0.76 |
| 1:I:143:TYR:CZ | 1:K:45:VAL:HG21 | 2.21 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:287:ILE:CD1 | 1:K:208:ILE:HD13 | 2.15 | 0.76 |
| 1:J:143:TYR:CZ | 1:L:45:VAL:HG21 | 2.21 | 0.76 |
| 1:K:236:LEU:HD12 | 1:K:237:GLU:N | 1.99 | 0.76 |
| 1:O:39:ARG:NE | 1:O:66:THR:HA | 2.00 | 0.76 |
| 1:P:143:TYR:CZ | 1:R:45:VAL:HG21 | 2.21 | 0.76 |
| 1:Q:173:HIS:CE1 | 1:R:268:GLY:HA3 | 2.19 | 0.76 |
| 1:T:54:VAL:HG12 | 1:T:55:GLY:N | 2.00 | 0.76 |
| 1:D:34:ILE:C | 1:D:54:VAL:HG21 | 2.06 | 0.76 |
| 1:D:143:TYR:CZ | 1:F:45:VAL:HG21 | 2.21 | 0.76 |
| 1:E:143:TYR:CZ | 1:G:45:VAL:HG21 | 2.21 | 0.76 |
| 1:Q:39:ARG:NE | 1:Q:66:THR:HA | 2.00 | 0.76 |
| 1:R:35:VAL:HG22 | 1:R:52:SER:HB2 | 1.66 | 0.76 |
| 1:S:34:ILE:C | 1:S:54:VAL:HG21 | 2.06 | 0.76 |
| 1:S:143:TYR:CZ | 1:U:45:VAL:HG21 | 2.21 | 0.76 |
| 1:T:39:ARG:NE | 1:T:66:THR:HA | 2.00 | 0.76 |
| 1:C:35:VAL:HG22 | 1:C:52:SER:HB2 | 1.66 | 0.76 |
| 1:D:39:ARG:NE | 1:D:66:THR:HA | 2.00 | 0.76 |
| 1:F:142:LEU:HD21 | 1:F:165:ILE:HD13 | 1.68 | 0.76 |
| 1:G:36:GLY:O | 1:G:52:SER:HA | 1.85 | 0.76 |
| 1:H:287:ILE:CD1 | 1:J:208:ILE:HD13 | 2.15 | 0.76 |
| 1:J:35:VAL:HG22 | 1:J:52:SER:HB2 | 1.66 | 0.76 |
| 1:Q:45:VAL:O | 1:Q:45:VAL:CG2 | 2.30 | 0.76 |
| 1:S:142:LEU:HD21 | 1:S:165:ILE:HD13 | 1.68 | 0.76 |
| 1:T:35:VAL:HG22 | 1:T:52:SER:HB2 | 1.66 | 0.76 |
| 1:U:39:ARG:NE | 1:U:66:THR:HA | 2.00 | 0.76 |
| 1:U:143:TYR:CZ | 1:W:45:VAL:HG21 | 2.21 | 0.76 |
| 1:G:39:ARG:NE | 1:G:66:THR:HA | 2.00 | 0.76 |
| 1:I:39:ARG:NE | 1:I:66:THR:HA | 2.00 | 0.76 |
| 1:L:36:GLY:O | 1:L:52:SER:HA | 1.85 | 0.76 |
| 1:Q:142:LEU:HD21 | 1:Q:165:ILE:HD13 | 1.68 | 0.76 |
| 1:R:287:ILE:CD1 | 1:T:208:ILE:HD13 | 2.15 | 0.76 |
| 1:A:36:GLY:O | 1:A:52:SER:HA | 1.85 | 0.76 |
| 1:C:36:GLY:O | 1:C:52:SER:HA | 1.85 | 0.76 |
| 1:C:287:ILE:CD1 | 1:E:208:ILE:HD13 | 2.15 | 0.76 |
| 1:H:143:TYR:CZ | 1:J:45:VAL:HG21 | 2.21 | 0.76 |
| 1:K:39:ARG:NE | 1:K:66:THR:HA | 2.00 | 0.76 |
| 1:M:34:ILE:C | 1:M:54:VAL:HG21 | 2.05 | 0.76 |
| 1:M:35:VAL:HG22 | 1:M:52:SER:HB2 | 1.66 | 0.76 |
| 1:M:143:TYR:CZ | 1:O:45:VAL:HG21 | 2.21 | 0.76 |
| 1:V:37:ARG:HG3 | 1:V:38:PRO:CD | 2.15 | 0.76 |
| 1:W:142:LEU:HD21 | 1:W:165:ILE:HD13 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:142:LEU:HD21 | 1:D:165:ILE:HD13 | 1.68 | 0.76 |
| 1:F:39:ARG:NE | 1:F:66:THR:HA | 2.00 | 0.76 |
| 1:G:143:TYR:CZ | 1:I:45:VAL:HG21 | 2.21 | 0.76 |
| 1:H:34:ILE:C | 1:H:54:VAL:HG21 | 2.06 | 0.76 |
| 1:H:39:ARG:NE | 1:H:66:THR:HA | 2.00 | 0.76 |
| 1:H:142:LEU:HD21 | 1:H:165:ILE:HD13 | 1.68 | 0.76 |
| 1:J:142:LEU:HD21 | 1:J:165:ILE:HD13 | 1.68 | 0.76 |
| 1:O:143:TYR:CZ | 1:Q:45:VAL:HG21 | 2.21 | 0.76 |
| 1:P:34:ILE:C | 1:P:54:VAL:HG21 | 2.06 | 0.76 |
| 1:S:357:ILE:HG12 | 1:S:370:VAL:CG2 | 2.07 | 0.76 |
| 1:T:143:TYR:CZ | 1:V:45:VAL:HG21 | 2.21 | 0.76 |
| 1:W:37:ARG:HG3 | 1:W:38:PRO:CD | 2.15 | 0.76 |
| 1:A:143:TYR:CZ | 1:C:45:VAL:HG21 | 2.21 | 0.76 |
| 1:B:35:VAL:HG22 | 1:B:52:SER:HB2 | 1.66 | 0.76 |
| 1:B:44:MET:HG3 | 1:B:45:VAL:H | 1.51 | 0.76 |
| 1:E:36:GLY:O | 1:E:52:SER:HA | 1.85 | 0.76 |
| 1:I:148:THR:O | 1:I:165:ILE:HG22 | 1.86 | 0.76 |
| 1:J:287:ILE:CD1 | 1:L:208:ILE:HD13 | 2.15 | 0.76 |
| 1:K:44:MET:HG3 | 1:K:45:VAL:H | 1.51 | 0.76 |
| 1:M:142:LEU:HD21 | 1:M:165:ILE:HD13 | 1.68 | 0.76 |
| 1:O:148:THR:O | 1:O:165:ILE:HG22 | 1.86 | 0.76 |
| 1:R:143:TYR:CZ | 1:T:45:VAL:HG21 | 2.21 | 0.76 |
| 1:S:39:ARG:NE | 1:S:66:THR:HA | 2.00 | 0.76 |
| 1:T:37:ARG:HG3 | 1:T:38:PRO:CD | 2.15 | 0.76 |
| 1:W:54:VAL:HG12 | 1:W:55:GLY:N | 2.00 | 0.76 |
| 1:G:54:VAL:HG12 | 1:G:55:GLY:N | 2.01 | 0.75 |
| 1:I:34:ILE:C | 1:I:54:VAL:HG21 | 2.06 | 0.75 |
| 1:K:143:TYR:CZ | 1:M:45:VAL:HG21 | 2.21 | 0.75 |
| 1:L:142:LEU:HD21 | 1:L:165:ILE:HD13 | 1.68 | 0.75 |
| 1:M:357:ILE:HG12 | 1:M:370:VAL:CG2 | 2.07 | 0.75 |
| 1:N:143:TYR:CZ | 1:P:45:VAL:HG21 | 2.21 | 0.75 |
| 1:U:142:LEU:HD21 | 1:U:165:ILE:HD13 | 1.68 | 0.75 |
| 1:D:36:GLY:O | 1:D:52:SER:HA | 1.85 | 0.75 |
| 1:F:35:VAL:HG22 | 1:F:52:SER:HB2 | 1.66 | 0.75 |
| 1:K:35:VAL:HG22 | 1:K:52:SER:HB2 | 1.66 | 0.75 |
| 1:K:36:GLY:O | 1:K:52:SER:HA | 1.85 | 0.75 |
| 1:L:143:TYR:CZ | 1:N:45:VAL:HG21 | 2.21 | 0.75 |
| 1:V:39:ARG:NE | 1:V:66:THR:HA | 2.00 | 0.75 |
| 1:B:142:LEU:HD21 | 1:B:165:ILE:HD13 | 1.68 | 0.75 |
| 1:D:148:THR:O | 1:D:165:ILE:HG22 | 1.86 | 0.75 |
| 1:G:35:VAL:HG22 | 1:G:52:SER:HB2 | 1.66 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:54:VAL:HG12 | 1:H:55:GLY:N | 2.00 | 0.75 |
| 1:M:36:GLY:O | 1:M:52:SER:HA | 1.85 | 0.75 |
| 1:O:44:MET:HG3 | 1:O:45:VAL:H | 1.51 | 0.75 |
| 1:O:142:LEU:HD21 | 1:O:165:ILE:HD13 | 1.68 | 0.75 |
| 1:R:37:ARG:HG3 | 1:R:38:PRO:CD | 2.15 | 0.75 |
| 1:U:37:ARG:HG3 | 1:U:38:PRO:CD | 2.15 | 0.75 |
| 1:C:34:ILE:C | 1:C:54:VAL:HG21 | 2.06 | 0.75 |
| 1:C:143:TYR:CZ | 1:E:45:VAL:HG21 | 2.21 | 0.75 |
| 1:I:36:GLY:O | 1:I:52:SER:HA | 1.85 | 0.75 |
| 1:I:54:VAL:HG12 | 1:I:55:GLY:N | 2.01 | 0.75 |
| 1:L:34:ILE:C | 1:L:54:VAL:HG21 | 2.06 | 0.75 |
| 1:M:148:THR:O | 1:M:165:ILE:HG22 | 1.86 | 0.75 |
| 1:N:148:THR:O | 1:N:165:ILE:HG22 | 1.86 | 0.75 |
| 1:O:35:VAL:HG22 | 1:O:52:SER:HB2 | 1.66 | 0.75 |
| 1:O:36:GLY:O | 1:O:52:SER:HA | 1.85 | 0.75 |
| 1:Q:143:TYR:CZ | 1:S:45:VAL:HG21 | 2.21 | 0.75 |
| 1:U:36:GLY:O | 1:U:52:SER:HA | 1.85 | 0.75 |
| 1:V:54:VAL:HG12 | 1:V:55:GLY:N | 2.00 | 0.75 |
| 1:B:143:TYR:CZ | 1:D:45:VAL:HG21 | 2.21 | 0.75 |
| 1:F:143:TYR:CZ | 1:H:45:VAL:HG21 | 2.21 | 0.75 |
| 1:J:54:VAL:HG12 | 1:J:55:GLY:N | 2.00 | 0.75 |
| 1:L:148:THR:O | 1:L:165:ILE:HG22 | 1.86 | 0.75 |
| 1:M:39:ARG:NE | 1:M:66:THR:HA | 2.00 | 0.75 |
| 1:N:39:ARG:NE | 1:N:66:THR:HA | 2.00 | 0.75 |
| 1:O:357:ILE:HG12 | 1:O:370:VAL:CG2 | 2.07 | 0.75 |
| 1:Q:142:LEU:HD11 | 1:Q:165:ILE:HD11 | 1.69 | 0.75 |
| 1:V:34:ILE:C | 1:V:54:VAL:HG21 | 2.06 | 0.75 |
| 1:W:35:VAL:HG22 | 1:W:52:SER:HB2 | 1.66 | 0.75 |
| 1:B:39:ARG:NE | 1:B:66:THR:HA | 2.00 | 0.75 |
| 1:C:54:VAL:HG12 | 1:C:55:GLY:N | 2.01 | 0.75 |
| 1:D:142:LEU:HD11 | 1:D:165:ILE:HD11 | 1.69 | 0.75 |
| 1:F:357:ILE:HG12 | 1:F:370:VAL:CG2 | 2.07 | 0.75 |
| 1:I:42:GLY:O | 1:I:43:VAL:HG12 | 1.87 | 0.75 |
| 1:J:36:GLY:O | 1:J:52:SER:HA | 1.85 | 0.75 |
| 1:K:142:LEU:HD11 | 1:K:165:ILE:HD11 | 1.69 | 0.75 |
| 1:P:148:THR:O | 1:P:165:ILE:HG22 | 1.86 | 0.75 |
| 1:Q:44:MET:HG3 | 1:Q:45:VAL:H | 1.52 | 0.75 |
| 1:Q:357:ILE:HG12 | 1:Q:370:VAL:CG2 | 2.07 | 0.75 |
| 1:U:44:MET:HG3 | 1:U:45:VAL:H | 1.51 | 0.75 |
| 1:E:39:ARG:NE | 1:E:66:THR:HA | 2.00 | 0.75 |
| 1:G:42:GLY:O | 1:G:43:VAL:HG12 | 1.87 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:148:THR:O | 1:J:165:ILE:HG22 | 1.86 | 0.75 |
| 1:R:54:VAL:HG12 | 1:R:55:GLY:N | 2.01 | 0.75 |
| 1:S:37:ARG:HG3 | 1:S:38:PRO:CD | 2.15 | 0.75 |
| 1:U:42:GLY:O | 1:U:43:VAL:HG12 | 1.87 | 0.75 |
| 1:E:42:GLY:O | 1:E:43:VAL:HG12 | 1.87 | 0.75 |
| 1:H:44:MET:HG3 | 1:H:45:VAL:H | 1.51 | 0.75 |
| 1:I:44:MET:HG3 | 1:I:45:VAL:H | 1.51 | 0.75 |
| 1:K:142:LEU:HD21 | 1:K:165:ILE:HD13 | 1.68 | 0.75 |
| 1:N:54:VAL:HG12 | 1:N:55:GLY:N | 2.00 | 0.75 |
| 1:N:290:ARG:CD | 1:P:244:ASP:HB2 | 2.12 | 0.75 |
| 1:B:357:ILE:HG12 | 1:B:370:VAL:CG2 | 2.07 | 0.75 |
| 1:E:44:MET:HG3 | 1:E:45:VAL:H | 1.51 | 0.75 |
| 1:F:142:LEU:HD11 | 1:F:165:ILE:HD11 | 1.69 | 0.75 |
| 1:K:42:GLY:O | 1:K:43:VAL:HG12 | 1.87 | 0.75 |
| 1:K:54:VAL:HG12 | 1:K:55:GLY:N | 2.00 | 0.75 |
| 1:M:45:VAL:O | 1:M:45:VAL:CG2 | 2.30 | 0.75 |
| 1:P:37:ARG:HG3 | 1:P:38:PRO:CD | 2.16 | 0.75 |
| 1:T:148:THR:O | 1:T:165:ILE:HG22 | 1.86 | 0.75 |
| 1:U:54:VAL:HG12 | 1:U:55:GLY:N | 2.01 | 0.75 |
| 1:V:35:VAL:HG22 | 1:V:52:SER:HB2 | 1.66 | 0.75 |
| 1:C:42:GLY:O | 1:C:43:VAL:HG12 | 1.87 | 0.74 |
| 1:D:44:MET:HG3 | 1:D:45:VAL:H | 1.51 | 0.74 |
| 1:D:357:ILE:HG12 | 1:D:370:VAL:CG2 | 2.07 | 0.74 |
| 1:J:39:ARG:HE | 1:J:66:THR:HA | 1.52 | 0.74 |
| 1:J:42:GLY:O | 1:J:43:VAL:HG12 | 1.87 | 0.74 |
| 1:R:148:THR:O | 1:R:165:ILE:HG22 | 1.86 | 0.74 |
| 1:S:42:GLY:O | 1:S:43:VAL:HG12 | 1.87 | 0.74 |
| 1:V:142:LEU:HD11 | 1:V:165:ILE:HD11 | 1.69 | 0.74 |
| 1:W:39:ARG:NE | 1:W:66:THR:HA | 2.00 | 0.74 |
| 1:D:35:VAL:HG22 | 1:D:52:SER:HB2 | 1.66 | 0.74 |
| 1:G:148:THR:O | 1:G:165:ILE:HG22 | 1.86 | 0.74 |
| 1:M:142:LEU:HD11 | 1:M:165:ILE:HD11 | 1.69 | 0.74 |
| 1:O:142:LEU:HD11 | 1:O:165:ILE:HD11 | 1.69 | 0.74 |
| 1:S:35:VAL:HG22 | 1:S:52:SER:HB2 | 1.66 | 0.74 |
| 1:T:44:MET:HG3 | 1:T:45:VAL:H | 1.51 | 0.74 |
| 1:U:142:LEU:HD11 | 1:U:165:ILE:HD11 | 1.69 | 0.74 |
| 1:V:44:MET:HG3 | 1:V:45:VAL:H | 1.51 | 0.74 |
| 1:A:142:LEU:HD21 | 1:A:165:ILE:HD13 | 1.68 | 0.74 |
| 1:A:148:THR:O | 1:A:165:ILE:HG22 | 1.86 | 0.74 |
| 1:B:42:GLY:O | 1:B:43:VAL:HG12 | 1.87 | 0.74 |
| 1:B:148:THR:O | 1:B:165:ILE:HG22 | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:142:LEU:HD11 | 1:G:165:ILE:HD11 | 1.69 | 0.74 |
| 1:H:148:THR:O | 1:H:165:ILE:HG22 | 1.86 | 0.74 |
| 1:L:42:GLY:O | 1:L:43:VAL:HG12 | 1.87 | 0.74 |
| 1:M:42:GLY:O | 1:M:43:VAL:HG12 | 1.87 | 0.74 |
| 1:N:142:LEU:HD21 | 1:N:165:ILE:HD13 | 1.68 | 0.74 |
| 1:P:39:ARG:HE | 1:P:66:THR:HA | 1.52 | 0.74 |
| 1:S:148:THR:O | 1:S:165:ILE:HG22 | 1.86 | 0.74 |
| 1:D:42:GLY:O | 1:D:43:VAL:HG12 | 1.87 | 0.74 |
| 1:Q:35:VAL:HG22 | 1:Q:52:SER:HB2 | 1.66 | 0.74 |
| 1:Q:37:ARG:HG3 | 1:Q:38:PRO:CD | 2.15 | 0.74 |
| 1:Q:54:VAL:HG12 | 1:Q:55:GLY:N | 2.01 | 0.74 |
| 1:Q:290:ARG:CD | 1:S:244:ASP:HB2 | 2.12 | 0.74 |
| 1:R:44:MET:HG3 | 1:R:45:VAL:H | 1.51 | 0.74 |
| 1:W:42:GLY:O | 1:W:43:VAL:HG12 | 1.87 | 0.74 |
| 1:W:148:THR:O | 1:W:165:ILE:HG22 | 1.86 | 0.74 |
| 1:F:44:MET:HG3 | 1:F:45:VAL:H | 1.51 | 0.74 |
| 1:I:35:VAL:HG22 | 1:I:52:SER:HB2 | 1.66 | 0.74 |
| 1:O:54:VAL:HG12 | 1:O:55:GLY:N | 2.01 | 0.74 |
| 1:U:148:THR:O | 1:U:165:ILE:HG22 | 1.86 | 0.74 |
| 1:A:42:GLY:O | 1:A:43:VAL:HG12 | 1.87 | 0.74 |
| 1:B:54:VAL:HG12 | 1:B:55:GLY:N | 2.01 | 0.74 |
| 1:F:148:THR:O | 1:F:165:ILE:HG22 | 1.86 | 0.74 |
| 1:H:180:LEU:HD12 | 1:H:181:ALA:N | 2.03 | 0.74 |
| 1:K:148:THR:O | 1:K:165:ILE:HG22 | 1.86 | 0.74 |
| 1:R:39:ARG:HE | 1:R:66:THR:HA | 1.52 | 0.74 |
| 1:B:142:LEU:HD11 | 1:B:165:ILE:HD11 | 1.69 | 0.74 |
| 1:F:180:LEU:HD12 | 1:F:181:ALA:N | 2.03 | 0.74 |
| 1:H:39:ARG:HE | 1:H:66:THR:HA | 1.52 | 0.74 |
| 1:J:180:LEU:HD12 | 1:J:181:ALA:N | 2.03 | 0.74 |
| 1:J:290:ARG:CD | 1:L:244:ASP:HB2 | 2.12 | 0.74 |
| 1:N:37:ARG:HG3 | 1:N:38:PRO:CD | 2.16 | 0.74 |
| 1:O:180:LEU:HD12 | 1:O:181:ALA:N | 2.03 | 0.74 |
| 1:S:39:ARG:HE | 1:S:66:THR:HA | 1.52 | 0.74 |
| 1:V:142:LEU:HD21 | 1:V:165:ILE:HD13 | 1.68 | 0.74 |
| 1:C:148:THR:O | 1:C:165:ILE:HG22 | 1.86 | 0.74 |
| 1:F:54:VAL:HG12 | 1:F:55:GLY:N | 2.01 | 0.74 |
| 1:G:44:MET:HG3 | 1:G:45:VAL:H | 1.51 | 0.74 |
| 1:H:42:GLY:O | 1:H:43:VAL:HG12 | 1.87 | 0.74 |
| 1:O:42:GLY:O | 1:O:43:VAL:HG12 | 1.87 | 0.74 |
| 1:P:142:LEU:HD21 | 1:P:165:ILE:HD13 | 1.68 | 0.74 |
| 1:S:54:VAL:HG12 | 1:S:55:GLY:N | 2.01 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:43:VAL:O | 1:A:44:MET:CB | 2.36 | 0.74 |
| 1:D:54:VAL:HG12 | 1:D:55:GLY:N | 2.00 | 0.74 |
| 1:E:142:LEU:HD21 | 1:E:165:ILE:HD13 | 1.68 | 0.74 |
| 1:J:142:LEU:HD11 | 1:J:165:ILE:HD11 | 1.69 | 0.74 |
| 1:L:43:VAL:O | 1:L:44:MET:CB | 2.36 | 0.74 |
| 1:M:180:LEU:HD12 | 1:M:181:ALA:N | 2.03 | 0.74 |
| 1:N:42:GLY:O | 1:N:43:VAL:HG12 | 1.87 | 0.74 |
| 1:O:290:ARG:CD | 1:Q:244:ASP:HB2 | 2.12 | 0.74 |
| 1:Q:42:GLY:O | 1:Q:43:VAL:HG12 | 1.87 | 0.74 |
| 1:Q:180:LEU:HD12 | 1:Q:181:ALA:N | 2.03 | 0.74 |
| 1:R:142:LEU:HD21 | 1:R:165:ILE:HD13 | 1.68 | 0.74 |
| 1:S:44:MET:HG3 | 1:S:45:VAL:H | 1.51 | 0.74 |
| 1:V:148:THR:O | 1:V:165:ILE:HG22 | 1.86 | 0.74 |
| 1:G:142:LEU:HD21 | 1:G:165:ILE:HD13 | 1.68 | 0.74 |
| 1:J:43:VAL:O | 1:J:44:MET:CB | 2.36 | 0.74 |
| 1:K:39:ARG:HE | 1:K:66:THR:HA | 1.52 | 0.74 |
| 1:M:54:VAL:HG12 | 1:M:55:GLY:N | 2.01 | 0.74 |
| 1:R:180:LEU:HD12 | 1:R:181:ALA:N | 2.03 | 0.74 |
| 1:T:142:LEU:HD21 | 1:T:165:ILE:HD13 | 1.68 | 0.74 |
| 1:C:43:VAL:O | 1:C:44:MET:CB | 2.36 | 0.73 |
| 1:C:142:LEU:HD21 | 1:C:165:ILE:HD13 | 1.68 | 0.73 |
| 1:D:180:LEU:HD12 | 1:D:181:ALA:N | 2.03 | 0.73 |
| 1:F:290:ARG:CD | 1:H:244:ASP:HB2 | 2.13 | 0.73 |
| 1:I:39:ARG:HE | 1:I:66:THR:HA | 1.52 | 0.73 |
| 1:I:142:LEU:HD21 | 1:I:165:ILE:HD13 | 1.68 | 0.73 |
| 1:P:42:GLY:O | 1:P:43:VAL:HG12 | 1.87 | 0.73 |
| 1:R:142:LEU:HD11 | 1:R:165:ILE:HD11 | 1.69 | 0.73 |
| 1:S:180:LEU:HD12 | 1:S:181:ALA:N | 2.03 | 0.73 |
| 1:V:180:LEU:HD12 | 1:V:181:ALA:N | 2.03 | 0.73 |
| 1:B:39:ARG:HE | 1:B:66:THR:HA | 1.52 | 0.73 |
| 1:B:287:ILE:HD11 | 1:D:208:ILE:CD1 | 2.19 | 0.73 |
| 1:E:287:ILE:HD11 | 1:G:208:ILE:CD1 | 2.19 | 0.73 |
| 1:G:39:ARG:HE | 1:G:66:THR:HA | 1.52 | 0.73 |
| 1:G:180:LEU:HD12 | 1:G:181:ALA:N | 2.03 | 0.73 |
| 1:G:287:ILE:HD11 | 1:I:208:ILE:CD1 | 2.19 | 0.73 |
| 1:L:180:LEU:HD12 | 1:L:181:ALA:N | 2.03 | 0.73 |
| 1:M:44:MET:HG3 | 1:M:45:VAL:H | 1.51 | 0.73 |
| 1:O:37:ARG:HG3 | 1:O:38:PRO:CD | 2.16 | 0.73 |
| 1:Q:148:THR:O | 1:Q:165:ILE:HG22 | 1.86 | 0.73 |
| 1:R:290:ARG:CD | 1:T:244:ASP:HB2 | 2.12 | 0.73 |
| 1:V:42:GLY:O | 1:V:43:VAL:HG12 | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:44:MET:HG3 | 1:A:45:VAL:H | 1.51 | 0.73 |
| 1:C:142:LEU:HD11 | 1:C:165:ILE:CD1 | 2.19 | 0.73 |
| 1:C:180:LEU:HD12 | 1:C:181:ALA:N | 2.03 | 0.73 |
| 1:E:142:LEU:HD11 | 1:E:165:ILE:CD1 | 2.19 | 0.73 |
| 1:E:180:LEU:HD12 | 1:E:181:ALA:N | 2.03 | 0.73 |
| 1:M:167:GLU:CD | 1:O:61:LYS:HE2 | 2.09 | 0.73 |
| 1:N:44:MET:HG3 | 1:N:45:VAL:H | 1.51 | 0.73 |
| 1:O:208:ILE:CD1 | 1:O:243:PRO:HD2 | 2.18 | 0.73 |
| 1:R:42:GLY:O | 1:R:43:VAL:HG12 | 1.87 | 0.73 |
| 1:U:43:VAL:O | 1:U:44:MET:CB | 2.36 | 0.73 |
| 1:A:142:LEU:HD11 | 1:A:165:ILE:CD1 | 2.19 | 0.73 |
| 1:A:180:LEU:HD12 | 1:A:181:ALA:N | 2.03 | 0.73 |
| 1:D:287:ILE:HD11 | 1:F:208:ILE:CD1 | 2.19 | 0.73 |
| 1:E:142:LEU:HD11 | 1:E:165:ILE:HD11 | 1.69 | 0.73 |
| 1:F:42:GLY:O | 1:F:43:VAL:HG12 | 1.87 | 0.73 |
| 1:G:142:LEU:HD11 | 1:G:165:ILE:CD1 | 2.19 | 0.73 |
| 1:G:290:ARG:CD | 1:I:244:ASP:HB2 | 2.12 | 0.73 |
| 1:K:180:LEU:HD12 | 1:K:181:ALA:N | 2.03 | 0.73 |
| 1:L:44:MET:HG3 | 1:L:45:VAL:H | 1.51 | 0.73 |
| 1:M:39:ARG:HE | 1:M:66:THR:HA | 1.52 | 0.73 |
| 1:R:43:VAL:O | 1:R:44:MET:CB | 2.36 | 0.73 |
| 1:T:142:LEU:HD11 | 1:T:165:ILE:CD1 | 2.19 | 0.73 |
| 1:U:290:ARG:CD | 1:W:244:ASP:HB2 | 2.12 | 0.73 |
| 1:W:142:LEU:HD11 | 1:W:165:ILE:HD11 | 1.69 | 0.73 |
| 1:B:180:LEU:HD12 | 1:B:181:ALA:N | 2.03 | 0.73 |
| 1:E:39:ARG:HE | 1:E:66:THR:HA | 1.52 | 0.73 |
| 1:F:34:ILE:HD13 | 1:F:67:LEU:HD13 | 1.71 | 0.73 |
| 1:I:287:ILE:HD11 | 1:K:208:ILE:CD1 | 2.19 | 0.73 |
| 1:J:142:LEU:HD11 | 1:J:165:ILE:CD1 | 2.19 | 0.73 |
| 1:L:142:LEU:HD11 | 1:L:165:ILE:CD1 | 2.19 | 0.73 |
| 1:M:34:ILE:HD13 | 1:M:67:LEU:HD13 | 1.71 | 0.73 |
| 1:N:43:VAL:O | 1:N:44:MET:CB | 2.36 | 0.73 |
| 1:N:287:ILE:HD11 | 1:P:208:ILE:CD1 | 2.19 | 0.73 |
| 1:P:142:LEU:HD11 | 1:P:165:ILE:CD1 | 2.19 | 0.73 |
| 1:P:223:PHE:CD1 | 1:P:259:GLU:HG2 | 2.24 | 0.73 |
| 1:R:223:PHE:CD1 | 1:R:259:GLU:HG2 | 2.24 | 0.73 |
| 1:S:142:LEU:HD11 | 1:S:165:ILE:HD11 | 1.69 | 0.73 |
| 1:S:223:PHE:CD1 | 1:S:259:GLU:HG2 | 2.24 | 0.73 |
| 1:U:180:LEU:HD12 | 1:U:181:ALA:N | 2.03 | 0.73 |
| 1:U:223:PHE:CD1 | 1:U:259:GLU:HG2 | 2.24 | 0.73 |
| 1:U:287:ILE:HD11 | 1:W:208:ILE:CD1 | 2.19 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:43:VAL:O | 1:W:44:MET:CB | 2.36 | 0.73 |
| 1:A:39:ARG:HE | 1:A:66:THR:HA | 1.52 | 0.73 |
| 1:C:287:ILE:HD11 | 1:E:208:ILE:CD1 | 2.19 | 0.73 |
| 1:E:148:THR:O | 1:E:165:ILE:HG22 | 1.86 | 0.73 |
| 1:G:167:GLU:CD | 1:I:61:LYS:HE2 | 2.09 | 0.73 |
| 1:I:142:LEU:HD11 | 1:I:165:ILE:HD11 | 1.69 | 0.73 |
| 1:L:37:ARG:HG3 | 1:L:38:PRO:CD | 2.15 | 0.73 |
| 1:N:142:LEU:HD11 | 1:N:165:ILE:CD1 | 2.19 | 0.73 |
| 1:P:287:ILE:HD11 | 1:R:208:ILE:CD1 | 2.19 | 0.73 |
| 1:Q:39:ARG:HE | 1:Q:66:THR:HA | 1.52 | 0.73 |
| 1:Q:223:PHE:CD1 | 1:Q:259:GLU:HG2 | 2.24 | 0.73 |
| 1:R:142:LEU:HD11 | 1:R:165:ILE:CD1 | 2.19 | 0.73 |
| 1:T:223:PHE:CD1 | 1:T:259:GLU:HG2 | 2.24 | 0.73 |
| 1:D:39:ARG:HE | 1:D:66:THR:HA | 1.52 | 0.73 |
| 1:D:290:ARG:CD | 1:F:244:ASP:HB2 | 2.12 | 0.73 |
| 1:E:208:ILE:CD1 | 1:E:243:PRO:HD2 | 2.18 | 0.73 |
| 1:H:34:ILE:HD13 | 1:H:67:LEU:HD13 | 1.71 | 0.73 |
| 1:H:142:LEU:HD11 | 1:H:165:ILE:HD11 | 1.69 | 0.73 |
| 1:I:142:LEU:HD11 | 1:I:165:ILE:CD1 | 2.19 | 0.73 |
| 1:K:287:ILE:HD11 | 1:M:208:ILE:CD1 | 2.19 | 0.73 |
| 1:L:142:LEU:HD11 | 1:L:165:ILE:HD11 | 1.69 | 0.73 |
| 1:L:287:ILE:HD11 | 1:N:208:ILE:CD1 | 2.19 | 0.73 |
| 1:N:180:LEU:HD12 | 1:N:181:ALA:N | 2.03 | 0.73 |
| 1:N:223:PHE:CD1 | 1:N:259:GLU:HG2 | 2.24 | 0.73 |
| 1:O:43:VAL:O | 1:O:44:MET:CB | 2.36 | 0.73 |
| 1:P:44:MET:HG3 | 1:P:45:VAL:H | 1.51 | 0.73 |
| 1:P:180:LEU:HD12 | 1:P:181:ALA:N | 2.03 | 0.73 |
| 1:T:43:VAL:O | 1:T:44:MET:CB | 2.36 | 0.73 |
| 1:T:180:LEU:HD12 | 1:T:181:ALA:N | 2.03 | 0.73 |
| 1:V:223:PHE:CD1 | 1:V:259:GLU:HG2 | 2.24 | 0.73 |
| 1:W:223:PHE:CD1 | 1:W:259:GLU:HG2 | 2.24 | 0.73 |
| 1:A:142:LEU:HD11 | 1:A:165:ILE:HD11 | 1.69 | 0.73 |
| 1:J:44:MET:HG3 | 1:J:45:VAL:H | 1.51 | 0.73 |
| 1:K:34:ILE:HD13 | 1:K:67:LEU:HD13 | 1.71 | 0.73 |
| 1:L:167:GLU:CD | 1:N:61:LYS:HE2 | 2.09 | 0.73 |
| 1:M:43:VAL:O | 1:M:44:MET:CB | 2.36 | 0.73 |
| 1:N:167:GLU:CD | 1:P:61:LYS:HE2 | 2.09 | 0.73 |
| 1:P:142:LEU:HD11 | 1:P:165:ILE:HD11 | 1.69 | 0.73 |
| 1:W:44:MET:HG3 | 1:W:45:VAL:H | 1.51 | 0.73 |
| 1:C:44:MET:HG3 | 1:C:45:VAL:H | 1.51 | 0.73 |
| 1:D:34:ILE:HD13 | 1:D:67:LEU:HD13 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:167:GLU:CD | 1:F:61:LYS:HE2 | 2.09 | 0.73 |
| 1:F:287:ILE:HD11 | 1:H:208:ILE:CD1 | 2.19 | 0.73 |
| 1:I:180:LEU:HD12 | 1:I:181:ALA:N | 2.03 | 0.73 |
| 1:J:34:ILE:HD13 | 1:J:67:LEU:HD13 | 1.71 | 0.73 |
| 1:J:167:GLU:CD | 1:L:61:LYS:HE2 | 2.09 | 0.73 |
| 1:K:142:LEU:HD11 | 1:K:165:ILE:CD1 | 2.19 | 0.73 |
| 1:L:223:PHE:CD1 | 1:L:259:GLU:HG2 | 2.24 | 0.73 |
| 1:M:37:ARG:HG3 | 1:M:38:PRO:CD | 2.16 | 0.73 |
| 1:N:39:ARG:HE | 1:N:66:THR:HA | 1.52 | 0.73 |
| 1:O:34:ILE:HD13 | 1:O:67:LEU:HD13 | 1.71 | 0.73 |
| 1:O:167:GLU:CD | 1:Q:61:LYS:HE2 | 2.09 | 0.73 |
| 1:Q:43:VAL:O | 1:Q:44:MET:CB | 2.36 | 0.73 |
| 1:R:287:ILE:HD11 | 1:T:208:ILE:CD1 | 2.19 | 0.73 |
| 1:S:287:ILE:HD11 | 1:U:208:ILE:CD1 | 2.19 | 0.73 |
| 1:T:42:GLY:O | 1:T:43:VAL:HG12 | 1.87 | 0.73 |
| 1:B:45:VAL:O | 1:B:45:VAL:CG2 | 2.30 | 0.73 |
| 1:H:142:LEU:HD11 | 1:H:165:ILE:CD1 | 2.19 | 0.73 |
| 1:J:223:PHE:CD1 | 1:J:259:GLU:HG2 | 2.24 | 0.73 |
| 1:K:43:VAL:O | 1:K:44:MET:CB | 2.36 | 0.73 |
| 1:K:167:GLU:CD | 1:M:61:LYS:HE2 | 2.09 | 0.73 |
| 1:P:43:VAL:O | 1:P:44:MET:CB | 2.36 | 0.73 |
| 1:P:208:ILE:CD1 | 1:P:243:PRO:HD2 | 2.18 | 0.73 |
| 1:T:167:GLU:CD | 1:V:61:LYS:HE2 | 2.09 | 0.73 |
| 1:V:43:VAL:O | 1:V:44:MET:CB | 2.36 | 0.73 |
| 1:W:142:LEU:HD11 | 1:W:165:ILE:CD1 | 2.19 | 0.73 |
| 1:F:39:ARG:HE | 1:F:66:THR:HA | 1.52 | 0.72 |
| 1:J:208:ILE:CD1 | 1:J:243:PRO:HD2 | 2.18 | 0.72 |
| 1:K:37:ARG:HG3 | 1:K:38:PRO:CD | 2.16 | 0.72 |
| 1:M:287:ILE:HD11 | 1:O:208:ILE:CD1 | 2.19 | 0.72 |
| 1:O:61:LYS:O | 1:O:64:ILE:HG22 | 1.89 | 0.72 |
| 1:O:223:PHE:CD1 | 1:O:259:GLU:HG2 | 2.24 | 0.72 |
| 1:T:142:LEU:HD11 | 1:T:165:ILE:HD11 | 1.69 | 0.72 |
| 1:U:142:LEU:HD11 | 1:U:165:ILE:CD1 | 2.19 | 0.72 |
| 1:W:39:ARG:HE | 1:W:66:THR:HA | 1.52 | 0.72 |
| 1:C:142:LEU:HD11 | 1:C:165:ILE:HD11 | 1.69 | 0.72 |
| 1:H:167:GLU:CD | 1:J:61:LYS:HE2 | 2.09 | 0.72 |
| 1:M:61:LYS:O | 1:M:64:ILE:HG22 | 1.90 | 0.72 |
| 1:S:167:GLU:CD | 1:U:61:LYS:HE2 | 2.09 | 0.72 |
| 1:B:223:PHE:CD1 | 1:B:259:GLU:HG2 | 2.24 | 0.72 |
| 1:C:39:ARG:HE | 1:C:66:THR:HA | 1.52 | 0.72 |
| 1:E:43:VAL:O | 1:E:44:MET:CB | 2.36 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:34:ILE:HD13 | 1:I:67:LEU:HD13 | 1.71 | 0.72 |
| 1:I:37:ARG:HG3 | 1:I:38:PRO:CD | 2.16 | 0.72 |
| 1:I:167:GLU:CD | 1:K:61:LYS:HE2 | 2.09 | 0.72 |
| 1:K:61:LYS:O | 1:K:64:ILE:HG22 | 1.90 | 0.72 |
| 1:N:142:LEU:HD11 | 1:N:165:ILE:HD11 | 1.69 | 0.72 |
| 1:P:167:GLU:CD | 1:R:61:LYS:HE2 | 2.09 | 0.72 |
| 1:Q:34:ILE:HD13 | 1:Q:67:LEU:HD13 | 1.71 | 0.72 |
| 1:U:244:ASP:OD1 | 1:U:246:GLN:HG3 | 1.90 | 0.72 |
| 1:V:142:LEU:HD11 | 1:V:165:ILE:CD1 | 2.19 | 0.72 |
| 1:W:180:LEU:HD12 | 1:W:181:ALA:N | 2.03 | 0.72 |
| 1:A:287:ILE:HD11 | 1:C:208:ILE:CD1 | 2.19 | 0.72 |
| 1:B:167:GLU:CD | 1:D:61:LYS:HE2 | 2.09 | 0.72 |
| 1:C:301:GLY:H | 1:C:335:ARG:HG3 | 1.55 | 0.72 |
| 1:D:223:PHE:CD1 | 1:D:259:GLU:HG2 | 2.24 | 0.72 |
| 1:E:167:GLU:CD | 1:G:61:LYS:HE2 | 2.09 | 0.72 |
| 1:F:167:GLU:CD | 1:H:61:LYS:HE2 | 2.09 | 0.72 |
| 1:F:244:ASP:OD1 | 1:F:246:GLN:HG3 | 1.89 | 0.72 |
| 1:H:223:PHE:CD1 | 1:H:259:GLU:HG2 | 2.24 | 0.72 |
| 1:J:39:ARG:HE | 1:J:66:THR:CA | 2.03 | 0.72 |
| 1:J:244:ASP:OD1 | 1:J:246:GLN:HG3 | 1.90 | 0.72 |
| 1:J:287:ILE:HD11 | 1:L:208:ILE:CD1 | 2.19 | 0.72 |
| 1:M:223:PHE:CD1 | 1:M:259:GLU:HG2 | 2.24 | 0.72 |
| 1:O:39:ARG:HE | 1:O:66:THR:HA | 1.52 | 0.72 |
| 1:Q:167:GLU:CD | 1:S:61:LYS:HE2 | 2.09 | 0.72 |
| 1:R:39:ARG:HE | 1:R:66:THR:CA | 2.03 | 0.72 |
| 1:S:43:VAL:O | 1:S:44:MET:CB | 2.36 | 0.72 |
| 1:S:142:LEU:HD11 | 1:S:165:ILE:CD1 | 2.19 | 0.72 |
| 1:V:43:VAL:O | 1:V:44:MET:HB3 | 1.90 | 0.72 |
| 1:W:39:ARG:HE | 1:W:66:THR:CA | 2.03 | 0.72 |
| 1:A:39:ARG:HE | 1:A:66:THR:CA | 2.03 | 0.72 |
| 1:B:43:VAL:O | 1:B:44:MET:CB | 2.36 | 0.72 |
| 1:B:43:VAL:O | 1:B:44:MET:HB3 | 1.90 | 0.72 |
| 1:D:301:GLY:H | 1:D:335:ARG:HG3 | 1.55 | 0.72 |
| 1:F:43:VAL:O | 1:F:44:MET:CB | 2.36 | 0.72 |
| 1:H:43:VAL:O | 1:H:44:MET:HB3 | 1.90 | 0.72 |
| 1:L:34:ILE:HD13 | 1:L:67:LEU:HD13 | 1.71 | 0.72 |
| 1:L:301:GLY:H | 1:L:335:ARG:HG3 | 1.55 | 0.72 |
| 1:O:287:ILE:HD11 | 1:Q:208:ILE:CD1 | 2.19 | 0.72 |
| 1:P:39:ARG:HE | 1:P:66:THR:CA | 2.03 | 0.72 |
| 1:P:43:VAL:O | 1:P:44:MET:HB3 | 1.90 | 0.72 |
| 1:Q:61:LYS:O | 1:Q:64:ILE:HG22 | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:287:ILE:HD11 | 1:S:208:ILE:CD1 | 2.19 | 0.72 |
| 1:S:43:VAL:O | 1:S:44:MET:HB3 | 1.89 | 0.72 |
| 1:S:236:LEU:HD13 | 1:S:251:GLY:HA2 | 1.72 | 0.72 |
| 1:S:244:ASP:OD1 | 1:S:246:GLN:HG3 | 1.90 | 0.72 |
| 1:T:39:ARG:HE | 1:T:66:THR:CA | 2.03 | 0.72 |
| 1:A:223:PHE:CD1 | 1:A:259:GLU:HG2 | 2.24 | 0.72 |
| 1:A:301:GLY:H | 1:A:335:ARG:HG3 | 1.55 | 0.72 |
| 1:G:39:ARG:HE | 1:G:66:THR:CA | 2.03 | 0.72 |
| 1:G:223:PHE:CD1 | 1:G:259:GLU:HG2 | 2.24 | 0.72 |
| 1:I:43:VAL:O | 1:I:44:MET:CB | 2.36 | 0.72 |
| 1:I:61:LYS:O | 1:I:64:ILE:HG22 | 1.90 | 0.72 |
| 1:Q:236:LEU:HD13 | 1:Q:251:GLY:HA2 | 1.72 | 0.72 |
| 1:T:287:ILE:HD11 | 1:V:208:ILE:CD1 | 2.19 | 0.72 |
| 1:U:167:GLU:CD | 1:W:61:LYS:HE2 | 2.09 | 0.72 |
| 1:U:301:GLY:H | 1:U:335:ARG:HG3 | 1.55 | 0.72 |
| 1:W:244:ASP:OD1 | 1:W:246:GLN:HG3 | 1.90 | 0.72 |
| 1:A:290:ARG:CD | 1:C:244:ASP:HB2 | 2.12 | 0.72 |
| 1:B:34:ILE:HD13 | 1:B:67:LEU:HD13 | 1.71 | 0.72 |
| 1:D:244:ASP:OD1 | 1:D:246:GLN:HG3 | 1.90 | 0.72 |
| 1:E:223:PHE:CD1 | 1:E:259:GLU:HG2 | 2.24 | 0.72 |
| 1:F:142:LEU:HD11 | 1:F:165:ILE:CD1 | 2.19 | 0.72 |
| 1:H:39:ARG:HE | 1:H:66:THR:CA | 2.03 | 0.72 |
| 1:I:39:ARG:HE | 1:I:66:THR:CA | 2.03 | 0.72 |
| 1:K:223:PHE:CD1 | 1:K:259:GLU:HG2 | 2.24 | 0.72 |
| 1:M:301:GLY:H | 1:M:335:ARG:HG3 | 1.55 | 0.72 |
| 1:T:43:VAL:O | 1:T:44:MET:HB3 | 1.90 | 0.72 |
| 1:W:301:GLY:H | 1:W:335:ARG:HG3 | 1.55 | 0.72 |
| 1:B:244:ASP:OD1 | 1:B:246:GLN:HG3 | 1.90 | 0.72 |
| 1:D:43:VAL:O | 1:D:44:MET:HB3 | 1.90 | 0.72 |
| 1:E:43:VAL:O | 1:E:44:MET:HB3 | 1.89 | 0.72 |
| 1:G:61:LYS:O | 1:G:64:ILE:HG22 | 1.90 | 0.72 |
| 1:J:37:ARG:HG3 | 1:J:38:PRO:CD | 2.16 | 0.72 |
| 1:L:244:ASP:OD1 | 1:L:246:GLN:HG3 | 1.89 | 0.72 |
| 1:N:43:VAL:O | 1:N:44:MET:HB3 | 1.90 | 0.72 |
| 1:N:301:GLY:H | 1:N:335:ARG:HG3 | 1.55 | 0.72 |
| 1:O:236:LEU:HD13 | 1:O:251:GLY:HA2 | 1.72 | 0.72 |
| 1:P:61:LYS:O | 1:P:64:ILE:HG22 | 1.90 | 0.72 |
| 1:R:43:VAL:O | 1:R:44:MET:HB3 | 1.90 | 0.72 |
| 1:R:61:LYS:O | 1:R:64:ILE:HG22 | 1.90 | 0.72 |
| 1:S:39:ARG:HE | 1:S:66:THR:CA | 2.03 | 0.72 |
| 1:U:61:LYS:O | 1:U:64:ILE:HG22 | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:61:LYS:O | 1:W:64:ILE:HG22 | 1.90 | 0.72 |
| 1:B:301:GLY:H | 1:B:335:ARG:HG3 | 1.55 | 0.72 |
| 1:C:167:GLU:CD | 1:E:61:LYS:HE2 | 2.09 | 0.72 |
| 1:C:223:PHE:CD1 | 1:C:259:GLU:HG2 | 2.24 | 0.72 |
| 1:F:223:PHE:CD1 | 1:F:259:GLU:HG2 | 2.24 | 0.72 |
| 1:F:301:GLY:H | 1:F:335:ARG:HG3 | 1.55 | 0.72 |
| 1:G:34:ILE:HD13 | 1:G:67:LEU:HD13 | 1.71 | 0.72 |
| 1:H:287:ILE:HD11 | 1:J:208:ILE:CD1 | 2.19 | 0.72 |
| 1:S:61:LYS:O | 1:S:64:ILE:HG22 | 1.90 | 0.72 |
| 1:U:39:ARG:HE | 1:U:66:THR:HA | 1.52 | 0.72 |
| 1:U:236:LEU:HD13 | 1:U:251:GLY:HA2 | 1.72 | 0.72 |
| 1:B:142:LEU:HD11 | 1:B:165:ILE:CD1 | 2.19 | 0.72 |
| 1:C:43:VAL:O | 1:C:44:MET:HB3 | 1.90 | 0.72 |
| 1:E:61:LYS:O | 1:E:64:ILE:HG22 | 1.90 | 0.72 |
| 1:F:43:VAL:O | 1:F:44:MET:HB3 | 1.89 | 0.72 |
| 1:I:208:ILE:CD1 | 1:I:243:PRO:HD2 | 2.18 | 0.72 |
| 1:L:39:ARG:HE | 1:L:66:THR:CA | 2.03 | 0.72 |
| 1:L:61:LYS:O | 1:L:64:ILE:HG22 | 1.90 | 0.72 |
| 1:Q:142:LEU:HD11 | 1:Q:165:ILE:CD1 | 2.19 | 0.72 |
| 1:R:167:GLU:CD | 1:T:61:LYS:HE2 | 2.09 | 0.72 |
| 1:S:34:ILE:HD13 | 1:S:67:LEU:HD13 | 1.71 | 0.72 |
| 1:U:39:ARG:HE | 1:U:66:THR:CA | 2.03 | 0.72 |
| 1:V:301:GLY:H | 1:V:335:ARG:HG3 | 1.55 | 0.72 |
| 1:A:34:ILE:CA | 1:A:54:VAL:HG11 | 2.20 | 0.71 |
| 1:A:167:GLU:CD | 1:C:61:LYS:HE2 | 2.09 | 0.71 |
| 1:D:43:VAL:O | 1:D:44:MET:CB | 2.36 | 0.71 |
| 1:D:142:LEU:HD11 | 1:D:165:ILE:CD1 | 2.19 | 0.71 |
| 1:G:37:ARG:HG3 | 1:G:38:PRO:CD | 2.15 | 0.71 |
| 1:I:223:PHE:CD1 | 1:I:259:GLU:HG2 | 2.24 | 0.71 |
| 1:L:34:ILE:CA | 1:L:54:VAL:HG11 | 2.20 | 0.71 |
| 1:N:34:ILE:HD13 | 1:N:67:LEU:HD13 | 1.71 | 0.71 |
| 1:N:61:LYS:O | 1:N:64:ILE:HG22 | 1.90 | 0.71 |
| 1:N:244:ASP:OD1 | 1:N:246:GLN:HG3 | 1.90 | 0.71 |
| 1:O:301:GLY:H | 1:O:335:ARG:HG3 | 1.55 | 0.71 |
| 1:Q:244:ASP:OD1 | 1:Q:246:GLN:HG3 | 1.90 | 0.71 |
| 1:T:61:LYS:O | 1:T:64:ILE:HG22 | 1.90 | 0.71 |
| 1:T:301:GLY:H | 1:T:335:ARG:HG3 | 1.55 | 0.71 |
| 1:E:39:ARG:HE | 1:E:66:THR:CA | 2.03 | 0.71 |
| 1:K:301:GLY:H | 1:K:335:ARG:HG3 | 1.55 | 0.71 |
| 1:M:290:ARG:CD | 1:O:244:ASP:HB2 | 2.12 | 0.71 |
| 1:C:39:ARG:HE | 1:C:66:THR:CA | 2.03 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:61:LYS:O | 1:C:64:ILE:HG22 | 1.90 | 0.71 |
| 1:E:301:GLY:H | 1:E:335:ARG:HG3 | 1.55 | 0.71 |
| 1:G:43:VAL:O | 1:G:44:MET:CB | 2.36 | 0.71 |
| 1:J:34:ILE:CA | 1:J:54:VAL:HG11 | 2.20 | 0.71 |
| 1:J:61:LYS:O | 1:J:64:ILE:HG22 | 1.90 | 0.71 |
| 1:J:236:LEU:HD13 | 1:J:251:GLY:HA2 | 1.72 | 0.71 |
| 1:J:301:GLY:H | 1:J:335:ARG:HG3 | 1.55 | 0.71 |
| 1:L:236:LEU:HD13 | 1:L:251:GLY:HA2 | 1.72 | 0.71 |
| 1:O:43:VAL:O | 1:O:44:MET:HB3 | 1.90 | 0.71 |
| 1:Q:39:ARG:HE | 1:Q:66:THR:CA | 2.03 | 0.71 |
| 1:T:39:ARG:HE | 1:T:66:THR:HA | 1.52 | 0.71 |
| 1:V:61:LYS:O | 1:V:64:ILE:HG22 | 1.90 | 0.71 |
| 1:W:34:ILE:HD13 | 1:W:67:LEU:HD13 | 1.71 | 0.71 |
| 1:H:244:ASP:OD1 | 1:H:246:GLN:HG3 | 1.90 | 0.71 |
| 1:H:290:ARG:CD | 1:J:244:ASP:HB2 | 2.12 | 0.71 |
| 1:H:301:GLY:H | 1:H:335:ARG:HG3 | 1.55 | 0.71 |
| 1:K:39:ARG:HE | 1:K:66:THR:CA | 2.03 | 0.71 |
| 1:M:142:LEU:HD11 | 1:M:165:ILE:CD1 | 2.19 | 0.71 |
| 1:N:236:LEU:HD13 | 1:N:251:GLY:HA2 | 1.72 | 0.71 |
| 1:O:244:ASP:OD1 | 1:O:246:GLN:HG3 | 1.90 | 0.71 |
| 1:P:34:ILE:CA | 1:P:54:VAL:HG11 | 2.20 | 0.71 |
| 1:S:208:ILE:CD1 | 1:S:243:PRO:HD2 | 2.18 | 0.71 |
| 1:T:143:TYR:CD2 | 1:T:346:LEU:HD13 | 2.26 | 0.71 |
| 1:V:39:ARG:HE | 1:V:66:THR:HA | 1.52 | 0.71 |
| 1:V:143:TYR:CD2 | 1:V:346:LEU:HD13 | 2.26 | 0.71 |
| 1:A:61:LYS:O | 1:A:64:ILE:HG22 | 1.90 | 0.71 |
| 1:B:39:ARG:HE | 1:B:66:THR:CA | 2.03 | 0.71 |
| 1:C:143:TYR:CD2 | 1:C:346:LEU:HD13 | 2.26 | 0.71 |
| 1:D:61:LYS:O | 1:D:64:ILE:HG22 | 1.90 | 0.71 |
| 1:E:34:ILE:HD13 | 1:E:67:LEU:HD13 | 1.71 | 0.71 |
| 1:M:143:TYR:CD2 | 1:M:346:LEU:HD13 | 2.26 | 0.71 |
| 1:M:236:LEU:HD13 | 1:M:251:GLY:HA2 | 1.72 | 0.71 |
| 1:O:143:TYR:CD2 | 1:O:346:LEU:HD13 | 2.26 | 0.71 |
| 1:W:34:ILE:CA | 1:W:54:VAL:HG11 | 2.20 | 0.71 |
| 1:W:236:LEU:HD13 | 1:W:251:GLY:HA2 | 1.72 | 0.71 |
| 1:F:39:ARG:HE | 1:F:66:THR:CA | 2.03 | 0.71 |
| 1:G:43:VAL:O | 1:G:44:MET:HB3 | 1.90 | 0.71 |
| 1:I:244:ASP:OD1 | 1:I:246:GLN:HG3 | 1.89 | 0.71 |
| 1:J:43:VAL:O | 1:J:44:MET:HB3 | 1.89 | 0.71 |
| 1:L:39:ARG:HE | 1:L:66:THR:HA | 1.53 | 0.71 |
| 1:R:34:ILE:CA | 1:R:54:VAL:HG11 | 2.20 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:301:GLY:H | 1:S:335:ARG:HG3 | 1.55 | 0.71 |
| 1:T:208:ILE:CD1 | 1:T:243:PRO:HD2 | 2.18 | 0.71 |
| 1:U:34:ILE:CA | 1:U:54:VAL:HG11 | 2.20 | 0.71 |
| 1:A:143:TYR:CD2 | 1:A:346:LEU:HD13 | 2.26 | 0.71 |
| 1:B:236:LEU:HD13 | 1:B:251:GLY:HA2 | 1.72 | 0.71 |
| 1:C:34:ILE:HD13 | 1:C:67:LEU:HD13 | 1.71 | 0.71 |
| 1:E:143:TYR:CD2 | 1:E:346:LEU:HD13 | 2.26 | 0.71 |
| 1:H:236:LEU:HD13 | 1:H:251:GLY:HA2 | 1.72 | 0.71 |
| 1:I:34:ILE:CA | 1:I:54:VAL:HG11 | 2.20 | 0.71 |
| 1:K:143:TYR:CD2 | 1:K:346:LEU:HD13 | 2.26 | 0.71 |
| 1:L:43:VAL:O | 1:L:44:MET:HB3 | 1.90 | 0.71 |
| 1:Q:43:VAL:O | 1:Q:44:MET:HB3 | 1.90 | 0.71 |
| 1:R:143:TYR:CD2 | 1:R:346:LEU:HD13 | 2.26 | 0.71 |
| 1:U:34:ILE:HD13 | 1:U:67:LEU:HD13 | 1.71 | 0.71 |
| 1:A:34:ILE:HD13 | 1:A:67:LEU:HD13 | 1.71 | 0.71 |
| 1:B:208:ILE:CD1 | 1:B:243:PRO:HD2 | 2.18 | 0.71 |
| 1:C:244:ASP:OD1 | 1:C:246:GLN:HG3 | 1.89 | 0.71 |
| 1:G:244:ASP:OD1 | 1:G:246:GLN:HG3 | 1.90 | 0.71 |
| 1:I:43:VAL:O | 1:I:44:MET:HB3 | 1.90 | 0.71 |
| 1:N:39:ARG:HE | 1:N:66:THR:CA | 2.03 | 0.71 |
| 1:P:244:ASP:OD1 | 1:P:246:GLN:HG3 | 1.90 | 0.71 |
| 1:R:301:GLY:H | 1:R:335:ARG:HG3 | 1.55 | 0.71 |
| 1:F:61:LYS:O | 1:F:64:ILE:HG22 | 1.90 | 0.71 |
| 1:H:43:VAL:O | 1:H:44:MET:CB | 2.36 | 0.71 |
| 1:O:39:ARG:HE | 1:O:66:THR:CA | 2.03 | 0.71 |
| 1:O:142:LEU:HD11 | 1:O:165:ILE:CD1 | 2.19 | 0.71 |
| 1:P:34:ILE:HD13 | 1:P:67:LEU:HD13 | 1.71 | 0.71 |
| 1:Q:301:GLY:H | 1:Q:335:ARG:HG3 | 1.55 | 0.71 |
| 1:S:290:ARG:CD | 1:U:244:ASP:HB2 | 2.12 | 0.71 |
| 1:T:34:ILE:HD13 | 1:T:67:LEU:HD13 | 1.71 | 0.71 |
| 1:V:39:ARG:HE | 1:V:66:THR:CA | 2.03 | 0.71 |
| 1:V:244:ASP:OD1 | 1:V:246:GLN:HG3 | 1.90 | 0.71 |
| 1:B:61:LYS:O | 1:B:64:ILE:HG22 | 1.90 | 0.71 |
| 1:E:34:ILE:CA | 1:E:54:VAL:HG11 | 2.20 | 0.71 |
| 1:F:34:ILE:CA | 1:F:54:VAL:HG11 | 2.20 | 0.71 |
| 1:G:34:ILE:CA | 1:G:54:VAL:HG11 | 2.20 | 0.71 |
| 1:H:208:ILE:CD1 | 1:H:243:PRO:HD2 | 2.18 | 0.71 |
| 1:L:290:ARG:CD | 1:N:244:ASP:HB2 | 2.12 | 0.71 |
| 1:P:236:LEU:HD13 | 1:P:251:GLY:HA2 | 1.72 | 0.71 |
| 1:Q:34:ILE:CA | 1:Q:54:VAL:HG11 | 2.20 | 0.71 |
| 1:Q:143:TYR:CD2 | 1:Q:346:LEU:HD13 | 2.26 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:34:ILE:HD13 | 1:R:67:LEU:HD13 | 1.71 | 0.71 |
| 1:B:34:ILE:CA | 1:B:54:VAL:HG11 | 2.20 | 0.70 |
| 1:B:290:ARG:CD | 1:D:244:ASP:HB2 | 2.12 | 0.70 |
| 1:K:34:ILE:CA | 1:K:54:VAL:HG11 | 2.20 | 0.70 |
| 1:M:43:VAL:O | 1:M:44:MET:HB3 | 1.90 | 0.70 |
| 1:O:34:ILE:CA | 1:O:54:VAL:HG11 | 2.20 | 0.70 |
| 1:P:143:TYR:CD2 | 1:P:346:LEU:HD13 | 2.26 | 0.70 |
| 1:W:43:VAL:O | 1:W:44:MET:HB3 | 1.90 | 0.70 |
| 1:W:143:TYR:CD2 | 1:W:346:LEU:HD13 | 2.26 | 0.70 |
| 1:C:34:ILE:CA | 1:C:54:VAL:HG11 | 2.20 | 0.70 |
| 1:D:39:ARG:HE | 1:D:66:THR:CA | 2.03 | 0.70 |
| 1:I:301:GLY:H | 1:I:335:ARG:HG3 | 1.55 | 0.70 |
| 1:K:236:LEU:HD13 | 1:K:251:GLY:HA2 | 1.72 | 0.70 |
| 1:R:244:ASP:OD1 | 1:R:246:GLN:HG3 | 1.90 | 0.70 |
| 1:S:34:ILE:CA | 1:S:54:VAL:HG11 | 2.20 | 0.70 |
| 1:V:34:ILE:HD13 | 1:V:67:LEU:HD13 | 1.71 | 0.70 |
| 1:E:37:ARG:HG3 | 1:E:38:PRO:CD | 2.15 | 0.70 |
| 1:F:143:TYR:CD2 | 1:F:346:LEU:HD13 | 2.26 | 0.70 |
| 1:H:143:TYR:CD2 | 1:H:346:LEU:HD13 | 2.26 | 0.70 |
| 1:J:143:TYR:CD2 | 1:J:346:LEU:HD13 | 2.26 | 0.70 |
| 1:K:244:ASP:OD1 | 1:K:246:GLN:HG3 | 1.90 | 0.70 |
| 1:M:208:ILE:CD1 | 1:M:243:PRO:HD2 | 2.18 | 0.70 |
| 1:N:34:ILE:CA | 1:N:54:VAL:HG11 | 2.20 | 0.70 |
| 1:P:301:GLY:H | 1:P:335:ARG:HG3 | 1.55 | 0.70 |
| 1:R:169:TYR:CE2 | 1:T:40:HIS:HB3 | 2.27 | 0.70 |
| 1:W:208:ILE:CD1 | 1:W:243:PRO:HD2 | 2.18 | 0.70 |
| 1:B:37:ARG:CG | 1:B:38:PRO:HD2 | 2.20 | 0.70 |
| 1:D:236:LEU:HD13 | 1:D:251:GLY:HA2 | 1.72 | 0.70 |
| 1:E:244:ASP:OD1 | 1:E:246:GLN:HG3 | 1.90 | 0.70 |
| 1:G:169:TYR:CE2 | 1:I:40:HIS:HB3 | 2.27 | 0.70 |
| 1:H:61:LYS:O | 1:H:64:ILE:HG22 | 1.90 | 0.70 |
| 1:I:169:TYR:CE2 | 1:K:40:HIS:HB3 | 2.27 | 0.70 |
| 1:K:43:VAL:O | 1:K:44:MET:HB3 | 1.90 | 0.70 |
| 1:M:169:TYR:CE2 | 1:O:40:HIS:HB3 | 2.27 | 0.70 |
| 1:M:244:ASP:OD1 | 1:M:246:GLN:HG3 | 1.90 | 0.70 |
| 1:N:208:ILE:CD1 | 1:N:243:PRO:HD2 | 2.18 | 0.70 |
| 1:P:169:TYR:CE2 | 1:R:40:HIS:HB3 | 2.27 | 0.70 |
| 1:R:236:LEU:CD1 | 1:R:237:GLU:HG2 | 2.22 | 0.70 |
| 1:T:236:LEU:HD13 | 1:T:251:GLY:HA2 | 1.72 | 0.70 |
| 1:U:143:TYR:CD2 | 1:U:346:LEU:HD13 | 2.26 | 0.70 |
| 1:B:169:TYR:CE2 | 1:D:40:HIS:HB3 | 2.27 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:236:LEU:CD1 | 1:B:237:GLU:HG2 | 2.22 | 0.70 |
| 1:E:236:LEU:CD1 | 1:E:237:GLU:HG2 | 2.22 | 0.70 |
| 1:F:37:ARG:CG | 1:F:38:PRO:HD2 | 2.20 | 0.70 |
| 1:F:236:LEU:HD13 | 1:F:251:GLY:HA2 | 1.72 | 0.70 |
| 1:G:143:TYR:CD2 | 1:G:346:LEU:HD13 | 2.26 | 0.70 |
| 1:I:143:TYR:CD2 | 1:I:346:LEU:HD13 | 2.26 | 0.70 |
| 1:M:39:ARG:HE | 1:M:66:THR:CA | 2.03 | 0.70 |
| 1:S:236:LEU:CD1 | 1:S:237:GLU:HG2 | 2.22 | 0.70 |
| 1:V:236:LEU:HD13 | 1:V:251:GLY:HA2 | 1.72 | 0.70 |
| 1:D:143:TYR:CD2 | 1:D:346:LEU:HD13 | 2.26 | 0.70 |
| 1:F:236:LEU:CD1 | 1:F:237:GLU:HG2 | 2.22 | 0.70 |
| 1:I:236:LEU:CD1 | 1:I:237:GLU:HG2 | 2.22 | 0.70 |
| 1:L:143:TYR:CD2 | 1:L:346:LEU:HD13 | 2.26 | 0.70 |
| 1:O:236:LEU:CD1 | 1:O:237:GLU:HG2 | 2.22 | 0.70 |
| 1:R:236:LEU:HD13 | 1:R:251:GLY:HA2 | 1.72 | 0.70 |
| 1:T:169:TYR:CE2 | 1:V:40:HIS:HB3 | 2.27 | 0.70 |
| 1:W:236:LEU:CD1 | 1:W:237:GLU:HG2 | 2.22 | 0.70 |
| 1:A:244:ASP:OD1 | 1:A:246:GLN:HG3 | 1.90 | 0.70 |
| 1:E:169:TYR:CE2 | 1:G:40:HIS:HB3 | 2.27 | 0.70 |
| 1:K:169:TYR:CE2 | 1:M:40:HIS:HB3 | 2.27 | 0.70 |
| 1:K:236:LEU:CD1 | 1:K:237:GLU:HG2 | 2.22 | 0.70 |
| 1:A:43:VAL:O | 1:A:44:MET:HB3 | 1.90 | 0.70 |
| 1:C:208:ILE:CD1 | 1:C:243:PRO:HD2 | 2.18 | 0.70 |
| 1:D:34:ILE:CA | 1:D:54:VAL:HG11 | 2.20 | 0.70 |
| 1:G:301:GLY:H | 1:G:335:ARG:HG3 | 1.55 | 0.70 |
| 1:R:37:ARG:CG | 1:R:38:PRO:HD2 | 2.20 | 0.70 |
| 1:S:143:TYR:CD2 | 1:S:346:LEU:HD13 | 2.26 | 0.70 |
| 1:V:34:ILE:CA | 1:V:54:VAL:HG11 | 2.20 | 0.70 |
| 1:V:236:LEU:CD1 | 1:V:237:GLU:HG2 | 2.22 | 0.70 |
| 1:C:143:TYR:CE1 | 1:E:45:VAL:HG21 | 2.27 | 0.70 |
| 1:C:236:LEU:CD1 | 1:C:237:GLU:HG2 | 2.22 | 0.70 |
| 1:D:169:TYR:CE2 | 1:F:40:HIS:HB3 | 2.27 | 0.70 |
| 1:H:34:ILE:CA | 1:H:54:VAL:HG11 | 2.20 | 0.70 |
| 1:J:143:TYR:CE1 | 1:L:45:VAL:HG21 | 2.27 | 0.70 |
| 1:J:236:LEU:CD1 | 1:J:237:GLU:HG2 | 2.22 | 0.70 |
| 1:M:34:ILE:CA | 1:M:54:VAL:HG11 | 2.20 | 0.70 |
| 1:M:37:ARG:CG | 1:M:38:PRO:HD2 | 2.20 | 0.70 |
| 1:N:169:TYR:CE2 | 1:P:40:HIS:HB3 | 2.27 | 0.70 |
| 1:N:236:LEU:CD1 | 1:N:237:GLU:HG2 | 2.22 | 0.70 |
| 1:P:143:TYR:CE1 | 1:R:45:VAL:HG21 | 2.27 | 0.70 |
| 1:T:244:ASP:OD1 | 1:T:246:GLN:HG3 | 1.89 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:43:VAL:O | 1:U:44:MET:HB3 | 1.90 | 0.70 |
| 1:U:143:TYR:CE1 | 1:W:45:VAL:HG21 | 2.27 | 0.70 |
| 1:A:34:ILE:HG22 | 1:A:35:VAL:N | 2.07 | 0.70 |
| 1:A:236:LEU:HD13 | 1:A:251:GLY:HA2 | 1.72 | 0.70 |
| 1:A:236:LEU:CD1 | 1:A:237:GLU:HG2 | 2.22 | 0.70 |
| 1:B:143:TYR:CD2 | 1:B:346:LEU:HD13 | 2.26 | 0.70 |
| 1:H:143:TYR:CE1 | 1:J:45:VAL:HG21 | 2.27 | 0.70 |
| 1:M:34:ILE:HG22 | 1:M:35:VAL:N | 2.07 | 0.70 |
| 1:P:34:ILE:HG22 | 1:P:35:VAL:N | 2.07 | 0.70 |
| 1:S:169:TYR:CE2 | 1:U:40:HIS:HB3 | 2.27 | 0.70 |
| 1:U:169:TYR:CE2 | 1:W:40:HIS:HB3 | 2.27 | 0.70 |
| 1:B:143:TYR:CE1 | 1:D:45:VAL:HG21 | 2.27 | 0.69 |
| 1:G:37:ARG:CG | 1:G:38:PRO:HD2 | 2.20 | 0.69 |
| 1:I:34:ILE:HG22 | 1:I:35:VAL:N | 2.07 | 0.69 |
| 1:L:236:LEU:CD1 | 1:L:237:GLU:HG2 | 2.22 | 0.69 |
| 1:Q:37:ARG:CG | 1:Q:38:PRO:HD2 | 2.20 | 0.69 |
| 1:Q:169:TYR:CE2 | 1:S:40:HIS:HB3 | 2.27 | 0.69 |
| 1:R:143:TYR:CE1 | 1:T:45:VAL:HG21 | 2.27 | 0.69 |
| 1:S:143:TYR:CE1 | 1:U:45:VAL:HG21 | 2.27 | 0.69 |
| 1:T:34:ILE:CA | 1:T:54:VAL:HG11 | 2.20 | 0.69 |
| 1:A:169:TYR:CE2 | 1:C:40:HIS:HB3 | 2.27 | 0.69 |
| 1:B:34:ILE:HG22 | 1:B:35:VAL:N | 2.07 | 0.69 |
| 1:D:143:TYR:CE1 | 1:F:45:VAL:HG21 | 2.27 | 0.69 |
| 1:E:34:ILE:HG22 | 1:E:35:VAL:N | 2.07 | 0.69 |
| 1:L:34:ILE:HG22 | 1:L:35:VAL:N | 2.07 | 0.69 |
| 1:M:143:TYR:CE1 | 1:O:45:VAL:HG21 | 2.27 | 0.69 |
| 1:N:143:TYR:CD2 | 1:N:346:LEU:HD13 | 2.26 | 0.69 |
| 1:N:143:TYR:CE1 | 1:P:45:VAL:HG21 | 2.27 | 0.69 |
| 1:P:236:LEU:CD1 | 1:P:237:GLU:HG2 | 2.22 | 0.69 |
| 1:E:143:TYR:CE1 | 1:G:45:VAL:HG21 | 2.27 | 0.69 |
| 1:H:50:LYS:HG3 | 1:H:53:TYR:CE2 | 2.28 | 0.69 |
| 1:I:236:LEU:HD13 | 1:I:251:GLY:HA2 | 1.72 | 0.69 |
| 1:L:169:TYR:CE2 | 1:N:40:HIS:HB3 | 2.27 | 0.69 |
| 1:T:34:ILE:HG22 | 1:T:35:VAL:N | 2.07 | 0.69 |
| 1:T:236:LEU:CD1 | 1:T:237:GLU:HG2 | 2.22 | 0.69 |
| 1:U:34:ILE:HG22 | 1:U:35:VAL:N | 2.07 | 0.69 |
| 1:F:143:TYR:CE1 | 1:H:45:VAL:HG21 | 2.27 | 0.69 |
| 1:G:58:ALA:CB | 1:G:65:LEU:HD22 | 2.23 | 0.69 |
| 1:G:143:TYR:CE1 | 1:I:45:VAL:HG21 | 2.27 | 0.69 |
| 1:H:58:ALA:CB | 1:H:65:LEU:HD22 | 2.23 | 0.69 |
| 1:H:236:LEU:CD1 | 1:H:237:GLU:HG2 | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:50:LYS:HG3 | 1:J:53:TYR:CE2 | 2.28 | 0.69 |
| 1:Q:34:ILE:HG22 | 1:Q:35:VAL:N | 2.07 | 0.69 |
| 1:Q:143:TYR:CE1 | 1:S:45:VAL:HG21 | 2.27 | 0.69 |
| 1:S:58:ALA:CB | 1:S:65:LEU:HD22 | 2.23 | 0.69 |
| 1:T:143:TYR:CE1 | 1:V:45:VAL:HG21 | 2.27 | 0.69 |
| 1:U:50:LYS:HG3 | 1:U:53:TYR:CE2 | 2.28 | 0.69 |
| 1:W:50:LYS:HG3 | 1:W:53:TYR:CE2 | 2.28 | 0.69 |
| 1:E:290:ARG:CD | 1:G:244:ASP:HB2 | 2.12 | 0.69 |
| 1:F:50:LYS:HG3 | 1:F:53:TYR:CE2 | 2.28 | 0.69 |
| 1:I:143:TYR:CE1 | 1:K:45:VAL:HG21 | 2.27 | 0.69 |
| 1:M:236:LEU:CD1 | 1:M:237:GLU:HG2 | 2.22 | 0.69 |
| 1:R:58:ALA:CB | 1:R:65:LEU:HD22 | 2.23 | 0.69 |
| 1:S:34:ILE:HG22 | 1:S:35:VAL:N | 2.07 | 0.69 |
| 1:S:50:LYS:HG3 | 1:S:53:TYR:CE2 | 2.28 | 0.69 |
| 1:A:50:LYS:HG3 | 1:A:53:TYR:CE2 | 2.28 | 0.69 |
| 1:D:50:LYS:HG3 | 1:D:53:TYR:CE2 | 2.28 | 0.69 |
| 1:F:169:TYR:CE2 | 1:H:40:HIS:HB3 | 2.27 | 0.69 |
| 1:G:236:LEU:HD13 | 1:G:251:GLY:HA2 | 1.72 | 0.69 |
| 1:L:50:LYS:HG3 | 1:L:53:TYR:CE2 | 2.28 | 0.69 |
| 1:N:50:LYS:HG3 | 1:N:53:TYR:CE2 | 2.28 | 0.69 |
| 1:N:58:ALA:CB | 1:N:65:LEU:HD22 | 2.23 | 0.69 |
| 1:O:143:TYR:CE1 | 1:Q:45:VAL:HG21 | 2.27 | 0.69 |
| 1:O:169:TYR:CE2 | 1:Q:40:HIS:HB3 | 2.27 | 0.69 |
| 1:A:58:ALA:CB | 1:A:65:LEU:HD22 | 2.23 | 0.69 |
| 1:C:50:LYS:HG3 | 1:C:53:TYR:CE2 | 2.28 | 0.69 |
| 1:Q:50:LYS:HG3 | 1:Q:53:TYR:CE2 | 2.28 | 0.69 |
| 1:A:143:TYR:CE1 | 1:C:45:VAL:HG21 | 2.27 | 0.69 |
| 1:B:50:LYS:HG3 | 1:B:53:TYR:CE2 | 2.28 | 0.69 |
| 1:B:58:ALA:CB | 1:B:65:LEU:HD22 | 2.23 | 0.69 |
| 1:C:58:ALA:CB | 1:C:65:LEU:HD22 | 2.23 | 0.69 |
| 1:C:169:TYR:CE2 | 1:E:40:HIS:HB3 | 2.27 | 0.69 |
| 1:C:236:LEU:HD13 | 1:C:251:GLY:HA2 | 1.72 | 0.69 |
| 1:D:236:LEU:CD1 | 1:D:237:GLU:HG2 | 2.22 | 0.69 |
| 1:E:50:LYS:HG3 | 1:E:53:TYR:CE2 | 2.28 | 0.69 |
| 1:E:236:LEU:HD13 | 1:E:251:GLY:HA2 | 1.72 | 0.69 |
| 1:F:34:ILE:HG22 | 1:F:35:VAL:N | 2.07 | 0.69 |
| 1:F:301:GLY:N | 1:F:335:ARG:HG3 | 2.08 | 0.69 |
| 1:G:50:LYS:HG3 | 1:G:53:TYR:CE2 | 2.28 | 0.69 |
| 1:G:236:LEU:CD1 | 1:G:237:GLU:HG2 | 2.22 | 0.69 |
| 1:J:169:TYR:CE2 | 1:L:40:HIS:HB3 | 2.27 | 0.69 |
| 1:L:58:ALA:CB | 1:L:65:LEU:HD22 | 2.23 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:143:TYR:CE1 | 1:N:45:VAL:HG21 | 2.27 | 0.69 |
| 1:L:208:ILE:HD11 | 1:L:243:PRO:CG | 2.23 | 0.69 |
| 1:M:58:ALA:CB | 1:M:65:LEU:HD22 | 2.23 | 0.69 |
| 1:N:208:ILE:HD11 | 1:N:243:PRO:CG | 2.23 | 0.69 |
| 1:O:50:LYS:HG3 | 1:O:53:TYR:CE2 | 2.28 | 0.69 |
| 1:P:50:LYS:HG3 | 1:P:53:TYR:CE2 | 2.28 | 0.69 |
| 1:P:290:ARG:CD | 1:R:244:ASP:HB2 | 2.13 | 0.69 |
| 1:Q:236:LEU:CD1 | 1:Q:237:GLU:HG2 | 2.22 | 0.69 |
| 1:R:34:ILE:HG22 | 1:R:35:VAL:N | 2.07 | 0.69 |
| 1:R:50:LYS:HG3 | 1:R:53:TYR:CE2 | 2.28 | 0.69 |
| 1:T:50:LYS:HG3 | 1:T:53:TYR:CE2 | 2.28 | 0.69 |
| 1:U:58:ALA:CB | 1:U:65:LEU:HD22 | 2.23 | 0.69 |
| 1:U:301:GLY:N | 1:U:335:ARG:HG3 | 2.08 | 0.69 |
| 1:V:58:ALA:CB | 1:V:65:LEU:HD22 | 2.23 | 0.69 |
| 1:A:301:GLY:N | 1:A:335:ARG:HG3 | 2.08 | 0.69 |
| 1:C:208:ILE:HD11 | 1:C:243:PRO:CG | 2.23 | 0.69 |
| 1:E:58:ALA:CB | 1:E:65:LEU:HD22 | 2.23 | 0.69 |
| 1:G:34:ILE:HG22 | 1:G:35:VAL:N | 2.07 | 0.69 |
| 1:J:34:ILE:HG22 | 1:J:35:VAL:N | 2.07 | 0.69 |
| 1:K:50:LYS:HG3 | 1:K:53:TYR:CE2 | 2.28 | 0.69 |
| 1:M:50:LYS:HG3 | 1:M:53:TYR:CE2 | 2.28 | 0.69 |
| 1:N:34:ILE:HG22 | 1:N:35:VAL:N | 2.07 | 0.69 |
| 1:P:208:ILE:HD11 | 1:P:243:PRO:CG | 2.23 | 0.69 |
| 1:T:301:GLY:N | 1:T:335:ARG:HG3 | 2.08 | 0.69 |
| 1:V:34:ILE:HG22 | 1:V:35:VAL:N | 2.07 | 0.69 |
| 1:V:301:GLY:N | 1:V:335:ARG:HG3 | 2.08 | 0.69 |
| 1:W:58:ALA:CB | 1:W:65:LEU:HD22 | 2.23 | 0.69 |
| 1:D:22:ALA:HB1 | 1:D:348:SER:HB3 | 1.75 | 0.69 |
| 1:D:58:ALA:CB | 1:D:65:LEU:HD22 | 2.23 | 0.69 |
| 1:E:208:ILE:HD11 | 1:E:243:PRO:CG | 2.23 | 0.69 |
| 1:H:22:ALA:HB1 | 1:H:348:SER:HB3 | 1.75 | 0.69 |
| 1:I:50:LYS:HG3 | 1:I:53:TYR:CE2 | 2.28 | 0.69 |
| 1:J:58:ALA:CB | 1:J:65:LEU:HD22 | 2.23 | 0.69 |
| 1:K:34:ILE:HG22 | 1:K:35:VAL:N | 2.07 | 0.69 |
| 1:O:22:ALA:HB1 | 1:O:348:SER:HB3 | 1.75 | 0.69 |
| 1:O:301:GLY:N | 1:O:335:ARG:HG3 | 2.08 | 0.69 |
| 1:Q:301:GLY:N | 1:Q:335:ARG:HG3 | 2.08 | 0.69 |
| 1:R:301:GLY:N | 1:R:335:ARG:HG3 | 2.08 | 0.69 |
| 1:V:50:LYS:HG3 | 1:V:53:TYR:CE2 | 2.28 | 0.69 |
| 1:W:34:ILE:HG22 | 1:W:35:VAL:N | 2.07 | 0.69 |
| 1:B:7:ALA:HB1 | 1:B:356:TRP:CH2 | 2.29 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:208:ILE:HD11 | 1:J:243:PRO:CG | 2.23 | 0.68 |
| 1:K:7:ALA:HB1 | 1:K:356:TRP:CH2 | 2.29 | 0.68 |
| 1:K:143:TYR:CE1 | 1:M:45:VAL:HG21 | 2.27 | 0.68 |
| 1:M:301:GLY:N | 1:M:335:ARG:HG3 | 2.08 | 0.68 |
| 1:N:22:ALA:HB1 | 1:N:348:SER:HB3 | 1.75 | 0.68 |
| 1:U:236:LEU:CD1 | 1:U:237:GLU:HG2 | 2.22 | 0.68 |
| 1:A:208:ILE:HD11 | 1:A:243:PRO:CG | 2.23 | 0.68 |
| 1:B:208:ILE:HD11 | 1:B:243:PRO:CG | 2.23 | 0.68 |
| 1:C:301:GLY:N | 1:C:335:ARG:HG3 | 2.08 | 0.68 |
| 1:G:208:ILE:HD11 | 1:G:243:PRO:CG | 2.23 | 0.68 |
| 1:H:169:TYR:CE2 | 1:J:40:HIS:HB3 | 2.27 | 0.68 |
| 1:K:58:ALA:CB | 1:K:65:LEU:HD22 | 2.23 | 0.68 |
| 1:L:301:GLY:N | 1:L:335:ARG:HG3 | 2.08 | 0.68 |
| 1:M:7:ALA:HB1 | 1:M:356:TRP:CH2 | 2.29 | 0.68 |
| 1:P:301:GLY:N | 1:P:335:ARG:HG3 | 2.08 | 0.68 |
| 1:Q:7:ALA:HB1 | 1:Q:356:TRP:CH2 | 2.29 | 0.68 |
| 1:S:22:ALA:HB1 | 1:S:348:SER:HB3 | 1.75 | 0.68 |
| 1:T:7:ALA:HB1 | 1:T:356:TRP:CH2 | 2.29 | 0.68 |
| 1:U:37:ARG:CG | 1:U:38:PRO:HD2 | 2.20 | 0.68 |
| 1:A:173:HIS:CE1 | 1:B:268:GLY:CA | 2.77 | 0.68 |
| 1:C:22:ALA:HB1 | 1:C:348:SER:HB3 | 1.75 | 0.68 |
| 1:C:34:ILE:HG22 | 1:C:35:VAL:N | 2.07 | 0.68 |
| 1:D:7:ALA:HB1 | 1:D:356:TRP:CH2 | 2.29 | 0.68 |
| 1:H:34:ILE:HG22 | 1:H:35:VAL:N | 2.07 | 0.68 |
| 1:I:7:ALA:HB1 | 1:I:356:TRP:CH2 | 2.28 | 0.68 |
| 1:I:58:ALA:CB | 1:I:65:LEU:HD22 | 2.23 | 0.68 |
| 1:J:37:ARG:CG | 1:J:38:PRO:HD2 | 2.20 | 0.68 |
| 1:O:34:ILE:HG22 | 1:O:35:VAL:N | 2.07 | 0.68 |
| 1:O:58:ALA:CB | 1:O:65:LEU:HD22 | 2.23 | 0.68 |
| 1:T:58:ALA:CB | 1:T:65:LEU:HD22 | 2.23 | 0.68 |
| 1:V:7:ALA:HB1 | 1:V:356:TRP:CH2 | 2.29 | 0.68 |
| 1:A:22:ALA:HB1 | 1:A:348:SER:HB3 | 1.75 | 0.68 |
| 1:E:173:HIS:CE1 | 1:F:268:GLY:CA | 2.77 | 0.68 |
| 1:L:173:HIS:CE1 | 1:M:268:GLY:CA | 2.77 | 0.68 |
| 1:N:173:HIS:CE1 | 1:O:268:GLY:CA | 2.77 | 0.68 |
| 1:P:58:ALA:CB | 1:P:65:LEU:HD22 | 2.23 | 0.68 |
| 1:R:173:HIS:CE1 | 1:S:268:GLY:CA | 2.77 | 0.68 |
| 1:S:301:GLY:N | 1:S:335:ARG:HG3 | 2.08 | 0.68 |
| 1:S:362:TYR:CE1 | 1:S:367:PRO:HB3 | 2.28 | 0.68 |
| 1:U:22:ALA:HB1 | 1:U:348:SER:HB3 | 1.75 | 0.68 |
| 1:U:173:HIS:CE1 | 1:V:268:GLY:CA | 2.77 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:208:ILE:CD1 | 1:A:243:PRO:HD2 | 2.18 | 0.68 |
| 1:F:58:ALA:CB | 1:F:65:LEU:HD22 | 2.23 | 0.68 |
| 1:H:173:HIS:CE1 | 1:I:268:GLY:CA | 2.77 | 0.68 |
| 1:J:301:GLY:N | 1:J:335:ARG:HG3 | 2.08 | 0.68 |
| 1:K:301:GLY:N | 1:K:335:ARG:HG3 | 2.08 | 0.68 |
| 1:L:22:ALA:HB1 | 1:L:348:SER:HB3 | 1.75 | 0.68 |
| 1:O:7:ALA:HB1 | 1:O:356:TRP:CH2 | 2.29 | 0.68 |
| 1:Q:208:ILE:CD1 | 1:Q:243:PRO:HD2 | 2.18 | 0.68 |
| 1:Q:362:TYR:CE1 | 1:Q:367:PRO:HB3 | 2.28 | 0.68 |
| 1:R:7:ALA:HB1 | 1:R:356:TRP:CH2 | 2.29 | 0.68 |
| 1:R:22:ALA:HB1 | 1:R:348:SER:HB3 | 1.75 | 0.68 |
| 1:R:208:ILE:HD11 | 1:R:243:PRO:CG | 2.23 | 0.68 |
| 1:B:301:GLY:N | 1:B:335:ARG:HG3 | 2.08 | 0.68 |
| 1:D:208:ILE:HD11 | 1:D:243:PRO:CG | 2.23 | 0.68 |
| 1:D:362:TYR:O | 1:D:366:GLY:HA2 | 1.94 | 0.68 |
| 1:G:362:TYR:CE1 | 1:G:367:PRO:HB3 | 2.28 | 0.68 |
| 1:G:362:TYR:O | 1:G:366:GLY:HA2 | 1.94 | 0.68 |
| 1:I:362:TYR:CE1 | 1:I:367:PRO:HB3 | 2.28 | 0.68 |
| 1:K:290:ARG:CD | 1:M:244:ASP:HB2 | 2.12 | 0.68 |
| 1:K:362:TYR:O | 1:K:366:GLY:HA2 | 1.94 | 0.68 |
| 1:Q:58:ALA:CB | 1:Q:65:LEU:HD22 | 2.23 | 0.68 |
| 1:F:362:TYR:O | 1:F:366:GLY:HA2 | 1.94 | 0.68 |
| 1:H:208:ILE:HD11 | 1:H:243:PRO:CG | 2.23 | 0.68 |
| 1:T:22:ALA:HB1 | 1:T:348:SER:HB3 | 1.75 | 0.68 |
| 1:U:208:ILE:HD11 | 1:U:243:PRO:CG | 2.23 | 0.68 |
| 1:V:362:TYR:O | 1:V:366:GLY:HA2 | 1.94 | 0.68 |
| 1:W:208:ILE:HD11 | 1:W:243:PRO:CG | 2.23 | 0.68 |
| 1:B:22:ALA:HB1 | 1:B:348:SER:HB3 | 1.75 | 0.68 |
| 1:E:362:TYR:CE1 | 1:E:367:PRO:HB3 | 2.28 | 0.68 |
| 1:F:7:ALA:HB1 | 1:F:356:TRP:CH2 | 2.29 | 0.68 |
| 1:F:208:ILE:CD1 | 1:F:243:PRO:HD2 | 2.18 | 0.68 |
| 1:I:22:ALA:HB1 | 1:I:348:SER:HB3 | 1.75 | 0.68 |
| 1:I:301:GLY:N | 1:I:335:ARG:HG3 | 2.08 | 0.68 |
| 1:I:362:TYR:O | 1:I:366:GLY:HA2 | 1.94 | 0.68 |
| 1:J:22:ALA:HB1 | 1:J:348:SER:HB3 | 1.75 | 0.68 |
| 1:J:173:HIS:CE1 | 1:K:268:GLY:CA | 2.77 | 0.68 |
| 1:J:362:TYR:O | 1:J:366:GLY:HA2 | 1.94 | 0.68 |
| 1:M:362:TYR:O | 1:M:366:GLY:HA2 | 1.94 | 0.68 |
| 1:O:208:ILE:HD11 | 1:O:243:PRO:CG | 2.23 | 0.68 |
| 1:O:362:TYR:CE1 | 1:O:367:PRO:HB3 | 2.28 | 0.68 |
| 1:P:38:PRO:CG | 1:P:49:GLN:HE22 | 2.07 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:208:ILE:HD11 | 1:Q:243:PRO:CG | 2.23 | 0.68 |
| 1:R:38:PRO:CG | 1:R:49:GLN:HE22 | 2.07 | 0.68 |
| 1:T:236:LEU:HD22 | 1:T:252:ASN:N | 2.09 | 0.68 |
| 1:U:7:ALA:HB1 | 1:U:356:TRP:CH2 | 2.29 | 0.68 |
| 1:W:7:ALA:HB1 | 1:W:356:TRP:CH2 | 2.29 | 0.68 |
| 1:W:362:TYR:O | 1:W:366:GLY:HA2 | 1.94 | 0.68 |
| 1:B:110:LEU:HD12 | 1:B:177:ARG:NH1 | 2.09 | 0.68 |
| 1:B:362:TYR:CE1 | 1:B:367:PRO:HB3 | 2.28 | 0.68 |
| 1:C:236:LEU:HD22 | 1:C:252:ASN:N | 2.09 | 0.68 |
| 1:D:110:LEU:HD12 | 1:D:177:ARG:NH1 | 2.09 | 0.68 |
| 1:F:208:ILE:HD11 | 1:F:243:PRO:CG | 2.23 | 0.68 |
| 1:G:22:ALA:HB1 | 1:G:348:SER:HB3 | 1.75 | 0.68 |
| 1:I:208:ILE:HD11 | 1:I:243:PRO:CG | 2.23 | 0.68 |
| 1:K:236:LEU:HD22 | 1:K:252:ASN:N | 2.09 | 0.68 |
| 1:M:22:ALA:HB1 | 1:M:348:SER:HB3 | 1.75 | 0.68 |
| 1:M:236:LEU:HD22 | 1:M:252:ASN:N | 2.09 | 0.68 |
| 1:P:173:HIS:CE1 | 1:Q:268:GLY:CA | 2.77 | 0.68 |
| 1:R:362:TYR:O | 1:R:366:GLY:HA2 | 1.94 | 0.68 |
| 1:S:7:ALA:HB1 | 1:S:356:TRP:CH2 | 2.29 | 0.68 |
| 1:S:58:ALA:HB1 | 1:S:65:LEU:CD2 | 2.24 | 0.68 |
| 1:U:362:TYR:O | 1:U:366:GLY:HA2 | 1.94 | 0.68 |
| 1:B:362:TYR:O | 1:B:366:GLY:HA2 | 1.94 | 0.68 |
| 1:F:173:HIS:CE1 | 1:G:268:GLY:CA | 2.77 | 0.68 |
| 1:G:7:ALA:HB1 | 1:G:356:TRP:CH2 | 2.29 | 0.68 |
| 1:M:208:ILE:HD11 | 1:M:243:PRO:CG | 2.23 | 0.68 |
| 1:N:38:PRO:CG | 1:N:49:GLN:HE22 | 2.07 | 0.68 |
| 1:O:58:ALA:HB1 | 1:O:65:LEU:CD2 | 2.25 | 0.68 |
| 1:Q:58:ALA:HB1 | 1:Q:65:LEU:CD2 | 2.24 | 0.68 |
| 1:R:236:LEU:HD22 | 1:R:252:ASN:N | 2.09 | 0.68 |
| 1:S:208:ILE:HD11 | 1:S:243:PRO:CG | 2.23 | 0.68 |
| 1:T:38:PRO:CG | 1:T:49:GLN:HE22 | 2.07 | 0.68 |
| 1:T:362:TYR:O | 1:T:366:GLY:HA2 | 1.94 | 0.68 |
| 1:U:362:TYR:CE1 | 1:U:367:PRO:HB3 | 2.28 | 0.68 |
| 1:V:208:ILE:HD11 | 1:V:243:PRO:CG | 2.23 | 0.68 |
| 1:V:236:LEU:HD22 | 1:V:252:ASN:N | 2.09 | 0.68 |
| 1:W:22:ALA:HB1 | 1:W:348:SER:HB3 | 1.75 | 0.68 |
| 1:C:110:LEU:HD12 | 1:C:177:ARG:NH1 | 2.09 | 0.67 |
| 1:C:362:TYR:O | 1:C:366:GLY:HA2 | 1.94 | 0.67 |
| 1:D:38:PRO:CG | 1:D:49:GLN:HE22 | 2.07 | 0.67 |
| 1:E:236:LEU:HD22 | 1:E:252:ASN:N | 2.09 | 0.67 |
| 1:E:301:GLY:N | 1:E:335:ARG:HG3 | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:110:LEU:HD12 | 1:F:177:ARG:NH1 | 2.09 | 0.67 |
| 1:L:38:PRO:CG | 1:L:49:GLN:HE22 | 2.07 | 0.67 |
| 1:M:58:ALA:HB1 | 1:M:65:LEU:CD2 | 2.25 | 0.67 |
| 1:O:236:LEU:HD22 | 1:O:252:ASN:N | 2.09 | 0.67 |
| 1:P:7:ALA:HB1 | 1:P:356:TRP:CH2 | 2.29 | 0.67 |
| 1:V:58:ALA:HB1 | 1:V:65:LEU:CD2 | 2.24 | 0.67 |
| 1:W:301:GLY:N | 1:W:335:ARG:HG3 | 2.08 | 0.67 |
| 1:B:38:PRO:CG | 1:B:49:GLN:HE22 | 2.07 | 0.67 |
| 1:B:236:LEU:HD22 | 1:B:252:ASN:N | 2.09 | 0.67 |
| 1:C:362:TYR:CE1 | 1:C:367:PRO:HB3 | 2.28 | 0.67 |
| 1:F:58:ALA:HB1 | 1:F:65:LEU:CD2 | 2.24 | 0.67 |
| 1:F:370:VAL:HG13 | 1:F:370:VAL:O | 1.95 | 0.67 |
| 1:G:143:TYR:O | 1:G:143:TYR:CD1 | 2.48 | 0.67 |
| 1:G:208:ILE:CD1 | 1:G:243:PRO:HD2 | 2.18 | 0.67 |
| 1:K:58:ALA:HB1 | 1:K:65:LEU:CD2 | 2.25 | 0.67 |
| 1:M:38:PRO:CG | 1:M:49:GLN:HE22 | 2.07 | 0.67 |
| 1:N:362:TYR:O | 1:N:366:GLY:HA2 | 1.94 | 0.67 |
| 1:P:37:ARG:CG | 1:P:38:PRO:HD2 | 2.20 | 0.67 |
| 1:P:362:TYR:O | 1:P:366:GLY:HA2 | 1.94 | 0.67 |
| 1:S:34:ILE:HD13 | 1:S:67:LEU:HD22 | 1.77 | 0.67 |
| 1:T:104:LEU:HB2 | 1:T:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:T:173:HIS:CE1 | 1:U:268:GLY:CA | 2.77 | 0.67 |
| 1:U:34:ILE:HD13 | 1:U:67:LEU:HD22 | 1.76 | 0.67 |
| 1:U:58:ALA:HB1 | 1:U:65:LEU:CD2 | 2.25 | 0.67 |
| 1:W:110:LEU:HD12 | 1:W:177:ARG:NH1 | 2.09 | 0.67 |
| 1:A:7:ALA:HB1 | 1:A:356:TRP:CH2 | 2.29 | 0.67 |
| 1:A:236:LEU:HD22 | 1:A:252:ASN:N | 2.09 | 0.67 |
| 1:B:173:HIS:CE1 | 1:C:268:GLY:CA | 2.77 | 0.67 |
| 1:D:34:ILE:HD13 | 1:D:67:LEU:HD22 | 1.77 | 0.67 |
| 1:D:34:ILE:HG22 | 1:D:35:VAL:N | 2.07 | 0.67 |
| 1:D:362:TYR:CE1 | 1:D:367:PRO:HB3 | 2.28 | 0.67 |
| 1:H:58:ALA:HB1 | 1:H:65:LEU:CD2 | 2.25 | 0.67 |
| 1:K:37:ARG:CG | 1:K:38:PRO:HD2 | 2.20 | 0.67 |
| 1:N:301:GLY:N | 1:N:335:ARG:HG3 | 2.08 | 0.67 |
| 1:O:362:TYR:O | 1:O:366:GLY:HA2 | 1.94 | 0.67 |
| 1:P:104:LEU:HB2 | 1:P:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:Q:22:ALA:HB1 | 1:Q:348:SER:HB3 | 1.75 | 0.67 |
| 1:R:104:LEU:HB2 | 1:R:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:V:37:ARG:CG | 1:V:38:PRO:HD2 | 2.20 | 0.67 |
| 1:V:104:LEU:HB2 | 1:V:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:V:143:TYR:O | 1:V:143:TYR:CD1 | 2.48 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:143:TYR:O | 1:C:143:TYR:CD1 | 2.48 | 0.67 |
| 1:C:173:HIS:CE1 | 1:D:268:GLY:CA | 2.77 | 0.67 |
| 1:D:58:ALA:HB1 | 1:D:65:LEU:CD2 | 2.25 | 0.67 |
| 1:D:236:LEU:HD22 | 1:D:252:ASN:N | 2.09 | 0.67 |
| 1:D:301:GLY:N | 1:D:335:ARG:HG3 | 2.08 | 0.67 |
| 1:G:110:LEU:HD12 | 1:G:177:ARG:NH1 | 2.09 | 0.67 |
| 1:G:301:GLY:N | 1:G:335:ARG:HG3 | 2.08 | 0.67 |
| 1:H:301:GLY:N | 1:H:335:ARG:HG3 | 2.08 | 0.67 |
| 1:H:362:TYR:O | 1:H:366:GLY:HA2 | 1.94 | 0.67 |
| 1:I:58:ALA:HB1 | 1:I:65:LEU:CD2 | 2.24 | 0.67 |
| 1:I:173:HIS:CE1 | 1:J:268:GLY:CA | 2.77 | 0.67 |
| 1:J:58:ALA:HB1 | 1:J:65:LEU:CD2 | 2.25 | 0.67 |
| 1:J:362:TYR:CE1 | 1:J:367:PRO:HB3 | 2.28 | 0.67 |
| 1:O:173:HIS:CE1 | 1:P:268:GLY:CA | 2.77 | 0.67 |
| 1:Q:370:VAL:HG13 | 1:Q:370:VAL:O | 1.95 | 0.67 |
| 1:R:110:LEU:HD12 | 1:R:177:ARG:NH1 | 2.09 | 0.67 |
| 1:R:143:TYR:O | 1:R:143:TYR:CD1 | 2.48 | 0.67 |
| 1:S:362:TYR:O | 1:S:366:GLY:HA2 | 1.94 | 0.67 |
| 1:S:370:VAL:O | 1:S:370:VAL:HG13 | 1.95 | 0.67 |
| 1:A:38:PRO:CG | 1:A:49:GLN:HE22 | 2.07 | 0.67 |
| 1:A:362:TYR:O | 1:A:366:GLY:HA2 | 1.94 | 0.67 |
| 1:B:58:ALA:HB1 | 1:B:65:LEU:CD2 | 2.24 | 0.67 |
| 1:C:7:ALA:HB1 | 1:C:356:TRP:CH2 | 2.29 | 0.67 |
| 1:F:34:ILE:HD13 | 1:F:67:LEU:HD22 | 1.77 | 0.67 |
| 1:H:7:ALA:HB1 | 1:H:356:TRP:CH2 | 2.28 | 0.67 |
| 1:I:236:LEU:HD22 | 1:I:252:ASN:N | 2.09 | 0.67 |
| 1:J:34:ILE:HD13 | 1:J:67:LEU:HD22 | 1.77 | 0.67 |
| 1:K:22:ALA:HB1 | 1:K:348:SER:HB3 | 1.75 | 0.67 |
| 1:K:38:PRO:CG | 1:K:49:GLN:HE22 | 2.07 | 0.67 |
| 1:K:110:LEU:HD12 | 1:K:177:ARG:NH1 | 2.09 | 0.67 |
| 1:K:143:TYR:O | 1:K:143:TYR:CD1 | 2.48 | 0.67 |
| 1:K:173:HIS:CE1 | 1:L:268:GLY:CA | 2.77 | 0.67 |
| 1:M:173:HIS:CE1 | 1:N:268:GLY:CA | 2.77 | 0.67 |
| 1:N:104:LEU:HB2 | 1:N:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:N:110:LEU:HD12 | 1:N:177:ARG:NH1 | 2.09 | 0.67 |
| 1:Q:173:HIS:CE1 | 1:R:268:GLY:CA | 2.77 | 0.67 |
| 1:Q:362:TYR:O | 1:Q:366:GLY:HA2 | 1.94 | 0.67 |
| 1:S:173:HIS:CE1 | 1:T:268:GLY:CA | 2.77 | 0.67 |
| 1:T:110:LEU:HD12 | 1:T:177:ARG:NH1 | 2.09 | 0.67 |
| 1:T:208:ILE:HD11 | 1:T:243:PRO:CG | 2.23 | 0.67 |
| 1:U:110:LEU:HD12 | 1:U:177:ARG:NH1 | 2.09 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:38:PRO:CG | 1:V:49:GLN:HE22 | 2.07 | 0.67 |
| 1:A:104:LEU:HB2 | 1:A:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:D:37:ARG:CG | 1:D:38:PRO:HD2 | 2.20 | 0.67 |
| 1:D:370:VAL:HG13 | 1:D:370:VAL:O | 1.95 | 0.67 |
| 1:E:7:ALA:HB1 | 1:E:356:TRP:CH2 | 2.29 | 0.67 |
| 1:E:37:ARG:CG | 1:E:38:PRO:HD2 | 2.20 | 0.67 |
| 1:F:22:ALA:HB1 | 1:F:348:SER:HB3 | 1.75 | 0.67 |
| 1:H:34:ILE:HD13 | 1:H:67:LEU:HD22 | 1.77 | 0.67 |
| 1:H:110:LEU:HD12 | 1:H:177:ARG:NH1 | 2.09 | 0.67 |
| 1:H:362:TYR:CE1 | 1:H:367:PRO:HB3 | 2.28 | 0.67 |
| 1:H:370:VAL:O | 1:H:370:VAL:HG13 | 1.95 | 0.67 |
| 1:J:38:PRO:CG | 1:J:49:GLN:HE22 | 2.07 | 0.67 |
| 1:K:208:ILE:HD11 | 1:K:243:PRO:CG | 2.23 | 0.67 |
| 1:M:110:LEU:HD12 | 1:M:177:ARG:NH1 | 2.09 | 0.67 |
| 1:N:7:ALA:HB1 | 1:N:356:TRP:CH2 | 2.29 | 0.67 |
| 1:O:34:ILE:HD13 | 1:O:67:LEU:HD22 | 1.77 | 0.67 |
| 1:P:236:LEU:HD22 | 1:P:252:ASN:N | 2.09 | 0.67 |
| 1:T:58:ALA:HB1 | 1:T:65:LEU:CD2 | 2.25 | 0.67 |
| 1:V:173:HIS:CE1 | 1:W:268:GLY:CA | 2.77 | 0.67 |
| 1:W:34:ILE:HD13 | 1:W:67:LEU:HD22 | 1.77 | 0.67 |
| 1:W:58:ALA:HB1 | 1:W:65:LEU:CD2 | 2.25 | 0.67 |
| 1:B:34:ILE:HD13 | 1:B:67:LEU:HD22 | 1.77 | 0.67 |
| 1:C:38:PRO:CG | 1:C:49:GLN:HE22 | 2.07 | 0.67 |
| 1:E:110:LEU:HD12 | 1:E:177:ARG:NH1 | 2.09 | 0.67 |
| 1:G:173:HIS:CE1 | 1:H:268:GLY:CA | 2.77 | 0.67 |
| 1:I:110:LEU:HD12 | 1:I:177:ARG:NH1 | 2.09 | 0.67 |
| 1:O:38:PRO:CG | 1:O:49:GLN:HE22 | 2.07 | 0.67 |
| 1:P:110:LEU:HD12 | 1:P:177:ARG:NH1 | 2.09 | 0.67 |
| 1:U:38:PRO:CG | 1:U:49:GLN:HE22 | 2.07 | 0.67 |
| 1:V:110:LEU:HD12 | 1:V:177:ARG:NH1 | 2.09 | 0.67 |
| 1:W:362:TYR:CE1 | 1:W:367:PRO:HB3 | 2.28 | 0.67 |
| 1:D:173:HIS:CE1 | 1:E:268:GLY:CA | 2.77 | 0.67 |
| 1:F:236:LEU:HD22 | 1:F:252:ASN:N | 2.09 | 0.67 |
| 1:L:34:ILE:HD13 | 1:L:67:LEU:HD22 | 1.77 | 0.67 |
| 1:L:236:LEU:HD22 | 1:L:252:ASN:N | 2.09 | 0.67 |
| 1:L:362:TYR:CE1 | 1:L:367:PRO:HB3 | 2.28 | 0.67 |
| 1:Q:34:ILE:HD13 | 1:Q:67:LEU:HD22 | 1.77 | 0.67 |
| 1:R:208:ILE:CD1 | 1:R:243:PRO:HD2 | 2.18 | 0.67 |
| 1:S:110:LEU:HD12 | 1:S:177:ARG:NH1 | 2.09 | 0.67 |
| 1:S:236:LEU:HD22 | 1:S:252:ASN:N | 2.09 | 0.67 |
| 1:V:208:ILE:CD1 | 1:V:243:PRO:HD2 | 2.18 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:104:LEU:HB2 | 1:W:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:B:104:LEU:HB2 | 1:B:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:C:104:LEU:HB2 | 1:C:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:F:38:PRO:CG | 1:F:49:GLN:HE22 | 2.07 | 0.67 |
| 1:H:39:ARG:NE | 1:H:66:THR:HB | 2.09 | 0.67 |
| 1:L:58:ALA:HB1 | 1:L:65:LEU:CD2 | 2.24 | 0.67 |
| 1:L:104:LEU:HB2 | 1:L:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:M:362:TYR:CE1 | 1:M:367:PRO:HB3 | 2.28 | 0.67 |
| 1:N:143:TYR:O | 1:N:143:TYR:CD1 | 2.48 | 0.67 |
| 1:U:104:LEU:HB2 | 1:U:356:TRP:CZ3 | 2.30 | 0.67 |
| 1:A:58:ALA:HB1 | 1:A:65:LEU:CD2 | 2.24 | 0.67 |
| 1:A:110:LEU:HD12 | 1:A:177:ARG:NH1 | 2.09 | 0.67 |
| 1:A:143:TYR:O | 1:A:143:TYR:CD1 | 2.48 | 0.67 |
| 1:A:362:TYR:CE1 | 1:A:367:PRO:HB3 | 2.28 | 0.67 |
| 1:F:362:TYR:CE1 | 1:F:367:PRO:HB3 | 2.28 | 0.67 |
| 1:H:236:LEU:HD22 | 1:H:252:ASN:N | 2.09 | 0.67 |
| 1:L:7:ALA:HB1 | 1:L:356:TRP:CH2 | 2.29 | 0.67 |
| 1:P:22:ALA:HB1 | 1:P:348:SER:HB3 | 1.75 | 0.67 |
| 1:Q:236:LEU:HD22 | 1:Q:252:ASN:N | 2.09 | 0.67 |
| 1:S:38:PRO:CG | 1:S:49:GLN:HE22 | 2.07 | 0.67 |
| 1:E:22:ALA:HB1 | 1:E:348:SER:HB3 | 1.75 | 0.66 |
| 1:E:104:LEU:HB2 | 1:E:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:G:58:ALA:HB1 | 1:G:65:LEU:CD2 | 2.25 | 0.66 |
| 1:L:208:ILE:CD1 | 1:L:243:PRO:HD2 | 2.18 | 0.66 |
| 1:M:143:TYR:O | 1:M:143:TYR:CD1 | 2.48 | 0.66 |
| 1:N:236:LEU:HD22 | 1:N:252:ASN:N | 2.09 | 0.66 |
| 1:O:110:LEU:HD12 | 1:O:177:ARG:NH1 | 2.09 | 0.66 |
| 1:O:370:VAL:HG13 | 1:O:370:VAL:O | 1.95 | 0.66 |
| 1:P:143:TYR:O | 1:P:143:TYR:CD1 | 2.48 | 0.66 |
| 1:Q:104:LEU:HB2 | 1:Q:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:S:104:LEU:HB2 | 1:S:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:W:38:PRO:CG | 1:W:49:GLN:HE22 | 2.07 | 0.66 |
| 1:B:34:ILE:HA | 1:B:68:LYS:O | 1.96 | 0.66 |
| 1:B:300:SER:CA | 1:B:335:ARG:HG3 | 2.25 | 0.66 |
| 1:E:38:PRO:CG | 1:E:49:GLN:HE22 | 2.07 | 0.66 |
| 1:I:34:ILE:HA | 1:I:68:LYS:O | 1.96 | 0.66 |
| 1:L:362:TYR:O | 1:L:366:GLY:HA2 | 1.94 | 0.66 |
| 1:M:34:ILE:HD13 | 1:M:67:LEU:HD22 | 1.77 | 0.66 |
| 1:M:300:SER:CA | 1:M:335:ARG:HG3 | 2.25 | 0.66 |
| 1:N:34:ILE:HD13 | 1:N:67:LEU:HD22 | 1.77 | 0.66 |
| 1:O:104:LEU:HB2 | 1:O:356:TRP:CZ3 | 2.30 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:34:ILE:HA | 1:Q:68:LYS:O | 1.96 | 0.66 |
| 1:W:236:LEU:HD22 | 1:W:252:ASN:N | 2.09 | 0.66 |
| 1:D:104:LEU:HB2 | 1:D:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:I:143:TYR:O | 1:I:143:TYR:CD1 | 2.48 | 0.66 |
| 1:J:7:ALA:HB1 | 1:J:356:TRP:CH2 | 2.29 | 0.66 |
| 1:J:236:LEU:HD22 | 1:J:252:ASN:N | 2.09 | 0.66 |
| 1:M:104:LEU:HB2 | 1:M:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:U:236:LEU:HD22 | 1:U:252:ASN:N | 2.09 | 0.66 |
| 1:U:370:VAL:O | 1:U:370:VAL:HG13 | 1.95 | 0.66 |
| 1:V:22:ALA:HB1 | 1:V:348:SER:HB3 | 1.75 | 0.66 |
| 1:V:34:ILE:HA | 1:V:68:LYS:O | 1.95 | 0.66 |
| 1:V:362:TYR:CE1 | 1:V:367:PRO:HB3 | 2.28 | 0.66 |
| 1:E:143:TYR:O | 1:E:143:TYR:CD1 | 2.48 | 0.66 |
| 1:G:34:ILE:HA | 1:G:68:LYS:O | 1.96 | 0.66 |
| 1:G:104:LEU:HB2 | 1:G:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:H:38:PRO:CG | 1:H:49:GLN:HE22 | 2.07 | 0.66 |
| 1:J:39:ARG:NE | 1:J:66:THR:HB | 2.09 | 0.66 |
| 1:J:104:LEU:HB2 | 1:J:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:J:110:LEU:HD12 | 1:J:177:ARG:NH1 | 2.09 | 0.66 |
| 1:L:110:LEU:HD12 | 1:L:177:ARG:NH1 | 2.09 | 0.66 |
| 1:L:143:TYR:O | 1:L:143:TYR:CD1 | 2.48 | 0.66 |
| 1:Q:39:ARG:NE | 1:Q:66:THR:HB | 2.09 | 0.66 |
| 1:R:58:ALA:HB1 | 1:R:65:LEU:CD2 | 2.25 | 0.66 |
| 1:S:39:ARG:NE | 1:S:66:THR:HB | 2.09 | 0.66 |
| 1:T:143:TYR:O | 1:T:143:TYR:CD1 | 2.48 | 0.66 |
| 1:D:34:ILE:HA | 1:D:68:LYS:O | 1.96 | 0.66 |
| 1:E:362:TYR:O | 1:E:366:GLY:HA2 | 1.94 | 0.66 |
| 1:G:236:LEU:HD22 | 1:G:252:ASN:N | 2.09 | 0.66 |
| 1:I:38:PRO:CG | 1:I:49:GLN:HE22 | 2.07 | 0.66 |
| 1:K:34:ILE:HD13 | 1:K:67:LEU:HD22 | 1.77 | 0.66 |
| 1:K:34:ILE:HA | 1:K:68:LYS:O | 1.96 | 0.66 |
| 1:N:362:TYR:CE1 | 1:N:367:PRO:HB3 | 2.28 | 0.66 |
| 1:O:39:ARG:NE | 1:O:66:THR:HB | 2.09 | 0.66 |
| 1:O:143:TYR:O | 1:O:143:TYR:CD1 | 2.48 | 0.66 |
| 1:Q:110:LEU:HD12 | 1:Q:177:ARG:NH1 | 2.09 | 0.66 |
| 1:R:34:ILE:HA | 1:R:68:LYS:O | 1.96 | 0.66 |
| 1:A:34:ILE:HD13 | 1:A:67:LEU:HD22 | 1.77 | 0.66 |
| 1:A:370:VAL:HG22 | 1:A:375:PHE:O | 1.96 | 0.66 |
| 1:B:143:TYR:O | 1:B:143:TYR:CD1 | 2.48 | 0.66 |
| 1:F:34:ILE:HA | 1:F:68:LYS:O | 1.96 | 0.66 |
| 1:F:370:VAL:HG22 | 1:F:375:PHE:O | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:300:SER:CA | 1:I:335:ARG:HG3 | 2.25 | 0.66 |
| 1:I:370:VAL:HG22 | 1:I:375:PHE:O | 1.96 | 0.66 |
| 1:K:104:LEU:HB2 | 1:K:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:M:34:ILE:HA | 1:M:68:LYS:O | 1.96 | 0.66 |
| 1:N:58:ALA:HB1 | 1:N:65:LEU:CD2 | 2.24 | 0.66 |
| 1:P:370:VAL:HG22 | 1:P:375:PHE:O | 1.96 | 0.66 |
| 1:Q:38:PRO:CG | 1:Q:49:GLN:HE22 | 2.07 | 0.66 |
| 1:S:34:ILE:HA | 1:S:68:LYS:O | 1.96 | 0.66 |
| 1:W:370:VAL:HG22 | 1:W:375:PHE:O | 1.96 | 0.66 |
| 1:I:104:LEU:HB2 | 1:I:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:J:143:TYR:O | 1:J:143:TYR:CD1 | 2.48 | 0.66 |
| 1:J:370:VAL:O | 1:J:370:VAL:HG13 | 1.95 | 0.66 |
| 1:O:37:ARG:CG | 1:O:38:PRO:HD2 | 2.20 | 0.66 |
| 1:Q:300:SER:CA | 1:Q:335:ARG:HG3 | 2.26 | 0.66 |
| 1:U:370:VAL:HG22 | 1:U:375:PHE:O | 1.96 | 0.66 |
| 1:C:58:ALA:HB1 | 1:C:65:LEU:CD2 | 2.25 | 0.66 |
| 1:G:38:PRO:CG | 1:G:49:GLN:HE22 | 2.07 | 0.66 |
| 1:H:370:VAL:HG22 | 1:H:375:PHE:O | 1.96 | 0.66 |
| 1:K:35:VAL:CA | 1:K:54:VAL:HG21 | 2.26 | 0.66 |
| 1:M:370:VAL:HG22 | 1:M:375:PHE:O | 1.96 | 0.66 |
| 1:N:370:VAL:HG22 | 1:N:375:PHE:O | 1.96 | 0.66 |
| 1:O:300:SER:CA | 1:O:335:ARG:HG3 | 2.25 | 0.66 |
| 1:O:370:VAL:HG22 | 1:O:375:PHE:O | 1.96 | 0.66 |
| 1:T:362:TYR:CE1 | 1:T:367:PRO:HB3 | 2.28 | 0.66 |
| 1:U:35:VAL:CA | 1:U:54:VAL:HG21 | 2.26 | 0.66 |
| 1:C:34:ILE:HD13 | 1:C:67:LEU:HD22 | 1.77 | 0.66 |
| 1:C:34:ILE:HA | 1:C:68:LYS:O | 1.96 | 0.66 |
| 1:D:143:TYR:O | 1:D:143:TYR:CD1 | 2.48 | 0.66 |
| 1:F:104:LEU:HB2 | 1:F:356:TRP:CZ3 | 2.30 | 0.66 |
| 1:K:362:TYR:CE1 | 1:K:367:PRO:HB3 | 2.28 | 0.66 |
| 1:L:35:VAL:CA | 1:L:54:VAL:HG21 | 2.26 | 0.66 |
| 1:M:35:VAL:CA | 1:M:54:VAL:HG21 | 2.26 | 0.66 |
| 1:Q:143:TYR:O | 1:Q:143:TYR:CD1 | 2.48 | 0.66 |
| 1:R:370:VAL:HG22 | 1:R:375:PHE:O | 1.96 | 0.66 |
| 1:S:300:SER:CA | 1:S:335:ARG:HG3 | 2.26 | 0.66 |
| 1:T:300:SER:CA | 1:T:335:ARG:HG3 | 2.25 | 0.66 |
| 1:U:34:ILE:HA | 1:U:68:LYS:O | 1.96 | 0.66 |
| 1:V:370:VAL:HG22 | 1:V:375:PHE:O | 1.96 | 0.66 |
| 1:W:35:VAL:CA | 1:W:54:VAL:HG21 | 2.26 | 0.66 |
| 1:B:370:VAL:O | 1:B:370:VAL:HG13 | 1.95 | 0.66 |
| 1:D:370:VAL:HG22 | 1:D:375:PHE:O | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:370:VAL:HG22 | 1:E:375:PHE:O | 1.96 | 0.66 |
| 1:F:35:VAL:CA | 1:F:54:VAL:HG21 | 2.26 | 0.66 |
| 1:F:300:SER:CA | 1:F:335:ARG:HG3 | 2.26 | 0.66 |
| 1:I:35:VAL:CA | 1:I:54:VAL:HG21 | 2.26 | 0.66 |
| 1:P:34:ILE:HD13 | 1:P:67:LEU:HD22 | 1.77 | 0.66 |
| 1:R:370:VAL:HG13 | 1:R:370:VAL:O | 1.95 | 0.66 |
| 1:S:35:VAL:CA | 1:S:54:VAL:HG21 | 2.26 | 0.66 |
| 1:W:143:TYR:O | 1:W:143:TYR:CD1 | 2.48 | 0.66 |
| 1:W:370:VAL:HG13 | 1:W:370:VAL:O | 1.95 | 0.66 |
| 1:D:35:VAL:CA | 1:D:54:VAL:HG21 | 2.26 | 0.65 |
| 1:E:34:ILE:HA | 1:E:68:LYS:O | 1.96 | 0.65 |
| 1:G:370:VAL:HG22 | 1:G:375:PHE:O | 1.96 | 0.65 |
| 1:H:35:VAL:CG1 | 1:H:68:LYS:HB2 | 2.22 | 0.65 |
| 1:H:143:TYR:O | 1:H:143:TYR:CD1 | 2.48 | 0.65 |
| 1:I:34:ILE:HD13 | 1:I:67:LEU:HD22 | 1.77 | 0.65 |
| 1:M:39:ARG:NE | 1:M:66:THR:HB | 2.09 | 0.65 |
| 1:N:35:VAL:CA | 1:N:54:VAL:HG21 | 2.26 | 0.65 |
| 1:P:34:ILE:HA | 1:P:68:LYS:O | 1.96 | 0.65 |
| 1:R:35:VAL:CA | 1:R:54:VAL:HG21 | 2.26 | 0.65 |
| 1:U:143:TYR:O | 1:U:143:TYR:CD1 | 2.48 | 0.65 |
| 1:C:370:VAL:HG22 | 1:C:375:PHE:O | 1.96 | 0.65 |
| 1:E:34:ILE:HD13 | 1:E:67:LEU:HD22 | 1.77 | 0.65 |
| 1:E:58:ALA:HB1 | 1:E:65:LEU:CD2 | 2.24 | 0.65 |
| 1:F:143:TYR:O | 1:F:143:TYR:CD1 | 2.48 | 0.65 |
| 1:J:34:ILE:HA | 1:J:68:LYS:O | 1.96 | 0.65 |
| 1:L:39:ARG:NE | 1:L:66:THR:HB | 2.09 | 0.65 |
| 1:N:370:VAL:HG13 | 1:N:370:VAL:O | 1.95 | 0.65 |
| 1:O:34:ILE:HA | 1:O:68:LYS:O | 1.96 | 0.65 |
| 1:T:35:VAL:CA | 1:T:54:VAL:HG21 | 2.26 | 0.65 |
| 1:T:370:VAL:HG22 | 1:T:375:PHE:O | 1.96 | 0.65 |
| 1:U:39:ARG:NE | 1:U:66:THR:HB | 2.09 | 0.65 |
| 1:D:300:SER:CA | 1:D:335:ARG:HG3 | 2.25 | 0.65 |
| 1:H:104:LEU:HB2 | 1:H:356:TRP:CZ3 | 2.30 | 0.65 |
| 1:L:370:VAL:HG13 | 1:L:370:VAL:O | 1.95 | 0.65 |
| 1:M:370:VAL:O | 1:M:370:VAL:HG13 | 1.95 | 0.65 |
| 1:R:34:ILE:HD13 | 1:R:67:LEU:HD22 | 1.76 | 0.65 |
| 1:S:143:TYR:O | 1:S:143:TYR:CD1 | 2.48 | 0.65 |
| 1:S:370:VAL:HG22 | 1:S:375:PHE:O | 1.96 | 0.65 |
| 1:T:34:ILE:HD13 | 1:T:67:LEU:HD22 | 1.77 | 0.65 |
| 1:T:34:ILE:HA | 1:T:68:LYS:O | 1.96 | 0.65 |
| 1:V:34:ILE:HD13 | 1:V:67:LEU:HD22 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:370:VAL:O | 1:V:370:VAL:HG13 | 1.95 | 0.65 |
| 1:W:34:ILE:HA | 1:W:68:LYS:O | 1.96 | 0.65 |
| 1:E:370:VAL:O | 1:E:370:VAL:HG13 | 1.95 | 0.65 |
| 1:G:300:SER:CA | 1:G:335:ARG:HG3 | 2.25 | 0.65 |
| 1:G:369:ILE:CG2 | 1:G:370:VAL:N | 2.60 | 0.65 |
| 1:K:208:ILE:CD1 | 1:K:243:PRO:HD2 | 2.18 | 0.65 |
| 1:N:34:ILE:HA | 1:N:68:LYS:O | 1.96 | 0.65 |
| 1:O:35:VAL:CA | 1:O:54:VAL:HG21 | 2.26 | 0.65 |
| 1:P:362:TYR:CE1 | 1:P:367:PRO:HB3 | 2.28 | 0.65 |
| 1:Q:35:VAL:CA | 1:Q:54:VAL:HG21 | 2.26 | 0.65 |
| 1:D:208:ILE:CD1 | 1:D:243:PRO:HD2 | 2.18 | 0.65 |
| 1:G:35:VAL:CA | 1:G:54:VAL:HG21 | 2.26 | 0.65 |
| 1:G:370:VAL:HG13 | 1:G:370:VAL:O | 1.95 | 0.65 |
| 1:H:300:SER:CA | 1:H:335:ARG:HG3 | 2.26 | 0.65 |
| 1:J:370:VAL:HG22 | 1:J:375:PHE:O | 1.96 | 0.65 |
| 1:K:300:SER:CA | 1:K:335:ARG:HG3 | 2.25 | 0.65 |
| 1:P:58:ALA:HB1 | 1:P:65:LEU:CD2 | 2.24 | 0.65 |
| 1:P:369:ILE:CG2 | 1:P:370:VAL:N | 2.60 | 0.65 |
| 1:P:370:VAL:O | 1:P:370:VAL:HG13 | 1.95 | 0.65 |
| 1:R:362:TYR:CE1 | 1:R:367:PRO:HB3 | 2.28 | 0.65 |
| 1:T:290:ARG:CD | 1:V:244:ASP:HB2 | 2.12 | 0.65 |
| 1:V:35:VAL:CA | 1:V:54:VAL:HG21 | 2.26 | 0.65 |
| 1:G:34:ILE:HD13 | 1:G:67:LEU:HD22 | 1.77 | 0.65 |
| 1:P:35:VAL:CA | 1:P:54:VAL:HG21 | 2.26 | 0.65 |
| 1:V:300:SER:CA | 1:V:335:ARG:HG3 | 2.26 | 0.65 |
| 1:V:369:ILE:CG2 | 1:V:370:VAL:N | 2.60 | 0.65 |
| 1:W:300:SER:CA | 1:W:335:ARG:HG3 | 2.25 | 0.65 |
| 1:A:39:ARG:NE | 1:A:66:THR:HB | 2.09 | 0.65 |
| 1:A:369:ILE:CG2 | 1:A:370:VAL:N | 2.60 | 0.65 |
| 1:B:35:VAL:CA | 1:B:54:VAL:HG21 | 2.26 | 0.65 |
| 1:L:34:ILE:HA | 1:L:68:LYS:O | 1.96 | 0.65 |
| 1:N:369:ILE:CG2 | 1:N:370:VAL:N | 2.60 | 0.65 |
| 1:D:58:ALA:O | 1:D:61:LYS:N | 2.30 | 0.65 |
| 1:E:369:ILE:CG2 | 1:E:370:VAL:N | 2.60 | 0.65 |
| 1:I:369:ILE:CG2 | 1:I:370:VAL:N | 2.60 | 0.65 |
| 1:K:370:VAL:HG22 | 1:K:375:PHE:O | 1.96 | 0.65 |
| 1:Q:35:VAL:CG1 | 1:Q:68:LYS:HB2 | 2.22 | 0.65 |
| 1:C:300:SER:CA | 1:C:335:ARG:HG3 | 2.25 | 0.65 |
| 1:I:370:VAL:HG13 | 1:I:370:VAL:O | 1.95 | 0.65 |
| 1:J:35:VAL:CG1 | 1:J:68:LYS:HB2 | 2.22 | 0.65 |
| 1:O:35:VAL:CG1 | 1:O:68:LYS:HB2 | 2.22 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:35:VAL:CA | 1:A:54:VAL:HG21 | 2.26 | 0.65 |
| 1:A:370:VAL:HG13 | 1:A:370:VAL:O | 1.95 | 0.65 |
| 1:C:35:VAL:CA | 1:C:54:VAL:HG21 | 2.26 | 0.65 |
| 1:C:58:ALA:O | 1:C:61:LYS:N | 2.30 | 0.65 |
| 1:E:300:SER:CA | 1:E:335:ARG:HG3 | 2.25 | 0.65 |
| 1:H:37:ARG:CG | 1:H:38:PRO:HD2 | 2.20 | 0.65 |
| 1:I:58:ALA:O | 1:I:61:LYS:N | 2.30 | 0.65 |
| 1:K:39:ARG:NE | 1:K:66:THR:HB | 2.09 | 0.65 |
| 1:O:58:ALA:O | 1:O:61:LYS:N | 2.30 | 0.65 |
| 1:R:300:SER:CA | 1:R:335:ARG:HG3 | 2.25 | 0.65 |
| 1:R:369:ILE:CG2 | 1:R:370:VAL:N | 2.60 | 0.65 |
| 1:S:35:VAL:CG1 | 1:S:68:LYS:HB2 | 2.22 | 0.65 |
| 1:T:58:ALA:O | 1:T:61:LYS:N | 2.30 | 0.65 |
| 1:Q:370:VAL:HG22 | 1:Q:375:PHE:O | 1.96 | 0.64 |
| 1:U:58:ALA:O | 1:U:61:LYS:N | 2.30 | 0.64 |
| 1:C:370:VAL:O | 1:C:370:VAL:HG13 | 1.95 | 0.64 |
| 1:I:290:ARG:CD | 1:K:244:ASP:HB2 | 2.12 | 0.64 |
| 1:L:300:SER:CA | 1:L:335:ARG:HG3 | 2.25 | 0.64 |
| 1:U:300:SER:CA | 1:U:335:ARG:HG3 | 2.25 | 0.64 |
| 1:W:39:ARG:NE | 1:W:66:THR:HB | 2.09 | 0.64 |
| 1:W:369:ILE:CG2 | 1:W:370:VAL:N | 2.60 | 0.64 |
| 1:A:34:ILE:HA | 1:A:68:LYS:O | 1.96 | 0.64 |
| 1:B:370:VAL:HG22 | 1:B:375:PHE:O | 1.96 | 0.64 |
| 1:E:58:ALA:O | 1:E:61:LYS:N | 2.30 | 0.64 |
| 1:F:58:ALA:O | 1:F:61:LYS:N | 2.30 | 0.64 |
| 1:K:370:VAL:O | 1:K:370:VAL:HG13 | 1.95 | 0.64 |
| 1:L:370:VAL:HG22 | 1:L:375:PHE:O | 1.96 | 0.64 |
| 1:N:37:ARG:CG | 1:N:38:PRO:HD2 | 2.20 | 0.64 |
| 1:N:300:SER:CA | 1:N:335:ARG:HG3 | 2.26 | 0.64 |
| 1:Q:369:ILE:CG2 | 1:Q:370:VAL:N | 2.60 | 0.64 |
| 1:S:37:ARG:CG | 1:S:38:PRO:HD2 | 2.20 | 0.64 |
| 1:T:369:ILE:CG2 | 1:T:370:VAL:N | 2.60 | 0.64 |
| 1:T:370:VAL:HG13 | 1:T:370:VAL:O | 1.95 | 0.64 |
| 1:B:7:ALA:HB1 | 1:B:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:E:35:VAL:CA | 1:E:54:VAL:HG21 | 2.26 | 0.64 |
| 1:L:37:ARG:CG | 1:L:38:PRO:HD2 | 2.20 | 0.64 |
| 1:M:35:VAL:CG1 | 1:M:68:LYS:HB2 | 2.22 | 0.64 |
| 1:N:58:ALA:O | 1:N:61:LYS:N | 2.30 | 0.64 |
| 1:Q:7:ALA:HB1 | 1:Q:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:T:7:ALA:HB1 | 1:T:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:V:58:ALA:O | 1:V:61:LYS:N | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:58:ALA:O | 1:W:61:LYS:N | 2.30 | 0.64 |
| 1:I:7:ALA:HB1 | 1:I:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:K:58:ALA:O | 1:K:61:LYS:N | 2.30 | 0.64 |
| 1:M:369:ILE:CG2 | 1:M:370:VAL:N | 2.60 | 0.64 |
| 1:N:39:ARG:NE | 1:N:66:THR:HB | 2.09 | 0.64 |
| 1:R:7:ALA:HB1 | 1:R:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:A:300:SER:CA | 1:A:335:ARG:HG3 | 2.25 | 0.64 |
| 1:B:369:ILE:CG2 | 1:B:370:VAL:N | 2.60 | 0.64 |
| 1:C:39:ARG:NE | 1:C:66:THR:HB | 2.09 | 0.64 |
| 1:C:369:ILE:CG2 | 1:C:370:VAL:N | 2.60 | 0.64 |
| 1:H:34:ILE:HA | 1:H:68:LYS:O | 1.96 | 0.64 |
| 1:H:35:VAL:CA | 1:H:54:VAL:HG21 | 2.26 | 0.64 |
| 1:H:369:ILE:CG2 | 1:H:370:VAL:N | 2.60 | 0.64 |
| 1:J:369:ILE:CG2 | 1:J:370:VAL:N | 2.60 | 0.64 |
| 1:Q:58:ALA:O | 1:Q:61:LYS:N | 2.30 | 0.64 |
| 1:U:7:ALA:HB1 | 1:U:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:V:39:ARG:NE | 1:V:66:THR:HB | 2.09 | 0.64 |
| 1:W:7:ALA:HB1 | 1:W:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:W:37:ARG:CG | 1:W:38:PRO:HD2 | 2.20 | 0.64 |
| 1:C:290:ARG:CD | 1:E:244:ASP:HB2 | 2.12 | 0.64 |
| 1:G:7:ALA:HB1 | 1:G:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:K:7:ALA:HB1 | 1:K:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:O:369:ILE:CG2 | 1:O:370:VAL:N | 2.60 | 0.64 |
| 1:P:300:SER:CA | 1:P:335:ARG:HG3 | 2.25 | 0.64 |
| 1:S:7:ALA:HB1 | 1:S:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:V:7:ALA:HB1 | 1:V:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:B:58:ALA:O | 1:B:61:LYS:N | 2.30 | 0.64 |
| 1:J:35:VAL:CA | 1:J:54:VAL:HG21 | 2.26 | 0.64 |
| 1:L:369:ILE:CG2 | 1:L:370:VAL:N | 2.60 | 0.64 |
| 1:O:7:ALA:HB1 | 1:O:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:P:7:ALA:HB1 | 1:P:356:TRP:CZ2 | 2.33 | 0.64 |
| 1:P:58:ALA:O | 1:P:61:LYS:N | 2.30 | 0.64 |
| 1:S:369:ILE:CG2 | 1:S:370:VAL:N | 2.60 | 0.64 |
| 1:U:35:VAL:CG1 | 1:U:68:LYS:HB2 | 2.22 | 0.64 |
| 1:U:208:ILE:CD1 | 1:U:243:PRO:HD2 | 2.18 | 0.64 |
| 1:F:369:ILE:CG2 | 1:F:370:VAL:N | 2.60 | 0.64 |
| 1:J:300:SER:CA | 1:J:335:ARG:HG3 | 2.26 | 0.64 |
| 1:K:35:VAL:CG1 | 1:K:68:LYS:HB2 | 2.22 | 0.64 |
| 1:M:58:ALA:O | 1:M:61:LYS:N | 2.30 | 0.64 |
| 1:A:37:ARG:CG | 1:A:38:PRO:HD2 | 2.20 | 0.63 |
| 1:A:298:VAL:HG12 | 1:A:335:ARG:HH11 | 1.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:34:ILE:HB | 1:B:54:VAL:HG13 | 1.79 | 0.63 |
| 1:C:7:ALA:HB1 | 1:C:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:F:334:GLU:HA | 1:F:334:GLU:OE2 | 1.98 | 0.63 |
| 1:G:58:ALA:O | 1:G:61:LYS:N | 2.30 | 0.63 |
| 1:H:7:ALA:HB1 | 1:H:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:K:369:ILE:CG2 | 1:K:370:VAL:N | 2.60 | 0.63 |
| 1:L:7:ALA:HB1 | 1:L:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:N:7:ALA:HB1 | 1:N:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:T:39:ARG:NE | 1:T:66:THR:HB | 2.09 | 0.63 |
| 1:D:369:ILE:CG2 | 1:D:370:VAL:N | 2.60 | 0.63 |
| 1:E:7:ALA:HB1 | 1:E:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:I:334:GLU:OE2 | 1:I:334:GLU:HA | 1.98 | 0.63 |
| 1:J:7:ALA:HB1 | 1:J:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:K:334:GLU:HA | 1:K:334:GLU:OE2 | 1.98 | 0.63 |
| 1:L:35:VAL:CG1 | 1:L:68:LYS:HB2 | 2.22 | 0.63 |
| 1:L:334:GLU:HA | 1:L:334:GLU:OE2 | 1.98 | 0.63 |
| 1:O:147:ARG:HH21 | 1:O:147:ARG:CG | 2.12 | 0.63 |
| 1:R:39:ARG:NE | 1:R:66:THR:HB | 2.09 | 0.63 |
| 1:U:369:ILE:CG2 | 1:U:370:VAL:N | 2.60 | 0.63 |
| 1:V:298:VAL:HG12 | 1:V:335:ARG:HH11 | 1.64 | 0.63 |
| 1:G:298:VAL:HG12 | 1:G:335:ARG:HH11 | 1.64 | 0.63 |
| 1:I:37:ARG:CG | 1:I:38:PRO:HD2 | 2.20 | 0.63 |
| 1:I:39:ARG:NE | 1:I:66:THR:HB | 2.09 | 0.63 |
| 1:K:34:ILE:HB | 1:K:54:VAL:HG13 | 1.80 | 0.63 |
| 1:K:104:LEU:HB2 | 1:K:356:TRP:HH2 | 1.62 | 0.63 |
| 1:M:7:ALA:HB1 | 1:M:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:M:147:ARG:HH21 | 1:M:147:ARG:CG | 2.12 | 0.63 |
| 1:P:298:VAL:HG12 | 1:P:335:ARG:HH11 | 1.64 | 0.63 |
| 1:S:334:GLU:HA | 1:S:334:GLU:OE2 | 1.98 | 0.63 |
| 1:V:147:ARG:HH21 | 1:V:147:ARG:CG | 2.12 | 0.63 |
| 1:V:334:GLU:HA | 1:V:334:GLU:OE2 | 1.98 | 0.63 |
| 1:W:147:ARG:HH21 | 1:W:147:ARG:CG | 2.12 | 0.63 |
| 1:W:298:VAL:HG12 | 1:W:335:ARG:HH11 | 1.64 | 0.63 |
| 1:B:37:ARG:HB2 | 1:B:51:ASP:O | 1.99 | 0.63 |
| 1:C:37:ARG:CG | 1:C:38:PRO:HD2 | 2.20 | 0.63 |
| 1:D:7:ALA:HB1 | 1:D:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:M:37:ARG:HB2 | 1:M:51:ASP:O | 1.99 | 0.63 |
| 1:M:298:VAL:HG12 | 1:M:335:ARG:HH11 | 1.64 | 0.63 |
| 1:O:298:VAL:HG12 | 1:O:335:ARG:HH11 | 1.64 | 0.63 |
| 1:Q:147:ARG:HH21 | 1:Q:147:ARG:CG | 2.12 | 0.63 |
| 1:T:37:ARG:CG | 1:T:38:PRO:HD2 | 2.20 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:334:GLU:HA | 1:U:334:GLU:OE2 | 1.98 | 0.63 |
| 1:D:104:LEU:HB2 | 1:D:356:TRP:HH2 | 1.63 | 0.63 |
| 1:E:39:ARG:NE | 1:E:66:THR:HB | 2.09 | 0.63 |
| 1:E:147:ARG:HH21 | 1:E:147:ARG:CG | 2.12 | 0.63 |
| 1:F:7:ALA:HB1 | 1:F:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:G:334:GLU:HA | 1:G:334:GLU:OE2 | 1.98 | 0.63 |
| 1:H:298:VAL:HG12 | 1:H:335:ARG:HH11 | 1.64 | 0.63 |
| 1:T:147:ARG:HH21 | 1:T:147:ARG:CG | 2.12 | 0.63 |
| 1:V:37:ARG:HB2 | 1:V:51:ASP:O | 1.99 | 0.63 |
| 1:A:7:ALA:HB1 | 1:A:356:TRP:CZ2 | 2.33 | 0.63 |
| 1:B:169:TYR:CE2 | 1:D:40:HIS:CB | 2.82 | 0.63 |
| 1:C:147:ARG:HH21 | 1:C:147:ARG:CG | 2.12 | 0.63 |
| 1:F:147:ARG:HH21 | 1:F:147:ARG:CG | 2.12 | 0.63 |
| 1:H:334:GLU:HA | 1:H:334:GLU:OE2 | 1.98 | 0.63 |
| 1:J:298:VAL:HG12 | 1:J:335:ARG:HH11 | 1.64 | 0.63 |
| 1:N:334:GLU:HA | 1:N:334:GLU:OE2 | 1.98 | 0.63 |
| 1:O:169:TYR:CE2 | 1:Q:40:HIS:CB | 2.82 | 0.63 |
| 1:P:169:TYR:CE2 | 1:R:40:HIS:CB | 2.82 | 0.63 |
| 1:Q:37:ARG:O | 1:Q:66:THR:HG22 | 1.99 | 0.63 |
| 1:R:169:TYR:CE2 | 1:T:40:HIS:CB | 2.82 | 0.63 |
| 1:U:147:ARG:HH21 | 1:U:147:ARG:CG | 2.12 | 0.63 |
| 1:A:37:ARG:O | 1:A:66:THR:HG22 | 1.99 | 0.63 |
| 1:B:39:ARG:NE | 1:B:66:THR:HB | 2.09 | 0.63 |
| 1:D:169:TYR:CE2 | 1:F:40:HIS:CB | 2.82 | 0.63 |
| 1:G:37:ARG:HB2 | 1:G:51:ASP:O | 1.99 | 0.63 |
| 1:H:58:ALA:O | 1:H:61:LYS:N | 2.30 | 0.63 |
| 1:I:35:VAL:CG1 | 1:I:68:LYS:HB2 | 2.22 | 0.63 |
| 1:M:169:TYR:CE2 | 1:O:40:HIS:CB | 2.82 | 0.63 |
| 1:N:298:VAL:HG12 | 1:N:335:ARG:HH11 | 1.64 | 0.63 |
| 1:P:39:ARG:NE | 1:P:66:THR:HB | 2.09 | 0.63 |
| 1:S:37:ARG:HB2 | 1:S:51:ASP:O | 1.99 | 0.63 |
| 1:T:169:TYR:CE2 | 1:V:40:HIS:CB | 2.82 | 0.63 |
| 1:T:334:GLU:OE2 | 1:T:334:GLU:HA | 1.98 | 0.63 |
| 1:V:37:ARG:O | 1:V:66:THR:HG22 | 1.99 | 0.63 |
| 1:A:147:ARG:HH21 | 1:A:147:ARG:CG | 2.12 | 0.63 |
| 1:B:37:ARG:O | 1:B:66:THR:HG22 | 1.99 | 0.63 |
| 1:C:37:ARG:O | 1:C:66:THR:HG22 | 1.99 | 0.63 |
| 1:H:37:ARG:O | 1:H:66:THR:HG22 | 1.99 | 0.63 |
| 1:H:147:ARG:HH21 | 1:H:147:ARG:CG | 2.12 | 0.63 |
| 1:K:169:TYR:CE2 | 1:M:40:HIS:CB | 2.82 | 0.63 |
| 1:M:334:GLU:HA | 1:M:334:GLU:OE2 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:147:ARG:HH21 | 1:S:147:ARG:CG | 2.12 | 0.63 |
| 1:A:334:GLU:OE2 | 1:A:334:GLU:HA | 1.98 | 0.63 |
| 1:D:37:ARG:HB2 | 1:D:51:ASP:O | 1.99 | 0.63 |
| 1:D:147:ARG:HH21 | 1:D:147:ARG:CG | 2.12 | 0.63 |
| 1:F:37:ARG:O | 1:F:66:THR:HG22 | 1.99 | 0.63 |
| 1:G:169:TYR:CE2 | 1:I:40:HIS:CB | 2.82 | 0.63 |
| 1:I:169:TYR:CE2 | 1:K:40:HIS:CB | 2.82 | 0.63 |
| 1:J:37:ARG:O | 1:J:66:THR:HG22 | 1.99 | 0.63 |
| 1:J:147:ARG:HH21 | 1:J:147:ARG:CG | 2.12 | 0.63 |
| 1:K:147:ARG:HH21 | 1:K:147:ARG:CG | 2.12 | 0.63 |
| 1:O:334:GLU:HA | 1:O:334:GLU:OE2 | 1.98 | 0.63 |
| 1:Q:169:TYR:CE2 | 1:S:40:HIS:CB | 2.82 | 0.63 |
| 1:S:37:ARG:O | 1:S:66:THR:HG22 | 1.99 | 0.63 |
| 1:V:35:VAL:CG1 | 1:V:68:LYS:HB2 | 2.22 | 0.63 |
| 1:W:35:VAL:CG1 | 1:W:68:LYS:HB2 | 2.22 | 0.63 |
| 1:B:334:GLU:HA | 1:B:334:GLU:OE2 | 1.98 | 0.62 |
| 1:E:37:ARG:O | 1:E:66:THR:HG22 | 1.99 | 0.62 |
| 1:I:298:VAL:HG12 | 1:I:335:ARG:HH11 | 1.64 | 0.62 |
| 1:J:334:GLU:HA | 1:J:334:GLU:OE2 | 1.98 | 0.62 |
| 1:K:37:ARG:HB2 | 1:K:51:ASP:O | 1.99 | 0.62 |
| 1:L:147:ARG:HH21 | 1:L:147:ARG:CG | 2.11 | 0.62 |
| 1:N:169:TYR:CE2 | 1:P:40:HIS:CB | 2.82 | 0.62 |
| 1:O:37:ARG:O | 1:O:66:THR:HG22 | 1.99 | 0.62 |
| 1:Q:37:ARG:HB2 | 1:Q:51:ASP:O | 1.99 | 0.62 |
| 1:T:298:VAL:HG12 | 1:T:335:ARG:HH11 | 1.64 | 0.62 |
| 1:C:298:VAL:HG12 | 1:C:335:ARG:HH11 | 1.64 | 0.62 |
| 1:E:169:TYR:CE2 | 1:G:40:HIS:CB | 2.82 | 0.62 |
| 1:F:169:TYR:CE2 | 1:H:40:HIS:CB | 2.82 | 0.62 |
| 1:F:298:VAL:HG12 | 1:F:335:ARG:HH11 | 1.64 | 0.62 |
| 1:G:147:ARG:HH21 | 1:G:147:ARG:CG | 2.12 | 0.62 |
| 1:M:37:ARG:O | 1:M:66:THR:HG22 | 1.99 | 0.62 |
| 1:O:37:ARG:HB2 | 1:O:51:ASP:O | 1.99 | 0.62 |
| 1:U:298:VAL:HG12 | 1:U:335:ARG:HH11 | 1.64 | 0.62 |
| 1:A:104:LEU:HB2 | 1:A:356:TRP:HH2 | 1.62 | 0.62 |
| 1:E:298:VAL:HG12 | 1:E:335:ARG:HH11 | 1.64 | 0.62 |
| 1:I:362:TYR:HA | 1:I:366:GLY:O | 2.00 | 0.62 |
| 1:J:37:ARG:HB2 | 1:J:51:ASP:O | 1.99 | 0.62 |
| 1:K:37:ARG:O | 1:K:66:THR:HG22 | 1.99 | 0.62 |
| 1:K:362:TYR:HA | 1:K:366:GLY:O | 2.00 | 0.62 |
| 1:L:37:ARG:HB2 | 1:L:51:ASP:O | 1.99 | 0.62 |
| 1:S:169:TYR:CE2 | 1:U:40:HIS:CB | 2.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:298:VAL:HG12 | 1:S:335:ARG:HH11 | 1.64 | 0.62 |
| 1:T:37:ARG:O | 1:T:66:THR:HG22 | 1.99 | 0.62 |
| 1:U:169:TYR:CE2 | 1:W:40:HIS:CB | 2.82 | 0.62 |
| 1:B:298:VAL:HG12 | 1:B:335:ARG:HH11 | 1.64 | 0.62 |
| 1:D:362:TYR:HA | 1:D:366:GLY:O | 2.00 | 0.62 |
| 1:E:334:GLU:HA | 1:E:334:GLU:OE2 | 1.98 | 0.62 |
| 1:I:147:ARG:HH21 | 1:I:147:ARG:CG | 2.12 | 0.62 |
| 1:L:169:TYR:CE2 | 1:N:40:HIS:CB | 2.82 | 0.62 |
| 1:M:362:TYR:HA | 1:M:366:GLY:O | 2.00 | 0.62 |
| 1:N:37:ARG:HB2 | 1:N:51:ASP:O | 1.99 | 0.62 |
| 1:Q:298:VAL:HG12 | 1:Q:335:ARG:HH11 | 1.64 | 0.62 |
| 1:R:58:ALA:O | 1:R:61:LYS:N | 2.30 | 0.62 |
| 1:S:58:ALA:O | 1:S:61:LYS:N | 2.30 | 0.62 |
| 1:T:34:ILE:HB | 1:T:54:VAL:HG13 | 1.80 | 0.62 |
| 1:B:147:ARG:HH21 | 1:B:147:ARG:CG | 2.12 | 0.62 |
| 1:C:104:LEU:HB2 | 1:C:356:TRP:HH2 | 1.63 | 0.62 |
| 1:G:37:ARG:O | 1:G:66:THR:HG22 | 1.99 | 0.62 |
| 1:H:37:ARG:HB2 | 1:H:51:ASP:O | 1.99 | 0.62 |
| 1:H:169:TYR:CE2 | 1:J:40:HIS:CB | 2.82 | 0.62 |
| 1:I:37:ARG:HB2 | 1:I:51:ASP:O | 1.99 | 0.62 |
| 1:L:37:ARG:O | 1:L:66:THR:HG22 | 1.99 | 0.62 |
| 1:N:147:ARG:HH21 | 1:N:147:ARG:CG | 2.12 | 0.62 |
| 1:O:362:TYR:HA | 1:O:366:GLY:O | 2.00 | 0.62 |
| 1:R:298:VAL:HG12 | 1:R:335:ARG:HH11 | 1.64 | 0.62 |
| 1:R:334:GLU:HA | 1:R:334:GLU:OE2 | 1.98 | 0.62 |
| 1:W:334:GLU:HA | 1:W:334:GLU:OE2 | 1.98 | 0.62 |
| 1:A:37:ARG:HB2 | 1:A:51:ASP:O | 1.99 | 0.62 |
| 1:C:37:ARG:HB2 | 1:C:51:ASP:O | 1.99 | 0.62 |
| 1:C:334:GLU:HA | 1:C:334:GLU:OE2 | 1.98 | 0.62 |
| 1:D:334:GLU:HA | 1:D:334:GLU:OE2 | 1.98 | 0.62 |
| 1:G:35:VAL:CG1 | 1:G:68:LYS:HB2 | 2.22 | 0.62 |
| 1:G:39:ARG:NE | 1:G:66:THR:HB | 2.09 | 0.62 |
| 1:G:133:TYR:HB2 | 1:G:356:TRP:CE3 | 2.35 | 0.62 |
| 1:G:362:TYR:HA | 1:G:366:GLY:O | 2.00 | 0.62 |
| 1:H:362:TYR:HA | 1:H:366:GLY:O | 2.00 | 0.62 |
| 1:I:133:TYR:HB2 | 1:I:356:TRP:CE3 | 2.35 | 0.62 |
| 1:J:362:TYR:HA | 1:J:366:GLY:O | 2.00 | 0.62 |
| 1:K:133:TYR:HB2 | 1:K:356:TRP:CE3 | 2.35 | 0.62 |
| 1:M:34:ILE:HB | 1:M:54:VAL:HG13 | 1.79 | 0.62 |
| 1:N:35:VAL:CG1 | 1:N:68:LYS:HB2 | 2.22 | 0.62 |
| 1:Q:334:GLU:OE2 | 1:Q:334:GLU:HA | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:362:TYR:HA | 1:Q:366:GLY:O | 2.00 | 0.62 |
| 1:W:37:ARG:O | 1:W:66:THR:HG22 | 1.99 | 0.62 |
| 1:A:35:VAL:CG1 | 1:A:68:LYS:HB2 | 2.22 | 0.62 |
| 1:A:169:TYR:CE2 | 1:C:40:HIS:CB | 2.82 | 0.62 |
| 1:C:169:TYR:CE2 | 1:E:40:HIS:CB | 2.82 | 0.62 |
| 1:D:34:ILE:HB | 1:D:54:VAL:HG13 | 1.80 | 0.62 |
| 1:D:39:ARG:NE | 1:D:66:THR:HB | 2.09 | 0.62 |
| 1:H:133:TYR:HB2 | 1:H:356:TRP:CE3 | 2.35 | 0.62 |
| 1:I:37:ARG:O | 1:I:66:THR:HG22 | 1.99 | 0.62 |
| 1:J:133:TYR:HB2 | 1:J:356:TRP:CE3 | 2.35 | 0.62 |
| 1:K:298:VAL:HG12 | 1:K:335:ARG:HH11 | 1.64 | 0.62 |
| 1:M:133:TYR:HB2 | 1:M:356:TRP:CE3 | 2.35 | 0.62 |
| 1:P:34:ILE:HB | 1:P:54:VAL:HG13 | 1.79 | 0.62 |
| 1:R:37:ARG:O | 1:R:66:THR:HG22 | 1.99 | 0.62 |
| 1:R:133:TYR:HB2 | 1:R:356:TRP:CE3 | 2.35 | 0.62 |
| 1:W:37:ARG:HB2 | 1:W:51:ASP:O | 1.99 | 0.62 |
| 1:D:37:ARG:O | 1:D:66:THR:HG22 | 1.99 | 0.62 |
| 1:E:37:ARG:HB2 | 1:E:51:ASP:O | 1.99 | 0.62 |
| 1:F:133:TYR:HB2 | 1:F:356:TRP:CE3 | 2.35 | 0.62 |
| 1:F:362:TYR:HA | 1:F:366:GLY:O | 2.00 | 0.62 |
| 1:N:133:TYR:HB2 | 1:N:356:TRP:CE3 | 2.35 | 0.62 |
| 1:P:37:ARG:HB2 | 1:P:51:ASP:O | 1.99 | 0.62 |
| 1:P:133:TYR:HB2 | 1:P:356:TRP:CE3 | 2.35 | 0.62 |
| 1:P:334:GLU:HA | 1:P:334:GLU:OE2 | 1.98 | 0.62 |
| 1:R:37:ARG:HB2 | 1:R:51:ASP:O | 1.99 | 0.62 |
| 1:T:44:MET:HG3 | 1:T:45:VAL:N | 2.15 | 0.62 |
| 1:B:104:LEU:HB2 | 1:B:356:TRP:HH2 | 1.62 | 0.62 |
| 1:L:133:TYR:HB2 | 1:L:356:TRP:CE3 | 2.35 | 0.62 |
| 1:L:362:TYR:HA | 1:L:366:GLY:O | 2.00 | 0.62 |
| 1:P:44:MET:HG3 | 1:P:45:VAL:N | 2.15 | 0.62 |
| 1:S:362:TYR:HA | 1:S:366:GLY:O | 2.00 | 0.62 |
| 1:C:35:VAL:CG1 | 1:C:68:LYS:HB2 | 2.22 | 0.62 |
| 1:D:133:TYR:HB2 | 1:D:356:TRP:CE3 | 2.35 | 0.62 |
| 1:E:35:VAL:CG1 | 1:E:68:LYS:HB2 | 2.22 | 0.62 |
| 1:E:133:TYR:HB2 | 1:E:356:TRP:CE3 | 2.35 | 0.62 |
| 1:E:362:TYR:HA | 1:E:366:GLY:O | 2.00 | 0.62 |
| 1:I:157:ASP:HB2 | 2:I:401:ADP:H5'1 | 1.82 | 0.62 |
| 1:M:44:MET:HG3 | 1:M:45:VAL:N | 2.15 | 0.62 |
| 1:O:133:TYR:HB2 | 1:O:356:TRP:CE3 | 2.35 | 0.62 |
| 1:O:133:TYR:OH | 1:O:375:PHE:HB2 | 2.00 | 0.62 |
| 1:T:133:TYR:HB2 | 1:T:356:TRP:CE3 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:133:TYR:HB2 | 1:W:356:TRP:CE3 | 2.35 | 0.62 |
| 1:C:44:MET:HG3 | 1:C:45:VAL:N | 2.15 | 0.61 |
| 1:F:37:ARG:HB2 | 1:F:51:ASP:O | 1.99 | 0.61 |
| 1:G:44:MET:HG3 | 1:G:45:VAL:N | 2.15 | 0.61 |
| 1:N:362:TYR:HA | 1:N:366:GLY:O | 2.00 | 0.61 |
| 1:P:147:ARG:HH21 | 1:P:147:ARG:CG | 2.12 | 0.61 |
| 1:T:35:VAL:CG1 | 1:T:68:LYS:HB2 | 2.22 | 0.61 |
| 1:B:35:VAL:CG1 | 1:B:68:LYS:HB2 | 2.22 | 0.61 |
| 1:B:133:TYR:HB2 | 1:B:356:TRP:CE3 | 2.35 | 0.61 |
| 1:C:133:TYR:HB2 | 1:C:356:TRP:CE3 | 2.35 | 0.61 |
| 1:D:133:TYR:OH | 1:D:375:PHE:HB2 | 2.00 | 0.61 |
| 1:I:44:MET:HG3 | 1:I:45:VAL:N | 2.15 | 0.61 |
| 1:J:169:TYR:CE2 | 1:L:40:HIS:CB | 2.82 | 0.61 |
| 1:L:298:VAL:HG12 | 1:L:335:ARG:HH11 | 1.64 | 0.61 |
| 1:N:37:ARG:O | 1:N:66:THR:HG22 | 1.99 | 0.61 |
| 1:O:157:ASP:HB2 | 2:O:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:Q:133:TYR:HB2 | 1:Q:356:TRP:CE3 | 2.35 | 0.61 |
| 1:S:44:MET:HG3 | 1:S:45:VAL:N | 2.15 | 0.61 |
| 1:S:133:TYR:HB2 | 1:S:356:TRP:CE3 | 2.35 | 0.61 |
| 1:T:37:ARG:HB2 | 1:T:51:ASP:O | 1.99 | 0.61 |
| 1:U:362:TYR:HA | 1:U:366:GLY:O | 2.00 | 0.61 |
| 1:V:157:ASP:HB2 | 2:V:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:A:44:MET:HG3 | 1:A:45:VAL:N | 2.15 | 0.61 |
| 1:B:157:ASP:HB2 | 2:B:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:I:104:LEU:HB2 | 1:I:356:TRP:HH2 | 1.63 | 0.61 |
| 1:I:133:TYR:OH | 1:I:375:PHE:HB2 | 2.00 | 0.61 |
| 1:J:44:MET:HG3 | 1:J:45:VAL:N | 2.15 | 0.61 |
| 1:K:157:ASP:HB2 | 2:K:401:ADP:H5'1 | 1.82 | 0.61 |
| 1:M:157:ASP:HB2 | 2:M:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:O:44:MET:HG3 | 1:O:45:VAL:N | 2.15 | 0.61 |
| 1:T:157:ASP:HB2 | 2:T:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:U:37:ARG:HB2 | 1:U:51:ASP:O | 1.99 | 0.61 |
| 1:U:37:ARG:O | 1:U:66:THR:HG22 | 1.99 | 0.61 |
| 1:V:34:ILE:HB | 1:V:54:VAL:HG13 | 1.80 | 0.61 |
| 1:V:362:TYR:HA | 1:V:366:GLY:O | 2.00 | 0.61 |
| 1:B:362:TYR:HA | 1:B:366:GLY:O | 2.00 | 0.61 |
| 1:D:35:VAL:CG1 | 1:D:68:LYS:HB2 | 2.22 | 0.61 |
| 1:D:157:ASP:HB2 | 2:D:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:D:298:VAL:HG12 | 1:D:335:ARG:HH11 | 1.64 | 0.61 |
| 1:E:44:MET:HG3 | 1:E:45:VAL:N | 2.15 | 0.61 |
| 1:F:44:MET:HG3 | 1:F:45:VAL:N | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:34:ILE:HB | 1:J:54:VAL:HG13 | 1.80 | 0.61 |
| 1:K:44:MET:HG3 | 1:K:45:VAL:N | 2.15 | 0.61 |
| 1:K:65:LEU:C | 1:K:65:LEU:HD12 | 2.21 | 0.61 |
| 1:L:104:LEU:HB2 | 1:L:356:TRP:HH2 | 1.62 | 0.61 |
| 1:O:65:LEU:C | 1:O:65:LEU:HD12 | 2.21 | 0.61 |
| 1:P:37:ARG:O | 1:P:66:THR:HG22 | 1.99 | 0.61 |
| 1:R:104:LEU:HB2 | 1:R:356:TRP:HH2 | 1.62 | 0.61 |
| 1:V:133:TYR:HB2 | 1:V:356:TRP:CE3 | 2.35 | 0.61 |
| 1:A:58:ALA:O | 1:A:61:LYS:N | 2.30 | 0.61 |
| 1:E:34:ILE:HB | 1:E:54:VAL:HG13 | 1.79 | 0.61 |
| 1:E:104:LEU:HB2 | 1:E:356:TRP:HH2 | 1.63 | 0.61 |
| 1:F:39:ARG:NE | 1:F:66:THR:HB | 2.09 | 0.61 |
| 1:H:324:THR:HG21 | 1:J:241:GLU:CD | 2.21 | 0.61 |
| 1:I:65:LEU:C | 1:I:65:LEU:HD12 | 2.21 | 0.61 |
| 1:J:58:ALA:O | 1:J:61:LYS:N | 2.30 | 0.61 |
| 1:P:362:TYR:HA | 1:P:366:GLY:O | 2.00 | 0.61 |
| 1:Q:157:ASP:HB2 | 2:Q:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:T:65:LEU:C | 1:T:65:LEU:HD12 | 2.21 | 0.61 |
| 1:U:133:TYR:HB2 | 1:U:356:TRP:CE3 | 2.35 | 0.61 |
| 1:V:65:LEU:C | 1:V:65:LEU:HD12 | 2.21 | 0.61 |
| 1:W:44:MET:HG3 | 1:W:45:VAL:N | 2.15 | 0.61 |
| 1:C:362:TYR:HA | 1:C:366:GLY:O | 2.00 | 0.61 |
| 1:D:44:MET:HG3 | 1:D:45:VAL:N | 2.15 | 0.61 |
| 1:G:157:ASP:HB2 | 2:G:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:H:34:ILE:HB | 1:H:54:VAL:HG13 | 1.80 | 0.61 |
| 1:L:58:ALA:O | 1:L:61:LYS:N | 2.30 | 0.61 |
| 1:N:44:MET:HG3 | 1:N:45:VAL:N | 2.15 | 0.61 |
| 1:P:65:LEU:HD12 | 1:P:65:LEU:C | 2.21 | 0.61 |
| 1:V:44:MET:HG3 | 1:V:45:VAL:N | 2.15 | 0.61 |
| 1:A:133:TYR:HB2 | 1:A:356:TRP:CE3 | 2.35 | 0.61 |
| 1:B:44:MET:HG3 | 1:B:45:VAL:N | 2.15 | 0.61 |
| 1:J:104:LEU:HB2 | 1:J:356:TRP:HH2 | 1.63 | 0.61 |
| 1:K:36:GLY:N | 1:K:54:VAL:HG23 | 2.16 | 0.61 |
| 1:L:44:MET:HG3 | 1:L:45:VAL:N | 2.15 | 0.61 |
| 1:M:65:LEU:HD12 | 1:M:65:LEU:C | 2.21 | 0.61 |
| 1:O:36:GLY:N | 1:O:54:VAL:HG23 | 2.16 | 0.61 |
| 1:R:65:LEU:C | 1:R:65:LEU:HD12 | 2.21 | 0.61 |
| 1:R:362:TYR:HA | 1:R:366:GLY:O | 2.00 | 0.61 |
| 1:T:104:LEU:HB2 | 1:T:356:TRP:HH2 | 1.62 | 0.61 |
| 1:T:133:TYR:OH | 1:T:375:PHE:HB2 | 2.00 | 0.61 |
| 1:U:36:GLY:N | 1:U:54:VAL:HG23 | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:36:GLY:N | 1:W:54:VAL:HG23 | 2.16 | 0.61 |
| 1:A:36:GLY:N | 1:A:54:VAL:HG23 | 2.16 | 0.61 |
| 1:A:65:LEU:C | 1:A:65:LEU:HD12 | 2.21 | 0.61 |
| 1:C:65:LEU:C | 1:C:65:LEU:HD12 | 2.21 | 0.61 |
| 1:G:65:LEU:C | 1:G:65:LEU:HD12 | 2.21 | 0.61 |
| 1:M:133:TYR:OH | 1:M:375:PHE:HB2 | 2.00 | 0.61 |
| 1:P:35:VAL:CG1 | 1:P:68:LYS:HB2 | 2.22 | 0.61 |
| 1:Q:133:TYR:OH | 1:Q:375:PHE:HB2 | 2.00 | 0.61 |
| 1:Q:324:THR:HG21 | 1:S:241:GLU:CD | 2.21 | 0.61 |
| 1:A:325:MET:CE | 1:C:244:ASP:O | 2.49 | 0.61 |
| 1:B:65:LEU:C | 1:B:65:LEU:HD12 | 2.21 | 0.61 |
| 1:B:324:THR:HG21 | 1:D:241:GLU:CD | 2.21 | 0.61 |
| 1:C:36:GLY:N | 1:C:54:VAL:HG23 | 2.16 | 0.61 |
| 1:F:35:VAL:CG1 | 1:F:68:LYS:HB2 | 2.22 | 0.61 |
| 1:F:133:TYR:OH | 1:F:375:PHE:HB2 | 2.00 | 0.61 |
| 1:J:61:LYS:HG2 | 1:J:64:ILE:HG21 | 1.83 | 0.61 |
| 1:J:324:THR:HG21 | 1:L:241:GLU:CD | 2.21 | 0.61 |
| 1:R:35:VAL:CG1 | 1:R:68:LYS:HB2 | 2.22 | 0.61 |
| 1:R:44:MET:HG3 | 1:R:45:VAL:N | 2.15 | 0.61 |
| 1:R:147:ARG:HH21 | 1:R:147:ARG:CG | 2.12 | 0.61 |
| 1:S:36:GLY:N | 1:S:54:VAL:HG23 | 2.16 | 0.61 |
| 1:S:324:THR:HG21 | 1:U:241:GLU:CD | 2.21 | 0.61 |
| 1:U:133:TYR:OH | 1:U:375:PHE:HB2 | 2.00 | 0.61 |
| 1:C:157:ASP:HB2 | 2:C:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:C:325:MET:CE | 1:E:244:ASP:O | 2.49 | 0.61 |
| 1:E:157:ASP:HB2 | 2:E:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:K:133:TYR:OH | 1:K:375:PHE:HB2 | 2.00 | 0.61 |
| 1:M:325:MET:CE | 1:O:244:ASP:O | 2.49 | 0.61 |
| 1:P:157:ASP:HB2 | 2:P:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:R:61:LYS:HG2 | 1:R:64:ILE:HG21 | 1.83 | 0.61 |
| 1:T:362:TYR:HA | 1:T:366:GLY:O | 2.00 | 0.61 |
| 1:U:157:ASP:HB2 | 2:U:401:ADP:H5'1 | 1.83 | 0.61 |
| 1:W:61:LYS:HG2 | 1:W:64:ILE:HG21 | 1.83 | 0.61 |
| 1:W:362:TYR:HA | 1:W:366:GLY:O | 2.00 | 0.61 |
| 1:B:325:MET:CE | 1:D:244:ASP:O | 2.49 | 0.60 |
| 1:C:61:LYS:HG2 | 1:C:64:ILE:HG21 | 1.83 | 0.60 |
| 1:E:36:GLY:N | 1:E:54:VAL:HG23 | 2.16 | 0.60 |
| 1:E:61:LYS:HG2 | 1:E:64:ILE:HG21 | 1.83 | 0.60 |
| 1:F:143:TYR:CD1 | 1:F:143:TYR:C | 2.75 | 0.60 |
| 1:F:324:THR:HG21 | 1:H:241:GLU:CD | 2.21 | 0.60 |
| 1:L:61:LYS:HG2 | 1:L:64:ILE:HG21 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:324:THR:HG21 | 1:P:241:GLU:CD | 2.21 | 0.60 |
| 1:P:61:LYS:HG2 | 1:P:64:ILE:HG21 | 1.83 | 0.60 |
| 1:Q:65:LEU:C | 1:Q:65:LEU:HD12 | 2.21 | 0.60 |
| 1:R:132:MET:O | 1:R:357:ILE:HB | 2.01 | 0.60 |
| 1:R:157:ASP:HB2 | 2:R:401:ADP:H5'1 | 1.83 | 0.60 |
| 1:R:325:MET:CE | 1:T:244:ASP:O | 2.49 | 0.60 |
| 1:S:157:ASP:HB2 | 2:S:401:ADP:H5'1 | 1.83 | 0.60 |
| 1:S:325:MET:CE | 1:U:244:ASP:O | 2.49 | 0.60 |
| 1:T:132:MET:O | 1:T:357:ILE:HB | 2.01 | 0.60 |
| 1:U:61:LYS:HG2 | 1:U:64:ILE:HG21 | 1.83 | 0.60 |
| 1:U:325:MET:CE | 1:W:244:ASP:O | 2.49 | 0.60 |
| 1:B:133:TYR:OH | 1:B:375:PHE:HB2 | 2.00 | 0.60 |
| 1:D:61:LYS:HG2 | 1:D:64:ILE:HG21 | 1.83 | 0.60 |
| 1:F:157:ASP:HB2 | 2:F:401:ADP:H5'1 | 1.83 | 0.60 |
| 1:H:65:LEU:C | 1:H:65:LEU:HD12 | 2.21 | 0.60 |
| 1:H:157:ASP:HB2 | 2:H:401:ADP:H5'1 | 1.83 | 0.60 |
| 1:J:132:MET:O | 1:J:357:ILE:HB | 2.01 | 0.60 |
| 1:P:104:LEU:HB2 | 1:P:356:TRP:HH2 | 1.63 | 0.60 |
| 1:P:325:MET:CE | 1:R:244:ASP:O | 2.49 | 0.60 |
| 1:Q:36:GLY:N | 1:Q:54:VAL:HG23 | 2.16 | 0.60 |
| 1:Q:61:LYS:HG2 | 1:Q:64:ILE:HG21 | 1.83 | 0.60 |
| 1:Q:132:MET:O | 1:Q:357:ILE:HB | 2.01 | 0.60 |
| 1:U:324:THR:HG21 | 1:W:241:GLU:CD | 2.21 | 0.60 |
| 1:V:36:GLY:N | 1:V:54:VAL:HG23 | 2.16 | 0.60 |
| 1:W:65:LEU:C | 1:W:65:LEU:HD12 | 2.21 | 0.60 |
| 1:A:324:THR:HG21 | 1:C:241:GLU:CD | 2.21 | 0.60 |
| 1:A:362:TYR:HA | 1:A:366:GLY:O | 2.00 | 0.60 |
| 1:D:324:THR:HG21 | 1:F:241:GLU:CD | 2.21 | 0.60 |
| 1:E:288:ASP:HA | 1:G:243:PRO:HB2 | 1.83 | 0.60 |
| 1:E:325:MET:CE | 1:G:244:ASP:O | 2.49 | 0.60 |
| 1:F:65:LEU:C | 1:F:65:LEU:HD12 | 2.21 | 0.60 |
| 1:G:133:TYR:OH | 1:G:375:PHE:HB2 | 2.00 | 0.60 |
| 1:H:61:LYS:HG2 | 1:H:64:ILE:HG21 | 1.83 | 0.60 |
| 1:I:288:ASP:HA | 1:K:243:PRO:HB2 | 1.83 | 0.60 |
| 1:I:325:MET:CE | 1:K:244:ASP:O | 2.49 | 0.60 |
| 1:M:34:ILE:CD1 | 1:M:67:LEU:HD22 | 2.31 | 0.60 |
| 1:N:325:MET:CE | 1:P:244:ASP:O | 2.49 | 0.60 |
| 1:O:132:MET:O | 1:O:357:ILE:HB | 2.01 | 0.60 |
| 1:P:132:MET:O | 1:P:357:ILE:HB | 2.02 | 0.60 |
| 1:Q:143:TYR:CD1 | 1:Q:143:TYR:C | 2.75 | 0.60 |
| 1:U:132:MET:O | 1:U:357:ILE:HB | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:16:LEU:HD23 | 1:V:32:PRO:HA | 1.83 | 0.60 |
| 1:V:132:MET:O | 1:V:357:ILE:HB | 2.01 | 0.60 |
| 1:A:61:LYS:HG2 | 1:A:64:ILE:HG21 | 1.83 | 0.60 |
| 1:A:157:ASP:HB2 | 2:A:401:ADP:H5'1 | 1.83 | 0.60 |
| 1:D:36:GLY:N | 1:D:54:VAL:HG23 | 2.16 | 0.60 |
| 1:F:34:ILE:HB | 1:F:54:VAL:HG13 | 1.79 | 0.60 |
| 1:F:61:LYS:HG2 | 1:F:64:ILE:HG21 | 1.83 | 0.60 |
| 1:G:36:GLY:N | 1:G:54:VAL:HG23 | 2.16 | 0.60 |
| 1:H:346:LEU:O | 1:H:349:LEU:HB2 | 2.02 | 0.60 |
| 1:I:346:LEU:O | 1:I:349:LEU:HB2 | 2.02 | 0.60 |
| 1:N:133:TYR:OH | 1:N:375:PHE:HB2 | 2.00 | 0.60 |
| 1:O:324:THR:HG21 | 1:Q:241:GLU:CD | 2.21 | 0.60 |
| 1:O:346:LEU:O | 1:O:349:LEU:HB2 | 2.02 | 0.60 |
| 1:Q:325:MET:CE | 1:S:244:ASP:O | 2.49 | 0.60 |
| 1:R:36:GLY:N | 1:R:54:VAL:HG23 | 2.16 | 0.60 |
| 1:R:288:ASP:HA | 1:T:243:PRO:HB2 | 1.83 | 0.60 |
| 1:R:346:LEU:O | 1:R:349:LEU:HB2 | 2.02 | 0.60 |
| 1:S:61:LYS:HG2 | 1:S:64:ILE:HG21 | 1.83 | 0.60 |
| 1:S:132:MET:O | 1:S:357:ILE:HB | 2.01 | 0.60 |
| 1:T:324:THR:HG21 | 1:V:241:GLU:CD | 2.21 | 0.60 |
| 1:T:325:MET:CE | 1:V:244:ASP:O | 2.49 | 0.60 |
| 1:U:34:ILE:HB | 1:U:54:VAL:HG13 | 1.79 | 0.60 |
| 1:U:143:TYR:CD1 | 1:U:143:TYR:C | 2.75 | 0.60 |
| 1:V:34:ILE:CD1 | 1:V:67:LEU:HD22 | 2.31 | 0.60 |
| 1:V:133:TYR:OH | 1:V:375:PHE:HB2 | 2.00 | 0.60 |
| 1:W:157:ASP:HB2 | 2:W:401:ADP:H5'1 | 1.83 | 0.60 |
| 1:C:133:TYR:OH | 1:C:375:PHE:HB2 | 2.00 | 0.60 |
| 1:I:36:GLY:N | 1:I:54:VAL:HG23 | 2.16 | 0.60 |
| 1:J:65:LEU:C | 1:J:65:LEU:HD12 | 2.21 | 0.60 |
| 1:J:133:TYR:OH | 1:J:375:PHE:HB2 | 2.00 | 0.60 |
| 1:J:157:ASP:HB2 | 2:J:401:ADP:H5'1 | 1.82 | 0.60 |
| 1:K:288:ASP:HA | 1:M:243:PRO:HB2 | 1.83 | 0.60 |
| 1:M:132:MET:O | 1:M:357:ILE:HB | 2.01 | 0.60 |
| 1:N:61:LYS:HG2 | 1:N:64:ILE:HG21 | 1.83 | 0.60 |
| 1:N:157:ASP:HB2 | 2:N:401:ADP:H5'1 | 1.83 | 0.60 |
| 1:P:36:GLY:N | 1:P:54:VAL:HG23 | 2.16 | 0.60 |
| 1:P:288:ASP:HA | 1:R:243:PRO:HB2 | 1.83 | 0.60 |
| 1:P:324:THR:HG21 | 1:R:241:GLU:CD | 2.21 | 0.60 |
| 1:S:133:TYR:OH | 1:S:375:PHE:HB2 | 2.00 | 0.60 |
| 1:T:36:GLY:N | 1:T:54:VAL:HG23 | 2.16 | 0.60 |
| 1:U:65:LEU:C | 1:U:65:LEU:HD12 | 2.21 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:346:LEU:O | 1:W:349:LEU:HB2 | 2.02 | 0.60 |
| 1:A:132:MET:O | 1:A:357:ILE:HB | 2.01 | 0.60 |
| 1:B:36:GLY:N | 1:B:54:VAL:HG23 | 2.16 | 0.60 |
| 1:B:346:LEU:O | 1:B:349:LEU:HB2 | 2.02 | 0.60 |
| 1:C:346:LEU:O | 1:C:349:LEU:HB2 | 2.02 | 0.60 |
| 1:G:61:LYS:HG2 | 1:G:64:ILE:HG21 | 1.83 | 0.60 |
| 1:G:325:MET:CE | 1:I:244:ASP:O | 2.49 | 0.60 |
| 1:I:34:ILE:CD1 | 1:I:67:LEU:HD22 | 2.31 | 0.60 |
| 1:K:16:LEU:HD23 | 1:K:32:PRO:HA | 1.83 | 0.60 |
| 1:L:132:MET:O | 1:L:357:ILE:HB | 2.01 | 0.60 |
| 1:L:325:MET:CE | 1:N:244:ASP:O | 2.49 | 0.60 |
| 1:N:132:MET:O | 1:N:357:ILE:HB | 2.01 | 0.60 |
| 1:U:34:ILE:CD1 | 1:U:67:LEU:HD22 | 2.31 | 0.60 |
| 1:B:61:LYS:HG2 | 1:B:64:ILE:HG21 | 1.83 | 0.60 |
| 1:C:288:ASP:HA | 1:E:243:PRO:HB2 | 1.83 | 0.60 |
| 1:F:36:GLY:N | 1:F:54:VAL:HG23 | 2.16 | 0.60 |
| 1:F:346:LEU:O | 1:F:349:LEU:HB2 | 2.02 | 0.60 |
| 1:G:16:LEU:HD23 | 1:G:32:PRO:HA | 1.83 | 0.60 |
| 1:G:288:ASP:HA | 1:I:243:PRO:HB2 | 1.84 | 0.60 |
| 1:H:104:LEU:HB2 | 1:H:356:TRP:HH2 | 1.63 | 0.60 |
| 1:I:61:LYS:HG2 | 1:I:64:ILE:HG21 | 1.83 | 0.60 |
| 1:K:132:MET:O | 1:K:357:ILE:HB | 2.01 | 0.60 |
| 1:K:325:MET:CE | 1:M:244:ASP:O | 2.49 | 0.60 |
| 1:N:36:GLY:N | 1:N:54:VAL:HG23 | 2.16 | 0.60 |
| 1:N:65:LEU:C | 1:N:65:LEU:HD12 | 2.21 | 0.60 |
| 1:O:61:LYS:HG2 | 1:O:64:ILE:HG21 | 1.83 | 0.60 |
| 1:P:346:LEU:O | 1:P:349:LEU:HB2 | 2.02 | 0.60 |
| 1:Q:346:LEU:O | 1:Q:349:LEU:HB2 | 2.02 | 0.60 |
| 1:R:34:ILE:CD1 | 1:R:67:LEU:HD22 | 2.31 | 0.60 |
| 1:R:324:THR:HG21 | 1:T:241:GLU:CD | 2.21 | 0.60 |
| 1:S:34:ILE:HB | 1:S:54:VAL:HG13 | 1.79 | 0.60 |
| 1:S:65:LEU:C | 1:S:65:LEU:HD12 | 2.21 | 0.60 |
| 1:U:44:MET:HG3 | 1:U:45:VAL:N | 2.15 | 0.60 |
| 1:A:346:LEU:O | 1:A:349:LEU:HB2 | 2.02 | 0.60 |
| 1:C:324:THR:CG2 | 1:E:241:GLU:OE2 | 2.50 | 0.60 |
| 1:D:65:LEU:C | 1:D:65:LEU:HD12 | 2.21 | 0.60 |
| 1:D:132:MET:O | 1:D:357:ILE:HB | 2.01 | 0.60 |
| 1:E:16:LEU:HD23 | 1:E:32:PRO:HA | 1.83 | 0.60 |
| 1:E:133:TYR:OH | 1:E:375:PHE:HB2 | 2.00 | 0.60 |
| 1:F:325:MET:CE | 1:H:244:ASP:O | 2.49 | 0.60 |
| 1:J:325:MET:CE | 1:L:244:ASP:O | 2.49 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:346:LEU:O | 1:K:349:LEU:HB2 | 2.02 | 0.60 |
| 1:L:65:LEU:C | 1:L:65:LEU:HD12 | 2.21 | 0.60 |
| 1:L:133:TYR:OH | 1:L:375:PHE:HB2 | 2.00 | 0.60 |
| 1:L:324:THR:HG21 | 1:N:241:GLU:CD | 2.21 | 0.60 |
| 1:M:16:LEU:HD23 | 1:M:32:PRO:HA | 1.83 | 0.60 |
| 1:O:34:ILE:HB | 1:O:54:VAL:HG13 | 1.80 | 0.60 |
| 1:P:133:TYR:OH | 1:P:375:PHE:HB2 | 2.00 | 0.60 |
| 1:T:61:LYS:HG2 | 1:T:64:ILE:HG21 | 1.83 | 0.60 |
| 1:U:346:LEU:O | 1:U:349:LEU:HB2 | 2.02 | 0.60 |
| 1:V:61:LYS:HG2 | 1:V:64:ILE:HG21 | 1.83 | 0.60 |
| 1:W:132:MET:O | 1:W:357:ILE:HB | 2.01 | 0.60 |
| 1:A:34:ILE:HB | 1:A:54:VAL:HG13 | 1.80 | 0.60 |
| 1:C:132:MET:O | 1:C:357:ILE:HB | 2.01 | 0.60 |
| 1:E:34:ILE:CD1 | 1:E:67:LEU:HD22 | 2.31 | 0.60 |
| 1:E:65:LEU:HD12 | 1:E:65:LEU:C | 2.21 | 0.60 |
| 1:G:34:ILE:CD1 | 1:G:67:LEU:HD22 | 2.32 | 0.60 |
| 1:H:133:TYR:OH | 1:H:375:PHE:HB2 | 2.00 | 0.60 |
| 1:I:132:MET:O | 1:I:357:ILE:HB | 2.01 | 0.60 |
| 1:I:324:THR:HG21 | 1:K:241:GLU:CD | 2.21 | 0.60 |
| 1:I:324:THR:CG2 | 1:K:241:GLU:OE2 | 2.50 | 0.60 |
| 1:J:143:TYR:CD1 | 1:J:143:TYR:C | 2.75 | 0.60 |
| 1:K:34:ILE:CD1 | 1:K:67:LEU:HD22 | 2.31 | 0.60 |
| 1:K:61:LYS:HG2 | 1:K:64:ILE:HG21 | 1.83 | 0.60 |
| 1:L:34:ILE:CD1 | 1:L:67:LEU:HD22 | 2.31 | 0.60 |
| 1:M:346:LEU:O | 1:M:349:LEU:HB2 | 2.02 | 0.60 |
| 1:N:34:ILE:CD1 | 1:N:67:LEU:HD22 | 2.31 | 0.60 |
| 1:R:133:TYR:OH | 1:R:375:PHE:HB2 | 2.00 | 0.60 |
| 1:R:324:THR:CG2 | 1:T:241:GLU:OE2 | 2.50 | 0.60 |
| 1:S:34:ILE:CD1 | 1:S:67:LEU:HD22 | 2.31 | 0.60 |
| 1:T:288:ASP:HA | 1:V:243:PRO:HB2 | 1.84 | 0.60 |
| 1:T:324:THR:CG2 | 1:V:241:GLU:OE2 | 2.50 | 0.60 |
| 1:T:346:LEU:O | 1:T:349:LEU:HB2 | 2.02 | 0.60 |
| 1:A:287:ILE:CD1 | 1:C:208:ILE:CD1 | 2.80 | 0.60 |
| 1:E:132:MET:O | 1:E:357:ILE:HB | 2.01 | 0.60 |
| 1:G:132:MET:O | 1:G:357:ILE:HB | 2.01 | 0.60 |
| 1:G:324:THR:HG21 | 1:I:241:GLU:CD | 2.21 | 0.60 |
| 1:H:36:GLY:N | 1:H:54:VAL:HG23 | 2.16 | 0.60 |
| 1:J:36:GLY:N | 1:J:54:VAL:HG23 | 2.16 | 0.60 |
| 1:J:346:LEU:O | 1:J:349:LEU:HB2 | 2.02 | 0.60 |
| 1:N:346:LEU:O | 1:N:349:LEU:HB2 | 2.02 | 0.60 |
| 1:O:325:MET:CE | 1:Q:244:ASP:O | 2.49 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:104:LEU:HB2 | 1:V:356:TRP:HH2 | 1.63 | 0.60 |
| 1:W:104:LEU:HB2 | 1:W:356:TRP:HH2 | 1.62 | 0.60 |
| 1:W:133:TYR:OH | 1:W:375:PHE:HB2 | 2.00 | 0.60 |
| 1:C:34:ILE:CD1 | 1:C:67:LEU:HD22 | 2.31 | 0.59 |
| 1:D:325:MET:CE | 1:F:244:ASP:O | 2.49 | 0.59 |
| 1:E:324:THR:CG2 | 1:G:241:GLU:OE2 | 2.50 | 0.59 |
| 1:E:346:LEU:O | 1:E:349:LEU:HB2 | 2.02 | 0.59 |
| 1:F:34:ILE:CD1 | 1:F:67:LEU:HD22 | 2.31 | 0.59 |
| 1:F:132:MET:O | 1:F:357:ILE:HB | 2.01 | 0.59 |
| 1:J:34:ILE:CD1 | 1:J:67:LEU:HD22 | 2.31 | 0.59 |
| 1:K:8:LEU:HB3 | 1:K:103:THR:HG23 | 1.84 | 0.59 |
| 1:L:36:GLY:N | 1:L:54:VAL:HG23 | 2.16 | 0.59 |
| 1:M:8:LEU:HB3 | 1:M:103:THR:HG23 | 1.84 | 0.59 |
| 1:O:8:LEU:HB3 | 1:O:103:THR:HG23 | 1.84 | 0.59 |
| 1:R:16:LEU:HD23 | 1:R:32:PRO:HA | 1.83 | 0.59 |
| 1:S:104:LEU:HB2 | 1:S:356:TRP:HH2 | 1.63 | 0.59 |
| 1:W:34:ILE:CD1 | 1:W:67:LEU:HD22 | 2.31 | 0.59 |
| 1:B:34:ILE:CD1 | 1:B:67:LEU:HD22 | 2.31 | 0.59 |
| 1:D:34:ILE:CD1 | 1:D:67:LEU:HD22 | 2.31 | 0.59 |
| 1:D:346:LEU:O | 1:D:349:LEU:HB2 | 2.02 | 0.59 |
| 1:G:324:THR:CG2 | 1:I:241:GLU:OE2 | 2.50 | 0.59 |
| 1:H:16:LEU:HD23 | 1:H:32:PRO:HA | 1.83 | 0.59 |
| 1:H:43:VAL:O | 1:H:44:MET:CG | 2.51 | 0.59 |
| 1:H:325:MET:CE | 1:J:244:ASP:O | 2.49 | 0.59 |
| 1:J:287:ILE:CD1 | 1:L:208:ILE:CD1 | 2.80 | 0.59 |
| 1:K:324:THR:HG21 | 1:M:241:GLU:CD | 2.21 | 0.59 |
| 1:L:43:VAL:O | 1:L:44:MET:CG | 2.51 | 0.59 |
| 1:L:157:ASP:HB2 | 2:L:401:ADP:H5'1 | 1.83 | 0.59 |
| 1:M:288:ASP:HA | 1:O:243:PRO:HB2 | 1.83 | 0.59 |
| 1:T:43:VAL:O | 1:T:44:MET:CG | 2.51 | 0.59 |
| 1:U:16:LEU:HD23 | 1:U:32:PRO:HA | 1.83 | 0.59 |
| 1:V:43:VAL:O | 1:V:44:MET:CG | 2.51 | 0.59 |
| 1:A:34:ILE:CD1 | 1:A:67:LEU:HD22 | 2.31 | 0.59 |
| 1:A:43:VAL:O | 1:A:44:MET:CG | 2.51 | 0.59 |
| 1:B:16:LEU:HD23 | 1:B:32:PRO:HA | 1.83 | 0.59 |
| 1:E:324:THR:HG21 | 1:G:241:GLU:CD | 2.21 | 0.59 |
| 1:F:16:LEU:HD23 | 1:F:32:PRO:HA | 1.83 | 0.59 |
| 1:F:43:VAL:O | 1:F:44:MET:CG | 2.51 | 0.59 |
| 1:G:104:LEU:HB2 | 1:G:356:TRP:HH2 | 1.63 | 0.59 |
| 1:H:132:MET:O | 1:H:357:ILE:HB | 2.01 | 0.59 |
| 1:I:34:ILE:HB | 1:I:54:VAL:HG13 | 1.79 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:43:VAL:O | 1:J:44:MET:CG | 2.51 | 0.59 |
| 1:L:16:LEU:HD23 | 1:L:32:PRO:HA | 1.83 | 0.59 |
| 1:L:34:ILE:HB | 1:L:54:VAL:HG13 | 1.80 | 0.59 |
| 1:M:36:GLY:N | 1:M:54:VAL:HG23 | 2.16 | 0.59 |
| 1:M:61:LYS:HG2 | 1:M:64:ILE:HG21 | 1.83 | 0.59 |
| 1:P:43:VAL:O | 1:P:44:MET:CG | 2.51 | 0.59 |
| 1:S:324:THR:CG2 | 1:U:241:GLU:OE2 | 2.50 | 0.59 |
| 1:W:16:LEU:HD23 | 1:W:32:PRO:HA | 1.83 | 0.59 |
| 1:A:133:TYR:OH | 1:A:375:PHE:HB2 | 2.00 | 0.59 |
| 1:B:208:ILE:HD11 | 1:B:243:PRO:HG2 | 1.85 | 0.59 |
| 1:E:43:VAL:O | 1:E:44:MET:CG | 2.51 | 0.59 |
| 1:H:44:MET:HG3 | 1:H:45:VAL:N | 2.15 | 0.59 |
| 1:I:8:LEU:HB3 | 1:I:103:THR:HG23 | 1.84 | 0.59 |
| 1:J:16:LEU:HD23 | 1:J:32:PRO:HA | 1.83 | 0.59 |
| 1:M:290:ARG:HH11 | 1:O:244:ASP:CB | 2.16 | 0.59 |
| 1:N:288:ASP:HA | 1:P:243:PRO:HB2 | 1.83 | 0.59 |
| 1:U:287:ILE:CD1 | 1:W:208:ILE:CD1 | 2.80 | 0.59 |
| 1:V:346:LEU:O | 1:V:349:LEU:HB2 | 2.02 | 0.59 |
| 1:A:324:THR:CG2 | 1:C:241:GLU:OE2 | 2.50 | 0.59 |
| 1:B:132:MET:O | 1:B:357:ILE:HB | 2.01 | 0.59 |
| 1:D:143:TYR:CD1 | 1:D:143:TYR:C | 2.75 | 0.59 |
| 1:G:346:LEU:O | 1:G:349:LEU:HB2 | 2.02 | 0.59 |
| 1:H:324:THR:CG2 | 1:J:241:GLU:OE2 | 2.50 | 0.59 |
| 1:I:361:GLU:HB3 | 1:I:369:ILE:CD1 | 2.14 | 0.59 |
| 1:J:324:THR:CG2 | 1:L:241:GLU:OE2 | 2.50 | 0.59 |
| 1:K:324:THR:CG2 | 1:M:241:GLU:OE2 | 2.50 | 0.59 |
| 1:N:324:THR:CG2 | 1:P:241:GLU:OE2 | 2.50 | 0.59 |
| 1:O:143:TYR:CD1 | 1:O:143:TYR:C | 2.75 | 0.59 |
| 1:P:16:LEU:HD23 | 1:P:32:PRO:HA | 1.83 | 0.59 |
| 1:Q:8:LEU:HB3 | 1:Q:103:THR:HG23 | 1.84 | 0.59 |
| 1:R:43:VAL:O | 1:R:44:MET:CG | 2.51 | 0.59 |
| 1:T:34:ILE:CD1 | 1:T:67:LEU:HD22 | 2.31 | 0.59 |
| 1:T:362:TYR:O | 1:T:366:GLY:CA | 2.51 | 0.59 |
| 1:W:43:VAL:O | 1:W:44:MET:CG | 2.51 | 0.59 |
| 1:A:288:ASP:HA | 1:C:243:PRO:HB2 | 1.84 | 0.59 |
| 1:B:288:ASP:HA | 1:D:243:PRO:HB2 | 1.83 | 0.59 |
| 1:C:64:ILE:HG23 | 1:C:65:LEU:N | 2.18 | 0.59 |
| 1:C:287:ILE:CD1 | 1:E:208:ILE:CD1 | 2.80 | 0.59 |
| 1:D:208:ILE:HD11 | 1:D:243:PRO:HG2 | 1.85 | 0.59 |
| 1:F:208:ILE:HD11 | 1:F:243:PRO:HG2 | 1.85 | 0.59 |
| 1:I:143:TYR:CD1 | 1:I:143:TYR:C | 2.75 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:287:ILE:HG13 | 1:J:288:ASP:OD1 | 2.03 | 0.59 |
| 1:K:143:TYR:CD1 | 1:K:143:TYR:C | 2.75 | 0.59 |
| 1:L:287:ILE:HG13 | 1:L:288:ASP:OD1 | 2.03 | 0.59 |
| 1:L:288:ASP:HA | 1:N:243:PRO:HB2 | 1.83 | 0.59 |
| 1:O:287:ILE:HG13 | 1:O:288:ASP:OD1 | 2.03 | 0.59 |
| 1:Q:34:ILE:CD1 | 1:Q:67:LEU:HD22 | 2.31 | 0.59 |
| 1:R:34:ILE:HB | 1:R:54:VAL:HG13 | 1.79 | 0.59 |
| 1:R:64:ILE:HG23 | 1:R:65:LEU:N | 2.18 | 0.59 |
| 1:U:324:THR:CG2 | 1:W:241:GLU:OE2 | 2.50 | 0.59 |
| 1:C:324:THR:HG21 | 1:E:241:GLU:CD | 2.21 | 0.59 |
| 1:D:43:VAL:O | 1:D:44:MET:CG | 2.51 | 0.59 |
| 1:D:287:ILE:HG13 | 1:D:288:ASP:OD1 | 2.03 | 0.59 |
| 1:D:290:ARG:HH11 | 1:F:244:ASP:CB | 2.16 | 0.59 |
| 1:E:143:TYR:CD1 | 1:E:143:TYR:C | 2.75 | 0.59 |
| 1:G:64:ILE:HG23 | 1:G:65:LEU:N | 2.18 | 0.59 |
| 1:H:34:ILE:CD1 | 1:H:67:LEU:HD22 | 2.32 | 0.59 |
| 1:H:287:ILE:HG13 | 1:H:288:ASP:OD1 | 2.03 | 0.59 |
| 1:L:346:LEU:O | 1:L:349:LEU:HB2 | 2.02 | 0.59 |
| 1:L:362:TYR:O | 1:L:366:GLY:CA | 2.51 | 0.59 |
| 1:N:43:VAL:O | 1:N:44:MET:CG | 2.51 | 0.59 |
| 1:N:104:LEU:HB2 | 1:N:356:TRP:HH2 | 1.63 | 0.59 |
| 1:N:362:TYR:O | 1:N:366:GLY:CA | 2.51 | 0.59 |
| 1:O:288:ASP:HA | 1:Q:243:PRO:HB2 | 1.84 | 0.59 |
| 1:P:34:ILE:CD1 | 1:P:67:LEU:HD22 | 2.31 | 0.59 |
| 1:R:362:TYR:O | 1:R:366:GLY:CA | 2.51 | 0.59 |
| 1:S:16:LEU:HD23 | 1:S:32:PRO:HA | 1.83 | 0.59 |
| 1:B:43:VAL:O | 1:B:44:MET:CG | 2.51 | 0.59 |
| 1:B:324:THR:CG2 | 1:D:241:GLU:OE2 | 2.50 | 0.59 |
| 1:C:362:TYR:O | 1:C:366:GLY:CA | 2.51 | 0.59 |
| 1:E:287:ILE:CD1 | 1:G:208:ILE:CD1 | 2.80 | 0.59 |
| 1:F:288:ASP:HA | 1:H:243:PRO:HB2 | 1.84 | 0.59 |
| 1:H:288:ASP:HA | 1:J:243:PRO:HB2 | 1.83 | 0.59 |
| 1:I:287:ILE:HG13 | 1:I:288:ASP:OD1 | 2.03 | 0.59 |
| 1:J:288:ASP:HA | 1:L:243:PRO:HB2 | 1.83 | 0.59 |
| 1:L:64:ILE:HG23 | 1:L:65:LEU:N | 2.18 | 0.59 |
| 1:N:287:ILE:HG13 | 1:N:288:ASP:OD1 | 2.03 | 0.59 |
| 1:P:287:ILE:CD1 | 1:R:208:ILE:CD1 | 2.80 | 0.59 |
| 1:Q:324:THR:CG2 | 1:S:241:GLU:OE2 | 2.50 | 0.59 |
| 1:S:361:GLU:HB3 | 1:S:369:ILE:CD1 | 2.14 | 0.59 |
| 1:T:143:TYR:CD1 | 1:T:143:TYR:C | 2.75 | 0.59 |
| 1:U:288:ASP:HA | 1:W:243:PRO:HB2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:16:LEU:HD23 | 1:A:32:PRO:HA | 1.83 | 0.59 |
| 1:A:362:TYR:O | 1:A:366:GLY:CA | 2.51 | 0.59 |
| 1:D:288:ASP:HA | 1:F:243:PRO:HB2 | 1.84 | 0.59 |
| 1:E:287:ILE:HG13 | 1:E:288:ASP:OD1 | 2.03 | 0.59 |
| 1:G:287:ILE:HG13 | 1:G:288:ASP:OD1 | 2.03 | 0.59 |
| 1:G:362:TYR:O | 1:G:366:GLY:CA | 2.51 | 0.59 |
| 1:L:8:LEU:HB3 | 1:L:103:THR:HG23 | 1.84 | 0.59 |
| 1:M:324:THR:HG21 | 1:O:241:GLU:CD | 2.21 | 0.59 |
| 1:O:34:ILE:CD1 | 1:O:67:LEU:HD22 | 2.31 | 0.59 |
| 1:O:223:PHE:CE1 | 1:O:259:GLU:HG2 | 2.38 | 0.59 |
| 1:P:287:ILE:HG13 | 1:P:288:ASP:OD1 | 2.03 | 0.59 |
| 1:P:362:TYR:O | 1:P:366:GLY:CA | 2.51 | 0.59 |
| 1:R:287:ILE:CD1 | 1:T:208:ILE:CD1 | 2.80 | 0.59 |
| 1:S:8:LEU:HB3 | 1:S:103:THR:HG23 | 1.84 | 0.59 |
| 1:S:287:ILE:CD1 | 1:U:208:ILE:CD1 | 2.80 | 0.59 |
| 1:S:288:ASP:HA | 1:U:243:PRO:HB2 | 1.83 | 0.59 |
| 1:S:346:LEU:O | 1:S:349:LEU:HB2 | 2.02 | 0.59 |
| 1:U:43:VAL:O | 1:U:44:MET:CG | 2.51 | 0.59 |
| 1:C:223:PHE:CE1 | 1:C:259:GLU:HG2 | 2.38 | 0.59 |
| 1:C:287:ILE:HG13 | 1:C:288:ASP:OD1 | 2.03 | 0.59 |
| 1:D:223:PHE:CE1 | 1:D:259:GLU:HG2 | 2.38 | 0.59 |
| 1:F:287:ILE:CD1 | 1:H:208:ILE:CD1 | 2.80 | 0.59 |
| 1:F:287:ILE:HG13 | 1:F:288:ASP:OD1 | 2.03 | 0.59 |
| 1:G:43:VAL:O | 1:G:44:MET:CG | 2.51 | 0.59 |
| 1:G:290:ARG:HH11 | 1:I:244:ASP:CB | 2.16 | 0.59 |
| 1:H:208:ILE:HD11 | 1:H:243:PRO:HG2 | 1.85 | 0.59 |
| 1:I:16:LEU:HD23 | 1:I:32:PRO:HA | 1.83 | 0.59 |
| 1:I:43:VAL:O | 1:I:44:MET:CG | 2.51 | 0.59 |
| 1:K:290:ARG:HH11 | 1:M:244:ASP:CB | 2.16 | 0.59 |
| 1:L:223:PHE:CE1 | 1:L:259:GLU:HG2 | 2.38 | 0.59 |
| 1:N:8:LEU:HB3 | 1:N:103:THR:HG23 | 1.84 | 0.59 |
| 1:Q:287:ILE:CD1 | 1:S:208:ILE:CD1 | 2.80 | 0.59 |
| 1:R:287:ILE:HG13 | 1:R:288:ASP:OD1 | 2.03 | 0.59 |
| 1:T:287:ILE:HG13 | 1:T:288:ASP:OD1 | 2.03 | 0.59 |
| 1:U:223:PHE:CE1 | 1:U:259:GLU:HG2 | 2.38 | 0.59 |
| 1:U:287:ILE:HG13 | 1:U:288:ASP:OD1 | 2.03 | 0.59 |
| 1:V:8:LEU:HB3 | 1:V:103:THR:HG23 | 1.84 | 0.59 |
| 1:W:64:ILE:HG23 | 1:W:65:LEU:N | 2.18 | 0.59 |
| 1:W:223:PHE:CE1 | 1:W:259:GLU:HG2 | 2.38 | 0.59 |
| 1:A:8:LEU:HB3 | 1:A:103:THR:HG23 | 1.84 | 0.58 |
| 1:A:64:ILE:HG23 | 1:A:65:LEU:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:143:TYR:CD1 | 1:A:143:TYR:C | 2.75 | 0.58 |
| 1:A:223:PHE:CE1 | 1:A:259:GLU:HG2 | 2.38 | 0.58 |
| 1:B:8:LEU:HB3 | 1:B:103:THR:HG23 | 1.84 | 0.58 |
| 1:E:362:TYR:O | 1:E:366:GLY:CA | 2.51 | 0.58 |
| 1:F:324:THR:CG2 | 1:H:241:GLU:OE2 | 2.50 | 0.58 |
| 1:I:223:PHE:CE1 | 1:I:259:GLU:HG2 | 2.38 | 0.58 |
| 1:I:362:TYR:O | 1:I:366:GLY:CA | 2.51 | 0.58 |
| 1:J:223:PHE:CE1 | 1:J:259:GLU:HG2 | 2.38 | 0.58 |
| 1:J:362:TYR:O | 1:J:366:GLY:CA | 2.51 | 0.58 |
| 1:N:16:LEU:HD23 | 1:N:32:PRO:HA | 1.83 | 0.58 |
| 1:N:64:ILE:HG23 | 1:N:65:LEU:N | 2.18 | 0.58 |
| 1:O:324:THR:CG2 | 1:Q:241:GLU:OE2 | 2.50 | 0.58 |
| 1:P:64:ILE:HG23 | 1:P:65:LEU:N | 2.18 | 0.58 |
| 1:P:223:PHE:CE1 | 1:P:259:GLU:HG2 | 2.38 | 0.58 |
| 1:P:324:THR:HG21 | 1:R:241:GLU:OE2 | 2.03 | 0.58 |
| 1:Q:16:LEU:HD23 | 1:Q:32:PRO:HA | 1.83 | 0.58 |
| 1:Q:288:ASP:HA | 1:S:243:PRO:HB2 | 1.84 | 0.58 |
| 1:S:43:VAL:O | 1:S:44:MET:CG | 2.51 | 0.58 |
| 1:S:143:TYR:CD1 | 1:S:143:TYR:C | 2.75 | 0.58 |
| 1:T:16:LEU:HD23 | 1:T:32:PRO:HA | 1.83 | 0.58 |
| 1:T:290:ARG:HH11 | 1:V:244:ASP:CB | 2.16 | 0.58 |
| 1:V:64:ILE:HG23 | 1:V:65:LEU:N | 2.18 | 0.58 |
| 1:V:143:TYR:CD1 | 1:V:143:TYR:C | 2.75 | 0.58 |
| 1:V:362:TYR:O | 1:V:366:GLY:CA | 2.51 | 0.58 |
| 1:C:43:VAL:O | 1:C:44:MET:CG | 2.51 | 0.58 |
| 1:D:16:LEU:HD23 | 1:D:32:PRO:HA | 1.83 | 0.58 |
| 1:D:324:THR:CG2 | 1:F:241:GLU:OE2 | 2.50 | 0.58 |
| 1:E:290:ARG:HH11 | 1:G:244:ASP:CB | 2.16 | 0.58 |
| 1:F:223:PHE:CE1 | 1:F:259:GLU:HG2 | 2.38 | 0.58 |
| 1:G:8:LEU:HB3 | 1:G:103:THR:HG23 | 1.84 | 0.58 |
| 1:K:223:PHE:CE1 | 1:K:259:GLU:HG2 | 2.38 | 0.58 |
| 1:L:324:THR:CG2 | 1:N:241:GLU:OE2 | 2.50 | 0.58 |
| 1:M:324:THR:CG2 | 1:O:241:GLU:OE2 | 2.50 | 0.58 |
| 1:N:324:THR:HG21 | 1:P:241:GLU:OE2 | 2.03 | 0.58 |
| 1:O:290:ARG:HH11 | 1:Q:244:ASP:CB | 2.16 | 0.58 |
| 1:P:324:THR:CG2 | 1:R:241:GLU:OE2 | 2.50 | 0.58 |
| 1:Q:223:PHE:CE1 | 1:Q:259:GLU:HG2 | 2.38 | 0.58 |
| 1:Q:287:ILE:HG13 | 1:Q:288:ASP:OD1 | 2.03 | 0.58 |
| 1:R:324:THR:HG21 | 1:T:241:GLU:OE2 | 2.03 | 0.58 |
| 1:T:8:LEU:HB3 | 1:T:103:THR:HG23 | 1.84 | 0.58 |
| 1:U:208:ILE:HD11 | 1:U:243:PRO:HG2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:208:ILE:HD11 | 1:W:243:PRO:HG2 | 1.85 | 0.58 |
| 1:A:287:ILE:HG13 | 1:A:288:ASP:OD1 | 2.03 | 0.58 |
| 1:E:223:PHE:CE1 | 1:E:259:GLU:HG2 | 2.38 | 0.58 |
| 1:G:143:TYR:CD1 | 1:G:143:TYR:C | 2.75 | 0.58 |
| 1:M:324:THR:HG21 | 1:O:241:GLU:OE2 | 2.03 | 0.58 |
| 1:N:223:PHE:CE1 | 1:N:259:GLU:HG2 | 2.38 | 0.58 |
| 1:O:38:PRO:CD | 1:O:49:GLN:HE22 | 2.17 | 0.58 |
| 1:P:143:TYR:CD1 | 1:P:143:TYR:C | 2.75 | 0.58 |
| 1:Q:44:MET:HG3 | 1:Q:45:VAL:N | 2.15 | 0.58 |
| 1:S:290:ARG:HH11 | 1:U:244:ASP:CB | 2.16 | 0.58 |
| 1:T:324:THR:HG21 | 1:V:241:GLU:OE2 | 2.03 | 0.58 |
| 1:V:287:ILE:HG13 | 1:V:288:ASP:OD1 | 2.03 | 0.58 |
| 1:W:34:ILE:HB | 1:W:54:VAL:HG13 | 1.79 | 0.58 |
| 1:A:336:LYS:CE | 2:A:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:B:38:PRO:CD | 1:B:49:GLN:HE22 | 2.17 | 0.58 |
| 1:F:104:LEU:HB2 | 1:F:356:TRP:HH2 | 1.63 | 0.58 |
| 1:H:143:TYR:CD1 | 1:H:143:TYR:C | 2.75 | 0.58 |
| 1:K:38:PRO:CD | 1:K:49:GLN:HE22 | 2.17 | 0.58 |
| 1:K:43:VAL:O | 1:K:44:MET:CG | 2.51 | 0.58 |
| 1:M:287:ILE:HG13 | 1:M:288:ASP:OD1 | 2.03 | 0.58 |
| 1:N:290:ARG:HH11 | 1:P:244:ASP:CB | 2.16 | 0.58 |
| 1:R:336:LYS:CE | 2:R:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:S:208:ILE:HD11 | 1:S:243:PRO:HG2 | 1.85 | 0.58 |
| 1:V:208:ILE:HD11 | 1:V:243:PRO:HG2 | 1.85 | 0.58 |
| 1:V:223:PHE:CE1 | 1:V:259:GLU:HG2 | 2.38 | 0.58 |
| 1:W:362:TYR:O | 1:W:366:GLY:CA | 2.51 | 0.58 |
| 1:B:290:ARG:HH11 | 1:D:244:ASP:CB | 2.16 | 0.58 |
| 1:E:324:THR:HG21 | 1:G:241:GLU:OE2 | 2.04 | 0.58 |
| 1:H:64:ILE:HG23 | 1:H:65:LEU:N | 2.18 | 0.58 |
| 1:H:287:ILE:CD1 | 1:J:208:ILE:CD1 | 2.80 | 0.58 |
| 1:H:362:TYR:O | 1:H:366:GLY:CA | 2.51 | 0.58 |
| 1:I:324:THR:HG21 | 1:K:241:GLU:OE2 | 2.04 | 0.58 |
| 1:J:8:LEU:HB3 | 1:J:103:THR:HG23 | 1.84 | 0.58 |
| 1:K:324:THR:HG21 | 1:M:241:GLU:OE2 | 2.04 | 0.58 |
| 1:L:324:THR:HG21 | 1:N:241:GLU:OE2 | 2.04 | 0.58 |
| 1:O:43:VAL:O | 1:O:44:MET:CG | 2.51 | 0.58 |
| 1:P:8:LEU:HB3 | 1:P:103:THR:HG23 | 1.84 | 0.58 |
| 1:P:290:ARG:HH11 | 1:R:244:ASP:CB | 2.16 | 0.58 |
| 1:P:336:LYS:CE | 2:P:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:R:8:LEU:HB3 | 1:R:103:THR:HG23 | 1.84 | 0.58 |
| 1:S:38:PRO:CD | 1:S:49:GLN:HE22 | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:64:ILE:HG23 | 1:B:65:LEU:N | 2.18 | 0.58 |
| 1:B:287:ILE:HG13 | 1:B:288:ASP:OD1 | 2.03 | 0.58 |
| 1:C:34:ILE:HB | 1:C:54:VAL:HG13 | 1.79 | 0.58 |
| 1:H:8:LEU:HB3 | 1:H:103:THR:HG23 | 1.84 | 0.58 |
| 1:H:290:ARG:HH11 | 1:J:244:ASP:CB | 2.16 | 0.58 |
| 1:I:290:ARG:HH11 | 1:K:244:ASP:CB | 2.16 | 0.58 |
| 1:J:208:ILE:HD11 | 1:J:243:PRO:HG2 | 1.85 | 0.58 |
| 1:K:287:ILE:HG13 | 1:K:288:ASP:OD1 | 2.03 | 0.58 |
| 1:K:362:TYR:O | 1:K:366:GLY:CA | 2.51 | 0.58 |
| 1:M:223:PHE:CE1 | 1:M:259:GLU:HG2 | 2.38 | 0.58 |
| 1:N:4:GLU:O | 1:N:5:THR:HB | 2.04 | 0.58 |
| 1:O:287:ILE:CD1 | 1:Q:208:ILE:CD1 | 2.80 | 0.58 |
| 1:O:324:THR:HG21 | 1:Q:241:GLU:OE2 | 2.04 | 0.58 |
| 1:O:362:TYR:O | 1:O:366:GLY:CA | 2.51 | 0.58 |
| 1:Q:38:PRO:CD | 1:Q:49:GLN:HE22 | 2.17 | 0.58 |
| 1:Q:208:ILE:HD11 | 1:Q:243:PRO:HG2 | 1.85 | 0.58 |
| 1:Q:290:ARG:HH11 | 1:S:244:ASP:CB | 2.16 | 0.58 |
| 1:T:223:PHE:CE1 | 1:T:259:GLU:HG2 | 2.38 | 0.58 |
| 1:W:8:LEU:HB3 | 1:W:103:THR:HG23 | 1.84 | 0.58 |
| 1:W:336:LYS:CE | 2:W:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:A:34:ILE:CG2 | 1:A:67:LEU:HB3 | 2.34 | 0.58 |
| 1:C:368:SER:O | 1:C:371:HIS:N | 2.37 | 0.58 |
| 1:F:336:LYS:CE | 2:F:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:H:336:LYS:CE | 2:H:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:J:290:ARG:HH11 | 1:L:244:ASP:CB | 2.16 | 0.58 |
| 1:J:324:THR:HG21 | 1:L:241:GLU:OE2 | 2.03 | 0.58 |
| 1:M:38:PRO:CD | 1:M:49:GLN:HE22 | 2.17 | 0.58 |
| 1:P:4:GLU:O | 1:P:5:THR:HB | 2.04 | 0.58 |
| 1:Q:43:VAL:O | 1:Q:44:MET:CG | 2.51 | 0.58 |
| 1:R:4:GLU:O | 1:R:5:THR:HB | 2.04 | 0.58 |
| 1:T:336:LYS:CE | 2:T:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:U:8:LEU:HB3 | 1:U:103:THR:HG23 | 1.84 | 0.58 |
| 1:U:362:TYR:O | 1:U:366:GLY:CA | 2.51 | 0.58 |
| 1:B:223:PHE:CE1 | 1:B:259:GLU:HG2 | 2.38 | 0.58 |
| 1:C:34:ILE:CG2 | 1:C:67:LEU:HB3 | 2.34 | 0.58 |
| 1:D:362:TYR:O | 1:D:366:GLY:CA | 2.51 | 0.58 |
| 1:I:38:PRO:CD | 1:I:49:GLN:HE22 | 2.17 | 0.58 |
| 1:J:4:GLU:O | 1:J:5:THR:HB | 2.04 | 0.58 |
| 1:N:287:ILE:CD1 | 1:P:208:ILE:CD1 | 2.80 | 0.58 |
| 1:O:16:LEU:HD23 | 1:O:32:PRO:HA | 1.83 | 0.58 |
| 1:R:143:TYR:CD1 | 1:R:143:TYR:C | 2.75 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:38:PRO:CD | 1:V:49:GLN:HE22 | 2.17 | 0.58 |
| 1:W:4:GLU:O | 1:W:5:THR:HB | 2.04 | 0.58 |
| 1:C:4:GLU:O | 1:C:5:THR:HB | 2.04 | 0.58 |
| 1:C:8:LEU:HB3 | 1:C:103:THR:HG23 | 1.84 | 0.58 |
| 1:C:16:LEU:HD23 | 1:C:32:PRO:HA | 1.83 | 0.58 |
| 1:G:34:ILE:HB | 1:G:54:VAL:HG13 | 1.79 | 0.58 |
| 1:G:324:THR:HG21 | 1:I:241:GLU:OE2 | 2.03 | 0.58 |
| 1:H:38:PRO:CD | 1:H:49:GLN:HE22 | 2.17 | 0.58 |
| 1:M:64:ILE:HG23 | 1:M:65:LEU:N | 2.18 | 0.58 |
| 1:O:208:ILE:HD11 | 1:O:243:PRO:HG2 | 1.85 | 0.58 |
| 1:Q:324:THR:HG21 | 1:S:241:GLU:OE2 | 2.04 | 0.58 |
| 1:R:223:PHE:CE1 | 1:R:259:GLU:HG2 | 2.38 | 0.58 |
| 1:R:368:SER:O | 1:R:371:HIS:N | 2.37 | 0.58 |
| 1:S:287:ILE:HG13 | 1:S:288:ASP:OD1 | 2.03 | 0.58 |
| 1:T:38:PRO:CD | 1:T:49:GLN:HE22 | 2.17 | 0.58 |
| 1:U:4:GLU:O | 1:U:5:THR:HB | 2.04 | 0.58 |
| 1:U:38:PRO:CD | 1:U:49:GLN:HE22 | 2.17 | 0.58 |
| 1:B:362:TYR:O | 1:B:366:GLY:CA | 2.51 | 0.58 |
| 1:C:336:LYS:CE | 2:C:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:D:8:LEU:HB3 | 1:D:103:THR:HG23 | 1.84 | 0.58 |
| 1:E:64:ILE:HG23 | 1:E:65:LEU:N | 2.18 | 0.58 |
| 1:F:290:ARG:HH11 | 1:H:244:ASP:CB | 2.16 | 0.58 |
| 1:G:287:ILE:CD1 | 1:I:208:ILE:CD1 | 2.80 | 0.58 |
| 1:I:4:GLU:O | 1:I:5:THR:HB | 2.04 | 0.58 |
| 1:K:64:ILE:HG23 | 1:K:65:LEU:N | 2.18 | 0.58 |
| 1:M:43:VAL:O | 1:M:44:MET:CG | 2.51 | 0.58 |
| 1:N:336:LYS:CE | 2:N:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:Q:64:ILE:HG23 | 1:Q:65:LEU:N | 2.18 | 0.58 |
| 1:Q:104:LEU:HB2 | 1:Q:356:TRP:HH2 | 1.63 | 0.58 |
| 1:R:34:ILE:CG2 | 1:R:67:LEU:HB3 | 2.34 | 0.58 |
| 1:S:34:ILE:HG21 | 1:S:67:LEU:CB | 2.34 | 0.58 |
| 1:S:223:PHE:CE1 | 1:S:259:GLU:HG2 | 2.38 | 0.58 |
| 1:S:362:TYR:O | 1:S:366:GLY:CA | 2.51 | 0.58 |
| 1:T:34:ILE:CG2 | 1:T:67:LEU:HB3 | 2.34 | 0.58 |
| 1:T:64:ILE:HG23 | 1:T:65:LEU:N | 2.18 | 0.58 |
| 1:U:34:ILE:HG21 | 1:U:67:LEU:CB | 2.34 | 0.58 |
| 1:U:336:LYS:CE | 2:U:401:ADP:H5'2 | 2.34 | 0.58 |
| 1:V:34:ILE:HG21 | 1:V:67:LEU:CB | 2.34 | 0.58 |
| 1:A:208:ILE:HD11 | 1:A:243:PRO:HG2 | 1.85 | 0.57 |
| 1:C:143:TYR:CD1 | 1:C:143:TYR:C | 2.75 | 0.57 |
| 1:C:208:ILE:HD11 | 1:C:243:PRO:HG2 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:324:THR:HG21 | 1:E:241:GLU:OE2 | 2.03 | 0.57 |
| 1:D:287:ILE:CD1 | 1:F:208:ILE:CD1 | 2.80 | 0.57 |
| 1:D:336:LYS:CE | 2:D:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:F:368:SER:O | 1:F:371:HIS:N | 2.37 | 0.57 |
| 1:G:208:ILE:HD11 | 1:G:243:PRO:HG2 | 1.85 | 0.57 |
| 1:I:336:LYS:CE | 2:I:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:J:38:PRO:CD | 1:J:49:GLN:HE22 | 2.17 | 0.57 |
| 1:J:64:ILE:HG23 | 1:J:65:LEU:N | 2.18 | 0.57 |
| 1:S:324:THR:HG21 | 1:U:241:GLU:OE2 | 2.03 | 0.57 |
| 1:T:208:ILE:HD11 | 1:T:243:PRO:HG2 | 1.85 | 0.57 |
| 1:W:34:ILE:HG21 | 1:W:67:LEU:CB | 2.34 | 0.57 |
| 1:B:34:ILE:HG21 | 1:B:67:LEU:CB | 2.34 | 0.57 |
| 1:C:290:ARG:HH11 | 1:E:244:ASP:CB | 2.16 | 0.57 |
| 1:D:34:ILE:HG21 | 1:D:67:LEU:CB | 2.34 | 0.57 |
| 1:D:38:PRO:CD | 1:D:49:GLN:HE22 | 2.17 | 0.57 |
| 1:D:64:ILE:HG23 | 1:D:65:LEU:N | 2.18 | 0.57 |
| 1:E:8:LEU:HB3 | 1:E:103:THR:HG23 | 1.84 | 0.57 |
| 1:F:8:LEU:HB3 | 1:F:103:THR:HG23 | 1.84 | 0.57 |
| 1:G:223:PHE:CE1 | 1:G:259:GLU:HG2 | 2.38 | 0.57 |
| 1:G:368:SER:O | 1:G:371:HIS:N | 2.37 | 0.57 |
| 1:H:223:PHE:CE1 | 1:H:259:GLU:HG2 | 2.38 | 0.57 |
| 1:I:208:ILE:HD11 | 1:I:243:PRO:HG2 | 1.85 | 0.57 |
| 1:J:336:LYS:CE | 2:J:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:K:336:LYS:CE | 2:K:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:K:368:SER:O | 1:K:371:HIS:N | 2.37 | 0.57 |
| 1:L:290:ARG:HH11 | 1:N:244:ASP:CB | 2.16 | 0.57 |
| 1:N:143:TYR:CD1 | 1:N:143:TYR:C | 2.75 | 0.57 |
| 1:Q:362:TYR:O | 1:Q:366:GLY:CA | 2.51 | 0.57 |
| 1:S:64:ILE:HG23 | 1:S:65:LEU:N | 2.18 | 0.57 |
| 1:T:4:GLU:O | 1:T:5:THR:HB | 2.04 | 0.57 |
| 1:U:368:SER:O | 1:U:371:HIS:N | 2.37 | 0.57 |
| 1:A:4:GLU:O | 1:A:5:THR:HB | 2.04 | 0.57 |
| 1:A:324:THR:HG21 | 1:C:241:GLU:OE2 | 2.03 | 0.57 |
| 1:C:40:HIS:O | 1:C:41:GLN:C | 2.43 | 0.57 |
| 1:D:324:THR:HG21 | 1:F:241:GLU:OE2 | 2.03 | 0.57 |
| 1:E:208:ILE:HD11 | 1:E:243:PRO:HG2 | 1.85 | 0.57 |
| 1:F:38:PRO:CD | 1:F:49:GLN:HE22 | 2.17 | 0.57 |
| 1:F:362:TYR:O | 1:F:366:GLY:CA | 2.51 | 0.57 |
| 1:G:4:GLU:O | 1:G:5:THR:HB | 2.04 | 0.57 |
| 1:K:4:GLU:O | 1:K:5:THR:HB | 2.04 | 0.57 |
| 1:M:336:LYS:CE | 2:M:401:ADP:H5'2 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:362:TYR:O | 1:M:366:GLY:CA | 2.51 | 0.57 |
| 1:Q:34:ILE:HB | 1:Q:54:VAL:HG13 | 1.80 | 0.57 |
| 1:Q:34:ILE:HG21 | 1:Q:67:LEU:CB | 2.34 | 0.57 |
| 1:R:290:ARG:HH11 | 1:T:244:ASP:CB | 2.16 | 0.57 |
| 1:T:34:ILE:HG21 | 1:T:67:LEU:CB | 2.34 | 0.57 |
| 1:V:34:ILE:CG2 | 1:V:67:LEU:HB3 | 2.34 | 0.57 |
| 1:V:368:SER:O | 1:V:371:HIS:N | 2.37 | 0.57 |
| 1:W:287:ILE:HG13 | 1:W:288:ASP:OD1 | 2.03 | 0.57 |
| 1:A:34:ILE:HG21 | 1:A:67:LEU:CB | 2.34 | 0.57 |
| 1:A:290:ARG:HH11 | 1:C:244:ASP:CB | 2.16 | 0.57 |
| 1:C:34:ILE:HG21 | 1:C:67:LEU:CB | 2.34 | 0.57 |
| 1:D:34:ILE:CG2 | 1:D:67:LEU:HB3 | 2.34 | 0.57 |
| 1:G:336:LYS:CE | 2:G:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:H:324:THR:HG21 | 1:J:241:GLU:OE2 | 2.03 | 0.57 |
| 1:K:208:ILE:HD11 | 1:K:243:PRO:HG2 | 1.85 | 0.57 |
| 1:L:208:ILE:HD11 | 1:L:243:PRO:HG2 | 1.85 | 0.57 |
| 1:L:361:GLU:HB3 | 1:L:369:ILE:CD1 | 2.14 | 0.57 |
| 1:N:34:ILE:HG21 | 1:N:67:LEU:CB | 2.34 | 0.57 |
| 1:N:40:HIS:O | 1:N:41:GLN:C | 2.43 | 0.57 |
| 1:O:34:ILE:CG2 | 1:O:67:LEU:HB3 | 2.34 | 0.57 |
| 1:P:34:ILE:HG21 | 1:P:67:LEU:CB | 2.34 | 0.57 |
| 1:Q:34:ILE:CG2 | 1:Q:67:LEU:HB3 | 2.34 | 0.57 |
| 1:R:40:HIS:O | 1:R:41:GLN:C | 2.43 | 0.57 |
| 1:U:290:ARG:HH11 | 1:W:244:ASP:CB | 2.16 | 0.57 |
| 1:U:324:THR:HG21 | 1:W:241:GLU:OE2 | 2.03 | 0.57 |
| 1:V:336:LYS:CE | 2:V:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:A:38:PRO:CD | 1:A:49:GLN:HE22 | 2.17 | 0.57 |
| 1:B:324:THR:HG21 | 1:D:241:GLU:OE2 | 2.03 | 0.57 |
| 1:B:368:SER:O | 1:B:371:HIS:N | 2.37 | 0.57 |
| 1:E:34:ILE:CG2 | 1:E:67:LEU:HB3 | 2.34 | 0.57 |
| 1:G:40:HIS:O | 1:G:41:GLN:C | 2.43 | 0.57 |
| 1:H:143:TYR:HD2 | 1:H:346:LEU:HD13 | 1.70 | 0.57 |
| 1:M:34:ILE:CG2 | 1:M:67:LEU:HB3 | 2.34 | 0.57 |
| 1:M:208:ILE:HD11 | 1:M:243:PRO:HG2 | 1.85 | 0.57 |
| 1:P:34:ILE:CG2 | 1:P:67:LEU:HB3 | 2.34 | 0.57 |
| 1:Q:368:SER:O | 1:Q:371:HIS:N | 2.37 | 0.57 |
| 1:R:34:ILE:HG21 | 1:R:67:LEU:CB | 2.34 | 0.57 |
| 1:S:34:ILE:CG2 | 1:S:67:LEU:HB3 | 2.34 | 0.57 |
| 1:T:287:ILE:CD1 | 1:V:208:ILE:CD1 | 2.80 | 0.57 |
| 1:V:4:GLU:O | 1:V:5:THR:HB | 2.04 | 0.57 |
| 1:B:34:ILE:CG2 | 1:B:67:LEU:HB3 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:34:ILE:HG21 | 1:E:67:LEU:CB | 2.34 | 0.57 |
| 1:F:4:GLU:O | 1:F:5:THR:HB | 2.04 | 0.57 |
| 1:F:143:TYR:HD2 | 1:F:346:LEU:HD13 | 1.70 | 0.57 |
| 1:G:34:ILE:HG21 | 1:G:67:LEU:CB | 2.34 | 0.57 |
| 1:J:40:HIS:O | 1:J:41:GLN:C | 2.43 | 0.57 |
| 1:M:34:ILE:HG21 | 1:M:67:LEU:CB | 2.34 | 0.57 |
| 1:M:104:LEU:HB2 | 1:M:356:TRP:HH2 | 1.63 | 0.57 |
| 1:R:38:PRO:CD | 1:R:49:GLN:HE22 | 2.17 | 0.57 |
| 1:U:104:LEU:HB2 | 1:U:356:TRP:HH2 | 1.63 | 0.57 |
| 1:B:336:LYS:CE | 2:B:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:C:38:PRO:CD | 1:C:49:GLN:HE22 | 2.17 | 0.57 |
| 1:D:4:GLU:O | 1:D:5:THR:HB | 2.04 | 0.57 |
| 1:F:34:ILE:HG21 | 1:F:67:LEU:CB | 2.34 | 0.57 |
| 1:F:34:ILE:CG2 | 1:F:67:LEU:HB3 | 2.34 | 0.57 |
| 1:H:4:GLU:O | 1:H:5:THR:HB | 2.04 | 0.57 |
| 1:J:34:ILE:CG2 | 1:J:67:LEU:HB3 | 2.34 | 0.57 |
| 1:J:143:TYR:HD2 | 1:J:346:LEU:HD13 | 1.70 | 0.57 |
| 1:L:34:ILE:HG21 | 1:L:67:LEU:CB | 2.34 | 0.57 |
| 1:L:38:PRO:CD | 1:L:49:GLN:HE22 | 2.17 | 0.57 |
| 1:O:34:ILE:HG21 | 1:O:67:LEU:CB | 2.34 | 0.57 |
| 1:O:64:ILE:HG23 | 1:O:65:LEU:N | 2.18 | 0.57 |
| 1:O:104:LEU:HB2 | 1:O:356:TRP:HH2 | 1.63 | 0.57 |
| 1:O:336:LYS:CE | 2:O:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:P:208:ILE:HD11 | 1:P:243:PRO:HG2 | 1.85 | 0.57 |
| 1:S:4:GLU:O | 1:S:5:THR:HB | 2.04 | 0.57 |
| 1:U:34:ILE:CG2 | 1:U:67:LEU:HB3 | 2.34 | 0.57 |
| 1:V:40:HIS:O | 1:V:41:GLN:C | 2.43 | 0.57 |
| 1:B:4:GLU:O | 1:B:5:THR:HB | 2.04 | 0.57 |
| 1:E:336:LYS:CE | 2:E:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:H:34:ILE:CG2 | 1:H:67:LEU:HB3 | 2.34 | 0.57 |
| 1:I:34:ILE:HG21 | 1:I:67:LEU:CB | 2.34 | 0.57 |
| 1:K:34:ILE:CG2 | 1:K:67:LEU:HB3 | 2.34 | 0.57 |
| 1:K:361:GLU:HB3 | 1:K:369:ILE:CD1 | 2.14 | 0.57 |
| 1:L:143:TYR:CD1 | 1:L:143:TYR:C | 2.75 | 0.57 |
| 1:M:287:ILE:CD1 | 1:O:208:ILE:CD1 | 2.80 | 0.57 |
| 1:N:208:ILE:HD11 | 1:N:243:PRO:HG2 | 1.85 | 0.57 |
| 1:W:34:ILE:CG2 | 1:W:67:LEU:HB3 | 2.34 | 0.57 |
| 1:E:38:PRO:CD | 1:E:49:GLN:HE22 | 2.17 | 0.57 |
| 1:G:38:PRO:CD | 1:G:49:GLN:HE22 | 2.17 | 0.57 |
| 1:K:34:ILE:HG21 | 1:K:67:LEU:CB | 2.34 | 0.57 |
| 1:L:336:LYS:CE | 2:L:401:ADP:H5'2 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:290:ARG:HH11 | 1:O:244:ASP:HB2 | 1.70 | 0.57 |
| 1:P:38:PRO:CD | 1:P:49:GLN:HE22 | 2.17 | 0.57 |
| 1:R:208:ILE:HD11 | 1:R:243:PRO:HG2 | 1.85 | 0.57 |
| 1:S:336:LYS:CE | 2:S:401:ADP:H5'2 | 2.34 | 0.57 |
| 1:D:143:TYR:HD2 | 1:D:346:LEU:HD13 | 1.70 | 0.57 |
| 1:F:324:THR:HG21 | 1:H:241:GLU:OE2 | 2.03 | 0.57 |
| 1:I:34:ILE:CG2 | 1:I:67:LEU:HB3 | 2.34 | 0.57 |
| 1:M:4:GLU:O | 1:M:5:THR:HB | 2.04 | 0.57 |
| 1:U:40:HIS:O | 1:U:41:GLN:C | 2.43 | 0.57 |
| 1:W:38:PRO:CD | 1:W:49:GLN:HE22 | 2.17 | 0.57 |
| 1:B:143:TYR:CZ | 1:D:45:VAL:CG2 | 2.88 | 0.56 |
| 1:D:143:TYR:CZ | 1:F:45:VAL:CG2 | 2.88 | 0.56 |
| 1:E:4:GLU:O | 1:E:5:THR:HB | 2.04 | 0.56 |
| 1:H:34:ILE:HG21 | 1:H:67:LEU:CB | 2.34 | 0.56 |
| 1:I:64:ILE:HG23 | 1:I:65:LEU:N | 2.18 | 0.56 |
| 1:K:40:HIS:O | 1:K:41:GLN:C | 2.43 | 0.56 |
| 1:L:34:ILE:CG2 | 1:L:67:LEU:HB3 | 2.34 | 0.56 |
| 1:N:34:ILE:CG2 | 1:N:67:LEU:HB3 | 2.34 | 0.56 |
| 1:N:38:PRO:CD | 1:N:49:GLN:HE22 | 2.17 | 0.56 |
| 1:T:290:ARG:HH11 | 1:V:244:ASP:HB2 | 1.70 | 0.56 |
| 1:B:287:ILE:CD1 | 1:D:208:ILE:CD1 | 2.80 | 0.56 |
| 1:G:34:ILE:CG2 | 1:G:67:LEU:HB3 | 2.34 | 0.56 |
| 1:N:361:GLU:HB3 | 1:N:369:ILE:CD1 | 2.14 | 0.56 |
| 1:O:290:ARG:HH11 | 1:Q:244:ASP:HB2 | 1.70 | 0.56 |
| 1:Q:290:ARG:HH11 | 1:S:244:ASP:HB2 | 1.70 | 0.56 |
| 1:Q:336:LYS:CE | 2:Q:401:ADP:H5'2 | 2.34 | 0.56 |
| 1:B:361:GLU:HB3 | 1:B:369:ILE:CD1 | 2.14 | 0.56 |
| 1:F:40:HIS:O | 1:F:41:GLN:C | 2.43 | 0.56 |
| 1:F:64:ILE:HG23 | 1:F:65:LEU:N | 2.18 | 0.56 |
| 1:F:143:TYR:CZ | 1:H:45:VAL:CG2 | 2.88 | 0.56 |
| 1:F:290:ARG:HH11 | 1:H:244:ASP:HB2 | 1.71 | 0.56 |
| 1:G:143:TYR:CZ | 1:I:45:VAL:CG2 | 2.88 | 0.56 |
| 1:J:34:ILE:HG21 | 1:J:67:LEU:CB | 2.34 | 0.56 |
| 1:K:287:ILE:CD1 | 1:M:208:ILE:CD1 | 2.80 | 0.56 |
| 1:L:4:GLU:O | 1:L:5:THR:HB | 2.04 | 0.56 |
| 1:L:143:TYR:HD2 | 1:L:346:LEU:HD13 | 1.70 | 0.56 |
| 1:M:368:SER:O | 1:M:371:HIS:N | 2.37 | 0.56 |
| 1:N:143:TYR:CZ | 1:P:45:VAL:CG2 | 2.88 | 0.56 |
| 1:O:4:GLU:O | 1:O:5:THR:HB | 2.04 | 0.56 |
| 1:O:143:TYR:HD2 | 1:O:346:LEU:HD13 | 1.70 | 0.56 |
| 1:Q:143:TYR:HD2 | 1:Q:346:LEU:HD13 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:290:ARG:HH11 | 1:U:244:ASP:HB2 | 1.70 | 0.56 |
| 1:T:40:HIS:O | 1:T:41:GLN:C | 2.43 | 0.56 |
| 1:U:64:ILE:HG23 | 1:U:65:LEU:N | 2.18 | 0.56 |
| 1:I:287:ILE:CD1 | 1:K:208:ILE:CD1 | 2.80 | 0.56 |
| 1:K:290:ARG:HH11 | 1:M:244:ASP:HB2 | 1.70 | 0.56 |
| 1:L:143:TYR:CZ | 1:N:45:VAL:CG2 | 2.88 | 0.56 |
| 1:P:40:HIS:O | 1:P:41:GLN:C | 2.43 | 0.56 |
| 1:P:116:ARG:HD3 | 1:P:370:VAL:HG13 | 1.88 | 0.56 |
| 1:A:40:HIS:O | 1:A:41:GLN:C | 2.43 | 0.56 |
| 1:C:116:ARG:HD3 | 1:C:370:VAL:HG13 | 1.88 | 0.56 |
| 1:D:290:ARG:HH11 | 1:F:244:ASP:HB2 | 1.70 | 0.56 |
| 1:E:40:HIS:O | 1:E:41:GLN:C | 2.43 | 0.56 |
| 1:E:290:ARG:HH11 | 1:G:244:ASP:HB2 | 1.70 | 0.56 |
| 1:I:40:HIS:O | 1:I:41:GLN:C | 2.43 | 0.56 |
| 1:M:40:HIS:O | 1:M:41:GLN:C | 2.43 | 0.56 |
| 1:P:361:GLU:HB3 | 1:P:369:ILE:CD1 | 2.14 | 0.56 |
| 1:Q:40:HIS:O | 1:Q:41:GLN:C | 2.43 | 0.56 |
| 1:A:143:TYR:HD2 | 1:A:346:LEU:HD13 | 1.70 | 0.56 |
| 1:C:290:ARG:HH11 | 1:E:244:ASP:HB2 | 1.70 | 0.56 |
| 1:E:116:ARG:HD3 | 1:E:370:VAL:HG13 | 1.88 | 0.56 |
| 1:E:368:SER:O | 1:E:371:HIS:N | 2.37 | 0.56 |
| 1:G:290:ARG:HH11 | 1:I:244:ASP:HB2 | 1.70 | 0.56 |
| 1:L:40:HIS:O | 1:L:41:GLN:C | 2.43 | 0.56 |
| 1:R:290:ARG:HH11 | 1:T:244:ASP:HB2 | 1.70 | 0.56 |
| 1:S:143:TYR:HD2 | 1:S:346:LEU:HD13 | 1.70 | 0.56 |
| 1:A:368:SER:O | 1:A:371:HIS:N | 2.37 | 0.56 |
| 1:H:290:ARG:HH11 | 1:J:244:ASP:HB2 | 1.71 | 0.56 |
| 1:I:368:SER:O | 1:I:371:HIS:N | 2.37 | 0.56 |
| 1:M:143:TYR:HD2 | 1:M:346:LEU:HD13 | 1.70 | 0.56 |
| 1:N:116:ARG:HD3 | 1:N:370:VAL:HG13 | 1.88 | 0.56 |
| 1:P:143:TYR:CZ | 1:R:45:VAL:CG2 | 2.88 | 0.56 |
| 1:Q:4:GLU:O | 1:Q:5:THR:HB | 2.04 | 0.56 |
| 1:B:40:HIS:O | 1:B:41:GLN:C | 2.43 | 0.56 |
| 1:B:143:TYR:HD2 | 1:B:346:LEU:HD13 | 1.70 | 0.56 |
| 1:E:143:TYR:CZ | 1:G:45:VAL:CG2 | 2.88 | 0.56 |
| 1:H:40:HIS:O | 1:H:41:GLN:C | 2.43 | 0.56 |
| 1:O:40:HIS:O | 1:O:41:GLN:C | 2.43 | 0.56 |
| 1:R:116:ARG:HD3 | 1:R:370:VAL:HG13 | 1.88 | 0.56 |
| 1:T:116:ARG:HD3 | 1:T:370:VAL:HG13 | 1.88 | 0.56 |
| 1:U:290:ARG:HH11 | 1:W:244:ASP:HB2 | 1.70 | 0.56 |
| 1:U:361:GLU:HB3 | 1:U:369:ILE:CD1 | 2.14 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:116:ARG:HD3 | 1:A:370:VAL:HG13 | 1.88 | 0.56 |
| 1:A:290:ARG:HH11 | 1:C:244:ASP:HB2 | 1.70 | 0.56 |
| 1:D:40:HIS:O | 1:D:41:GLN:C | 2.43 | 0.56 |
| 1:J:143:TYR:CZ | 1:L:45:VAL:CG2 | 2.88 | 0.56 |
| 1:J:290:ARG:HH11 | 1:L:244:ASP:HB2 | 1.70 | 0.56 |
| 1:P:368:SER:O | 1:P:371:HIS:N | 2.37 | 0.56 |
| 1:W:40:HIS:O | 1:W:41:GLN:C | 2.43 | 0.56 |
| 1:C:143:TYR:CZ | 1:E:45:VAL:CG2 | 2.88 | 0.56 |
| 1:G:116:ARG:HD3 | 1:G:370:VAL:HG13 | 1.88 | 0.56 |
| 1:I:290:ARG:HH11 | 1:K:244:ASP:HB2 | 1.70 | 0.56 |
| 1:L:290:ARG:HH11 | 1:N:244:ASP:HB2 | 1.70 | 0.56 |
| 1:N:34:ILE:HB | 1:N:54:VAL:HG13 | 1.80 | 0.56 |
| 1:T:143:TYR:CZ | 1:V:45:VAL:CG2 | 2.88 | 0.56 |
| 1:V:116:ARG:HD3 | 1:V:370:VAL:HG13 | 1.88 | 0.56 |
| 1:W:143:TYR:CD1 | 1:W:143:TYR:C | 2.75 | 0.56 |
| 1:F:362:TYR:HE1 | 1:F:367:PRO:CB | 2.19 | 0.55 |
| 1:J:34:ILE:CG2 | 1:J:67:LEU:HD22 | 2.28 | 0.55 |
| 1:K:121:GLN:HA | 1:K:362:TYR:OH | 2.07 | 0.55 |
| 1:R:325:MET:HE3 | 1:T:244:ASP:O | 2.06 | 0.55 |
| 1:R:361:GLU:HB3 | 1:R:369:ILE:CD1 | 2.14 | 0.55 |
| 1:S:40:HIS:O | 1:S:41:GLN:C | 2.43 | 0.55 |
| 1:S:143:TYR:CZ | 1:U:45:VAL:CG2 | 2.88 | 0.55 |
| 1:T:368:SER:O | 1:T:371:HIS:N | 2.37 | 0.55 |
| 1:U:143:TYR:CZ | 1:W:45:VAL:CG2 | 2.88 | 0.55 |
| 1:A:143:TYR:CZ | 1:C:45:VAL:CG2 | 2.88 | 0.55 |
| 1:B:290:ARG:HH11 | 1:D:244:ASP:HB2 | 1.71 | 0.55 |
| 1:B:362:TYR:HE1 | 1:B:367:PRO:CB | 2.19 | 0.55 |
| 1:D:325:MET:HE3 | 1:F:244:ASP:O | 2.06 | 0.55 |
| 1:F:325:MET:HE3 | 1:H:244:ASP:O | 2.07 | 0.55 |
| 1:J:121:GLN:HA | 1:J:362:TYR:OH | 2.07 | 0.55 |
| 1:K:37:ARG:CG | 1:K:38:PRO:CD | 2.83 | 0.55 |
| 1:L:54:VAL:O | 1:L:55:GLY:C | 2.45 | 0.55 |
| 1:L:116:ARG:HD3 | 1:L:370:VAL:HG13 | 1.88 | 0.55 |
| 1:L:121:GLN:HA | 1:L:362:TYR:OH | 2.07 | 0.55 |
| 1:Q:116:ARG:HD3 | 1:Q:370:VAL:HG13 | 1.88 | 0.55 |
| 1:Q:121:GLN:HA | 1:Q:362:TYR:OH | 2.07 | 0.55 |
| 1:Q:143:TYR:CZ | 1:S:45:VAL:CG2 | 2.88 | 0.55 |
| 1:T:121:GLN:HA | 1:T:362:TYR:OH | 2.07 | 0.55 |
| 1:A:54:VAL:O | 1:A:55:GLY:C | 2.45 | 0.55 |
| 1:A:110:LEU:HD12 | 1:A:177:ARG:HH11 | 1.72 | 0.55 |
| 1:C:110:LEU:HD12 | 1:C:177:ARG:HH11 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:121:GLN:HA | 1:C:362:TYR:OH | 2.07 | 0.55 |
| 1:C:143:TYR:HD2 | 1:C:346:LEU:HD13 | 1.70 | 0.55 |
| 1:D:116:ARG:HD3 | 1:D:370:VAL:HG13 | 1.88 | 0.55 |
| 1:I:116:ARG:HD3 | 1:I:370:VAL:HG13 | 1.88 | 0.55 |
| 1:I:325:MET:HE3 | 1:K:244:ASP:O | 2.07 | 0.55 |
| 1:L:368:SER:O | 1:L:371:HIS:N | 2.37 | 0.55 |
| 1:N:121:GLN:HA | 1:N:362:TYR:OH | 2.07 | 0.55 |
| 1:N:290:ARG:HH11 | 1:P:244:ASP:HB2 | 1.70 | 0.55 |
| 1:S:121:GLN:HA | 1:S:362:TYR:OH | 2.07 | 0.55 |
| 1:T:325:MET:HE3 | 1:V:244:ASP:O | 2.06 | 0.55 |
| 1:U:143:TYR:HD2 | 1:U:346:LEU:HD13 | 1.70 | 0.55 |
| 1:W:54:VAL:O | 1:W:55:GLY:C | 2.45 | 0.55 |
| 1:B:121:GLN:HA | 1:B:362:TYR:OH | 2.07 | 0.55 |
| 1:K:325:MET:HE3 | 1:M:244:ASP:O | 2.07 | 0.55 |
| 1:M:325:MET:HE3 | 1:O:244:ASP:O | 2.07 | 0.55 |
| 1:O:116:ARG:HD3 | 1:O:370:VAL:HG13 | 1.88 | 0.55 |
| 1:A:325:MET:HE3 | 1:C:244:ASP:O | 2.06 | 0.55 |
| 1:B:116:ARG:HD3 | 1:B:370:VAL:HG13 | 1.88 | 0.55 |
| 1:B:325:MET:HE3 | 1:D:244:ASP:O | 2.07 | 0.55 |
| 1:E:121:GLN:HA | 1:E:362:TYR:OH | 2.07 | 0.55 |
| 1:F:54:VAL:O | 1:F:55:GLY:C | 2.45 | 0.55 |
| 1:H:325:MET:HE3 | 1:J:244:ASP:O | 2.06 | 0.55 |
| 1:J:37:ARG:CG | 1:J:38:PRO:CD | 2.83 | 0.55 |
| 1:J:116:ARG:HD3 | 1:J:370:VAL:HG13 | 1.88 | 0.55 |
| 1:N:143:TYR:CZ | 1:N:345:ILE:HG22 | 2.42 | 0.55 |
| 1:T:110:LEU:HD12 | 1:T:177:ARG:HH11 | 1.72 | 0.55 |
| 1:U:121:GLN:HA | 1:U:362:TYR:OH | 2.07 | 0.55 |
| 1:V:110:LEU:HD12 | 1:V:177:ARG:HH11 | 1.72 | 0.55 |
| 1:B:32:PRO:HG3 | 1:B:59:GLN:NE2 | 2.22 | 0.55 |
| 1:E:37:ARG:CG | 1:E:38:PRO:CD | 2.83 | 0.55 |
| 1:E:143:TYR:CZ | 1:E:345:ILE:HG22 | 2.42 | 0.55 |
| 1:E:325:MET:HE3 | 1:G:244:ASP:O | 2.06 | 0.55 |
| 1:H:54:VAL:O | 1:H:55:GLY:C | 2.45 | 0.55 |
| 1:H:121:GLN:HA | 1:H:362:TYR:OH | 2.07 | 0.55 |
| 1:K:143:TYR:HD2 | 1:K:346:LEU:HD13 | 1.70 | 0.55 |
| 1:O:121:GLN:HA | 1:O:362:TYR:OH | 2.07 | 0.55 |
| 1:O:143:TYR:CZ | 1:Q:45:VAL:CG2 | 2.88 | 0.55 |
| 1:P:121:GLN:HA | 1:P:362:TYR:OH | 2.07 | 0.55 |
| 1:P:143:TYR:CZ | 1:P:345:ILE:HG22 | 2.42 | 0.55 |
| 1:Q:32:PRO:HG3 | 1:Q:59:GLN:NE2 | 2.22 | 0.55 |
| 1:R:7:ALA:CB | 1:R:347:ALA:HB1 | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:54:VAL:O | 1:R:55:GLY:C | 2.45 | 0.55 |
| 1:R:143:TYR:CZ | 1:T:45:VAL:CG2 | 2.88 | 0.55 |
| 1:T:7:ALA:CB | 1:T:347:ALA:HB1 | 2.37 | 0.55 |
| 1:T:143:TYR:CZ | 1:T:345:ILE:HG22 | 2.42 | 0.55 |
| 1:U:32:PRO:HG3 | 1:U:59:GLN:NE2 | 2.22 | 0.55 |
| 1:U:143:TYR:CZ | 1:U:345:ILE:HG22 | 2.42 | 0.55 |
| 1:W:7:ALA:CB | 1:W:347:ALA:HB1 | 2.37 | 0.55 |
| 1:A:7:ALA:CB | 1:A:347:ALA:HB1 | 2.37 | 0.55 |
| 1:F:116:ARG:HD3 | 1:F:370:VAL:HG13 | 1.88 | 0.55 |
| 1:H:143:TYR:CZ | 1:H:345:ILE:HG22 | 2.42 | 0.55 |
| 1:I:34:ILE:CG2 | 1:I:67:LEU:HD22 | 2.27 | 0.55 |
| 1:I:121:GLN:HA | 1:I:362:TYR:OH | 2.07 | 0.55 |
| 1:J:32:PRO:HG3 | 1:J:59:GLN:NE2 | 2.22 | 0.55 |
| 1:N:143:TYR:HD2 | 1:N:346:LEU:HD13 | 1.70 | 0.55 |
| 1:P:290:ARG:HH11 | 1:R:244:ASP:HB2 | 1.70 | 0.55 |
| 1:Q:236:LEU:HD12 | 1:Q:237:GLU:CG | 2.37 | 0.55 |
| 1:R:121:GLN:HA | 1:R:362:TYR:OH | 2.07 | 0.55 |
| 1:U:7:ALA:CB | 1:U:347:ALA:HB1 | 2.37 | 0.55 |
| 1:V:7:ALA:CB | 1:V:347:ALA:HB1 | 2.37 | 0.55 |
| 1:V:121:GLN:HA | 1:V:362:TYR:OH | 2.07 | 0.55 |
| 1:W:116:ARG:HD3 | 1:W:370:VAL:HG13 | 1.88 | 0.55 |
| 1:W:121:GLN:HA | 1:W:362:TYR:OH | 2.07 | 0.55 |
| 1:W:143:TYR:CZ | 1:W:345:ILE:HG22 | 2.42 | 0.55 |
| 1:W:236:LEU:HD12 | 1:W:237:GLU:CG | 2.37 | 0.55 |
| 1:A:32:PRO:HG3 | 1:A:59:GLN:NE2 | 2.22 | 0.55 |
| 1:C:325:MET:HE3 | 1:E:244:ASP:O | 2.07 | 0.55 |
| 1:F:32:PRO:HG3 | 1:F:59:GLN:NE2 | 2.22 | 0.55 |
| 1:F:143:TYR:CZ | 1:F:345:ILE:HG22 | 2.42 | 0.55 |
| 1:H:143:TYR:CZ | 1:J:45:VAL:CG2 | 2.88 | 0.55 |
| 1:L:143:TYR:CZ | 1:L:345:ILE:HG22 | 2.42 | 0.55 |
| 1:M:32:PRO:HG3 | 1:M:59:GLN:NE2 | 2.22 | 0.55 |
| 1:M:110:LEU:HD12 | 1:M:177:ARG:HH11 | 1.72 | 0.55 |
| 1:M:121:GLN:HA | 1:M:362:TYR:OH | 2.07 | 0.55 |
| 1:M:143:TYR:CZ | 1:O:45:VAL:CG2 | 2.88 | 0.55 |
| 1:N:37:ARG:CG | 1:N:38:PRO:CD | 2.83 | 0.55 |
| 1:N:54:VAL:O | 1:N:55:GLY:C | 2.45 | 0.55 |
| 1:O:7:ALA:CB | 1:O:347:ALA:HB1 | 2.37 | 0.55 |
| 1:O:236:LEU:HD12 | 1:O:237:GLU:CG | 2.37 | 0.55 |
| 1:P:7:ALA:CB | 1:P:347:ALA:HB1 | 2.37 | 0.55 |
| 1:P:54:VAL:O | 1:P:55:GLY:C | 2.45 | 0.55 |
| 1:R:110:LEU:HD12 | 1:R:177:ARG:HH11 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:143:TYR:CZ | 1:R:345:ILE:HG22 | 2.42 | 0.55 |
| 1:S:7:ALA:CB | 1:S:347:ALA:HB1 | 2.37 | 0.55 |
| 1:S:147:ARG:NH2 | 1:S:147:ARG:HG3 | 2.22 | 0.55 |
| 1:S:236:LEU:HD12 | 1:S:237:GLU:CG | 2.37 | 0.55 |
| 1:U:34:ILE:CG2 | 1:U:67:LEU:HD22 | 2.28 | 0.55 |
| 1:U:236:LEU:HD12 | 1:U:237:GLU:CG | 2.37 | 0.55 |
| 1:C:7:ALA:CB | 1:C:347:ALA:HB1 | 2.37 | 0.55 |
| 1:C:54:VAL:O | 1:C:55:GLY:C | 2.45 | 0.55 |
| 1:E:7:ALA:CB | 1:E:347:ALA:HB1 | 2.37 | 0.55 |
| 1:F:121:GLN:HA | 1:F:362:TYR:OH | 2.07 | 0.55 |
| 1:G:7:ALA:CB | 1:G:347:ALA:HB1 | 2.37 | 0.55 |
| 1:H:368:SER:O | 1:H:371:HIS:N | 2.37 | 0.55 |
| 1:K:116:ARG:HD3 | 1:K:370:VAL:HG13 | 1.88 | 0.55 |
| 1:K:143:TYR:CZ | 1:K:345:ILE:HG22 | 2.42 | 0.55 |
| 1:M:7:ALA:CB | 1:M:347:ALA:HB1 | 2.37 | 0.55 |
| 1:N:7:ALA:CB | 1:N:347:ALA:HB1 | 2.37 | 0.55 |
| 1:N:147:ARG:NH2 | 1:N:147:ARG:HG3 | 2.22 | 0.55 |
| 1:R:32:PRO:HG3 | 1:R:59:GLN:NE2 | 2.22 | 0.55 |
| 1:S:54:VAL:O | 1:S:55:GLY:C | 2.45 | 0.55 |
| 1:T:32:PRO:HG3 | 1:T:59:GLN:NE2 | 2.22 | 0.55 |
| 1:T:361:GLU:HB3 | 1:T:369:ILE:CD1 | 2.14 | 0.55 |
| 1:U:116:ARG:HD3 | 1:U:370:VAL:HG13 | 1.88 | 0.55 |
| 1:V:143:TYR:HD2 | 1:V:346:LEU:HD13 | 1.70 | 0.55 |
| 1:C:236:LEU:HD12 | 1:C:237:GLU:CG | 2.37 | 0.55 |
| 1:D:236:LEU:HD12 | 1:D:237:GLU:CG | 2.37 | 0.55 |
| 1:E:110:LEU:HD12 | 1:E:177:ARG:HH11 | 1.72 | 0.55 |
| 1:E:362:TYR:HE1 | 1:E:367:PRO:CB | 2.19 | 0.55 |
| 1:G:54:VAL:O | 1:G:55:GLY:C | 2.45 | 0.55 |
| 1:G:143:TYR:CZ | 1:G:345:ILE:HG22 | 2.42 | 0.55 |
| 1:H:116:ARG:HD3 | 1:H:370:VAL:HG13 | 1.88 | 0.55 |
| 1:H:147:ARG:NH2 | 1:H:147:ARG:HG3 | 2.22 | 0.55 |
| 1:K:7:ALA:CB | 1:K:347:ALA:HB1 | 2.37 | 0.55 |
| 1:K:143:TYR:HD1 | 1:K:143:TYR:C | 2.09 | 0.55 |
| 1:L:32:PRO:HG3 | 1:L:59:GLN:NE2 | 2.22 | 0.55 |
| 1:M:143:TYR:CZ | 1:M:345:ILE:HG22 | 2.42 | 0.55 |
| 1:M:236:LEU:HD12 | 1:M:237:GLU:CG | 2.37 | 0.55 |
| 1:N:32:PRO:HG3 | 1:N:59:GLN:NE2 | 2.22 | 0.55 |
| 1:P:32:PRO:HG3 | 1:P:59:GLN:NE2 | 2.22 | 0.55 |
| 1:Q:7:ALA:CB | 1:Q:347:ALA:HB1 | 2.37 | 0.55 |
| 1:Q:54:VAL:O | 1:Q:55:GLY:C | 2.45 | 0.55 |
| 1:S:116:ARG:HD3 | 1:S:370:VAL:HG13 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:37:ARG:CG | 1:U:38:PRO:CD | 2.83 | 0.55 |
| 1:W:368:SER:O | 1:W:371:HIS:N | 2.37 | 0.55 |
| 1:A:121:GLN:HA | 1:A:362:TYR:OH | 2.07 | 0.54 |
| 1:C:143:TYR:CZ | 1:C:345:ILE:HG22 | 2.42 | 0.54 |
| 1:D:147:ARG:HG3 | 1:D:147:ARG:NH2 | 2.22 | 0.54 |
| 1:H:236:LEU:HD12 | 1:H:237:GLU:CG | 2.37 | 0.54 |
| 1:I:38:PRO:HB2 | 1:I:41:GLN:HB2 | 1.89 | 0.54 |
| 1:J:54:VAL:O | 1:J:55:GLY:C | 2.45 | 0.54 |
| 1:J:236:LEU:HD12 | 1:J:237:GLU:CG | 2.37 | 0.54 |
| 1:K:32:PRO:HG3 | 1:K:59:GLN:NE2 | 2.22 | 0.54 |
| 1:O:32:PRO:HG3 | 1:O:59:GLN:NE2 | 2.22 | 0.54 |
| 1:O:110:LEU:HD12 | 1:O:177:ARG:HH11 | 1.72 | 0.54 |
| 1:T:37:ARG:CG | 1:T:38:PRO:CD | 2.83 | 0.54 |
| 1:B:7:ALA:CB | 1:B:347:ALA:HB1 | 2.37 | 0.54 |
| 1:B:236:LEU:HD12 | 1:B:237:GLU:CG | 2.37 | 0.54 |
| 1:C:147:ARG:NH2 | 1:C:147:ARG:HG3 | 2.22 | 0.54 |
| 1:D:34:ILE:HG21 | 1:D:67:LEU:HB3 | 1.89 | 0.54 |
| 1:E:236:LEU:HD12 | 1:E:237:GLU:CG | 2.37 | 0.54 |
| 1:F:236:LEU:HD12 | 1:F:237:GLU:CG | 2.37 | 0.54 |
| 1:G:121:GLN:HA | 1:G:362:TYR:OH | 2.07 | 0.54 |
| 1:H:34:ILE:HG21 | 1:H:67:LEU:HB3 | 1.90 | 0.54 |
| 1:J:325:MET:HE3 | 1:L:244:ASP:O | 2.06 | 0.54 |
| 1:K:8:LEU:HB2 | 1:K:103:THR:OG1 | 2.08 | 0.54 |
| 1:K:143:TYR:CZ | 1:M:45:VAL:CG2 | 2.88 | 0.54 |
| 1:L:236:LEU:HD12 | 1:L:237:GLU:CG | 2.37 | 0.54 |
| 1:M:116:ARG:HD3 | 1:M:370:VAL:HG13 | 1.88 | 0.54 |
| 1:P:236:LEU:HD12 | 1:P:237:GLU:CG | 2.37 | 0.54 |
| 1:T:143:TYR:HD2 | 1:T:346:LEU:HD13 | 1.70 | 0.54 |
| 1:V:32:PRO:HG3 | 1:V:59:GLN:NE2 | 2.22 | 0.54 |
| 1:W:147:ARG:HG3 | 1:W:147:ARG:NH2 | 2.22 | 0.54 |
| 1:A:143:TYR:CZ | 1:A:345:ILE:HG22 | 2.42 | 0.54 |
| 1:B:223:PHE:CZ | 1:B:266:PHE:HZ | 2.26 | 0.54 |
| 1:D:34:ILE:CG2 | 1:D:67:LEU:HD22 | 2.28 | 0.54 |
| 1:D:106:THR:HG22 | 1:D:140:LEU:CD1 | 2.38 | 0.54 |
| 1:E:54:VAL:O | 1:E:55:GLY:C | 2.45 | 0.54 |
| 1:F:37:ARG:CG | 1:F:38:PRO:CD | 2.83 | 0.54 |
| 1:G:8:LEU:HB2 | 1:G:103:THR:OG1 | 2.08 | 0.54 |
| 1:G:300:SER:HA | 1:G:335:ARG:HG2 | 1.89 | 0.54 |
| 1:I:7:ALA:CB | 1:I:347:ALA:HB1 | 2.37 | 0.54 |
| 1:I:34:ILE:HG21 | 1:I:67:LEU:HB3 | 1.90 | 0.54 |
| 1:J:147:ARG:NH2 | 1:J:147:ARG:HG3 | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:38:PRO:HB2 | 1:K:41:GLN:HB2 | 1.89 | 0.54 |
| 1:L:7:ALA:CB | 1:L:347:ALA:HB1 | 2.37 | 0.54 |
| 1:L:106:THR:HG22 | 1:L:140:LEU:CD1 | 2.38 | 0.54 |
| 1:N:106:THR:HG22 | 1:N:140:LEU:CD1 | 2.38 | 0.54 |
| 1:N:236:LEU:HD12 | 1:N:237:GLU:CG | 2.37 | 0.54 |
| 1:U:34:ILE:HG21 | 1:U:67:LEU:HB3 | 1.90 | 0.54 |
| 1:U:54:VAL:O | 1:U:55:GLY:C | 2.45 | 0.54 |
| 1:V:236:LEU:HD12 | 1:V:237:GLU:CG | 2.37 | 0.54 |
| 1:W:143:TYR:HD2 | 1:W:346:LEU:HD13 | 1.70 | 0.54 |
| 1:W:236:LEU:HD12 | 1:W:237:GLU:HG2 | 1.90 | 0.54 |
| 1:W:362:TYR:HE1 | 1:W:367:PRO:CB | 2.19 | 0.54 |
| 1:A:236:LEU:HD12 | 1:A:237:GLU:CG | 2.37 | 0.54 |
| 1:B:7:ALA:CB | 1:B:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:C:223:PHE:CZ | 1:C:266:PHE:HZ | 2.26 | 0.54 |
| 1:C:236:LEU:HD12 | 1:C:237:GLU:HG2 | 1.90 | 0.54 |
| 1:D:32:PRO:HG3 | 1:D:59:GLN:NE2 | 2.22 | 0.54 |
| 1:D:143:TYR:CZ | 1:D:345:ILE:HG22 | 2.42 | 0.54 |
| 1:E:32:PRO:HG3 | 1:E:59:GLN:NE2 | 2.22 | 0.54 |
| 1:F:106:THR:HG22 | 1:F:140:LEU:CD1 | 2.38 | 0.54 |
| 1:G:38:PRO:HB2 | 1:G:41:GLN:HB2 | 1.89 | 0.54 |
| 1:H:106:THR:HG22 | 1:H:140:LEU:CD1 | 2.38 | 0.54 |
| 1:H:110:LEU:HD12 | 1:H:177:ARG:HH11 | 1.72 | 0.54 |
| 1:I:32:PRO:HG3 | 1:I:59:GLN:NE2 | 2.22 | 0.54 |
| 1:J:34:ILE:HG21 | 1:J:67:LEU:HB3 | 1.90 | 0.54 |
| 1:J:106:THR:HG22 | 1:J:140:LEU:CD1 | 2.38 | 0.54 |
| 1:K:7:ALA:CB | 1:K:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:K:110:LEU:HD12 | 1:K:177:ARG:HH11 | 1.72 | 0.54 |
| 1:M:223:PHE:CZ | 1:M:266:PHE:HZ | 2.26 | 0.54 |
| 1:N:223:PHE:CZ | 1:N:266:PHE:HZ | 2.26 | 0.54 |
| 1:N:236:LEU:HD12 | 1:N:237:GLU:HG2 | 1.90 | 0.54 |
| 1:O:7:ALA:CB | 1:O:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:O:8:LEU:HB2 | 1:O:103:THR:OG1 | 2.08 | 0.54 |
| 1:O:143:TYR:CZ | 1:O:345:ILE:HG22 | 2.42 | 0.54 |
| 1:P:34:ILE:CG2 | 1:P:67:LEU:HD22 | 2.27 | 0.54 |
| 1:P:325:MET:HE3 | 1:R:244:ASP:O | 2.06 | 0.54 |
| 1:Q:325:MET:HE3 | 1:S:244:ASP:O | 2.06 | 0.54 |
| 1:T:54:VAL:O | 1:T:55:GLY:C | 2.45 | 0.54 |
| 1:V:7:ALA:CB | 1:V:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:V:8:LEU:HB2 | 1:V:103:THR:OG1 | 2.08 | 0.54 |
| 1:V:34:ILE:HG21 | 1:V:67:LEU:HB3 | 1.90 | 0.54 |
| 1:V:38:PRO:HB2 | 1:V:41:GLN:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:143:TYR:CZ | 1:V:345:ILE:HG22 | 2.42 | 0.54 |
| 1:W:34:ILE:HG21 | 1:W:67:LEU:HB3 | 1.90 | 0.54 |
| 1:A:236:LEU:HD12 | 1:A:237:GLU:HG2 | 1.90 | 0.54 |
| 1:E:143:TYR:HD2 | 1:E:346:LEU:HD13 | 1.70 | 0.54 |
| 1:E:223:PHE:CZ | 1:E:266:PHE:HZ | 2.26 | 0.54 |
| 1:G:32:PRO:HG3 | 1:G:59:GLN:NE2 | 2.22 | 0.54 |
| 1:G:34:ILE:HG21 | 1:G:67:LEU:HB3 | 1.90 | 0.54 |
| 1:I:7:ALA:CB | 1:I:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:I:143:TYR:CZ | 1:I:345:ILE:HG22 | 2.42 | 0.54 |
| 1:J:110:LEU:HD12 | 1:J:177:ARG:HH11 | 1.72 | 0.54 |
| 1:J:143:TYR:CZ | 1:J:345:ILE:HG22 | 2.42 | 0.54 |
| 1:K:34:ILE:HG21 | 1:K:67:LEU:HB3 | 1.90 | 0.54 |
| 1:K:223:PHE:CZ | 1:K:266:PHE:HZ | 2.26 | 0.54 |
| 1:L:147:ARG:HG3 | 1:L:147:ARG:NH2 | 2.22 | 0.54 |
| 1:L:236:LEU:HD12 | 1:L:237:GLU:HG2 | 1.90 | 0.54 |
| 1:M:7:ALA:CB | 1:M:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:M:34:ILE:HG21 | 1:M:67:LEU:HB3 | 1.90 | 0.54 |
| 1:O:34:ILE:HG21 | 1:O:67:LEU:HB3 | 1.90 | 0.54 |
| 1:O:37:ARG:CG | 1:O:38:PRO:CD | 2.83 | 0.54 |
| 1:R:147:ARG:NH2 | 1:R:147:ARG:HG3 | 2.22 | 0.54 |
| 1:S:143:TYR:CZ | 1:S:345:ILE:HG22 | 2.42 | 0.54 |
| 1:T:7:ALA:CB | 1:T:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:T:34:ILE:HG21 | 1:T:67:LEU:HB3 | 1.90 | 0.54 |
| 1:V:223:PHE:CZ | 1:V:266:PHE:HZ | 2.26 | 0.54 |
| 1:A:34:ILE:HG21 | 1:A:67:LEU:HB3 | 1.90 | 0.54 |
| 1:A:223:PHE:CZ | 1:A:266:PHE:HZ | 2.26 | 0.54 |
| 1:B:34:ILE:HG21 | 1:B:67:LEU:HB3 | 1.90 | 0.54 |
| 1:B:106:THR:HG22 | 1:B:140:LEU:CD1 | 2.38 | 0.54 |
| 1:C:32:PRO:HG3 | 1:C:59:GLN:NE2 | 2.22 | 0.54 |
| 1:C:34:ILE:HG21 | 1:C:67:LEU:HB3 | 1.90 | 0.54 |
| 1:C:37:ARG:CG | 1:C:38:PRO:CD | 2.83 | 0.54 |
| 1:D:7:ALA:CB | 1:D:347:ALA:HB1 | 2.37 | 0.54 |
| 1:D:54:VAL:O | 1:D:55:GLY:C | 2.45 | 0.54 |
| 1:D:121:GLN:HA | 1:D:362:TYR:OH | 2.07 | 0.54 |
| 1:D:223:PHE:CZ | 1:D:266:PHE:HZ | 2.26 | 0.54 |
| 1:E:8:LEU:HB2 | 1:E:103:THR:OG1 | 2.08 | 0.54 |
| 1:I:54:VAL:O | 1:I:55:GLY:C | 2.45 | 0.54 |
| 1:L:287:ILE:CD1 | 1:N:208:ILE:CD1 | 2.80 | 0.54 |
| 1:O:54:VAL:O | 1:O:55:GLY:C | 2.45 | 0.54 |
| 1:O:147:ARG:HG3 | 1:O:147:ARG:NH2 | 2.22 | 0.54 |
| 1:O:325:MET:HE3 | 1:Q:244:ASP:O | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:106:THR:HG22 | 1:P:140:LEU:CD1 | 2.38 | 0.54 |
| 1:P:223:PHE:CZ | 1:P:266:PHE:HZ | 2.26 | 0.54 |
| 1:Q:7:ALA:CB | 1:Q:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:Q:34:ILE:HG21 | 1:Q:67:LEU:HB3 | 1.90 | 0.54 |
| 1:R:8:LEU:HB2 | 1:R:103:THR:OG1 | 2.08 | 0.54 |
| 1:R:143:TYR:HD2 | 1:R:346:LEU:HD13 | 1.70 | 0.54 |
| 1:R:236:LEU:HD12 | 1:R:237:GLU:CG | 2.37 | 0.54 |
| 1:T:38:PRO:HB2 | 1:T:41:GLN:HB2 | 1.89 | 0.54 |
| 1:B:8:LEU:HB2 | 1:B:103:THR:OG1 | 2.08 | 0.54 |
| 1:D:7:ALA:CB | 1:D:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:D:368:SER:O | 1:D:371:HIS:N | 2.37 | 0.54 |
| 1:E:236:LEU:HD12 | 1:E:237:GLU:HG2 | 1.90 | 0.54 |
| 1:G:236:LEU:HD12 | 1:G:237:GLU:CG | 2.37 | 0.54 |
| 1:H:32:PRO:HG3 | 1:H:59:GLN:NE2 | 2.22 | 0.54 |
| 1:I:8:LEU:HB2 | 1:I:103:THR:OG1 | 2.08 | 0.54 |
| 1:I:106:THR:HG22 | 1:I:140:LEU:CD1 | 2.38 | 0.54 |
| 1:J:7:ALA:CB | 1:J:347:ALA:HB1 | 2.37 | 0.54 |
| 1:J:143:TYR:HD1 | 1:J:143:TYR:C | 2.09 | 0.54 |
| 1:K:106:THR:HG22 | 1:K:140:LEU:CD1 | 2.38 | 0.54 |
| 1:K:236:LEU:HD12 | 1:K:237:GLU:CG | 2.37 | 0.54 |
| 1:L:110:LEU:HD12 | 1:L:177:ARG:HH11 | 1.72 | 0.54 |
| 1:L:223:PHE:CZ | 1:L:266:PHE:HZ | 2.26 | 0.54 |
| 1:O:223:PHE:CZ | 1:O:266:PHE:HZ | 2.26 | 0.54 |
| 1:R:223:PHE:CZ | 1:R:266:PHE:HZ | 2.26 | 0.54 |
| 1:T:223:PHE:CZ | 1:T:266:PHE:HZ | 2.26 | 0.54 |
| 1:W:32:PRO:HG3 | 1:W:59:GLN:NE2 | 2.22 | 0.54 |
| 1:C:8:LEU:HB2 | 1:C:103:THR:OG1 | 2.08 | 0.54 |
| 1:C:140:LEU:HD22 | 1:C:343:GLY:HA2 | 1.90 | 0.54 |
| 1:D:143:TYR:HD1 | 1:D:143:TYR:C | 2.09 | 0.54 |
| 1:F:7:ALA:CB | 1:F:347:ALA:HB1 | 2.37 | 0.54 |
| 1:F:34:ILE:HG21 | 1:F:67:LEU:HB3 | 1.90 | 0.54 |
| 1:F:147:ARG:HG3 | 1:F:147:ARG:NH2 | 2.22 | 0.54 |
| 1:H:360:GLN:O | 1:H:364:GLU:HG3 | 2.08 | 0.54 |
| 1:I:143:TYR:CZ | 1:K:45:VAL:CG2 | 2.88 | 0.54 |
| 1:L:140:LEU:HD22 | 1:L:343:GLY:HA2 | 1.90 | 0.54 |
| 1:M:38:PRO:HB2 | 1:M:41:GLN:HB2 | 1.89 | 0.54 |
| 1:N:147:ARG:CG | 1:N:147:ARG:NH2 | 2.71 | 0.54 |
| 1:P:110:LEU:HD12 | 1:P:177:ARG:HH11 | 1.72 | 0.54 |
| 1:Q:110:LEU:HD12 | 1:Q:177:ARG:HH11 | 1.72 | 0.54 |
| 1:S:7:ALA:CB | 1:S:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:S:34:ILE:HG21 | 1:S:67:LEU:HB3 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:325:MET:HE3 | 1:U:244:ASP:O | 2.08 | 0.54 |
| 1:S:368:SER:O | 1:S:371:HIS:N | 2.37 | 0.54 |
| 1:U:223:PHE:CZ | 1:U:266:PHE:HZ | 2.26 | 0.54 |
| 1:U:236:LEU:HD12 | 1:U:237:GLU:HG2 | 1.90 | 0.54 |
| 1:U:325:MET:HE3 | 1:W:244:ASP:O | 2.07 | 0.54 |
| 1:W:223:PHE:CZ | 1:W:266:PHE:HZ | 2.26 | 0.54 |
| 1:A:147:ARG:HG3 | 1:A:147:ARG:NH2 | 2.22 | 0.54 |
| 1:B:38:PRO:HB2 | 1:B:41:GLN:HB2 | 1.89 | 0.54 |
| 1:B:54:VAL:O | 1:B:55:GLY:C | 2.45 | 0.54 |
| 1:B:143:TYR:CZ | 1:B:345:ILE:HG22 | 2.42 | 0.54 |
| 1:E:300:SER:HA | 1:E:335:ARG:HG2 | 1.89 | 0.54 |
| 1:G:56:ASP:C | 1:G:56:ASP:OD1 | 2.47 | 0.54 |
| 1:G:110:LEU:HD12 | 1:G:177:ARG:HH11 | 1.72 | 0.54 |
| 1:G:360:GLN:O | 1:G:364:GLU:HG3 | 2.08 | 0.54 |
| 1:H:7:ALA:CB | 1:H:347:ALA:HB1 | 2.37 | 0.54 |
| 1:I:236:LEU:HD12 | 1:I:237:GLU:CG | 2.37 | 0.54 |
| 1:K:56:ASP:C | 1:K:56:ASP:OD1 | 2.47 | 0.54 |
| 1:N:34:ILE:HG21 | 1:N:67:LEU:HB3 | 1.90 | 0.54 |
| 1:N:140:LEU:HD22 | 1:N:343:GLY:HA2 | 1.90 | 0.54 |
| 1:O:34:ILE:CG2 | 1:O:67:LEU:HD22 | 2.27 | 0.54 |
| 1:O:38:PRO:HB2 | 1:O:41:GLN:HB2 | 1.89 | 0.54 |
| 1:P:34:ILE:HG21 | 1:P:67:LEU:HB3 | 1.90 | 0.54 |
| 1:P:236:LEU:HD12 | 1:P:237:GLU:HG2 | 1.90 | 0.54 |
| 1:R:140:LEU:HD22 | 1:R:343:GLY:HA2 | 1.90 | 0.54 |
| 1:S:360:GLN:O | 1:S:364:GLU:HG3 | 2.08 | 0.54 |
| 1:S:362:TYR:HE1 | 1:S:367:PRO:CB | 2.19 | 0.54 |
| 1:T:106:THR:HG22 | 1:T:140:LEU:CD1 | 2.38 | 0.54 |
| 1:V:56:ASP:C | 1:V:56:ASP:OD1 | 2.47 | 0.54 |
| 1:V:360:GLN:O | 1:V:364:GLU:HG3 | 2.08 | 0.54 |
| 1:D:8:LEU:HB2 | 1:D:103:THR:OG1 | 2.08 | 0.54 |
| 1:D:116:ARG:HH12 | 1:D:375:PHE:HA | 1.73 | 0.54 |
| 1:E:34:ILE:HG21 | 1:E:67:LEU:HB3 | 1.90 | 0.54 |
| 1:E:38:PRO:HB2 | 1:E:41:GLN:HB2 | 1.89 | 0.54 |
| 1:E:106:THR:HG22 | 1:E:140:LEU:CD1 | 2.38 | 0.54 |
| 1:F:56:ASP:C | 1:F:56:ASP:OD1 | 2.47 | 0.54 |
| 1:F:110:LEU:HD12 | 1:F:177:ARG:HH11 | 1.72 | 0.54 |
| 1:F:223:PHE:CZ | 1:F:266:PHE:HZ | 2.26 | 0.54 |
| 1:F:360:GLN:O | 1:F:364:GLU:HG3 | 2.08 | 0.54 |
| 1:H:135:ALA:HB1 | 1:H:140:LEU:HD21 | 1.90 | 0.54 |
| 1:I:34:ILE:CG2 | 1:I:68:LYS:H | 2.21 | 0.54 |
| 1:J:223:PHE:O | 1:J:227:MET:HG2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:223:PHE:CZ | 1:J:266:PHE:HZ | 2.26 | 0.54 |
| 1:J:236:LEU:HD12 | 1:J:237:GLU:HG2 | 1.90 | 0.54 |
| 1:J:360:GLN:O | 1:J:364:GLU:HG3 | 2.08 | 0.54 |
| 1:L:34:ILE:HG21 | 1:L:67:LEU:HB3 | 1.90 | 0.54 |
| 1:L:325:MET:HE3 | 1:N:244:ASP:O | 2.07 | 0.54 |
| 1:M:223:PHE:O | 1:M:227:MET:HG2 | 2.08 | 0.54 |
| 1:N:8:LEU:HB2 | 1:N:103:THR:OG1 | 2.08 | 0.54 |
| 1:N:325:MET:HE3 | 1:P:244:ASP:O | 2.07 | 0.54 |
| 1:P:8:LEU:HB2 | 1:P:103:THR:OG1 | 2.08 | 0.54 |
| 1:R:7:ALA:CB | 1:R:356:TRP:CZ2 | 2.91 | 0.54 |
| 1:R:32:PRO:CG | 1:R:55:GLY:O | 2.55 | 0.54 |
| 1:R:34:ILE:HG21 | 1:R:67:LEU:HB3 | 1.90 | 0.54 |
| 1:R:56:ASP:OD1 | 1:R:56:ASP:C | 2.47 | 0.54 |
| 1:R:106:THR:HG22 | 1:R:140:LEU:CD1 | 2.38 | 0.54 |
| 1:S:223:PHE:CZ | 1:S:266:PHE:HZ | 2.26 | 0.54 |
| 1:S:236:LEU:HD12 | 1:S:237:GLU:HG2 | 1.90 | 0.54 |
| 1:T:8:LEU:HB2 | 1:T:103:THR:OG1 | 2.08 | 0.54 |
| 1:T:32:PRO:CG | 1:T:55:GLY:O | 2.55 | 0.54 |
| 1:T:236:LEU:HD12 | 1:T:237:GLU:CG | 2.37 | 0.54 |
| 1:U:56:ASP:C | 1:U:56:ASP:OD1 | 2.47 | 0.54 |
| 1:U:147:ARG:NH2 | 1:U:147:ARG:HG3 | 2.22 | 0.54 |
| 1:U:360:GLN:O | 1:U:364:GLU:HG3 | 2.08 | 0.54 |
| 1:V:34:ILE:CG2 | 1:V:68:LYS:H | 2.21 | 0.54 |
| 1:V:236:LEU:HD12 | 1:V:237:GLU:HG2 | 1.90 | 0.54 |
| 1:V:362:TYR:HE1 | 1:V:367:PRO:CB | 2.19 | 0.54 |
| 1:W:106:THR:HG22 | 1:W:140:LEU:CD1 | 2.38 | 0.54 |
| 1:W:110:LEU:HD12 | 1:W:177:ARG:HH11 | 1.72 | 0.54 |
| 1:A:135:ALA:HB1 | 1:A:140:LEU:HD21 | 1.91 | 0.53 |
| 1:A:140:LEU:HD22 | 1:A:343:GLY:HA2 | 1.90 | 0.53 |
| 1:C:56:ASP:C | 1:C:56:ASP:OD1 | 2.47 | 0.53 |
| 1:E:7:ALA:CB | 1:E:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:E:223:PHE:O | 1:E:227:MET:HG2 | 2.09 | 0.53 |
| 1:F:116:ARG:HH12 | 1:F:375:PHE:HA | 1.74 | 0.53 |
| 1:G:147:ARG:HG3 | 1:G:147:ARG:NH2 | 2.22 | 0.53 |
| 1:G:325:MET:HE3 | 1:I:244:ASP:O | 2.07 | 0.53 |
| 1:I:32:PRO:CG | 1:I:55:GLY:O | 2.55 | 0.53 |
| 1:I:116:ARG:HH12 | 1:I:375:PHE:HA | 1.74 | 0.53 |
| 1:I:360:GLN:O | 1:I:364:GLU:HG3 | 2.08 | 0.53 |
| 1:J:38:PRO:HB2 | 1:J:41:GLN:HB2 | 1.89 | 0.53 |
| 1:K:34:ILE:CG2 | 1:K:68:LYS:H | 2.21 | 0.53 |
| 1:L:135:ALA:HB1 | 1:L:140:LEU:HD21 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:362:TYR:HE1 | 1:L:367:PRO:CB | 2.19 | 0.53 |
| 1:M:361:GLU:HB3 | 1:M:369:ILE:CD1 | 2.14 | 0.53 |
| 1:N:135:ALA:HB1 | 1:N:140:LEU:HD21 | 1.91 | 0.53 |
| 1:O:208:ILE:HG22 | 1:O:209:VAL:N | 2.23 | 0.53 |
| 1:Q:8:LEU:HB2 | 1:Q:103:THR:OG1 | 2.08 | 0.53 |
| 1:Q:208:ILE:HG22 | 1:Q:209:VAL:N | 2.23 | 0.53 |
| 1:S:32:PRO:HG3 | 1:S:59:GLN:NE2 | 2.22 | 0.53 |
| 1:S:135:ALA:HB1 | 1:S:140:LEU:HD21 | 1.90 | 0.53 |
| 1:S:208:ILE:HG22 | 1:S:209:VAL:N | 2.23 | 0.53 |
| 1:T:223:PHE:O | 1:T:227:MET:HG2 | 2.08 | 0.53 |
| 1:W:360:GLN:O | 1:W:364:GLU:HG3 | 2.08 | 0.53 |
| 1:C:106:THR:HG22 | 1:C:140:LEU:CD1 | 2.38 | 0.53 |
| 1:D:56:ASP:C | 1:D:56:ASP:OD1 | 2.47 | 0.53 |
| 1:D:173:HIS:CE1 | 1:E:267:ILE:C | 2.82 | 0.53 |
| 1:E:140:LEU:HD22 | 1:E:343:GLY:HA2 | 1.90 | 0.53 |
| 1:G:32:PRO:CG | 1:G:55:GLY:O | 2.55 | 0.53 |
| 1:G:223:PHE:CZ | 1:G:266:PHE:HZ | 2.26 | 0.53 |
| 1:H:38:PRO:HB2 | 1:H:41:GLN:HB2 | 1.89 | 0.53 |
| 1:I:143:TYR:HD2 | 1:I:346:LEU:HD13 | 1.70 | 0.53 |
| 1:J:56:ASP:OD1 | 1:J:56:ASP:C | 2.47 | 0.53 |
| 1:J:147:ARG:CG | 1:J:147:ARG:NH2 | 2.71 | 0.53 |
| 1:L:7:ALA:CB | 1:L:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:L:223:PHE:O | 1:L:227:MET:HG2 | 2.08 | 0.53 |
| 1:L:360:GLN:O | 1:L:364:GLU:HG3 | 2.08 | 0.53 |
| 1:M:208:ILE:HG22 | 1:M:209:VAL:N | 2.23 | 0.53 |
| 1:O:362:TYR:HE1 | 1:O:367:PRO:CB | 2.19 | 0.53 |
| 1:P:140:LEU:HD22 | 1:P:343:GLY:HA2 | 1.90 | 0.53 |
| 1:P:143:TYR:HD2 | 1:P:346:LEU:HD13 | 1.70 | 0.53 |
| 1:P:173:HIS:CE1 | 1:Q:267:ILE:C | 2.82 | 0.53 |
| 1:Q:38:PRO:HB2 | 1:Q:41:GLN:HB2 | 1.89 | 0.53 |
| 1:Q:56:ASP:C | 1:Q:56:ASP:OD1 | 2.47 | 0.53 |
| 1:Q:223:PHE:O | 1:Q:227:MET:HG2 | 2.08 | 0.53 |
| 1:Q:360:GLN:O | 1:Q:364:GLU:HG3 | 2.08 | 0.53 |
| 1:R:38:PRO:HB2 | 1:R:41:GLN:HB2 | 1.89 | 0.53 |
| 1:U:7:ALA:CB | 1:U:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:U:135:ALA:HB1 | 1:U:140:LEU:HD21 | 1.91 | 0.53 |
| 1:U:208:ILE:HG22 | 1:U:209:VAL:N | 2.23 | 0.53 |
| 1:W:140:LEU:HD22 | 1:W:343:GLY:HA2 | 1.90 | 0.53 |
| 1:W:361:GLU:HB3 | 1:W:369:ILE:CD1 | 2.14 | 0.53 |
| 1:B:34:ILE:CG2 | 1:B:68:LYS:H | 2.21 | 0.53 |
| 1:B:143:TYR:CD1 | 1:B:143:TYR:C | 2.75 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:7:ALA:CB | 1:C:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:C:223:PHE:O | 1:C:227:MET:HG2 | 2.08 | 0.53 |
| 1:D:236:LEU:HD12 | 1:D:237:GLU:HG2 | 1.90 | 0.53 |
| 1:D:360:GLN:O | 1:D:364:GLU:HG3 | 2.08 | 0.53 |
| 1:G:7:ALA:CB | 1:G:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:G:116:ARG:HH12 | 1:G:375:PHE:HA | 1.74 | 0.53 |
| 1:G:236:LEU:HD12 | 1:G:237:GLU:HG2 | 1.90 | 0.53 |
| 1:G:336:LYS:HE2 | 2:G:401:ADP:C5' | 2.38 | 0.53 |
| 1:I:173:HIS:CE1 | 1:J:267:ILE:C | 2.82 | 0.53 |
| 1:I:223:PHE:CZ | 1:I:266:PHE:HZ | 2.26 | 0.53 |
| 1:I:223:PHE:O | 1:I:227:MET:HG2 | 2.08 | 0.53 |
| 1:K:54:VAL:O | 1:K:55:GLY:C | 2.45 | 0.53 |
| 1:K:116:ARG:HH12 | 1:K:375:PHE:HA | 1.74 | 0.53 |
| 1:N:56:ASP:C | 1:N:56:ASP:OD1 | 2.47 | 0.53 |
| 1:O:56:ASP:C | 1:O:56:ASP:OD1 | 2.47 | 0.53 |
| 1:O:142:LEU:HD21 | 1:O:165:ILE:CD1 | 2.38 | 0.53 |
| 1:P:360:GLN:O | 1:P:364:GLU:HG3 | 2.08 | 0.53 |
| 1:Q:143:TYR:CZ | 1:Q:345:ILE:HG22 | 2.42 | 0.53 |
| 1:R:173:HIS:CE1 | 1:S:267:ILE:C | 2.82 | 0.53 |
| 1:S:8:LEU:HB2 | 1:S:103:THR:OG1 | 2.08 | 0.53 |
| 1:S:106:THR:HG22 | 1:S:140:LEU:CD1 | 2.38 | 0.53 |
| 1:S:173:HIS:CE1 | 1:T:267:ILE:C | 2.82 | 0.53 |
| 1:S:223:PHE:O | 1:S:227:MET:HG2 | 2.09 | 0.53 |
| 1:T:173:HIS:CE1 | 1:U:267:ILE:C | 2.82 | 0.53 |
| 1:U:106:THR:HG22 | 1:U:140:LEU:CD1 | 2.38 | 0.53 |
| 1:U:336:LYS:HE2 | 2:U:401:ADP:C5' | 2.38 | 0.53 |
| 1:V:223:PHE:O | 1:V:227:MET:HG2 | 2.08 | 0.53 |
| 1:A:173:HIS:CE1 | 1:B:267:ILE:C | 2.82 | 0.53 |
| 1:B:223:PHE:O | 1:B:227:MET:HG2 | 2.08 | 0.53 |
| 1:B:236:LEU:HD12 | 1:B:237:GLU:HG2 | 1.90 | 0.53 |
| 1:E:173:HIS:CE1 | 1:F:267:ILE:C | 2.82 | 0.53 |
| 1:E:360:GLN:O | 1:E:364:GLU:HG3 | 2.08 | 0.53 |
| 1:F:7:ALA:CB | 1:F:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:F:135:ALA:HB1 | 1:F:140:LEU:HD21 | 1.91 | 0.53 |
| 1:H:142:LEU:HD21 | 1:H:165:ILE:CD1 | 2.38 | 0.53 |
| 1:H:223:PHE:CZ | 1:H:266:PHE:HZ | 2.26 | 0.53 |
| 1:I:110:LEU:HD12 | 1:I:177:ARG:HH11 | 1.72 | 0.53 |
| 1:J:135:ALA:HB1 | 1:J:140:LEU:HD21 | 1.91 | 0.53 |
| 1:L:38:PRO:HB2 | 1:L:41:GLN:HB2 | 1.89 | 0.53 |
| 1:M:34:ILE:CG2 | 1:M:68:LYS:H | 2.21 | 0.53 |
| 1:N:7:ALA:CB | 1:N:356:TRP:CZ2 | 2.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:173:HIS:CE1 | 1:P:267:ILE:C | 2.82 | 0.53 |
| 1:S:56:ASP:C | 1:S:56:ASP:OD1 | 2.47 | 0.53 |
| 1:T:34:ILE:CG2 | 1:T:68:LYS:H | 2.21 | 0.53 |
| 1:T:208:ILE:HG22 | 1:T:209:VAL:N | 2.23 | 0.53 |
| 1:V:147:ARG:NH2 | 1:V:147:ARG:HG3 | 2.22 | 0.53 |
| 1:W:38:PRO:HB2 | 1:W:41:GLN:HB2 | 1.89 | 0.53 |
| 1:A:7:ALA:CB | 1:A:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:B:56:ASP:OD1 | 1:B:56:ASP:C | 2.47 | 0.53 |
| 1:B:116:ARG:HH12 | 1:B:375:PHE:HA | 1.74 | 0.53 |
| 1:C:143:TYR:HD1 | 1:C:143:TYR:C | 2.09 | 0.53 |
| 1:D:38:PRO:HB2 | 1:D:41:GLN:HB2 | 1.89 | 0.53 |
| 1:D:223:PHE:O | 1:D:227:MET:HG2 | 2.09 | 0.53 |
| 1:F:173:HIS:CE1 | 1:G:267:ILE:C | 2.82 | 0.53 |
| 1:G:34:ILE:CG2 | 1:G:68:LYS:H | 2.21 | 0.53 |
| 1:G:140:LEU:HD22 | 1:G:343:GLY:HA2 | 1.90 | 0.53 |
| 1:H:140:LEU:HD22 | 1:H:343:GLY:HA2 | 1.90 | 0.53 |
| 1:H:173:HIS:CE1 | 1:I:267:ILE:C | 2.82 | 0.53 |
| 1:H:223:PHE:O | 1:H:227:MET:HG2 | 2.08 | 0.53 |
| 1:J:7:ALA:CB | 1:J:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:J:140:LEU:HD22 | 1:J:343:GLY:HA2 | 1.90 | 0.53 |
| 1:K:147:ARG:NH2 | 1:K:147:ARG:HG3 | 2.22 | 0.53 |
| 1:K:223:PHE:O | 1:K:227:MET:HG2 | 2.08 | 0.53 |
| 1:L:8:LEU:HB2 | 1:L:103:THR:OG1 | 2.08 | 0.53 |
| 1:L:37:ARG:CG | 1:L:38:PRO:CD | 2.83 | 0.53 |
| 1:M:360:GLN:O | 1:M:364:GLU:HG3 | 2.08 | 0.53 |
| 1:N:173:HIS:CE1 | 1:O:267:ILE:C | 2.82 | 0.53 |
| 1:N:360:GLN:O | 1:N:364:GLU:HG3 | 2.08 | 0.53 |
| 1:O:116:ARG:HH12 | 1:O:375:PHE:HA | 1.74 | 0.53 |
| 1:O:360:GLN:O | 1:O:364:GLU:HG3 | 2.08 | 0.53 |
| 1:P:38:PRO:HB2 | 1:P:41:GLN:HB2 | 1.89 | 0.53 |
| 1:P:147:ARG:NH2 | 1:P:147:ARG:HG3 | 2.22 | 0.53 |
| 1:Q:106:THR:HG22 | 1:Q:140:LEU:CD1 | 2.38 | 0.53 |
| 1:Q:116:ARG:HH12 | 1:Q:375:PHE:HA | 1.74 | 0.53 |
| 1:Q:147:ARG:HG3 | 1:Q:147:ARG:NH2 | 2.22 | 0.53 |
| 1:R:37:ARG:CG | 1:R:38:PRO:CD | 2.83 | 0.53 |
| 1:R:223:PHE:O | 1:R:227:MET:HG2 | 2.09 | 0.53 |
| 1:T:140:LEU:HD22 | 1:T:343:GLY:HA2 | 1.90 | 0.53 |
| 1:T:360:GLN:O | 1:T:364:GLU:HG3 | 2.08 | 0.53 |
| 1:V:54:VAL:O | 1:V:55:GLY:C | 2.45 | 0.53 |
| 1:W:7:ALA:CB | 1:W:356:TRP:CZ2 | 2.91 | 0.53 |
| 1:W:208:ILE:HG22 | 1:W:209:VAL:N | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:8:LEU:HB2 | 1:A:103:THR:OG1 | 2.08 | 0.53 |
| 1:A:362:TYR:HE1 | 1:A:367:PRO:CB | 2.19 | 0.53 |
| 1:C:135:ALA:HB1 | 1:C:140:LEU:HD21 | 1.91 | 0.53 |
| 1:D:110:LEU:HD12 | 1:D:177:ARG:HH11 | 1.72 | 0.53 |
| 1:F:38:PRO:HB2 | 1:F:41:GLN:HB2 | 1.89 | 0.53 |
| 1:F:147:ARG:CG | 1:F:147:ARG:NH2 | 2.71 | 0.53 |
| 1:G:223:PHE:O | 1:G:227:MET:HG2 | 2.08 | 0.53 |
| 1:H:116:ARG:HH12 | 1:H:375:PHE:HA | 1.74 | 0.53 |
| 1:H:236:LEU:HD12 | 1:H:237:GLU:HG2 | 1.90 | 0.53 |
| 1:O:106:THR:HG22 | 1:O:140:LEU:CD1 | 2.38 | 0.53 |
| 1:O:236:LEU:HD12 | 1:O:237:GLU:HG2 | 1.90 | 0.53 |
| 1:O:368:SER:O | 1:O:371:HIS:N | 2.37 | 0.53 |
| 1:Q:236:LEU:HD12 | 1:Q:237:GLU:HG2 | 1.90 | 0.53 |
| 1:S:336:LYS:HE2 | 2:S:401:ADP:C5' | 2.38 | 0.53 |
| 1:U:147:ARG:CG | 1:U:147:ARG:NH2 | 2.71 | 0.53 |
| 1:U:173:HIS:CE1 | 1:V:267:ILE:C | 2.82 | 0.53 |
| 1:V:142:LEU:HD21 | 1:V:165:ILE:CD1 | 2.38 | 0.53 |
| 1:W:37:ARG:CG | 1:W:38:PRO:CD | 2.83 | 0.53 |
| 1:W:135:ALA:HB1 | 1:W:140:LEU:HD21 | 1.91 | 0.53 |
| 1:W:147:ARG:CG | 1:W:147:ARG:NH2 | 2.71 | 0.53 |
| 1:A:32:PRO:CG | 1:A:55:GLY:O | 2.55 | 0.53 |
| 1:A:360:GLN:O | 1:A:364:GLU:HG3 | 2.08 | 0.53 |
| 1:C:32:PRO:CG | 1:C:55:GLY:O | 2.55 | 0.53 |
| 1:C:38:PRO:HB2 | 1:C:41:GLN:HB2 | 1.90 | 0.53 |
| 1:D:34:ILE:CG2 | 1:D:68:LYS:H | 2.21 | 0.53 |
| 1:E:34:ILE:CG2 | 1:E:67:LEU:HD22 | 2.27 | 0.53 |
| 1:E:135:ALA:HB1 | 1:E:140:LEU:HD21 | 1.91 | 0.53 |
| 1:F:236:LEU:HD12 | 1:F:237:GLU:HG2 | 1.90 | 0.53 |
| 1:H:56:ASP:C | 1:H:56:ASP:OD1 | 2.47 | 0.53 |
| 1:H:143:TYR:CE2 | 1:J:45:VAL:HG21 | 2.44 | 0.53 |
| 1:I:37:ARG:CG | 1:I:38:PRO:CD | 2.83 | 0.53 |
| 1:I:208:ILE:HG22 | 1:I:209:VAL:N | 2.24 | 0.53 |
| 1:I:336:LYS:HE2 | 2:I:401:ADP:C5' | 2.38 | 0.53 |
| 1:J:299:MET:HE1 | 1:J:304:THR:HB | 1.91 | 0.53 |
| 1:K:173:HIS:CE1 | 1:L:267:ILE:C | 2.82 | 0.53 |
| 1:M:54:VAL:O | 1:M:55:GLY:C | 2.45 | 0.53 |
| 1:M:56:ASP:C | 1:M:56:ASP:OD1 | 2.47 | 0.53 |
| 1:M:116:ARG:HH12 | 1:M:375:PHE:HA | 1.74 | 0.53 |
| 1:M:143:TYR:CE2 | 1:O:45:VAL:HG21 | 2.44 | 0.53 |
| 1:M:236:LEU:HD12 | 1:M:237:GLU:HG2 | 1.90 | 0.53 |
| 1:N:110:LEU:HD12 | 1:N:177:ARG:HH11 | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:223:PHE:O | 1:N:227:MET:HG2 | 2.08 | 0.53 |
| 1:P:135:ALA:HB1 | 1:P:140:LEU:HD21 | 1.91 | 0.53 |
| 1:R:34:ILE:CG2 | 1:R:68:LYS:H | 2.21 | 0.53 |
| 1:R:135:ALA:HB1 | 1:R:140:LEU:HD21 | 1.91 | 0.53 |
| 1:R:236:LEU:HD12 | 1:R:237:GLU:HG2 | 1.90 | 0.53 |
| 1:T:236:LEU:HD12 | 1:T:237:GLU:HG2 | 1.90 | 0.53 |
| 1:U:8:LEU:HB2 | 1:U:103:THR:OG1 | 2.08 | 0.53 |
| 1:W:34:ILE:CG2 | 1:W:68:LYS:H | 2.21 | 0.53 |
| 1:W:223:PHE:O | 1:W:227:MET:HG2 | 2.08 | 0.53 |
| 1:A:37:ARG:CG | 1:A:38:PRO:CD | 2.83 | 0.53 |
| 1:A:106:THR:HG22 | 1:A:140:LEU:CD1 | 2.38 | 0.53 |
| 1:B:208:ILE:HG22 | 1:B:209:VAL:N | 2.23 | 0.53 |
| 1:C:173:HIS:CE1 | 1:D:267:ILE:C | 2.82 | 0.53 |
| 1:D:208:ILE:HG22 | 1:D:209:VAL:N | 2.23 | 0.53 |
| 1:E:56:ASP:C | 1:E:56:ASP:OD1 | 2.47 | 0.53 |
| 1:E:116:ARG:HH12 | 1:E:375:PHE:HA | 1.74 | 0.53 |
| 1:F:143:TYR:CE2 | 1:H:45:VAL:HG21 | 2.44 | 0.53 |
| 1:G:106:THR:HG22 | 1:G:140:LEU:CD1 | 2.38 | 0.53 |
| 1:G:173:HIS:CE1 | 1:H:267:ILE:C | 2.82 | 0.53 |
| 1:H:8:LEU:HB2 | 1:H:103:THR:OG1 | 2.08 | 0.53 |
| 1:I:147:ARG:HG3 | 1:I:147:ARG:NH2 | 2.22 | 0.53 |
| 1:I:236:LEU:HD12 | 1:I:237:GLU:HG2 | 1.90 | 0.53 |
| 1:L:300:SER:HA | 1:L:335:ARG:HG2 | 1.89 | 0.53 |
| 1:M:173:HIS:CE1 | 1:N:267:ILE:C | 2.82 | 0.53 |
| 1:P:32:PRO:CG | 1:P:55:GLY:O | 2.55 | 0.53 |
| 1:P:37:ARG:CG | 1:P:38:PRO:CD | 2.83 | 0.53 |
| 1:Q:135:ALA:HB1 | 1:Q:140:LEU:HD21 | 1.90 | 0.53 |
| 1:Q:223:PHE:CZ | 1:Q:266:PHE:HZ | 2.26 | 0.53 |
| 1:S:110:LEU:HD12 | 1:S:177:ARG:HH11 | 1.72 | 0.53 |
| 1:T:135:ALA:HB1 | 1:T:140:LEU:HD21 | 1.91 | 0.53 |
| 1:V:140:LEU:HD22 | 1:V:343:GLY:HA2 | 1.90 | 0.53 |
| 1:V:361:GLU:HB3 | 1:V:369:ILE:CD1 | 2.14 | 0.53 |
| 1:W:8:LEU:HB2 | 1:W:103:THR:OG1 | 2.08 | 0.53 |
| 1:B:360:GLN:O | 1:B:364:GLU:HG3 | 2.08 | 0.53 |
| 1:E:147:ARG:CG | 1:E:147:ARG:NH2 | 2.71 | 0.53 |
| 1:F:208:ILE:HG22 | 1:F:209:VAL:N | 2.24 | 0.53 |
| 1:G:135:ALA:HB1 | 1:G:140:LEU:HD21 | 1.90 | 0.53 |
| 1:H:208:ILE:HG22 | 1:H:209:VAL:N | 2.23 | 0.53 |
| 1:I:140:LEU:HD22 | 1:I:343:GLY:HA2 | 1.90 | 0.53 |
| 1:J:173:HIS:CE1 | 1:K:267:ILE:C | 2.82 | 0.53 |
| 1:K:34:ILE:CG2 | 1:K:67:LEU:HD22 | 2.27 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:236:LEU:HD12 | 1:K:237:GLU:HG2 | 1.90 | 0.53 |
| 1:K:362:TYR:HE1 | 1:K:367:PRO:CB | 2.19 | 0.53 |
| 1:M:142:LEU:HD21 | 1:M:165:ILE:CD1 | 2.38 | 0.53 |
| 1:N:38:PRO:HB2 | 1:N:41:GLN:HB2 | 1.89 | 0.53 |
| 1:O:34:ILE:CG2 | 1:O:68:LYS:H | 2.21 | 0.53 |
| 1:O:143:TYR:CE2 | 1:Q:45:VAL:HG21 | 2.44 | 0.53 |
| 1:Q:173:HIS:CE1 | 1:R:267:ILE:C | 2.82 | 0.53 |
| 1:T:299:MET:HE1 | 1:T:304:THR:HB | 1.91 | 0.53 |
| 1:U:38:PRO:HB2 | 1:U:41:GLN:HB2 | 1.89 | 0.53 |
| 1:U:143:TYR:CE2 | 1:W:45:VAL:HG21 | 2.44 | 0.53 |
| 1:V:32:PRO:CG | 1:V:55:GLY:O | 2.55 | 0.53 |
| 1:V:173:HIS:CE1 | 1:W:267:ILE:C | 2.82 | 0.53 |
| 1:A:38:PRO:HB2 | 1:A:41:GLN:HB2 | 1.90 | 0.53 |
| 1:A:56:ASP:C | 1:A:56:ASP:OD1 | 2.47 | 0.53 |
| 1:B:135:ALA:HB1 | 1:B:140:LEU:HD21 | 1.91 | 0.53 |
| 1:B:173:HIS:CE1 | 1:C:267:ILE:C | 2.82 | 0.53 |
| 1:C:142:LEU:HD21 | 1:C:165:ILE:CD1 | 2.39 | 0.53 |
| 1:C:300:SER:HA | 1:C:335:ARG:HG2 | 1.89 | 0.53 |
| 1:J:8:LEU:HB2 | 1:J:103:THR:OG1 | 2.08 | 0.53 |
| 1:J:208:ILE:HG22 | 1:J:209:VAL:N | 2.23 | 0.53 |
| 1:J:368:SER:O | 1:J:371:HIS:N | 2.37 | 0.53 |
| 1:K:32:PRO:CG | 1:K:55:GLY:O | 2.55 | 0.53 |
| 1:K:208:ILE:HG22 | 1:K:209:VAL:N | 2.24 | 0.53 |
| 1:L:173:HIS:CE1 | 1:M:267:ILE:C | 2.82 | 0.53 |
| 1:M:8:LEU:HB2 | 1:M:103:THR:OG1 | 2.08 | 0.53 |
| 1:M:106:THR:HG22 | 1:M:140:LEU:CD1 | 2.38 | 0.53 |
| 1:N:34:ILE:CG2 | 1:N:68:LYS:H | 2.21 | 0.53 |
| 1:O:140:LEU:HD22 | 1:O:343:GLY:HA2 | 1.90 | 0.53 |
| 1:T:34:ILE:CG2 | 1:T:67:LEU:HD22 | 2.28 | 0.53 |
| 1:V:106:THR:HG22 | 1:V:140:LEU:CD1 | 2.38 | 0.53 |
| 1:W:56:ASP:C | 1:W:56:ASP:OD1 | 2.47 | 0.53 |
| 1:B:147:ARG:NH2 | 1:B:147:ARG:HG3 | 2.22 | 0.52 |
| 1:B:169:TYR:CZ | 1:B:172:PRO:HD3 | 2.45 | 0.52 |
| 1:D:135:ALA:HB1 | 1:D:140:LEU:HD21 | 1.91 | 0.52 |
| 1:D:169:TYR:CZ | 1:D:172:PRO:HD3 | 2.45 | 0.52 |
| 1:E:32:PRO:CG | 1:E:55:GLY:O | 2.55 | 0.52 |
| 1:F:142:LEU:HD21 | 1:F:165:ILE:CD1 | 2.39 | 0.52 |
| 1:H:7:ALA:CB | 1:H:356:TRP:CZ2 | 2.91 | 0.52 |
| 1:H:300:SER:HA | 1:H:335:ARG:HG2 | 1.89 | 0.52 |
| 1:H:362:TYR:HE1 | 1:H:367:PRO:CB | 2.19 | 0.52 |
| 1:J:116:ARG:HH12 | 1:J:375:PHE:HA | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:300:SER:HA | 1:J:335:ARG:HG2 | 1.89 | 0.52 |
| 1:O:135:ALA:HB1 | 1:O:140:LEU:HD21 | 1.91 | 0.52 |
| 1:P:34:ILE:CG2 | 1:P:68:LYS:H | 2.21 | 0.52 |
| 1:P:56:ASP:C | 1:P:56:ASP:OD1 | 2.47 | 0.52 |
| 1:P:208:ILE:HG22 | 1:P:209:VAL:N | 2.23 | 0.52 |
| 1:S:38:PRO:HB2 | 1:S:41:GLN:HB2 | 1.89 | 0.52 |
| 1:S:116:ARG:HH12 | 1:S:375:PHE:HA | 1.74 | 0.52 |
| 1:U:140:LEU:HD22 | 1:U:343:GLY:HA2 | 1.90 | 0.52 |
| 1:V:336:LYS:HE2 | 2:V:401:ADP:C5' | 2.38 | 0.52 |
| 1:A:142:LEU:HD21 | 1:A:165:ILE:CD1 | 2.39 | 0.52 |
| 1:A:223:PHE:O | 1:A:227:MET:HG2 | 2.08 | 0.52 |
| 1:B:140:LEU:HD22 | 1:B:343:GLY:HA2 | 1.90 | 0.52 |
| 1:B:336:LYS:HE2 | 2:B:401:ADP:C5' | 2.38 | 0.52 |
| 1:C:360:GLN:O | 1:C:364:GLU:HG3 | 2.08 | 0.52 |
| 1:D:300:SER:HA | 1:D:335:ARG:HG2 | 1.89 | 0.52 |
| 1:D:336:LYS:HE2 | 2:D:401:ADP:C5' | 2.38 | 0.52 |
| 1:D:361:GLU:HB3 | 1:D:369:ILE:CD1 | 2.14 | 0.52 |
| 1:E:34:ILE:CG2 | 1:E:68:LYS:H | 2.21 | 0.52 |
| 1:F:300:SER:HA | 1:F:335:ARG:HG2 | 1.89 | 0.52 |
| 1:G:143:TYR:HD2 | 1:G:346:LEU:HD13 | 1.70 | 0.52 |
| 1:I:56:ASP:C | 1:I:56:ASP:OD1 | 2.47 | 0.52 |
| 1:J:143:TYR:CE2 | 1:L:45:VAL:HG21 | 2.44 | 0.52 |
| 1:J:169:TYR:CZ | 1:J:172:PRO:HD3 | 2.45 | 0.52 |
| 1:K:143:TYR:CE2 | 1:M:45:VAL:HG21 | 2.44 | 0.52 |
| 1:L:56:ASP:C | 1:L:56:ASP:OD1 | 2.47 | 0.52 |
| 1:M:169:TYR:CZ | 1:M:172:PRO:HD3 | 2.45 | 0.52 |
| 1:P:7:ALA:CB | 1:P:356:TRP:CZ2 | 2.91 | 0.52 |
| 1:Q:147:ARG:CG | 1:Q:147:ARG:NH2 | 2.71 | 0.52 |
| 1:S:140:LEU:HD22 | 1:S:343:GLY:HA2 | 1.90 | 0.52 |
| 1:S:169:TYR:CZ | 1:S:172:PRO:HD3 | 2.45 | 0.52 |
| 1:T:56:ASP:C | 1:T:56:ASP:OD1 | 2.47 | 0.52 |
| 1:T:142:LEU:HD21 | 1:T:165:ILE:CD1 | 2.38 | 0.52 |
| 1:U:34:ILE:CG2 | 1:U:68:LYS:H | 2.21 | 0.52 |
| 1:W:54:VAL:CG1 | 1:W:55:GLY:N | 2.72 | 0.52 |
| 1:A:208:ILE:HG22 | 1:A:209:VAL:N | 2.23 | 0.52 |
| 1:C:362:TYR:HE1 | 1:C:367:PRO:CB | 2.19 | 0.52 |
| 1:D:37:ARG:CG | 1:D:38:PRO:CD | 2.83 | 0.52 |
| 1:D:143:TYR:CE2 | 1:F:45:VAL:HG21 | 2.44 | 0.52 |
| 1:D:299:MET:HE1 | 1:D:304:THR:HB | 1.91 | 0.52 |
| 1:E:147:ARG:NH2 | 1:E:147:ARG:HG3 | 2.22 | 0.52 |
| 1:F:8:LEU:HB2 | 1:F:103:THR:OG1 | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:34:ILE:CG2 | 1:F:68:LYS:H | 2.21 | 0.52 |
| 1:F:336:LYS:HE2 | 2:F:401:ADP:C5' | 2.38 | 0.52 |
| 1:G:208:ILE:HG22 | 1:G:209:VAL:N | 2.23 | 0.52 |
| 1:K:169:TYR:CZ | 1:K:172:PRO:HD3 | 2.45 | 0.52 |
| 1:L:147:ARG:CG | 1:L:147:ARG:NH2 | 2.71 | 0.52 |
| 1:M:147:ARG:NH2 | 1:M:147:ARG:HG3 | 2.22 | 0.52 |
| 1:N:143:TYR:CE2 | 1:P:45:VAL:HG21 | 2.44 | 0.52 |
| 1:O:223:PHE:O | 1:O:227:MET:HG2 | 2.08 | 0.52 |
| 1:Q:34:ILE:CG2 | 1:Q:68:LYS:H | 2.21 | 0.52 |
| 1:Q:169:TYR:CZ | 1:Q:172:PRO:HD3 | 2.45 | 0.52 |
| 1:R:208:ILE:HG22 | 1:R:209:VAL:N | 2.23 | 0.52 |
| 1:R:362:TYR:HE1 | 1:R:367:PRO:CB | 2.19 | 0.52 |
| 1:S:37:ARG:CG | 1:S:38:PRO:CD | 2.83 | 0.52 |
| 1:T:169:TYR:CZ | 1:T:172:PRO:HD3 | 2.45 | 0.52 |
| 1:T:362:TYR:HD1 | 1:T:367:PRO:HA | 1.75 | 0.52 |
| 1:V:362:TYR:HD1 | 1:V:367:PRO:HA | 1.75 | 0.52 |
| 1:A:143:TYR:CE2 | 1:C:45:VAL:HG21 | 2.44 | 0.52 |
| 1:B:110:LEU:HD12 | 1:B:177:ARG:HH11 | 1.72 | 0.52 |
| 1:C:116:ARG:HH12 | 1:C:375:PHE:HA | 1.74 | 0.52 |
| 1:D:140:LEU:HD22 | 1:D:343:GLY:HA2 | 1.90 | 0.52 |
| 1:E:362:TYR:HD1 | 1:E:367:PRO:HA | 1.75 | 0.52 |
| 1:G:54:VAL:CG1 | 1:G:55:GLY:N | 2.72 | 0.52 |
| 1:J:164:PRO:HG3 | 1:J:174:ALA:HB1 | 1.92 | 0.52 |
| 1:K:336:LYS:HE2 | 2:K:401:ADP:C5' | 2.38 | 0.52 |
| 1:K:360:GLN:O | 1:K:364:GLU:HG3 | 2.08 | 0.52 |
| 1:L:208:ILE:HG22 | 1:L:209:VAL:N | 2.23 | 0.52 |
| 1:M:37:ARG:CG | 1:M:38:PRO:CD | 2.83 | 0.52 |
| 1:M:135:ALA:HB1 | 1:M:140:LEU:HD21 | 1.91 | 0.52 |
| 1:M:362:TYR:HD1 | 1:M:367:PRO:HA | 1.75 | 0.52 |
| 1:P:147:ARG:CG | 1:P:147:ARG:NH2 | 2.71 | 0.52 |
| 1:Q:37:ARG:CG | 1:Q:38:PRO:CD | 2.83 | 0.52 |
| 1:Q:336:LYS:HE2 | 2:Q:401:ADP:C5' | 2.38 | 0.52 |
| 1:R:360:GLN:O | 1:R:364:GLU:HG3 | 2.08 | 0.52 |
| 1:T:143:TYR:CE2 | 1:V:45:VAL:HG21 | 2.44 | 0.52 |
| 1:T:147:ARG:HG3 | 1:T:147:ARG:NH2 | 2.22 | 0.52 |
| 1:U:223:PHE:O | 1:U:227:MET:HG2 | 2.08 | 0.52 |
| 1:B:300:SER:HA | 1:B:335:ARG:HG2 | 1.89 | 0.52 |
| 1:C:208:ILE:HG22 | 1:C:209:VAL:N | 2.23 | 0.52 |
| 1:E:169:TYR:CZ | 1:E:172:PRO:HD3 | 2.45 | 0.52 |
| 1:G:143:TYR:CE2 | 1:I:45:VAL:HG21 | 2.44 | 0.52 |
| 1:I:135:ALA:HB1 | 1:I:140:LEU:HD21 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:34:ILE:CG2 | 1:L:68:LYS:H | 2.21 | 0.52 |
| 1:L:169:TYR:CZ | 1:L:172:PRO:HD3 | 2.44 | 0.52 |
| 1:P:223:PHE:O | 1:P:227:MET:HG2 | 2.08 | 0.52 |
| 1:P:362:TYR:HD1 | 1:P:367:PRO:HA | 1.75 | 0.52 |
| 1:T:143:TYR:HD1 | 1:T:143:TYR:C | 2.09 | 0.52 |
| 1:U:116:ARG:HH12 | 1:U:375:PHE:HA | 1.74 | 0.52 |
| 1:V:135:ALA:HB1 | 1:V:140:LEU:HD21 | 1.91 | 0.52 |
| 1:W:116:ARG:HH12 | 1:W:375:PHE:HA | 1.74 | 0.52 |
| 1:A:34:ILE:CG2 | 1:A:68:LYS:H | 2.21 | 0.52 |
| 1:A:147:ARG:CG | 1:A:147:ARG:NH2 | 2.71 | 0.52 |
| 1:C:169:TYR:CZ | 1:C:172:PRO:HD3 | 2.45 | 0.52 |
| 1:D:362:TYR:HD1 | 1:D:367:PRO:HA | 1.74 | 0.52 |
| 1:E:143:TYR:CE2 | 1:G:45:VAL:HG21 | 2.44 | 0.52 |
| 1:F:169:TYR:CZ | 1:F:172:PRO:HD3 | 2.45 | 0.52 |
| 1:F:223:PHE:O | 1:F:227:MET:HG2 | 2.09 | 0.52 |
| 1:F:362:TYR:HD1 | 1:F:367:PRO:HA | 1.75 | 0.52 |
| 1:H:34:ILE:CG2 | 1:H:68:LYS:H | 2.21 | 0.52 |
| 1:H:37:ARG:CG | 1:H:38:PRO:CD | 2.83 | 0.52 |
| 1:H:169:TYR:CZ | 1:H:172:PRO:HD3 | 2.45 | 0.52 |
| 1:K:39:ARG:NE | 1:K:66:THR:CA | 2.69 | 0.52 |
| 1:K:362:TYR:HD1 | 1:K:367:PRO:HA | 1.75 | 0.52 |
| 1:L:116:ARG:HH12 | 1:L:375:PHE:HA | 1.74 | 0.52 |
| 1:L:164:PRO:HG3 | 1:L:174:ALA:HB1 | 1.92 | 0.52 |
| 1:M:140:LEU:HD22 | 1:M:343:GLY:HA2 | 1.90 | 0.52 |
| 1:N:208:ILE:HG22 | 1:N:209:VAL:N | 2.23 | 0.52 |
| 1:P:143:TYR:CE2 | 1:R:45:VAL:HG21 | 2.44 | 0.52 |
| 1:Q:143:TYR:CE2 | 1:S:45:VAL:HG21 | 2.44 | 0.52 |
| 1:R:169:TYR:CZ | 1:R:172:PRO:HD3 | 2.45 | 0.52 |
| 1:S:143:TYR:CE2 | 1:U:45:VAL:HG21 | 2.44 | 0.52 |
| 1:T:336:LYS:HE2 | 2:T:401:ADP:C5' | 2.38 | 0.52 |
| 1:V:164:PRO:HG2 | 1:V:174:ALA:HB3 | 1.92 | 0.52 |
| 1:V:208:ILE:HG22 | 1:V:209:VAL:N | 2.24 | 0.52 |
| 1:W:169:TYR:CZ | 1:W:172:PRO:HD3 | 2.45 | 0.52 |
| 1:W:362:TYR:HD1 | 1:W:367:PRO:HA | 1.75 | 0.52 |
| 1:A:164:PRO:HG3 | 1:A:174:ALA:HB1 | 1.92 | 0.52 |
| 1:B:167:GLU:OE1 | 1:D:61:LYS:CE | 2.58 | 0.52 |
| 1:C:164:PRO:HG3 | 1:C:174:ALA:HB1 | 1.92 | 0.52 |
| 1:D:362:TYR:HE1 | 1:D:367:PRO:CB | 2.19 | 0.52 |
| 1:F:140:LEU:HD22 | 1:F:343:GLY:HA2 | 1.90 | 0.52 |
| 1:H:164:PRO:HG3 | 1:H:174:ALA:HB1 | 1.92 | 0.52 |
| 1:H:336:LYS:HE2 | 2:H:401:ADP:C5' | 2.38 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:164:PRO:HG2 | 1:I:174:ALA:HB3 | 1.92 | 0.52 |
| 1:K:135:ALA:HB1 | 1:K:140:LEU:HD21 | 1.91 | 0.52 |
| 1:K:140:LEU:HD22 | 1:K:343:GLY:HA2 | 1.90 | 0.52 |
| 1:L:32:PRO:CG | 1:L:55:GLY:O | 2.55 | 0.52 |
| 1:M:143:TYR:CD1 | 1:M:143:TYR:C | 2.75 | 0.52 |
| 1:O:362:TYR:HD1 | 1:O:367:PRO:HA | 1.75 | 0.52 |
| 1:R:362:TYR:HD1 | 1:R:367:PRO:HA | 1.75 | 0.52 |
| 1:U:110:LEU:HD12 | 1:U:177:ARG:HH11 | 1.72 | 0.52 |
| 1:V:116:ARG:HH12 | 1:V:375:PHE:HA | 1.74 | 0.52 |
| 1:V:169:TYR:CZ | 1:V:172:PRO:HD3 | 2.45 | 0.52 |
| 1:V:300:SER:HA | 1:V:335:ARG:HG2 | 1.89 | 0.52 |
| 1:A:362:TYR:HD1 | 1:A:367:PRO:HA | 1.75 | 0.52 |
| 1:C:362:TYR:HD1 | 1:C:367:PRO:HA | 1.75 | 0.52 |
| 1:G:169:TYR:CZ | 1:G:172:PRO:HD3 | 2.45 | 0.52 |
| 1:I:169:TYR:CZ | 1:I:172:PRO:HD3 | 2.45 | 0.52 |
| 1:M:164:PRO:HG2 | 1:M:174:ALA:HB3 | 1.92 | 0.52 |
| 1:O:164:PRO:HG2 | 1:O:174:ALA:HB3 | 1.92 | 0.52 |
| 1:P:362:TYR:HE1 | 1:P:367:PRO:CB | 2.19 | 0.52 |
| 1:S:34:ILE:CG2 | 1:S:68:LYS:H | 2.21 | 0.52 |
| 1:U:169:TYR:CZ | 1:U:172:PRO:HD3 | 2.45 | 0.52 |
| 1:A:116:ARG:HH12 | 1:A:375:PHE:HA | 1.74 | 0.52 |
| 1:B:164:PRO:HG2 | 1:B:174:ALA:HB3 | 1.92 | 0.52 |
| 1:D:36:GLY:HA3 | 1:D:66:THR:O | 2.10 | 0.52 |
| 1:D:167:GLU:OE1 | 1:F:61:LYS:CE | 2.58 | 0.52 |
| 1:E:164:PRO:HG3 | 1:E:174:ALA:HB1 | 1.92 | 0.52 |
| 1:F:164:PRO:HG3 | 1:F:174:ALA:HB1 | 1.92 | 0.52 |
| 1:H:362:TYR:HD1 | 1:H:367:PRO:HA | 1.75 | 0.52 |
| 1:I:362:TYR:HD1 | 1:I:367:PRO:HA | 1.75 | 0.52 |
| 1:K:142:LEU:HD21 | 1:K:165:ILE:CD1 | 2.39 | 0.52 |
| 1:K:164:PRO:HG2 | 1:K:174:ALA:HB3 | 1.92 | 0.52 |
| 1:K:167:GLU:OE1 | 1:M:61:LYS:CE | 2.58 | 0.52 |
| 1:N:32:PRO:CG | 1:N:55:GLY:O | 2.55 | 0.52 |
| 1:P:116:ARG:HH12 | 1:P:375:PHE:HA | 1.74 | 0.52 |
| 1:R:116:ARG:HH12 | 1:R:375:PHE:HA | 1.74 | 0.52 |
| 1:T:167:GLU:OE1 | 1:V:61:LYS:CE | 2.58 | 0.52 |
| 1:W:142:LEU:HD21 | 1:W:165:ILE:CD1 | 2.38 | 0.52 |
| 1:B:58:ALA:CA | 1:B:65:LEU:CD2 | 2.89 | 0.52 |
| 1:G:37:ARG:CG | 1:G:38:PRO:CD | 2.83 | 0.52 |
| 1:G:164:PRO:HG2 | 1:G:174:ALA:HB3 | 1.92 | 0.52 |
| 1:I:143:TYR:CE2 | 1:K:45:VAL:HG21 | 2.44 | 0.52 |
| 1:J:34:ILE:CG2 | 1:J:68:LYS:H | 2.21 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:143:TYR:CE2 | 1:N:45:VAL:HG21 | 2.44 | 0.52 |
| 1:M:58:ALA:CA | 1:M:65:LEU:CD2 | 2.88 | 0.52 |
| 1:N:116:ARG:HH12 | 1:N:375:PHE:HA | 1.74 | 0.52 |
| 1:R:36:GLY:HA3 | 1:R:66:THR:O | 2.10 | 0.52 |
| 1:S:36:GLY:HA3 | 1:S:66:THR:O | 2.10 | 0.52 |
| 1:T:164:PRO:HG2 | 1:T:174:ALA:HB3 | 1.92 | 0.52 |
| 1:W:2:GLU:HA | 1:W:2:GLU:OE2 | 2.10 | 0.52 |
| 1:A:300:SER:HA | 1:A:335:ARG:HG2 | 1.89 | 0.51 |
| 1:B:143:TYR:CE2 | 1:D:45:VAL:HG21 | 2.44 | 0.51 |
| 1:C:36:GLY:HA3 | 1:C:66:THR:O | 2.10 | 0.51 |
| 1:D:142:LEU:HD21 | 1:D:165:ILE:CD1 | 2.39 | 0.51 |
| 1:E:143:TYR:HD1 | 1:E:143:TYR:C | 2.09 | 0.51 |
| 1:F:36:GLY:HA3 | 1:F:66:THR:O | 2.10 | 0.51 |
| 1:G:36:GLY:HA3 | 1:G:66:THR:O | 2.10 | 0.51 |
| 1:I:58:ALA:CA | 1:I:65:LEU:CD2 | 2.88 | 0.51 |
| 1:K:58:ALA:CA | 1:K:65:LEU:CD2 | 2.89 | 0.51 |
| 1:N:368:SER:O | 1:N:371:HIS:N | 2.37 | 0.51 |
| 1:O:36:GLY:HA3 | 1:O:66:THR:O | 2.10 | 0.51 |
| 1:O:167:GLU:OE1 | 1:Q:61:LYS:CE | 2.58 | 0.51 |
| 1:R:142:LEU:HD21 | 1:R:165:ILE:CD1 | 2.38 | 0.51 |
| 1:W:230:ALA:HA | 1:W:233:SER:HB2 | 1.92 | 0.51 |
| 1:A:169:TYR:CZ | 1:A:172:PRO:HD3 | 2.45 | 0.51 |
| 1:C:22:ALA:HB1 | 1:C:348:SER:CB | 2.41 | 0.51 |
| 1:D:58:ALA:CA | 1:D:65:LEU:CD2 | 2.89 | 0.51 |
| 1:F:167:GLU:OE1 | 1:H:61:LYS:CE | 2.58 | 0.51 |
| 1:H:230:ALA:HA | 1:H:233:SER:HB2 | 1.92 | 0.51 |
| 1:I:362:TYR:HE1 | 1:I:367:PRO:CB | 2.19 | 0.51 |
| 1:J:230:ALA:HA | 1:J:233:SER:HB2 | 1.92 | 0.51 |
| 1:N:164:PRO:HG3 | 1:N:174:ALA:HB1 | 1.92 | 0.51 |
| 1:O:58:ALA:CA | 1:O:65:LEU:CD2 | 2.89 | 0.51 |
| 1:O:169:TYR:CZ | 1:O:172:PRO:HD3 | 2.45 | 0.51 |
| 1:O:336:LYS:HE2 | 2:O:401:ADP:C5' | 2.38 | 0.51 |
| 1:P:36:GLY:HA3 | 1:P:66:THR:O | 2.10 | 0.51 |
| 1:Q:58:ALA:CA | 1:Q:65:LEU:CD2 | 2.89 | 0.51 |
| 1:Q:164:PRO:HG2 | 1:Q:174:ALA:HB3 | 1.92 | 0.51 |
| 1:R:22:ALA:HB1 | 1:R:348:SER:CB | 2.41 | 0.51 |
| 1:R:167:GLU:OE1 | 1:T:61:LYS:CE | 2.58 | 0.51 |
| 1:S:58:ALA:CA | 1:S:65:LEU:CD2 | 2.88 | 0.51 |
| 1:V:39:ARG:HG2 | 1:V:66:THR:HB | 1.92 | 0.51 |
| 1:A:230:ALA:HA | 1:A:233:SER:HB2 | 1.92 | 0.51 |
| 1:B:22:ALA:HB1 | 1:B:348:SER:CB | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:362:TYR:HD1 | 1:B:367:PRO:HA | 1.75 | 0.51 |
| 1:D:164:PRO:HG2 | 1:D:174:ALA:HB3 | 1.92 | 0.51 |
| 1:G:167:GLU:OE1 | 1:I:61:LYS:CE | 2.58 | 0.51 |
| 1:H:2:GLU:OE2 | 1:H:2:GLU:HA | 2.11 | 0.51 |
| 1:J:22:ALA:HB1 | 1:J:348:SER:CB | 2.41 | 0.51 |
| 1:N:167:GLU:OE1 | 1:P:61:LYS:CE | 2.58 | 0.51 |
| 1:N:230:ALA:HA | 1:N:233:SER:HB2 | 1.92 | 0.51 |
| 1:N:362:TYR:HD1 | 1:N:367:PRO:HA | 1.75 | 0.51 |
| 1:O:169:TYR:OH | 1:Q:40:HIS:HB3 | 2.10 | 0.51 |
| 1:Q:22:ALA:HB1 | 1:Q:348:SER:CB | 2.41 | 0.51 |
| 1:Q:140:LEU:HD22 | 1:Q:343:GLY:HA2 | 1.90 | 0.51 |
| 1:Q:332:PRO:HG2 | 1:Q:335:ARG:NE | 2.26 | 0.51 |
| 1:R:34:ILE:CG2 | 1:R:35:VAL:N | 2.74 | 0.51 |
| 1:T:34:ILE:CG2 | 1:T:35:VAL:N | 2.74 | 0.51 |
| 1:T:332:PRO:HG2 | 1:T:335:ARG:NE | 2.26 | 0.51 |
| 1:U:230:ALA:HA | 1:U:233:SER:HB2 | 1.92 | 0.51 |
| 1:V:58:ALA:CA | 1:V:65:LEU:CD2 | 2.88 | 0.51 |
| 1:W:164:PRO:HG3 | 1:W:174:ALA:HB1 | 1.92 | 0.51 |
| 1:B:36:GLY:HA3 | 1:B:66:THR:O | 2.10 | 0.51 |
| 1:C:34:ILE:CG2 | 1:C:35:VAL:N | 2.74 | 0.51 |
| 1:E:22:ALA:HB1 | 1:E:348:SER:CB | 2.41 | 0.51 |
| 1:F:58:ALA:CA | 1:F:65:LEU:CD2 | 2.89 | 0.51 |
| 1:G:2:GLU:OE2 | 1:G:2:GLU:HA | 2.10 | 0.51 |
| 1:G:164:PRO:HG3 | 1:G:174:ALA:HB1 | 1.92 | 0.51 |
| 1:G:362:TYR:HE1 | 1:G:367:PRO:CB | 2.19 | 0.51 |
| 1:H:22:ALA:HB1 | 1:H:348:SER:CB | 2.41 | 0.51 |
| 1:H:36:GLY:HA3 | 1:H:66:THR:O | 2.10 | 0.51 |
| 1:H:167:GLU:OE1 | 1:J:61:LYS:CE | 2.58 | 0.51 |
| 1:H:332:PRO:HG2 | 1:H:335:ARG:NE | 2.26 | 0.51 |
| 1:I:39:ARG:HG2 | 1:I:66:THR:HB | 1.93 | 0.51 |
| 1:I:167:GLU:OE1 | 1:K:61:LYS:CE | 2.58 | 0.51 |
| 1:K:34:ILE:CG2 | 1:K:35:VAL:N | 2.74 | 0.51 |
| 1:L:230:ALA:HA | 1:L:233:SER:HB2 | 1.92 | 0.51 |
| 1:L:362:TYR:HD1 | 1:L:367:PRO:HA | 1.75 | 0.51 |
| 1:M:336:LYS:HE2 | 2:M:401:ADP:C5' | 2.38 | 0.51 |
| 1:O:32:PRO:CG | 1:O:55:GLY:O | 2.55 | 0.51 |
| 1:O:332:PRO:HG2 | 1:O:335:ARG:NE | 2.26 | 0.51 |
| 1:P:169:TYR:CZ | 1:P:172:PRO:HD3 | 2.45 | 0.51 |
| 1:R:332:PRO:HG2 | 1:R:335:ARG:NE | 2.26 | 0.51 |
| 1:U:58:ALA:CA | 1:U:65:LEU:CD2 | 2.89 | 0.51 |
| 1:U:362:TYR:HD1 | 1:U:367:PRO:HA | 1.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2:GLU:HA | 1:C:2:GLU:OE2 | 2.10 | 0.51 |
| 1:C:34:ILE:CG2 | 1:C:68:LYS:H | 2.21 | 0.51 |
| 1:D:164:PRO:HG3 | 1:D:174:ALA:HB1 | 1.92 | 0.51 |
| 1:E:167:GLU:OE1 | 1:G:61:LYS:CE | 2.58 | 0.51 |
| 1:E:208:ILE:HG22 | 1:E:209:VAL:N | 2.24 | 0.51 |
| 1:F:332:PRO:HG2 | 1:F:335:ARG:NE | 2.26 | 0.51 |
| 1:G:58:ALA:CA | 1:G:65:LEU:CD2 | 2.88 | 0.51 |
| 1:J:362:TYR:HD1 | 1:J:367:PRO:HA | 1.75 | 0.51 |
| 1:L:167:GLU:OE1 | 1:N:61:LYS:CE | 2.58 | 0.51 |
| 1:M:169:TYR:OH | 1:O:40:HIS:HB3 | 2.10 | 0.51 |
| 1:P:230:ALA:HA | 1:P:233:SER:HB2 | 1.92 | 0.51 |
| 1:Q:169:TYR:OH | 1:S:40:HIS:HB3 | 2.10 | 0.51 |
| 1:Q:362:TYR:HD1 | 1:Q:367:PRO:HA | 1.75 | 0.51 |
| 1:S:164:PRO:HG2 | 1:S:174:ALA:HB3 | 1.92 | 0.51 |
| 1:S:332:PRO:HG2 | 1:S:335:ARG:NE | 2.26 | 0.51 |
| 1:T:22:ALA:HB1 | 1:T:348:SER:CB | 2.41 | 0.51 |
| 1:T:116:ARG:HH12 | 1:T:375:PHE:HA | 1.74 | 0.51 |
| 1:T:362:TYR:HE1 | 1:T:367:PRO:CB | 2.19 | 0.51 |
| 1:U:36:GLY:HA3 | 1:U:66:THR:O | 2.10 | 0.51 |
| 1:V:36:GLY:HA3 | 1:V:66:THR:O | 2.10 | 0.51 |
| 1:V:37:ARG:CG | 1:V:38:PRO:CD | 2.83 | 0.51 |
| 1:A:36:GLY:HA3 | 1:A:66:THR:O | 2.10 | 0.51 |
| 1:A:332:PRO:HG2 | 1:A:335:ARG:NE | 2.26 | 0.51 |
| 1:C:143:TYR:CE2 | 1:E:45:VAL:HG21 | 2.44 | 0.51 |
| 1:C:167:GLU:OE1 | 1:E:61:LYS:CE | 2.58 | 0.51 |
| 1:C:230:ALA:HA | 1:C:233:SER:HB2 | 1.92 | 0.51 |
| 1:E:34:ILE:CG2 | 1:E:35:VAL:N | 2.74 | 0.51 |
| 1:I:34:ILE:CG2 | 1:I:35:VAL:N | 2.74 | 0.51 |
| 1:I:36:GLY:HA3 | 1:I:66:THR:O | 2.10 | 0.51 |
| 1:J:32:PRO:CG | 1:J:55:GLY:O | 2.55 | 0.51 |
| 1:J:332:PRO:HG2 | 1:J:335:ARG:NE | 2.26 | 0.51 |
| 1:K:2:GLU:OE2 | 1:K:2:GLU:HA | 2.10 | 0.51 |
| 1:K:22:ALA:HB1 | 1:K:348:SER:CB | 2.41 | 0.51 |
| 1:L:22:ALA:HB1 | 1:L:348:SER:CB | 2.41 | 0.51 |
| 1:L:169:TYR:OH | 1:N:40:HIS:HB3 | 2.10 | 0.51 |
| 1:M:34:ILE:HG23 | 1:M:68:LYS:N | 2.26 | 0.51 |
| 1:M:36:GLY:HA3 | 1:M:66:THR:O | 2.10 | 0.51 |
| 1:N:54:VAL:CG1 | 1:N:55:GLY:N | 2.72 | 0.51 |
| 1:N:169:TYR:CZ | 1:N:172:PRO:HD3 | 2.45 | 0.51 |
| 1:N:169:TYR:OH | 1:P:40:HIS:HB3 | 2.10 | 0.51 |
| 1:O:34:ILE:HG23 | 1:O:68:LYS:N | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:167:GLU:OE1 | 1:R:61:LYS:CE | 2.58 | 0.51 |
| 1:Q:167:GLU:OE1 | 1:S:61:LYS:CE | 2.58 | 0.51 |
| 1:R:143:TYR:CE2 | 1:T:45:VAL:HG21 | 2.44 | 0.51 |
| 1:S:2:GLU:OE2 | 1:S:2:GLU:HA | 2.10 | 0.51 |
| 1:T:36:GLY:HA3 | 1:T:66:THR:O | 2.10 | 0.51 |
| 1:T:58:ALA:CA | 1:T:65:LEU:CD2 | 2.88 | 0.51 |
| 1:V:2:GLU:HA | 1:V:2:GLU:OE2 | 2.11 | 0.51 |
| 1:V:332:PRO:HG2 | 1:V:335:ARG:NE | 2.26 | 0.51 |
| 1:W:36:GLY:HA3 | 1:W:66:THR:O | 2.10 | 0.51 |
| 1:E:164:PRO:HG2 | 1:E:174:ALA:HB3 | 1.92 | 0.51 |
| 1:E:169:TYR:OH | 1:G:40:HIS:HB3 | 2.10 | 0.51 |
| 1:F:230:ALA:HA | 1:F:233:SER:HB2 | 1.92 | 0.51 |
| 1:J:167:GLU:OE1 | 1:L:61:LYS:CE | 2.58 | 0.51 |
| 1:J:336:LYS:HE2 | 2:J:401:ADP:C5' | 2.38 | 0.51 |
| 1:K:34:ILE:HG23 | 1:K:68:LYS:N | 2.26 | 0.51 |
| 1:L:34:ILE:HG23 | 1:L:68:LYS:N | 2.26 | 0.51 |
| 1:M:39:ARG:HG2 | 1:M:66:THR:HB | 1.93 | 0.51 |
| 1:M:164:PRO:HG3 | 1:M:174:ALA:HB1 | 1.92 | 0.51 |
| 1:M:332:PRO:HG2 | 1:M:335:ARG:NE | 2.26 | 0.51 |
| 1:N:36:GLY:HA3 | 1:N:66:THR:O | 2.10 | 0.51 |
| 1:P:34:ILE:HG12 | 1:P:69:TYR:CE1 | 2.46 | 0.51 |
| 1:S:169:TYR:OH | 1:U:40:HIS:HB3 | 2.10 | 0.51 |
| 1:T:300:SER:HA | 1:T:335:ARG:HG2 | 1.89 | 0.51 |
| 1:W:34:ILE:HG23 | 1:W:68:LYS:N | 2.26 | 0.51 |
| 1:C:332:PRO:HG2 | 1:C:335:ARG:NE | 2.26 | 0.51 |
| 1:D:34:ILE:HG12 | 1:D:69:TYR:CE1 | 2.46 | 0.51 |
| 1:D:332:PRO:HG2 | 1:D:335:ARG:NE | 2.26 | 0.51 |
| 1:G:34:ILE:HG12 | 1:G:69:TYR:CE1 | 2.46 | 0.51 |
| 1:H:58:ALA:CA | 1:H:65:LEU:CD2 | 2.89 | 0.51 |
| 1:J:361:GLU:HB3 | 1:J:369:ILE:CD1 | 2.14 | 0.51 |
| 1:M:32:PRO:CG | 1:M:55:GLY:O | 2.55 | 0.51 |
| 1:N:2:GLU:HA | 1:N:2:GLU:OE2 | 2.10 | 0.51 |
| 1:O:347:ALA:HA | 1:O:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:R:2:GLU:HA | 1:R:2:GLU:OE2 | 2.11 | 0.51 |
| 1:R:34:ILE:HG23 | 1:R:68:LYS:N | 2.26 | 0.51 |
| 1:S:230:ALA:HA | 1:S:233:SER:HB2 | 1.92 | 0.51 |
| 1:T:34:ILE:HG23 | 1:T:68:LYS:N | 2.26 | 0.51 |
| 1:U:34:ILE:HG12 | 1:U:69:TYR:CE1 | 2.46 | 0.51 |
| 1:W:32:PRO:CG | 1:W:55:GLY:O | 2.55 | 0.51 |
| 1:W:58:ALA:CA | 1:W:65:LEU:CD2 | 2.89 | 0.51 |
| 1:A:34:ILE:CG2 | 1:A:35:VAL:N | 2.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:169:TYR:OH | 1:D:40:HIS:HB3 | 2.10 | 0.51 |
| 1:C:34:ILE:HG23 | 1:C:68:LYS:N | 2.26 | 0.51 |
| 1:C:164:PRO:HG2 | 1:C:174:ALA:HB3 | 1.92 | 0.51 |
| 1:D:2:GLU:HA | 1:D:2:GLU:OE2 | 2.11 | 0.51 |
| 1:D:169:TYR:OH | 1:F:40:HIS:HB3 | 2.10 | 0.51 |
| 1:F:164:PRO:HG2 | 1:F:174:ALA:HB3 | 1.92 | 0.51 |
| 1:H:34:ILE:HG23 | 1:H:68:LYS:N | 2.26 | 0.51 |
| 1:I:34:ILE:HG23 | 1:I:68:LYS:N | 2.26 | 0.51 |
| 1:K:164:PRO:HG3 | 1:K:174:ALA:HB1 | 1.92 | 0.51 |
| 1:K:169:TYR:OH | 1:M:40:HIS:HB3 | 2.10 | 0.51 |
| 1:K:332:PRO:HG2 | 1:K:335:ARG:NE | 2.26 | 0.51 |
| 1:L:34:ILE:CG2 | 1:L:35:VAL:N | 2.74 | 0.51 |
| 1:P:164:PRO:HG3 | 1:P:174:ALA:HB1 | 1.92 | 0.51 |
| 1:P:332:PRO:HG2 | 1:P:335:ARG:NE | 2.26 | 0.51 |
| 1:P:347:ALA:HA | 1:P:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:Q:34:ILE:HG23 | 1:Q:68:LYS:N | 2.26 | 0.51 |
| 1:Q:347:ALA:HA | 1:Q:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:R:39:ARG:HG2 | 1:R:66:THR:HB | 1.93 | 0.51 |
| 1:R:347:ALA:HA | 1:R:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:S:22:ALA:HB1 | 1:S:348:SER:CB | 2.41 | 0.51 |
| 1:S:167:GLU:OE1 | 1:U:61:LYS:CE | 2.58 | 0.51 |
| 1:S:347:ALA:HA | 1:S:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:T:347:ALA:HA | 1:T:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:V:34:ILE:CG2 | 1:V:35:VAL:N | 2.74 | 0.51 |
| 1:V:347:ALA:HA | 1:V:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:E:39:ARG:HG2 | 1:E:66:THR:HB | 1.93 | 0.51 |
| 1:E:54:VAL:CG1 | 1:E:55:GLY:N | 2.72 | 0.51 |
| 1:G:169:TYR:OH | 1:I:40:HIS:HB3 | 2.10 | 0.51 |
| 1:H:34:ILE:HG12 | 1:H:69:TYR:CE1 | 2.46 | 0.51 |
| 1:J:34:ILE:HG12 | 1:J:69:TYR:CE1 | 2.46 | 0.51 |
| 1:J:58:ALA:CA | 1:J:65:LEU:CD2 | 2.89 | 0.51 |
| 1:K:36:GLY:HA3 | 1:K:66:THR:O | 2.10 | 0.51 |
| 1:M:34:ILE:CG2 | 1:M:35:VAL:N | 2.74 | 0.51 |
| 1:M:167:GLU:OE1 | 1:O:61:LYS:CE | 2.58 | 0.51 |
| 1:N:34:ILE:HG23 | 1:N:68:LYS:N | 2.26 | 0.51 |
| 1:O:2:GLU:OE2 | 1:O:2:GLU:HA | 2.11 | 0.51 |
| 1:O:34:ILE:HG12 | 1:O:69:TYR:CE1 | 2.46 | 0.51 |
| 1:P:34:ILE:HG23 | 1:P:68:LYS:N | 2.26 | 0.51 |
| 1:P:142:LEU:HD21 | 1:P:165:ILE:CD1 | 2.38 | 0.51 |
| 1:R:164:PRO:HG2 | 1:R:174:ALA:HB3 | 1.92 | 0.51 |
| 1:U:142:LEU:HD21 | 1:U:165:ILE:CD1 | 2.38 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:347:ALA:HA | 1:W:356:TRP:CZ2 | 2.46 | 0.51 |
| 1:A:167:GLU:OE1 | 1:C:61:LYS:CE | 2.58 | 0.50 |
| 1:B:34:ILE:CG2 | 1:B:35:VAL:N | 2.74 | 0.50 |
| 1:B:37:ARG:CG | 1:B:38:PRO:CD | 2.83 | 0.50 |
| 1:B:39:ARG:HG2 | 1:B:66:THR:HB | 1.93 | 0.50 |
| 1:D:22:ALA:HB1 | 1:D:348:SER:CB | 2.41 | 0.50 |
| 1:E:34:ILE:HG12 | 1:E:69:TYR:CE1 | 2.46 | 0.50 |
| 1:E:230:ALA:HA | 1:E:233:SER:HB2 | 1.92 | 0.50 |
| 1:F:34:ILE:HG23 | 1:F:68:LYS:N | 2.26 | 0.50 |
| 1:F:169:TYR:OH | 1:H:40:HIS:HB3 | 2.10 | 0.50 |
| 1:I:332:PRO:HG2 | 1:I:335:ARG:NE | 2.26 | 0.50 |
| 1:J:2:GLU:OE2 | 1:J:2:GLU:HA | 2.10 | 0.50 |
| 1:J:164:PRO:HG2 | 1:J:174:ALA:HB3 | 1.92 | 0.50 |
| 1:J:169:TYR:OH | 1:L:40:HIS:HB3 | 2.10 | 0.50 |
| 1:K:34:ILE:HG12 | 1:K:69:TYR:CE1 | 2.46 | 0.50 |
| 1:K:39:ARG:HG2 | 1:K:66:THR:HB | 1.93 | 0.50 |
| 1:L:34:ILE:CG2 | 1:L:67:LEU:HD22 | 2.28 | 0.50 |
| 1:N:34:ILE:CG2 | 1:N:35:VAL:N | 2.74 | 0.50 |
| 1:N:164:PRO:HG2 | 1:N:174:ALA:HB3 | 1.92 | 0.50 |
| 1:N:347:ALA:HA | 1:N:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:P:164:PRO:HG2 | 1:P:174:ALA:HB3 | 1.92 | 0.50 |
| 1:P:369:ILE:C | 1:P:371:HIS:H | 2.15 | 0.50 |
| 1:Q:32:PRO:CG | 1:Q:55:GLY:O | 2.55 | 0.50 |
| 1:Q:34:ILE:HG12 | 1:Q:69:TYR:CE1 | 2.46 | 0.50 |
| 1:S:34:ILE:HG23 | 1:S:68:LYS:N | 2.26 | 0.50 |
| 1:T:169:TYR:OH | 1:V:40:HIS:HB3 | 2.10 | 0.50 |
| 1:U:34:ILE:HG23 | 1:U:68:LYS:N | 2.26 | 0.50 |
| 1:U:164:PRO:HG2 | 1:U:174:ALA:HB3 | 1.92 | 0.50 |
| 1:U:164:PRO:HG3 | 1:U:174:ALA:HB1 | 1.92 | 0.50 |
| 1:U:347:ALA:HA | 1:U:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:V:34:ILE:HG23 | 1:V:68:LYS:N | 2.26 | 0.50 |
| 1:V:34:ILE:HG12 | 1:V:69:TYR:CE1 | 2.46 | 0.50 |
| 1:W:164:PRO:HG2 | 1:W:174:ALA:HB3 | 1.92 | 0.50 |
| 1:A:58:ALA:CA | 1:A:65:LEU:CD2 | 2.89 | 0.50 |
| 1:C:58:ALA:CA | 1:C:65:LEU:CD2 | 2.89 | 0.50 |
| 1:C:169:TYR:OH | 1:E:40:HIS:HB3 | 2.10 | 0.50 |
| 1:G:362:TYR:HD1 | 1:G:367:PRO:HA | 1.75 | 0.50 |
| 1:I:164:PRO:HG3 | 1:I:174:ALA:HB1 | 1.92 | 0.50 |
| 1:I:230:ALA:HA | 1:I:233:SER:HB2 | 1.92 | 0.50 |
| 1:K:230:ALA:HA | 1:K:233:SER:HB2 | 1.92 | 0.50 |
| 1:M:347:ALA:HA | 1:M:356:TRP:CZ2 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:34:ILE:HG12 | 1:N:69:TYR:CE1 | 2.46 | 0.50 |
| 1:N:369:ILE:C | 1:N:371:HIS:H | 2.15 | 0.50 |
| 1:Q:36:GLY:HA3 | 1:Q:66:THR:O | 2.10 | 0.50 |
| 1:R:58:ALA:CA | 1:R:65:LEU:CD2 | 2.89 | 0.50 |
| 1:R:230:ALA:HA | 1:R:233:SER:HB2 | 1.93 | 0.50 |
| 1:U:32:PRO:CG | 1:U:55:GLY:O | 2.55 | 0.50 |
| 1:U:167:GLU:OE1 | 1:W:61:LYS:CE | 2.58 | 0.50 |
| 1:U:332:PRO:HG2 | 1:U:335:ARG:NE | 2.26 | 0.50 |
| 1:A:34:ILE:CG2 | 1:A:67:LEU:HD22 | 2.27 | 0.50 |
| 1:A:164:PRO:HG2 | 1:A:174:ALA:HB3 | 1.92 | 0.50 |
| 1:B:142:LEU:HD21 | 1:B:165:ILE:CD1 | 2.39 | 0.50 |
| 1:B:164:PRO:HG3 | 1:B:174:ALA:HB1 | 1.92 | 0.50 |
| 1:D:32:PRO:CG | 1:D:55:GLY:O | 2.55 | 0.50 |
| 1:D:230:ALA:HA | 1:D:233:SER:HB2 | 1.92 | 0.50 |
| 1:E:36:GLY:HA3 | 1:E:66:THR:O | 2.10 | 0.50 |
| 1:E:58:ALA:CA | 1:E:65:LEU:CD2 | 2.89 | 0.50 |
| 1:H:164:PRO:HG2 | 1:H:174:ALA:HB3 | 1.92 | 0.50 |
| 1:I:34:ILE:HG12 | 1:I:69:TYR:CE1 | 2.46 | 0.50 |
| 1:I:347:ALA:HA | 1:I:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:J:34:ILE:HG23 | 1:J:68:LYS:N | 2.26 | 0.50 |
| 1:J:36:GLY:HA3 | 1:J:66:THR:O | 2.10 | 0.50 |
| 1:K:347:ALA:HA | 1:K:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:L:58:ALA:CA | 1:L:65:LEU:CD2 | 2.89 | 0.50 |
| 1:L:164:PRO:HG2 | 1:L:174:ALA:HB3 | 1.92 | 0.50 |
| 1:L:332:PRO:HG2 | 1:L:335:ARG:NE | 2.26 | 0.50 |
| 1:M:230:ALA:HA | 1:M:233:SER:HB2 | 1.92 | 0.50 |
| 1:N:22:ALA:HB1 | 1:N:348:SER:CB | 2.41 | 0.50 |
| 1:O:164:PRO:HG3 | 1:O:174:ALA:HB1 | 1.92 | 0.50 |
| 1:P:34:ILE:CG2 | 1:P:35:VAL:N | 2.74 | 0.50 |
| 1:P:169:TYR:OH | 1:R:40:HIS:HB3 | 2.10 | 0.50 |
| 1:Q:34:ILE:HD13 | 1:Q:67:LEU:CD1 | 2.41 | 0.50 |
| 1:Q:39:ARG:HG2 | 1:Q:66:THR:HB | 1.93 | 0.50 |
| 1:R:34:ILE:HG12 | 1:R:69:TYR:CE1 | 2.46 | 0.50 |
| 1:S:34:ILE:HG12 | 1:S:69:TYR:CE1 | 2.46 | 0.50 |
| 1:S:37:ARG:CG | 1:S:38:PRO:N | 2.75 | 0.50 |
| 1:A:34:ILE:HG12 | 1:A:69:TYR:CE1 | 2.46 | 0.50 |
| 1:A:347:ALA:HA | 1:A:356:TRP:CZ2 | 2.47 | 0.50 |
| 1:D:34:ILE:HG23 | 1:D:68:LYS:N | 2.26 | 0.50 |
| 1:D:37:ARG:CG | 1:D:38:PRO:N | 2.75 | 0.50 |
| 1:F:34:ILE:HD13 | 1:F:67:LEU:CD1 | 2.41 | 0.50 |
| 1:F:34:ILE:CG2 | 1:F:67:LEU:HD22 | 2.28 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:34:ILE:HG12 | 1:F:69:TYR:CE1 | 2.46 | 0.50 |
| 1:G:34:ILE:CG2 | 1:G:35:VAL:N | 2.74 | 0.50 |
| 1:G:34:ILE:HG23 | 1:G:68:LYS:N | 2.26 | 0.50 |
| 1:G:347:ALA:HA | 1:G:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:H:169:TYR:OH | 1:J:40:HIS:HB3 | 2.10 | 0.50 |
| 1:I:142:LEU:HD21 | 1:I:165:ILE:CD1 | 2.39 | 0.50 |
| 1:I:369:ILE:C | 1:I:371:HIS:H | 2.15 | 0.50 |
| 1:L:347:ALA:HA | 1:L:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:L:369:ILE:C | 1:L:371:HIS:H | 2.15 | 0.50 |
| 1:Q:230:ALA:HA | 1:Q:233:SER:HB2 | 1.92 | 0.50 |
| 1:R:369:ILE:C | 1:R:371:HIS:H | 2.15 | 0.50 |
| 1:S:164:PRO:HG3 | 1:S:174:ALA:HB1 | 1.92 | 0.50 |
| 1:U:169:TYR:OH | 1:W:40:HIS:HB3 | 2.10 | 0.50 |
| 1:W:37:ARG:CG | 1:W:38:PRO:N | 2.75 | 0.50 |
| 1:A:34:ILE:HG23 | 1:A:68:LYS:N | 2.26 | 0.50 |
| 1:B:40:HIS:O | 1:B:41:GLN:O | 2.30 | 0.50 |
| 1:C:290:ARG:NH1 | 1:E:244:ASP:OD1 | 2.45 | 0.50 |
| 1:D:40:HIS:O | 1:D:41:GLN:O | 2.30 | 0.50 |
| 1:E:332:PRO:HG2 | 1:E:335:ARG:NE | 2.26 | 0.50 |
| 1:E:347:ALA:HA | 1:E:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:F:32:PRO:CG | 1:F:55:GLY:O | 2.55 | 0.50 |
| 1:G:22:ALA:HB1 | 1:G:348:SER:CB | 2.41 | 0.50 |
| 1:G:332:PRO:HG2 | 1:G:335:ARG:NE | 2.26 | 0.50 |
| 1:H:37:ARG:CG | 1:H:38:PRO:N | 2.75 | 0.50 |
| 1:H:39:ARG:HG2 | 1:H:66:THR:HB | 1.92 | 0.50 |
| 1:H:147:ARG:CG | 1:H:147:ARG:NH2 | 2.71 | 0.50 |
| 1:J:34:ILE:CG2 | 1:J:35:VAL:N | 2.74 | 0.50 |
| 1:K:369:ILE:C | 1:K:371:HIS:H | 2.15 | 0.50 |
| 1:N:58:ALA:CA | 1:N:65:LEU:CD2 | 2.88 | 0.50 |
| 1:N:362:TYR:HE1 | 1:N:367:PRO:CB | 2.19 | 0.50 |
| 1:O:34:ILE:HD13 | 1:O:67:LEU:CD1 | 2.41 | 0.50 |
| 1:O:39:ARG:HG2 | 1:O:66:THR:HB | 1.93 | 0.50 |
| 1:O:40:HIS:O | 1:O:41:GLN:O | 2.30 | 0.50 |
| 1:O:361:GLU:HB3 | 1:O:369:ILE:CD1 | 2.14 | 0.50 |
| 1:S:362:TYR:HD1 | 1:S:367:PRO:HA | 1.75 | 0.50 |
| 1:T:164:PRO:HG3 | 1:T:174:ALA:HB1 | 1.92 | 0.50 |
| 1:V:164:PRO:HG3 | 1:V:174:ALA:HB1 | 1.92 | 0.50 |
| 1:W:34:ILE:CG2 | 1:W:67:LEU:HD22 | 2.27 | 0.50 |
| 1:B:332:PRO:HG2 | 1:B:335:ARG:NE | 2.26 | 0.50 |
| 1:D:34:ILE:HD13 | 1:D:67:LEU:CD1 | 2.41 | 0.50 |
| 1:D:34:ILE:CG2 | 1:D:35:VAL:N | 2.74 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:39:ARG:HG2 | 1:D:66:THR:HB | 1.93 | 0.50 |
| 1:G:39:ARG:HG2 | 1:G:66:THR:HB | 1.93 | 0.50 |
| 1:J:37:ARG:CG | 1:J:38:PRO:N | 2.75 | 0.50 |
| 1:J:39:ARG:HG2 | 1:J:66:THR:HB | 1.93 | 0.50 |
| 1:J:362:TYR:HE1 | 1:J:367:PRO:CB | 2.19 | 0.50 |
| 1:K:290:ARG:NH1 | 1:M:244:ASP:OD1 | 2.45 | 0.50 |
| 1:L:36:GLY:HA3 | 1:L:66:THR:O | 2.10 | 0.50 |
| 1:M:40:HIS:O | 1:M:41:GLN:O | 2.30 | 0.50 |
| 1:N:287:ILE:HG13 | 1:N:288:ASP:N | 2.27 | 0.50 |
| 1:O:230:ALA:HA | 1:O:233:SER:HB2 | 1.92 | 0.50 |
| 1:Q:164:PRO:HG3 | 1:Q:174:ALA:HB1 | 1.92 | 0.50 |
| 1:R:164:PRO:HG3 | 1:R:174:ALA:HB1 | 1.92 | 0.50 |
| 1:R:169:TYR:OH | 1:T:40:HIS:HB3 | 2.10 | 0.50 |
| 1:R:287:ILE:HG13 | 1:R:288:ASP:N | 2.27 | 0.50 |
| 1:R:290:ARG:NH1 | 1:T:244:ASP:OD1 | 2.45 | 0.50 |
| 1:A:290:ARG:NH1 | 1:C:244:ASP:OD1 | 2.45 | 0.50 |
| 1:B:32:PRO:CG | 1:B:55:GLY:O | 2.55 | 0.50 |
| 1:B:230:ALA:HA | 1:B:233:SER:HB2 | 1.92 | 0.50 |
| 1:B:347:ALA:HA | 1:B:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:E:34:ILE:HG23 | 1:E:68:LYS:N | 2.26 | 0.50 |
| 1:F:40:HIS:O | 1:F:41:GLN:O | 2.30 | 0.50 |
| 1:G:230:ALA:HA | 1:G:233:SER:HB2 | 1.92 | 0.50 |
| 1:G:290:ARG:NH1 | 1:I:244:ASP:OD1 | 2.45 | 0.50 |
| 1:I:169:TYR:OH | 1:K:40:HIS:HB3 | 2.10 | 0.50 |
| 1:I:290:ARG:NH1 | 1:K:244:ASP:OD1 | 2.45 | 0.50 |
| 1:J:347:ALA:HA | 1:J:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:K:40:HIS:O | 1:K:41:GLN:O | 2.30 | 0.50 |
| 1:M:22:ALA:HB1 | 1:M:348:SER:CB | 2.41 | 0.50 |
| 1:P:290:ARG:NH1 | 1:R:244:ASP:OD1 | 2.45 | 0.50 |
| 1:Q:34:ILE:CG2 | 1:Q:35:VAL:N | 2.74 | 0.50 |
| 1:Q:40:HIS:O | 1:Q:41:GLN:O | 2.30 | 0.50 |
| 1:T:369:ILE:C | 1:T:371:HIS:H | 2.15 | 0.50 |
| 1:U:39:ARG:HG2 | 1:U:66:THR:HB | 1.93 | 0.50 |
| 1:W:332:PRO:HG2 | 1:W:335:ARG:NE | 2.26 | 0.50 |
| 1:A:169:TYR:OH | 1:C:40:HIS:HB3 | 2.10 | 0.50 |
| 1:A:369:ILE:C | 1:A:371:HIS:H | 2.15 | 0.50 |
| 1:C:34:ILE:HG12 | 1:C:69:TYR:CE1 | 2.46 | 0.50 |
| 1:C:347:ALA:HA | 1:C:356:TRP:CZ2 | 2.47 | 0.50 |
| 1:J:40:HIS:O | 1:J:41:GLN:O | 2.30 | 0.50 |
| 1:N:37:ARG:CG | 1:N:38:PRO:N | 2.75 | 0.50 |
| 1:N:290:ARG:NH1 | 1:P:244:ASP:OD1 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:332:PRO:HG2 | 1:N:335:ARG:NE | 2.26 | 0.50 |
| 1:O:35:VAL:CA | 1:O:54:VAL:CG2 | 2.90 | 0.50 |
| 1:P:58:ALA:CA | 1:P:65:LEU:CD2 | 2.89 | 0.50 |
| 1:R:300:SER:HA | 1:R:335:ARG:HG2 | 1.89 | 0.50 |
| 1:S:34:ILE:CG2 | 1:S:35:VAL:N | 2.74 | 0.50 |
| 1:S:40:HIS:O | 1:S:41:GLN:O | 2.30 | 0.50 |
| 1:T:35:VAL:CA | 1:T:54:VAL:CG2 | 2.90 | 0.50 |
| 1:V:34:ILE:CG2 | 1:V:67:LEU:HD22 | 2.28 | 0.50 |
| 1:V:35:VAL:CA | 1:V:54:VAL:CG2 | 2.90 | 0.50 |
| 1:V:299:MET:HE1 | 1:V:304:THR:HB | 1.94 | 0.50 |
| 1:W:40:HIS:O | 1:W:41:GLN:O | 2.30 | 0.50 |
| 1:B:34:ILE:HG23 | 1:B:68:LYS:N | 2.26 | 0.50 |
| 1:B:290:ARG:NH1 | 1:D:244:ASP:OD1 | 2.45 | 0.50 |
| 1:H:40:HIS:O | 1:H:41:GLN:O | 2.30 | 0.50 |
| 1:H:347:ALA:HA | 1:H:356:TRP:CZ2 | 2.46 | 0.50 |
| 1:I:37:ARG:CG | 1:I:38:PRO:N | 2.75 | 0.50 |
| 1:L:37:ARG:CG | 1:L:38:PRO:N | 2.75 | 0.50 |
| 1:L:40:HIS:O | 1:L:41:GLN:O | 2.30 | 0.50 |
| 1:L:287:ILE:HG13 | 1:L:288:ASP:N | 2.27 | 0.50 |
| 1:M:34:ILE:HG12 | 1:M:69:TYR:CE1 | 2.46 | 0.50 |
| 1:M:369:ILE:C | 1:M:371:HIS:H | 2.15 | 0.50 |
| 1:O:290:ARG:NH1 | 1:Q:244:ASP:OD1 | 2.45 | 0.50 |
| 1:P:287:ILE:HG13 | 1:P:288:ASP:N | 2.27 | 0.50 |
| 1:Q:35:VAL:CA | 1:Q:54:VAL:CG2 | 2.90 | 0.50 |
| 1:T:34:ILE:HG12 | 1:T:69:TYR:CE1 | 2.46 | 0.50 |
| 1:U:2:GLU:HA | 1:U:2:GLU:OE2 | 2.10 | 0.50 |
| 1:U:40:HIS:O | 1:U:41:GLN:O | 2.30 | 0.50 |
| 1:W:39:ARG:HG2 | 1:W:66:THR:HB | 1.93 | 0.50 |
| 1:C:35:VAL:CA | 1:C:54:VAL:CG2 | 2.90 | 0.49 |
| 1:C:37:ARG:CG | 1:C:38:PRO:N | 2.75 | 0.49 |
| 1:C:39:ARG:HG2 | 1:C:66:THR:HB | 1.93 | 0.49 |
| 1:D:347:ALA:HA | 1:D:356:TRP:CZ2 | 2.46 | 0.49 |
| 1:E:35:VAL:CA | 1:E:54:VAL:CG2 | 2.90 | 0.49 |
| 1:F:2:GLU:OE2 | 1:F:2:GLU:HA | 2.10 | 0.49 |
| 1:G:369:ILE:C | 1:G:371:HIS:H | 2.15 | 0.49 |
| 1:J:369:ILE:C | 1:J:371:HIS:H | 2.15 | 0.49 |
| 1:M:34:ILE:CG2 | 1:M:67:LEU:HD22 | 2.28 | 0.49 |
| 1:M:35:VAL:CA | 1:M:54:VAL:CG2 | 2.90 | 0.49 |
| 1:O:37:ARG:CG | 1:O:38:PRO:N | 2.75 | 0.49 |
| 1:Q:290:ARG:NH1 | 1:S:244:ASP:OD1 | 2.45 | 0.49 |
| 1:R:35:VAL:CA | 1:R:54:VAL:CG2 | 2.90 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:230:ALA:HA | 1:T:233:SER:HB2 | 1.92 | 0.49 |
| 1:U:34:ILE:CG2 | 1:U:35:VAL:N | 2.74 | 0.49 |
| 1:U:37:ARG:CG | 1:U:38:PRO:N | 2.75 | 0.49 |
| 1:V:22:ALA:HB1 | 1:V:348:SER:CB | 2.41 | 0.49 |
| 1:W:34:ILE:HG12 | 1:W:69:TYR:CE1 | 2.46 | 0.49 |
| 1:W:300:SER:HA | 1:W:335:ARG:HG2 | 1.89 | 0.49 |
| 1:B:34:ILE:HG12 | 1:B:69:TYR:CE1 | 2.46 | 0.49 |
| 1:B:35:VAL:CA | 1:B:54:VAL:CG2 | 2.90 | 0.49 |
| 1:F:37:ARG:CG | 1:F:38:PRO:N | 2.75 | 0.49 |
| 1:H:287:ILE:HG22 | 1:H:290:ARG:CZ | 2.43 | 0.49 |
| 1:J:133:TYR:HH | 1:J:375:PHE:HD1 | 1.60 | 0.49 |
| 1:L:39:ARG:HG2 | 1:L:66:THR:HB | 1.93 | 0.49 |
| 1:M:147:ARG:CG | 1:M:147:ARG:NH2 | 2.71 | 0.49 |
| 1:N:40:HIS:O | 1:N:41:GLN:O | 2.30 | 0.49 |
| 1:N:142:LEU:HD21 | 1:N:165:ILE:CD1 | 2.39 | 0.49 |
| 1:O:34:ILE:CG2 | 1:O:35:VAL:N | 2.74 | 0.49 |
| 1:U:34:ILE:HD13 | 1:U:67:LEU:CD1 | 2.41 | 0.49 |
| 1:V:230:ALA:HA | 1:V:233:SER:HB2 | 1.92 | 0.49 |
| 1:A:40:HIS:O | 1:A:41:GLN:O | 2.30 | 0.49 |
| 1:B:287:ILE:HG22 | 1:B:290:ARG:CZ | 2.43 | 0.49 |
| 1:D:44:MET:CG | 1:D:45:VAL:N | 2.75 | 0.49 |
| 1:F:347:ALA:HA | 1:F:356:TRP:CZ2 | 2.46 | 0.49 |
| 1:G:287:ILE:HG13 | 1:G:288:ASP:N | 2.27 | 0.49 |
| 1:I:40:HIS:O | 1:I:41:GLN:O | 2.30 | 0.49 |
| 1:K:34:ILE:HD13 | 1:K:67:LEU:CD1 | 2.41 | 0.49 |
| 1:K:147:ARG:CG | 1:K:147:ARG:NH2 | 2.71 | 0.49 |
| 1:K:287:ILE:HG22 | 1:K:290:ARG:CZ | 2.43 | 0.49 |
| 1:L:34:ILE:HG12 | 1:L:69:TYR:CE1 | 2.46 | 0.49 |
| 1:O:287:ILE:HG22 | 1:O:290:ARG:CZ | 2.43 | 0.49 |
| 1:P:34:ILE:HG22 | 1:P:35:VAL:H | 1.78 | 0.49 |
| 1:S:39:ARG:HG2 | 1:S:66:THR:HB | 1.93 | 0.49 |
| 1:S:44:MET:CG | 1:S:45:VAL:N | 2.76 | 0.49 |
| 1:T:37:ARG:CG | 1:T:38:PRO:N | 2.75 | 0.49 |
| 1:U:287:ILE:HG22 | 1:U:290:ARG:CZ | 2.43 | 0.49 |
| 1:V:40:HIS:O | 1:V:41:GLN:O | 2.30 | 0.49 |
| 1:A:35:VAL:CA | 1:A:54:VAL:CG2 | 2.90 | 0.49 |
| 1:G:35:VAL:CA | 1:G:54:VAL:CG2 | 2.90 | 0.49 |
| 1:H:34:ILE:CG2 | 1:H:35:VAL:N | 2.74 | 0.49 |
| 1:J:287:ILE:HG13 | 1:J:288:ASP:N | 2.27 | 0.49 |
| 1:L:287:ILE:HG22 | 1:L:290:ARG:CZ | 2.43 | 0.49 |
| 1:O:369:ILE:C | 1:O:371:HIS:H | 2.15 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:37:ARG:CG | 1:R:38:PRO:N | 2.75 | 0.49 |
| 1:S:35:VAL:CA | 1:S:54:VAL:CG2 | 2.90 | 0.49 |
| 1:T:227:MET:HA | 1:T:227:MET:HE3 | 1.95 | 0.49 |
| 1:U:22:ALA:HB1 | 1:U:348:SER:CB | 2.41 | 0.49 |
| 1:V:43:VAL:O | 1:V:44:MET:HG2 | 2.13 | 0.49 |
| 1:V:369:ILE:C | 1:V:371:HIS:H | 2.15 | 0.49 |
| 1:B:34:ILE:HD13 | 1:B:67:LEU:CD1 | 2.41 | 0.49 |
| 1:C:369:ILE:C | 1:C:371:HIS:H | 2.15 | 0.49 |
| 1:E:287:ILE:HG13 | 1:E:288:ASP:N | 2.27 | 0.49 |
| 1:F:22:ALA:HB1 | 1:F:348:SER:CB | 2.41 | 0.49 |
| 1:F:39:ARG:HG2 | 1:F:66:THR:HB | 1.93 | 0.49 |
| 1:F:299:MET:HE1 | 1:F:304:THR:HB | 1.94 | 0.49 |
| 1:G:37:ARG:CG | 1:G:38:PRO:N | 2.75 | 0.49 |
| 1:G:40:HIS:O | 1:G:41:GLN:O | 2.30 | 0.49 |
| 1:H:43:VAL:O | 1:H:44:MET:HG2 | 2.13 | 0.49 |
| 1:I:34:ILE:HG22 | 1:I:35:VAL:H | 1.78 | 0.49 |
| 1:J:43:VAL:O | 1:J:44:MET:HG2 | 2.13 | 0.49 |
| 1:J:290:ARG:NH1 | 1:L:244:ASP:OD1 | 2.45 | 0.49 |
| 1:L:43:VAL:O | 1:L:44:MET:HG2 | 2.13 | 0.49 |
| 1:M:290:ARG:NH1 | 1:O:244:ASP:OD1 | 2.45 | 0.49 |
| 1:P:35:VAL:CA | 1:P:54:VAL:CG2 | 2.90 | 0.49 |
| 1:P:40:HIS:O | 1:P:41:GLN:O | 2.30 | 0.49 |
| 1:R:34:ILE:HG22 | 1:R:35:VAL:H | 1.78 | 0.49 |
| 1:S:34:ILE:HD13 | 1:S:67:LEU:CD1 | 2.41 | 0.49 |
| 1:T:290:ARG:NH1 | 1:V:244:ASP:OD1 | 2.45 | 0.49 |
| 1:U:369:ILE:C | 1:U:371:HIS:H | 2.15 | 0.49 |
| 1:W:34:ILE:HD13 | 1:W:67:LEU:CD1 | 2.41 | 0.49 |
| 1:W:34:ILE:CG2 | 1:W:35:VAL:N | 2.74 | 0.49 |
| 1:W:43:VAL:O | 1:W:44:MET:HG2 | 2.13 | 0.49 |
| 1:W:369:ILE:C | 1:W:371:HIS:H | 2.15 | 0.49 |
| 1:A:37:ARG:CG | 1:A:38:PRO:N | 2.75 | 0.49 |
| 1:C:40:HIS:O | 1:C:41:GLN:O | 2.30 | 0.49 |
| 1:F:34:ILE:CG2 | 1:F:35:VAL:N | 2.74 | 0.49 |
| 1:H:32:PRO:CG | 1:H:55:GLY:O | 2.55 | 0.49 |
| 1:H:290:ARG:NH1 | 1:J:244:ASP:OD1 | 2.45 | 0.49 |
| 1:K:35:VAL:CA | 1:K:54:VAL:CG2 | 2.90 | 0.49 |
| 1:K:43:VAL:O | 1:K:44:MET:HG2 | 2.13 | 0.49 |
| 1:M:299:MET:HE1 | 1:M:304:THR:HB | 1.94 | 0.49 |
| 1:N:39:ARG:HG2 | 1:N:66:THR:HB | 1.93 | 0.49 |
| 1:N:287:ILE:HG22 | 1:N:290:ARG:CZ | 2.43 | 0.49 |
| 1:Q:287:ILE:HG22 | 1:Q:290:ARG:CZ | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:142:LEU:HD21 | 1:S:165:ILE:CD1 | 2.38 | 0.49 |
| 1:S:147:ARG:CG | 1:S:147:ARG:NH2 | 2.71 | 0.49 |
| 1:T:39:ARG:HG2 | 1:T:66:THR:HB | 1.93 | 0.49 |
| 1:T:40:HIS:O | 1:T:41:GLN:O | 2.30 | 0.49 |
| 1:T:43:VAL:O | 1:T:44:MET:HG2 | 2.13 | 0.49 |
| 1:T:287:ILE:HG13 | 1:T:288:ASP:N | 2.27 | 0.49 |
| 1:D:147:ARG:CG | 1:D:147:ARG:NH2 | 2.71 | 0.49 |
| 1:D:290:ARG:NH1 | 1:F:244:ASP:OD1 | 2.45 | 0.49 |
| 1:F:361:GLU:HB3 | 1:F:369:ILE:CD1 | 2.14 | 0.49 |
| 1:G:34:ILE:HG22 | 1:G:35:VAL:H | 1.78 | 0.49 |
| 1:H:270:GLU:O | 1:H:270:GLU:CD | 2.51 | 0.49 |
| 1:I:287:ILE:HG13 | 1:I:288:ASP:N | 2.27 | 0.49 |
| 1:K:8:LEU:HB2 | 1:K:103:THR:HA | 1.95 | 0.49 |
| 1:P:22:ALA:HB1 | 1:P:348:SER:CB | 2.41 | 0.49 |
| 1:P:39:ARG:HG2 | 1:P:66:THR:HB | 1.93 | 0.49 |
| 1:Q:299:MET:HE1 | 1:Q:304:THR:HB | 1.94 | 0.49 |
| 1:Q:369:ILE:C | 1:Q:371:HIS:H | 2.15 | 0.49 |
| 1:R:40:HIS:O | 1:R:41:GLN:O | 2.30 | 0.49 |
| 1:S:290:ARG:NH1 | 1:U:244:ASP:OD1 | 2.45 | 0.49 |
| 1:S:369:ILE:C | 1:S:371:HIS:H | 2.15 | 0.49 |
| 1:U:44:MET:CG | 1:U:45:VAL:N | 2.75 | 0.49 |
| 1:V:37:ARG:CG | 1:V:38:PRO:N | 2.75 | 0.49 |
| 1:A:39:ARG:HG2 | 1:A:66:THR:HB | 1.93 | 0.49 |
| 1:B:147:ARG:CG | 1:B:147:ARG:NH2 | 2.71 | 0.49 |
| 1:B:287:ILE:HG13 | 1:B:288:ASP:N | 2.27 | 0.49 |
| 1:C:287:ILE:HG22 | 1:C:290:ARG:CZ | 2.43 | 0.49 |
| 1:D:287:ILE:HG22 | 1:D:290:ARG:CZ | 2.43 | 0.49 |
| 1:E:37:ARG:CG | 1:E:38:PRO:N | 2.75 | 0.49 |
| 1:E:40:HIS:O | 1:E:41:GLN:O | 2.30 | 0.49 |
| 1:E:369:ILE:C | 1:E:371:HIS:H | 2.15 | 0.49 |
| 1:F:287:ILE:HG22 | 1:F:290:ARG:CZ | 2.43 | 0.49 |
| 1:F:290:ARG:NH1 | 1:H:244:ASP:OD1 | 2.45 | 0.49 |
| 1:G:287:ILE:HG22 | 1:G:290:ARG:CZ | 2.43 | 0.49 |
| 1:L:290:ARG:NH1 | 1:N:244:ASP:OD1 | 2.45 | 0.49 |
| 1:M:58:ALA:HA | 1:M:65:LEU:CD2 | 2.43 | 0.49 |
| 1:N:270:GLU:O | 1:N:270:GLU:CD | 2.51 | 0.49 |
| 1:O:298:VAL:HG12 | 1:O:335:ARG:NH1 | 2.28 | 0.49 |
| 1:Q:37:ARG:CG | 1:Q:38:PRO:N | 2.75 | 0.49 |
| 1:Q:43:VAL:O | 1:Q:44:MET:HG2 | 2.13 | 0.49 |
| 1:S:32:PRO:CG | 1:S:55:GLY:O | 2.55 | 0.49 |
| 1:S:43:VAL:O | 1:S:44:MET:HG2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:287:ILE:HG22 | 1:T:290:ARG:CZ | 2.43 | 0.49 |
| 1:U:300:SER:HA | 1:U:335:ARG:HG2 | 1.89 | 0.49 |
| 1:V:8:LEU:HB2 | 1:V:103:THR:HA | 1.95 | 0.49 |
| 1:W:287:ILE:HG22 | 1:W:290:ARG:CZ | 2.43 | 0.49 |
| 1:C:270:GLU:O | 1:C:270:GLU:CD | 2.51 | 0.49 |
| 1:D:43:VAL:O | 1:D:44:MET:HG2 | 2.13 | 0.49 |
| 1:F:298:VAL:HG12 | 1:F:335:ARG:NH1 | 2.28 | 0.49 |
| 1:G:43:VAL:O | 1:G:44:MET:HG2 | 2.13 | 0.49 |
| 1:G:142:LEU:HD21 | 1:G:165:ILE:CD1 | 2.38 | 0.49 |
| 1:G:147:ARG:CG | 1:G:147:ARG:NH2 | 2.71 | 0.49 |
| 1:H:34:ILE:HD13 | 1:H:67:LEU:CD1 | 2.41 | 0.49 |
| 1:H:287:ILE:HG13 | 1:H:288:ASP:N | 2.27 | 0.49 |
| 1:I:8:LEU:HB2 | 1:I:103:THR:HA | 1.95 | 0.49 |
| 1:I:35:VAL:CA | 1:I:54:VAL:CG2 | 2.90 | 0.49 |
| 1:I:287:ILE:HG22 | 1:I:290:ARG:CZ | 2.43 | 0.49 |
| 1:J:34:ILE:HD13 | 1:J:67:LEU:CD1 | 2.41 | 0.49 |
| 1:M:37:ARG:CG | 1:M:38:PRO:N | 2.75 | 0.49 |
| 1:P:287:ILE:HG22 | 1:P:290:ARG:CZ | 2.43 | 0.49 |
| 1:Q:298:VAL:HG12 | 1:Q:335:ARG:NH1 | 2.28 | 0.49 |
| 1:S:270:GLU:O | 1:S:270:GLU:CD | 2.52 | 0.49 |
| 1:U:290:ARG:NH1 | 1:W:244:ASP:OD1 | 2.45 | 0.49 |
| 1:U:362:TYR:HE1 | 1:U:367:PRO:CB | 2.19 | 0.49 |
| 1:V:39:ARG:NE | 1:V:66:THR:CA | 2.69 | 0.49 |
| 1:V:147:ARG:CG | 1:V:147:ARG:NH2 | 2.71 | 0.49 |
| 1:W:270:GLU:O | 1:W:270:GLU:CD | 2.51 | 0.49 |
| 1:A:43:VAL:O | 1:A:44:MET:HG2 | 2.13 | 0.49 |
| 1:B:8:LEU:HB2 | 1:B:103:THR:HA | 1.95 | 0.49 |
| 1:B:270:GLU:O | 1:B:270:GLU:CD | 2.51 | 0.49 |
| 1:C:287:ILE:HG13 | 1:C:288:ASP:N | 2.27 | 0.49 |
| 1:E:270:GLU:CD | 1:E:270:GLU:O | 2.52 | 0.49 |
| 1:E:290:ARG:NH1 | 1:G:244:ASP:OD1 | 2.45 | 0.49 |
| 1:F:44:MET:CG | 1:F:45:VAL:N | 2.76 | 0.49 |
| 1:H:58:ALA:HA | 1:H:65:LEU:CD2 | 2.43 | 0.49 |
| 1:H:298:VAL:HG12 | 1:H:335:ARG:NH1 | 2.28 | 0.49 |
| 1:H:369:ILE:C | 1:H:371:HIS:H | 2.15 | 0.49 |
| 1:I:147:ARG:CG | 1:I:147:ARG:NH2 | 2.71 | 0.49 |
| 1:J:180:LEU:HD12 | 1:J:181:ALA:O | 2.13 | 0.49 |
| 1:K:37:ARG:CG | 1:K:38:PRO:N | 2.75 | 0.49 |
| 1:L:35:VAL:CA | 1:L:54:VAL:CG2 | 2.90 | 0.49 |
| 1:M:34:ILE:HD13 | 1:M:67:LEU:CD1 | 2.41 | 0.49 |
| 1:N:34:ILE:HG22 | 1:N:35:VAL:H | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:35:VAL:CA | 1:N:54:VAL:CG2 | 2.90 | 0.49 |
| 1:O:43:VAL:O | 1:O:44:MET:HG2 | 2.13 | 0.49 |
| 1:O:58:ALA:HA | 1:O:65:LEU:CD2 | 2.43 | 0.49 |
| 1:P:43:VAL:O | 1:P:44:MET:HG2 | 2.13 | 0.49 |
| 1:Q:2:GLU:OE2 | 1:Q:2:GLU:HA | 2.10 | 0.49 |
| 1:T:8:LEU:HB2 | 1:T:103:THR:HA | 1.95 | 0.49 |
| 1:T:270:GLU:O | 1:T:270:GLU:CD | 2.51 | 0.49 |
| 1:U:58:ALA:HA | 1:U:65:LEU:CD2 | 2.43 | 0.49 |
| 1:V:180:LEU:HD12 | 1:V:181:ALA:O | 2.13 | 0.49 |
| 1:V:287:ILE:HG13 | 1:V:288:ASP:N | 2.27 | 0.49 |
| 1:W:34:ILE:HG22 | 1:W:35:VAL:H | 1.78 | 0.49 |
| 1:A:22:ALA:HB1 | 1:A:348:SER:CB | 2.41 | 0.48 |
| 1:B:2:GLU:HA | 1:B:2:GLU:OE2 | 2.11 | 0.48 |
| 1:C:54:VAL:CG1 | 1:C:55:GLY:N | 2.72 | 0.48 |
| 1:D:298:VAL:HG12 | 1:D:335:ARG:NH1 | 2.28 | 0.48 |
| 1:E:180:LEU:HD12 | 1:E:181:ALA:O | 2.13 | 0.48 |
| 1:F:58:ALA:HA | 1:F:65:LEU:CD2 | 2.43 | 0.48 |
| 1:J:287:ILE:HG22 | 1:J:290:ARG:CZ | 2.43 | 0.48 |
| 1:K:58:ALA:HA | 1:K:65:LEU:CD2 | 2.43 | 0.48 |
| 1:K:180:LEU:HD12 | 1:K:181:ALA:O | 2.13 | 0.48 |
| 1:M:8:LEU:HB2 | 1:M:103:THR:HA | 1.95 | 0.48 |
| 1:M:298:VAL:HG12 | 1:M:335:ARG:NH1 | 2.28 | 0.48 |
| 1:Q:270:GLU:O | 1:Q:270:GLU:CD | 2.51 | 0.48 |
| 1:S:8:LEU:HB2 | 1:S:103:THR:HA | 1.95 | 0.48 |
| 1:S:287:ILE:HG13 | 1:S:288:ASP:N | 2.27 | 0.48 |
| 1:S:287:ILE:HG22 | 1:S:290:ARG:CZ | 2.43 | 0.48 |
| 1:T:58:ALA:HA | 1:T:65:LEU:CD2 | 2.43 | 0.48 |
| 1:U:8:LEU:HB2 | 1:U:103:THR:HA | 1.95 | 0.48 |
| 1:U:34:ILE:HG22 | 1:U:35:VAL:H | 1.78 | 0.48 |
| 1:U:180:LEU:HD12 | 1:U:181:ALA:O | 2.13 | 0.48 |
| 1:V:34:ILE:HD13 | 1:V:67:LEU:CD1 | 2.41 | 0.48 |
| 1:W:35:VAL:CA | 1:W:54:VAL:CG2 | 2.90 | 0.48 |
| 1:A:287:ILE:HG22 | 1:A:290:ARG:CZ | 2.43 | 0.48 |
| 1:A:299:MET:HE1 | 1:A:304:THR:HB | 1.96 | 0.48 |
| 1:B:37:ARG:CG | 1:B:38:PRO:N | 2.75 | 0.48 |
| 1:B:58:ALA:CB | 1:B:65:LEU:CD2 | 2.90 | 0.48 |
| 1:B:173:HIS:NE2 | 1:C:267:ILE:C | 2.67 | 0.48 |
| 1:C:147:ARG:CG | 1:C:147:ARG:NH2 | 2.71 | 0.48 |
| 1:D:173:HIS:NE2 | 1:E:267:ILE:C | 2.67 | 0.48 |
| 1:D:270:GLU:O | 1:D:270:GLU:CD | 2.51 | 0.48 |
| 1:D:287:ILE:HG13 | 1:D:288:ASP:N | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:173:HIS:NE2 | 1:G:267:ILE:C | 2.67 | 0.48 |
| 1:G:173:HIS:NE2 | 1:H:267:ILE:C | 2.67 | 0.48 |
| 1:I:34:ILE:HD13 | 1:I:67:LEU:CD1 | 2.41 | 0.48 |
| 1:M:43:VAL:O | 1:M:44:MET:HG2 | 2.13 | 0.48 |
| 1:M:173:HIS:NE2 | 1:N:267:ILE:C | 2.67 | 0.48 |
| 1:M:227:MET:HA | 1:M:227:MET:HE3 | 1.95 | 0.48 |
| 1:O:173:HIS:NE2 | 1:P:267:ILE:C | 2.67 | 0.48 |
| 1:P:180:LEU:HD12 | 1:P:181:ALA:O | 2.13 | 0.48 |
| 1:Q:34:ILE:HG22 | 1:Q:35:VAL:H | 1.78 | 0.48 |
| 1:Q:287:ILE:HG13 | 1:Q:288:ASP:N | 2.27 | 0.48 |
| 1:W:8:LEU:HB2 | 1:W:103:THR:HA | 1.95 | 0.48 |
| 1:W:58:ALA:HA | 1:W:65:LEU:CD2 | 2.43 | 0.48 |
| 1:W:223:PHE:CD1 | 1:W:259:GLU:CG | 2.96 | 0.48 |
| 1:A:34:ILE:HG22 | 1:A:54:VAL:HG21 | 1.95 | 0.48 |
| 1:C:34:ILE:HG22 | 1:C:54:VAL:HG21 | 1.96 | 0.48 |
| 1:D:58:ALA:HA | 1:D:65:LEU:CD2 | 2.43 | 0.48 |
| 1:E:43:VAL:O | 1:E:44:MET:HG2 | 2.13 | 0.48 |
| 1:G:39:ARG:NE | 1:G:66:THR:CA | 2.69 | 0.48 |
| 1:H:35:VAL:CA | 1:H:54:VAL:CG2 | 2.90 | 0.48 |
| 1:H:173:HIS:NE2 | 1:I:267:ILE:C | 2.67 | 0.48 |
| 1:I:43:VAL:O | 1:I:44:MET:HG2 | 2.13 | 0.48 |
| 1:K:270:GLU:O | 1:K:270:GLU:CD | 2.51 | 0.48 |
| 1:K:287:ILE:HG13 | 1:K:288:ASP:N | 2.27 | 0.48 |
| 1:L:34:ILE:HD13 | 1:L:67:LEU:CD1 | 2.41 | 0.48 |
| 1:O:147:ARG:CG | 1:O:147:ARG:NH2 | 2.71 | 0.48 |
| 1:O:227:MET:HA | 1:O:227:MET:HE3 | 1.95 | 0.48 |
| 1:P:270:GLU:O | 1:P:270:GLU:CD | 2.51 | 0.48 |
| 1:Q:34:ILE:CG2 | 1:Q:67:LEU:HD22 | 2.28 | 0.48 |
| 1:Q:173:HIS:NE2 | 1:R:267:ILE:C | 2.67 | 0.48 |
| 1:Q:362:TYR:HE1 | 1:Q:367:PRO:CB | 2.19 | 0.48 |
| 1:R:43:VAL:O | 1:R:44:MET:HG2 | 2.13 | 0.48 |
| 1:R:270:GLU:O | 1:R:270:GLU:CD | 2.52 | 0.48 |
| 1:S:34:ILE:HG22 | 1:S:35:VAL:H | 1.78 | 0.48 |
| 1:S:173:HIS:NE2 | 1:T:267:ILE:C | 2.67 | 0.48 |
| 1:U:223:PHE:CD1 | 1:U:259:GLU:CG | 2.96 | 0.48 |
| 1:V:58:ALA:HA | 1:V:65:LEU:CD2 | 2.43 | 0.48 |
| 1:V:287:ILE:HG22 | 1:V:290:ARG:CZ | 2.43 | 0.48 |
| 1:V:298:VAL:HG12 | 1:V:335:ARG:NH1 | 2.28 | 0.48 |
| 1:A:287:ILE:HG13 | 1:A:288:ASP:N | 2.27 | 0.48 |
| 1:A:298:VAL:HG12 | 1:A:335:ARG:NH1 | 2.28 | 0.48 |
| 1:C:34:ILE:CG2 | 1:C:67:LEU:HD22 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:180:LEU:HD12 | 1:D:181:ALA:O | 2.13 | 0.48 |
| 1:E:34:ILE:HG22 | 1:E:35:VAL:H | 1.78 | 0.48 |
| 1:E:287:ILE:HG22 | 1:E:290:ARG:CZ | 2.43 | 0.48 |
| 1:I:173:HIS:NE2 | 1:J:267:ILE:C | 2.67 | 0.48 |
| 1:J:270:GLU:O | 1:J:270:GLU:CD | 2.52 | 0.48 |
| 1:J:298:VAL:HG12 | 1:J:335:ARG:NH1 | 2.28 | 0.48 |
| 1:K:173:HIS:NE2 | 1:L:267:ILE:C | 2.67 | 0.48 |
| 1:L:142:LEU:HD21 | 1:L:165:ILE:CD1 | 2.38 | 0.48 |
| 1:L:270:GLU:O | 1:L:270:GLU:CD | 2.51 | 0.48 |
| 1:M:287:ILE:HG22 | 1:M:290:ARG:CZ | 2.43 | 0.48 |
| 1:O:34:ILE:HG23 | 1:O:68:LYS:H | 1.79 | 0.48 |
| 1:Q:142:LEU:HD21 | 1:Q:165:ILE:CD1 | 2.39 | 0.48 |
| 1:Q:223:PHE:CD1 | 1:Q:259:GLU:CG | 2.96 | 0.48 |
| 1:R:8:LEU:HB2 | 1:R:103:THR:HA | 1.95 | 0.48 |
| 1:R:147:ARG:CG | 1:R:147:ARG:NH2 | 2.71 | 0.48 |
| 1:R:287:ILE:HG22 | 1:R:290:ARG:CZ | 2.43 | 0.48 |
| 1:S:34:ILE:HG23 | 1:S:68:LYS:H | 1.79 | 0.48 |
| 1:S:58:ALA:HA | 1:S:65:LEU:CD2 | 2.43 | 0.48 |
| 1:U:34:ILE:HG23 | 1:U:68:LYS:H | 1.79 | 0.48 |
| 1:V:270:GLU:O | 1:V:270:GLU:CD | 2.51 | 0.48 |
| 1:W:298:VAL:HG12 | 1:W:335:ARG:NH1 | 2.28 | 0.48 |
| 1:W:335:ARG:O | 1:W:338:SER:HB3 | 2.14 | 0.48 |
| 1:A:34:ILE:HG23 | 1:A:68:LYS:H | 1.79 | 0.48 |
| 1:C:223:PHE:CD1 | 1:C:259:GLU:CG | 2.96 | 0.48 |
| 1:D:8:LEU:HB2 | 1:D:103:THR:HA | 1.95 | 0.48 |
| 1:E:34:ILE:HG22 | 1:E:54:VAL:HG21 | 1.96 | 0.48 |
| 1:E:34:ILE:HG23 | 1:E:68:LYS:H | 1.79 | 0.48 |
| 1:F:43:VAL:O | 1:F:44:MET:HG2 | 2.13 | 0.48 |
| 1:F:270:GLU:O | 1:F:270:GLU:CD | 2.51 | 0.48 |
| 1:F:287:ILE:HG13 | 1:F:288:ASP:N | 2.27 | 0.48 |
| 1:G:8:LEU:HB2 | 1:G:103:THR:HA | 1.95 | 0.48 |
| 1:G:180:LEU:HD12 | 1:G:181:ALA:O | 2.13 | 0.48 |
| 1:J:35:VAL:CA | 1:J:54:VAL:CG2 | 2.90 | 0.48 |
| 1:N:34:ILE:HG23 | 1:N:68:LYS:H | 1.79 | 0.48 |
| 1:O:223:PHE:CD1 | 1:O:259:GLU:CG | 2.96 | 0.48 |
| 1:P:300:SER:HA | 1:P:335:ARG:HG2 | 1.89 | 0.48 |
| 1:Q:58:ALA:HA | 1:Q:65:LEU:CD2 | 2.43 | 0.48 |
| 1:Q:236:LEU:HD22 | 1:Q:251:GLY:C | 2.34 | 0.48 |
| 1:R:173:HIS:NE2 | 1:S:267:ILE:C | 2.67 | 0.48 |
| 1:S:223:PHE:CD1 | 1:S:259:GLU:CG | 2.96 | 0.48 |
| 1:S:298:VAL:HG12 | 1:S:335:ARG:NH1 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:300:SER:HA | 1:S:335:ARG:HG2 | 1.89 | 0.48 |
| 1:S:335:ARG:O | 1:S:338:SER:HB3 | 2.13 | 0.48 |
| 1:V:173:HIS:NE2 | 1:W:267:ILE:C | 2.67 | 0.48 |
| 1:W:34:ILE:HG23 | 1:W:68:LYS:H | 1.79 | 0.48 |
| 1:B:180:LEU:HD12 | 1:B:181:ALA:O | 2.13 | 0.48 |
| 1:B:369:ILE:C | 1:B:371:HIS:H | 2.15 | 0.48 |
| 1:C:43:VAL:O | 1:C:44:MET:HG2 | 2.13 | 0.48 |
| 1:C:227:MET:HA | 1:C:227:MET:HE3 | 1.95 | 0.48 |
| 1:D:34:ILE:HG23 | 1:D:68:LYS:H | 1.79 | 0.48 |
| 1:I:31:PHE:HA | 1:I:32:PRO:HD3 | 1.65 | 0.48 |
| 1:I:58:ALA:HA | 1:I:65:LEU:CD2 | 2.43 | 0.48 |
| 1:J:39:ARG:NE | 1:J:66:THR:CA | 2.69 | 0.48 |
| 1:L:34:ILE:HG22 | 1:L:35:VAL:H | 1.78 | 0.48 |
| 1:M:58:ALA:CB | 1:M:65:LEU:CD2 | 2.90 | 0.48 |
| 1:M:270:GLU:O | 1:M:270:GLU:CD | 2.52 | 0.48 |
| 1:O:180:LEU:HD12 | 1:O:181:ALA:O | 2.13 | 0.48 |
| 1:O:236:LEU:HD22 | 1:O:251:GLY:C | 2.34 | 0.48 |
| 1:U:335:ARG:O | 1:U:338:SER:HB3 | 2.14 | 0.48 |
| 1:A:361:GLU:HB3 | 1:A:369:ILE:CD1 | 2.14 | 0.48 |
| 1:A:369:ILE:HG22 | 1:A:370:VAL:N | 2.29 | 0.48 |
| 1:B:58:ALA:HA | 1:B:65:LEU:CD2 | 2.43 | 0.48 |
| 1:C:34:ILE:HG23 | 1:C:68:LYS:H | 1.79 | 0.48 |
| 1:D:58:ALA:CB | 1:D:65:LEU:CD2 | 2.90 | 0.48 |
| 1:F:34:ILE:HG23 | 1:F:68:LYS:H | 1.79 | 0.48 |
| 1:F:35:VAL:CA | 1:F:54:VAL:CG2 | 2.90 | 0.48 |
| 1:F:369:ILE:C | 1:F:371:HIS:H | 2.15 | 0.48 |
| 1:G:58:ALA:CB | 1:G:65:LEU:CD2 | 2.90 | 0.48 |
| 1:H:8:LEU:HB2 | 1:H:103:THR:HA | 1.95 | 0.48 |
| 1:H:180:LEU:HD12 | 1:H:181:ALA:O | 2.13 | 0.48 |
| 1:I:2:GLU:OE2 | 1:I:2:GLU:HA | 2.10 | 0.48 |
| 1:J:8:LEU:HB2 | 1:J:103:THR:HA | 1.95 | 0.48 |
| 1:K:298:VAL:HG12 | 1:K:335:ARG:NH1 | 2.28 | 0.48 |
| 1:M:2:GLU:OE2 | 1:M:2:GLU:HA | 2.11 | 0.48 |
| 1:M:223:PHE:CD1 | 1:M:259:GLU:CG | 2.96 | 0.48 |
| 1:M:287:ILE:HG13 | 1:M:288:ASP:N | 2.27 | 0.48 |
| 1:N:43:VAL:O | 1:N:44:MET:HG2 | 2.13 | 0.48 |
| 1:N:180:LEU:HD12 | 1:N:181:ALA:O | 2.13 | 0.48 |
| 1:O:8:LEU:HB2 | 1:O:103:THR:HA | 1.95 | 0.48 |
| 1:Q:335:ARG:O | 1:Q:338:SER:HB3 | 2.13 | 0.48 |
| 1:R:58:ALA:HA | 1:R:65:LEU:CD2 | 2.43 | 0.48 |
| 1:R:180:LEU:HD12 | 1:R:181:ALA:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:180:LEU:HD12 | 1:S:181:ALA:O | 2.13 | 0.48 |
| 1:T:34:ILE:HG22 | 1:T:54:VAL:HG21 | 1.96 | 0.48 |
| 1:T:298:VAL:HG12 | 1:T:335:ARG:NH1 | 2.28 | 0.48 |
| 1:V:34:ILE:HG23 | 1:V:68:LYS:H | 1.79 | 0.48 |
| 1:D:35:VAL:CA | 1:D:54:VAL:CG2 | 2.90 | 0.48 |
| 1:E:173:HIS:NE2 | 1:F:267:ILE:C | 2.67 | 0.48 |
| 1:G:34:ILE:HG22 | 1:G:54:VAL:HG21 | 1.96 | 0.48 |
| 1:G:369:ILE:HG22 | 1:G:370:VAL:N | 2.29 | 0.48 |
| 1:I:8:LEU:O | 1:I:104:LEU:N | 2.47 | 0.48 |
| 1:I:270:GLU:O | 1:I:270:GLU:CD | 2.52 | 0.48 |
| 1:J:58:ALA:HA | 1:J:65:LEU:CD2 | 2.43 | 0.48 |
| 1:L:8:LEU:HB2 | 1:L:103:THR:HA | 1.95 | 0.48 |
| 1:M:34:ILE:HG23 | 1:M:68:LYS:H | 1.79 | 0.48 |
| 1:M:362:TYR:HE1 | 1:M:367:PRO:CB | 2.19 | 0.48 |
| 1:N:173:HIS:NE2 | 1:O:267:ILE:C | 2.67 | 0.48 |
| 1:N:335:ARG:O | 1:N:338:SER:HB3 | 2.14 | 0.48 |
| 1:P:8:LEU:HB2 | 1:P:103:THR:HA | 1.95 | 0.48 |
| 1:P:369:ILE:HG22 | 1:P:370:VAL:N | 2.29 | 0.48 |
| 1:Q:180:LEU:HD12 | 1:Q:181:ALA:O | 2.13 | 0.48 |
| 1:R:44:MET:CG | 1:R:45:VAL:N | 2.75 | 0.48 |
| 1:T:173:HIS:NE2 | 1:U:267:ILE:C | 2.67 | 0.48 |
| 1:U:58:ALA:CB | 1:U:65:LEU:CD2 | 2.90 | 0.48 |
| 1:U:173:HIS:NE2 | 1:V:267:ILE:C | 2.67 | 0.48 |
| 1:U:270:GLU:O | 1:U:270:GLU:CD | 2.52 | 0.48 |
| 1:V:34:ILE:HG22 | 1:V:54:VAL:HG21 | 1.96 | 0.48 |
| 1:A:58:ALA:HA | 1:A:65:LEU:CD2 | 2.43 | 0.48 |
| 1:A:288:ASP:OD2 | 1:C:204:ALA:HB1 | 2.14 | 0.48 |
| 1:B:298:VAL:HG12 | 1:B:335:ARG:NH1 | 2.28 | 0.48 |
| 1:C:288:ASP:OD2 | 1:E:204:ALA:HB1 | 2.14 | 0.48 |
| 1:C:335:ARG:O | 1:C:338:SER:HB3 | 2.14 | 0.48 |
| 1:E:34:ILE:HD13 | 1:E:67:LEU:CD1 | 2.41 | 0.48 |
| 1:F:180:LEU:HD12 | 1:F:181:ALA:O | 2.13 | 0.48 |
| 1:G:58:ALA:HA | 1:G:65:LEU:CD2 | 2.43 | 0.48 |
| 1:J:236:LEU:HD22 | 1:J:251:GLY:C | 2.34 | 0.48 |
| 1:K:223:PHE:CD1 | 1:K:259:GLU:CG | 2.96 | 0.48 |
| 1:L:236:LEU:HD22 | 1:L:251:GLY:C | 2.34 | 0.48 |
| 1:L:335:ARG:O | 1:L:338:SER:HB3 | 2.14 | 0.48 |
| 1:M:180:LEU:O | 1:M:180:LEU:HG | 2.11 | 0.48 |
| 1:O:335:ARG:O | 1:O:338:SER:HB3 | 2.14 | 0.48 |
| 1:P:37:ARG:CG | 1:P:38:PRO:N | 2.75 | 0.48 |
| 1:P:173:HIS:NE2 | 1:Q:267:ILE:C | 2.67 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:34:ILE:HG22 | 1:R:54:VAL:HG21 | 1.95 | 0.48 |
| 1:S:58:ALA:CB | 1:S:65:LEU:CD2 | 2.90 | 0.48 |
| 1:S:236:LEU:HD22 | 1:S:251:GLY:C | 2.34 | 0.48 |
| 1:T:34:ILE:HD13 | 1:T:67:LEU:CD1 | 2.41 | 0.48 |
| 1:T:180:LEU:HD12 | 1:T:181:ALA:O | 2.13 | 0.48 |
| 1:U:227:MET:HA | 1:U:227:MET:HE3 | 1.95 | 0.48 |
| 1:V:227:MET:HA | 1:V:227:MET:HE3 | 1.96 | 0.48 |
| 1:V:369:ILE:HG22 | 1:V:370:VAL:N | 2.29 | 0.48 |
| 1:A:34:ILE:HD13 | 1:A:67:LEU:CD1 | 2.41 | 0.48 |
| 1:A:270:GLU:O | 1:A:270:GLU:CD | 2.51 | 0.48 |
| 1:B:31:PHE:HA | 1:B:32:PRO:HD3 | 1.66 | 0.48 |
| 1:C:58:ALA:HA | 1:C:65:LEU:CD2 | 2.43 | 0.48 |
| 1:C:180:LEU:HD12 | 1:C:181:ALA:O | 2.13 | 0.48 |
| 1:C:298:VAL:HG12 | 1:C:335:ARG:NH1 | 2.28 | 0.48 |
| 1:D:288:ASP:OD2 | 1:F:204:ALA:HB1 | 2.14 | 0.48 |
| 1:E:58:ALA:CB | 1:E:65:LEU:CD2 | 2.90 | 0.48 |
| 1:E:223:PHE:CD1 | 1:E:259:GLU:CG | 2.96 | 0.48 |
| 1:E:335:ARG:O | 1:E:338:SER:HB3 | 2.14 | 0.48 |
| 1:G:270:GLU:O | 1:G:270:GLU:CD | 2.52 | 0.48 |
| 1:H:58:ALA:O | 1:H:59:GLN:C | 2.52 | 0.48 |
| 1:H:236:LEU:HD22 | 1:H:251:GLY:C | 2.34 | 0.48 |
| 1:H:288:ASP:OD2 | 1:J:204:ALA:HB1 | 2.14 | 0.48 |
| 1:I:22:ALA:HB1 | 1:I:348:SER:CB | 2.41 | 0.48 |
| 1:I:180:LEU:HD12 | 1:I:181:ALA:O | 2.13 | 0.48 |
| 1:I:227:MET:HA | 1:I:227:MET:HE3 | 1.96 | 0.48 |
| 1:J:335:ARG:O | 1:J:338:SER:HB3 | 2.14 | 0.48 |
| 1:J:369:ILE:HG22 | 1:J:370:VAL:N | 2.29 | 0.48 |
| 1:L:34:ILE:HG23 | 1:L:68:LYS:H | 1.79 | 0.48 |
| 1:L:288:ASP:OD2 | 1:N:204:ALA:HB1 | 2.14 | 0.48 |
| 1:M:335:ARG:O | 1:M:338:SER:HB3 | 2.14 | 0.48 |
| 1:M:369:ILE:HG22 | 1:M:370:VAL:N | 2.29 | 0.48 |
| 1:N:8:LEU:HB2 | 1:N:103:THR:HA | 1.95 | 0.48 |
| 1:O:22:ALA:HB1 | 1:O:348:SER:CB | 2.41 | 0.48 |
| 1:O:288:ASP:OD2 | 1:Q:204:ALA:HB1 | 2.14 | 0.48 |
| 1:P:288:ASP:OD2 | 1:R:204:ALA:HB1 | 2.14 | 0.48 |
| 1:P:335:ARG:O | 1:P:338:SER:HB3 | 2.14 | 0.48 |
| 1:Q:34:ILE:HG23 | 1:Q:68:LYS:H | 1.79 | 0.48 |
| 1:R:298:VAL:HG12 | 1:R:335:ARG:NH1 | 2.28 | 0.48 |
| 1:S:58:ALA:O | 1:S:59:GLN:C | 2.53 | 0.48 |
| 1:T:8:LEU:O | 1:T:104:LEU:N | 2.47 | 0.48 |
| 1:T:44:MET:CG | 1:T:45:VAL:N | 2.75 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:236:LEU:HD11 | 1:T:237:GLU:HG2 | 1.96 | 0.48 |
| 1:U:35:VAL:CA | 1:U:54:VAL:CG2 | 2.90 | 0.48 |
| 1:U:43:VAL:O | 1:U:44:MET:HG2 | 2.13 | 0.48 |
| 1:U:287:ILE:HG13 | 1:U:288:ASP:N | 2.27 | 0.48 |
| 1:W:22:ALA:HB1 | 1:W:348:SER:CB | 2.41 | 0.48 |
| 1:A:58:ALA:O | 1:A:59:GLN:C | 2.53 | 0.47 |
| 1:A:180:LEU:HD12 | 1:A:181:ALA:O | 2.14 | 0.47 |
| 1:A:335:ARG:O | 1:A:338:SER:HB3 | 2.14 | 0.47 |
| 1:D:58:ALA:O | 1:D:59:GLN:C | 2.53 | 0.47 |
| 1:D:369:ILE:C | 1:D:371:HIS:H | 2.15 | 0.47 |
| 1:E:8:LEU:HB2 | 1:E:103:THR:HA | 1.95 | 0.47 |
| 1:G:223:PHE:CD1 | 1:G:259:GLU:CG | 2.96 | 0.47 |
| 1:G:236:LEU:HD22 | 1:G:251:GLY:C | 2.34 | 0.47 |
| 1:G:236:LEU:HD11 | 1:G:237:GLU:HG2 | 1.96 | 0.47 |
| 1:H:236:LEU:HD11 | 1:H:237:GLU:HG2 | 1.96 | 0.47 |
| 1:I:223:PHE:CD1 | 1:I:259:GLU:CG | 2.96 | 0.47 |
| 1:J:173:HIS:NE2 | 1:K:267:ILE:C | 2.67 | 0.47 |
| 1:J:236:LEU:HD11 | 1:J:237:GLU:HG2 | 1.96 | 0.47 |
| 1:K:58:ALA:CB | 1:K:65:LEU:CD2 | 2.90 | 0.47 |
| 1:L:58:ALA:O | 1:L:59:GLN:C | 2.53 | 0.47 |
| 1:L:180:LEU:HD12 | 1:L:181:ALA:O | 2.13 | 0.47 |
| 1:N:236:LEU:HD22 | 1:N:251:GLY:C | 2.34 | 0.47 |
| 1:O:34:ILE:HG22 | 1:O:35:VAL:H | 1.78 | 0.47 |
| 1:O:287:ILE:HG13 | 1:O:288:ASP:N | 2.27 | 0.47 |
| 1:P:44:MET:CG | 1:P:45:VAL:N | 2.76 | 0.47 |
| 1:P:58:ALA:O | 1:P:59:GLN:C | 2.53 | 0.47 |
| 1:Q:58:ALA:CB | 1:Q:65:LEU:CD2 | 2.90 | 0.47 |
| 1:Q:288:ASP:OD2 | 1:S:204:ALA:HB1 | 2.14 | 0.47 |
| 1:S:288:ASP:OD2 | 1:U:204:ALA:HB1 | 2.14 | 0.47 |
| 1:T:34:ILE:HG23 | 1:T:68:LYS:H | 1.79 | 0.47 |
| 1:V:8:LEU:O | 1:V:104:LEU:N | 2.47 | 0.47 |
| 1:W:58:ALA:O | 1:W:59:GLN:C | 2.53 | 0.47 |
| 1:W:287:ILE:HG13 | 1:W:288:ASP:N | 2.27 | 0.47 |
| 1:A:173:HIS:NE2 | 1:B:267:ILE:C | 2.67 | 0.47 |
| 1:A:287:ILE:HD12 | 1:C:208:ILE:HD13 | 1.96 | 0.47 |
| 1:E:2:GLU:OE2 | 1:E:2:GLU:HA | 2.11 | 0.47 |
| 1:E:58:ALA:HA | 1:E:65:LEU:CD2 | 2.43 | 0.47 |
| 1:E:236:LEU:HD22 | 1:E:251:GLY:C | 2.34 | 0.47 |
| 1:E:236:LEU:HD11 | 1:E:237:GLU:HG2 | 1.96 | 0.47 |
| 1:E:288:ASP:OD2 | 1:G:204:ALA:HB1 | 2.14 | 0.47 |
| 1:G:34:ILE:HG23 | 1:G:68:LYS:H | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:236:LEU:HD22 | 1:I:251:GLY:C | 2.34 | 0.47 |
| 1:I:369:ILE:HG22 | 1:I:370:VAL:N | 2.29 | 0.47 |
| 1:J:288:ASP:OD2 | 1:L:204:ALA:HB1 | 2.14 | 0.47 |
| 1:K:8:LEU:O | 1:K:104:LEU:N | 2.47 | 0.47 |
| 1:L:287:ILE:HD12 | 1:N:208:ILE:HD13 | 1.96 | 0.47 |
| 1:N:143:TYR:CZ | 1:N:345:ILE:CG2 | 2.98 | 0.47 |
| 1:N:236:LEU:HD11 | 1:N:237:GLU:HG2 | 1.96 | 0.47 |
| 1:O:58:ALA:O | 1:O:59:GLN:C | 2.53 | 0.47 |
| 1:O:270:GLU:O | 1:O:270:GLU:CD | 2.51 | 0.47 |
| 1:P:34:ILE:HD13 | 1:P:67:LEU:CD1 | 2.41 | 0.47 |
| 1:P:34:ILE:HG23 | 1:P:68:LYS:H | 1.79 | 0.47 |
| 1:P:236:LEU:HD11 | 1:P:237:GLU:HG2 | 1.96 | 0.47 |
| 1:P:298:VAL:HG12 | 1:P:335:ARG:NH1 | 2.28 | 0.47 |
| 1:Q:8:LEU:HB2 | 1:Q:103:THR:HA | 1.95 | 0.47 |
| 1:Q:300:SER:HA | 1:Q:335:ARG:HG2 | 1.89 | 0.47 |
| 1:R:227:MET:HA | 1:R:227:MET:HE3 | 1.96 | 0.47 |
| 1:R:236:LEU:HD11 | 1:R:237:GLU:HG2 | 1.97 | 0.47 |
| 1:R:369:ILE:HG22 | 1:R:370:VAL:N | 2.29 | 0.47 |
| 1:U:236:LEU:HD11 | 1:U:237:GLU:HG2 | 1.97 | 0.47 |
| 1:W:236:LEU:HD11 | 1:W:237:GLU:HG2 | 1.96 | 0.47 |
| 1:B:43:VAL:O | 1:B:44:MET:HG2 | 2.13 | 0.47 |
| 1:B:58:ALA:O | 1:B:59:GLN:C | 2.53 | 0.47 |
| 1:C:236:LEU:HD11 | 1:C:237:GLU:HG2 | 1.96 | 0.47 |
| 1:E:58:ALA:O | 1:E:59:GLN:C | 2.53 | 0.47 |
| 1:E:298:VAL:HG12 | 1:E:335:ARG:NH1 | 2.28 | 0.47 |
| 1:F:8:LEU:HB2 | 1:F:103:THR:HA | 1.95 | 0.47 |
| 1:F:236:LEU:HD22 | 1:F:251:GLY:C | 2.34 | 0.47 |
| 1:F:288:ASP:OD2 | 1:H:204:ALA:HB1 | 2.14 | 0.47 |
| 1:G:335:ARG:O | 1:G:338:SER:HB3 | 2.14 | 0.47 |
| 1:H:34:ILE:CG2 | 1:H:67:LEU:HD22 | 2.28 | 0.47 |
| 1:L:34:ILE:HG22 | 1:L:54:VAL:HG21 | 1.95 | 0.47 |
| 1:L:236:LEU:HD11 | 1:L:237:GLU:HG2 | 1.97 | 0.47 |
| 1:L:298:VAL:HG12 | 1:L:335:ARG:NH1 | 2.28 | 0.47 |
| 1:M:180:LEU:HD12 | 1:M:181:ALA:O | 2.13 | 0.47 |
| 1:M:236:LEU:HD22 | 1:M:251:GLY:C | 2.34 | 0.47 |
| 1:N:298:VAL:HG12 | 1:N:335:ARG:NH1 | 2.28 | 0.47 |
| 1:O:8:LEU:O | 1:O:104:LEU:N | 2.47 | 0.47 |
| 1:P:58:ALA:HA | 1:P:65:LEU:CD2 | 2.43 | 0.47 |
| 1:P:143:TYR:CZ | 1:P:345:ILE:CG2 | 2.98 | 0.47 |
| 1:R:34:ILE:CG2 | 1:R:67:LEU:HD22 | 2.28 | 0.47 |
| 1:U:236:LEU:HD22 | 1:U:251:GLY:C | 2.34 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:335:ARG:O | 1:V:338:SER:HB3 | 2.14 | 0.47 |
| 1:W:34:ILE:HG22 | 1:W:54:VAL:HG21 | 1.96 | 0.47 |
| 1:W:180:LEU:HD12 | 1:W:181:ALA:O | 2.13 | 0.47 |
| 1:A:236:LEU:HD11 | 1:A:237:GLU:HG2 | 1.96 | 0.47 |
| 1:B:34:ILE:HG23 | 1:B:68:LYS:H | 1.79 | 0.47 |
| 1:C:361:GLU:HB3 | 1:C:369:ILE:CD1 | 2.14 | 0.47 |
| 1:E:8:LEU:O | 1:E:104:LEU:N | 2.47 | 0.47 |
| 1:F:288:ASP:OD1 | 1:H:208:ILE:HD12 | 2.15 | 0.47 |
| 1:G:34:ILE:HD13 | 1:G:67:LEU:CD1 | 2.41 | 0.47 |
| 1:I:34:ILE:HG22 | 1:I:54:VAL:HG21 | 1.95 | 0.47 |
| 1:J:34:ILE:HG22 | 1:J:54:VAL:HG21 | 1.96 | 0.47 |
| 1:K:288:ASP:OD1 | 1:M:208:ILE:HD12 | 2.15 | 0.47 |
| 1:L:143:TYR:CZ | 1:L:345:ILE:CG2 | 2.98 | 0.47 |
| 1:M:288:ASP:OD2 | 1:O:204:ALA:HB1 | 2.14 | 0.47 |
| 1:N:299:MET:HE1 | 1:N:304:THR:HB | 1.97 | 0.47 |
| 1:P:236:LEU:HD22 | 1:P:251:GLY:C | 2.34 | 0.47 |
| 1:R:58:ALA:O | 1:R:59:GLN:C | 2.53 | 0.47 |
| 1:T:2:GLU:HA | 1:T:2:GLU:OE2 | 2.10 | 0.47 |
| 1:T:288:ASP:OD2 | 1:V:204:ALA:HB1 | 2.14 | 0.47 |
| 1:W:143:TYR:CZ | 1:W:345:ILE:CG2 | 2.98 | 0.47 |
| 1:C:34:ILE:HG22 | 1:C:35:VAL:H | 1.78 | 0.47 |
| 1:C:58:ALA:O | 1:C:59:GLN:C | 2.53 | 0.47 |
| 1:D:335:ARG:O | 1:D:338:SER:HB3 | 2.13 | 0.47 |
| 1:E:335:ARG:HA | 1:E:335:ARG:HD3 | 1.39 | 0.47 |
| 1:H:143:TYR:CZ | 1:H:345:ILE:CG2 | 2.98 | 0.47 |
| 1:H:335:ARG:O | 1:H:338:SER:HB3 | 2.14 | 0.47 |
| 1:J:34:ILE:HG22 | 1:J:35:VAL:H | 1.78 | 0.47 |
| 1:K:34:ILE:HG23 | 1:K:68:LYS:H | 1.79 | 0.47 |
| 1:K:335:ARG:O | 1:K:338:SER:HB3 | 2.14 | 0.47 |
| 1:L:288:ASP:OD1 | 1:N:208:ILE:HD12 | 2.15 | 0.47 |
| 1:M:58:ALA:O | 1:M:59:GLN:C | 2.53 | 0.47 |
| 1:N:58:ALA:O | 1:N:59:GLN:C | 2.53 | 0.47 |
| 1:N:134:VAL:O | 1:N:375:PHE:OXT | 2.33 | 0.47 |
| 1:O:335:ARG:HA | 1:O:335:ARG:HD3 | 1.39 | 0.47 |
| 1:Q:58:ALA:O | 1:Q:59:GLN:C | 2.53 | 0.47 |
| 1:R:34:ILE:HG23 | 1:R:68:LYS:H | 1.79 | 0.47 |
| 1:R:143:TYR:CZ | 1:R:345:ILE:CG2 | 2.98 | 0.47 |
| 1:S:134:VAL:O | 1:S:375:PHE:OXT | 2.33 | 0.47 |
| 1:T:169:TYR:CD1 | 1:V:42:GLY:HA3 | 2.50 | 0.47 |
| 1:U:143:TYR:CZ | 1:U:345:ILE:CG2 | 2.98 | 0.47 |
| 1:U:298:VAL:HG12 | 1:U:335:ARG:NH1 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:134:VAL:O | 1:W:375:PHE:OXT | 2.33 | 0.47 |
| 1:A:2:GLU:OE2 | 1:A:2:GLU:HA | 2.10 | 0.47 |
| 1:B:236:LEU:HD22 | 1:B:251:GLY:C | 2.34 | 0.47 |
| 1:B:335:ARG:O | 1:B:338:SER:HB3 | 2.14 | 0.47 |
| 1:C:8:LEU:HB2 | 1:C:103:THR:HA | 1.95 | 0.47 |
| 1:C:173:HIS:NE2 | 1:D:267:ILE:C | 2.67 | 0.47 |
| 1:C:236:LEU:HD22 | 1:C:251:GLY:C | 2.34 | 0.47 |
| 1:D:369:ILE:HG22 | 1:D:370:VAL:N | 2.29 | 0.47 |
| 1:E:169:TYR:CD1 | 1:G:42:GLY:HA3 | 2.50 | 0.47 |
| 1:F:134:VAL:O | 1:F:375:PHE:OXT | 2.33 | 0.47 |
| 1:G:58:ALA:O | 1:G:59:GLN:C | 2.53 | 0.47 |
| 1:H:14:SER:HB2 | 1:H:183:ARG:HH22 | 1.80 | 0.47 |
| 1:H:34:ILE:HG22 | 1:H:54:VAL:HG21 | 1.95 | 0.47 |
| 1:H:134:VAL:O | 1:H:375:PHE:OXT | 2.33 | 0.47 |
| 1:I:298:VAL:HG12 | 1:I:335:ARG:NH1 | 2.28 | 0.47 |
| 1:J:134:VAL:O | 1:J:375:PHE:OXT | 2.33 | 0.47 |
| 1:J:143:TYR:CZ | 1:J:345:ILE:CG2 | 2.98 | 0.47 |
| 1:K:58:ALA:O | 1:K:59:GLN:C | 2.53 | 0.47 |
| 1:K:61:LYS:HG2 | 1:K:64:ILE:CG2 | 2.45 | 0.47 |
| 1:L:58:ALA:HA | 1:L:65:LEU:CD2 | 2.43 | 0.47 |
| 1:L:134:VAL:O | 1:L:375:PHE:OXT | 2.33 | 0.47 |
| 1:M:8:LEU:O | 1:M:104:LEU:N | 2.47 | 0.47 |
| 1:M:288:ASP:OD1 | 1:O:208:ILE:HD12 | 2.15 | 0.47 |
| 1:N:369:ILE:HG22 | 1:N:370:VAL:N | 2.29 | 0.47 |
| 1:P:34:ILE:HG22 | 1:P:54:VAL:HG21 | 1.96 | 0.47 |
| 1:Q:34:ILE:HG22 | 1:Q:54:VAL:HG21 | 1.95 | 0.47 |
| 1:Q:134:VAL:O | 1:Q:375:PHE:OXT | 2.33 | 0.47 |
| 1:Q:288:ASP:OD1 | 1:S:208:ILE:HD12 | 2.15 | 0.47 |
| 1:Q:369:ILE:HG22 | 1:Q:370:VAL:N | 2.29 | 0.47 |
| 1:R:37:ARG:O | 1:R:66:THR:CG2 | 2.63 | 0.47 |
| 1:S:369:ILE:HG22 | 1:S:370:VAL:N | 2.29 | 0.47 |
| 1:T:335:ARG:O | 1:T:338:SER:HB3 | 2.13 | 0.47 |
| 1:U:134:VAL:O | 1:U:375:PHE:OXT | 2.33 | 0.47 |
| 1:V:44:MET:CG | 1:V:45:VAL:N | 2.76 | 0.47 |
| 1:V:58:ALA:O | 1:V:59:GLN:C | 2.53 | 0.47 |
| 1:A:8:LEU:HB2 | 1:A:103:THR:HA | 1.95 | 0.47 |
| 1:A:14:SER:HB2 | 1:A:183:ARG:HH22 | 1.80 | 0.47 |
| 1:A:134:VAL:O | 1:A:375:PHE:OXT | 2.33 | 0.47 |
| 1:B:288:ASP:OD1 | 1:D:208:ILE:HD12 | 2.15 | 0.47 |
| 1:C:169:TYR:CD1 | 1:E:42:GLY:HA3 | 2.50 | 0.47 |
| 1:C:288:ASP:OD1 | 1:E:208:ILE:HD12 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:299:MET:HE1 | 1:C:304:THR:HB | 1.97 | 0.47 |
| 1:C:369:ILE:HG22 | 1:C:370:VAL:N | 2.29 | 0.47 |
| 1:D:14:SER:HB2 | 1:D:183:ARG:HH22 | 1.80 | 0.47 |
| 1:D:34:ILE:HG22 | 1:D:54:VAL:HG21 | 1.95 | 0.47 |
| 1:D:61:LYS:HG2 | 1:D:64:ILE:CG2 | 2.45 | 0.47 |
| 1:D:134:VAL:O | 1:D:375:PHE:OXT | 2.33 | 0.47 |
| 1:E:142:LEU:HD21 | 1:E:165:ILE:CD1 | 2.39 | 0.47 |
| 1:E:143:TYR:CZ | 1:E:345:ILE:CG2 | 2.98 | 0.47 |
| 1:E:288:ASP:OD1 | 1:G:208:ILE:HD12 | 2.15 | 0.47 |
| 1:E:369:ILE:HG22 | 1:E:370:VAL:N | 2.29 | 0.47 |
| 1:E:369:ILE:HG23 | 1:E:370:VAL:N | 2.30 | 0.47 |
| 1:F:14:SER:HB2 | 1:F:183:ARG:HH22 | 1.80 | 0.47 |
| 1:F:58:ALA:O | 1:F:59:GLN:C | 2.53 | 0.47 |
| 1:F:143:TYR:CZ | 1:F:345:ILE:CG2 | 2.98 | 0.47 |
| 1:F:236:LEU:HD11 | 1:F:237:GLU:HG2 | 1.97 | 0.47 |
| 1:F:335:ARG:O | 1:F:338:SER:HB3 | 2.14 | 0.47 |
| 1:G:37:ARG:O | 1:G:66:THR:CG2 | 2.63 | 0.47 |
| 1:G:169:TYR:CD1 | 1:I:42:GLY:HA3 | 2.50 | 0.47 |
| 1:G:290:ARG:HB2 | 1:I:244:ASP:HA | 1.97 | 0.47 |
| 1:G:298:VAL:HG12 | 1:G:335:ARG:NH1 | 2.28 | 0.47 |
| 1:H:335:ARG:HA | 1:H:335:ARG:HD3 | 1.39 | 0.47 |
| 1:I:37:ARG:O | 1:I:66:THR:CG2 | 2.63 | 0.47 |
| 1:I:58:ALA:O | 1:I:59:GLN:C | 2.53 | 0.47 |
| 1:I:169:TYR:CD1 | 1:K:42:GLY:HA3 | 2.50 | 0.47 |
| 1:J:14:SER:HB2 | 1:J:183:ARG:HH22 | 1.80 | 0.47 |
| 1:J:37:ARG:O | 1:J:66:THR:CG2 | 2.63 | 0.47 |
| 1:J:223:PHE:CD1 | 1:J:259:GLU:CG | 2.96 | 0.47 |
| 1:K:14:SER:HB2 | 1:K:183:ARG:HH22 | 1.80 | 0.47 |
| 1:K:169:TYR:CD1 | 1:M:42:GLY:HA3 | 2.50 | 0.47 |
| 1:K:236:LEU:HD22 | 1:K:251:GLY:C | 2.34 | 0.47 |
| 1:L:173:HIS:NE2 | 1:M:267:ILE:C | 2.67 | 0.47 |
| 1:L:223:PHE:CD1 | 1:L:259:GLU:CG | 2.96 | 0.47 |
| 1:L:336:LYS:HE2 | 2:L:401:ADP:C5' | 2.38 | 0.47 |
| 1:L:369:ILE:HG22 | 1:L:370:VAL:N | 2.29 | 0.47 |
| 1:M:14:SER:HB2 | 1:M:183:ARG:HH22 | 1.80 | 0.47 |
| 1:M:61:LYS:HG2 | 1:M:64:ILE:CG2 | 2.45 | 0.47 |
| 1:N:34:ILE:HG22 | 1:N:54:VAL:HG21 | 1.96 | 0.47 |
| 1:N:44:MET:CG | 1:N:45:VAL:N | 2.75 | 0.47 |
| 1:N:58:ALA:HA | 1:N:65:LEU:CD2 | 2.43 | 0.47 |
| 1:N:288:ASP:OD1 | 1:P:208:ILE:HD12 | 2.15 | 0.47 |
| 1:N:336:LYS:HE2 | 2:N:401:ADP:C5' | 2.38 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:369:ILE:HG23 | 1:N:370:VAL:N | 2.30 | 0.47 |
| 1:O:14:SER:HB2 | 1:O:183:ARG:HH22 | 1.80 | 0.47 |
| 1:O:369:ILE:HG22 | 1:O:370:VAL:N | 2.29 | 0.47 |
| 1:P:37:ARG:O | 1:P:66:THR:CG2 | 2.63 | 0.47 |
| 1:P:134:VAL:O | 1:P:375:PHE:OXT | 2.33 | 0.47 |
| 1:P:180:LEU:O | 1:P:180:LEU:HG | 2.11 | 0.47 |
| 1:Q:14:SER:HB2 | 1:Q:183:ARG:HH22 | 1.80 | 0.47 |
| 1:R:34:ILE:HD13 | 1:R:67:LEU:CD1 | 2.41 | 0.47 |
| 1:R:169:TYR:CD1 | 1:T:42:GLY:HA3 | 2.50 | 0.47 |
| 1:R:288:ASP:OD2 | 1:T:204:ALA:HB1 | 2.14 | 0.47 |
| 1:R:299:MET:HE1 | 1:R:304:THR:HB | 1.97 | 0.47 |
| 1:R:335:ARG:O | 1:R:338:SER:HB3 | 2.14 | 0.47 |
| 1:T:58:ALA:O | 1:T:59:GLN:C | 2.53 | 0.47 |
| 1:T:369:ILE:HG23 | 1:T:370:VAL:N | 2.30 | 0.47 |
| 1:W:14:SER:HB2 | 1:W:183:ARG:HH22 | 1.80 | 0.47 |
| 1:A:37:ARG:O | 1:A:66:THR:CG2 | 2.63 | 0.47 |
| 1:A:39:ARG:NE | 1:A:66:THR:CA | 2.69 | 0.47 |
| 1:B:34:ILE:HG22 | 1:B:54:VAL:HG21 | 1.95 | 0.47 |
| 1:B:134:VAL:O | 1:B:375:PHE:OXT | 2.33 | 0.47 |
| 1:C:8:LEU:O | 1:C:104:LEU:N | 2.47 | 0.47 |
| 1:C:14:SER:HB2 | 1:C:183:ARG:HH22 | 1.80 | 0.47 |
| 1:C:143:TYR:CZ | 1:C:345:ILE:CG2 | 2.98 | 0.47 |
| 1:D:31:PHE:HA | 1:D:32:PRO:HD3 | 1.66 | 0.47 |
| 1:D:227:MET:HA | 1:D:227:MET:HE3 | 1.96 | 0.47 |
| 1:F:34:ILE:HG22 | 1:F:54:VAL:HG21 | 1.96 | 0.47 |
| 1:F:106:THR:HB | 1:F:137:GLN:HG2 | 1.97 | 0.47 |
| 1:G:143:TYR:CZ | 1:G:345:ILE:CG2 | 2.98 | 0.47 |
| 1:H:223:PHE:CD1 | 1:H:259:GLU:CG | 2.96 | 0.47 |
| 1:H:288:ASP:OD1 | 1:J:208:ILE:HD12 | 2.15 | 0.47 |
| 1:I:61:LYS:HG2 | 1:I:64:ILE:CG2 | 2.45 | 0.47 |
| 1:J:58:ALA:O | 1:J:59:GLN:C | 2.52 | 0.47 |
| 1:O:134:VAL:O | 1:O:375:PHE:OXT | 2.33 | 0.47 |
| 1:R:290:ARG:HB2 | 1:T:244:ASP:HA | 1.97 | 0.47 |
| 1:S:34:ILE:HG22 | 1:S:54:VAL:HG21 | 1.96 | 0.47 |
| 1:T:236:LEU:HD22 | 1:T:251:GLY:C | 2.34 | 0.47 |
| 1:U:34:ILE:HG22 | 1:U:54:VAL:HG21 | 1.95 | 0.47 |
| 1:U:369:ILE:HG22 | 1:U:370:VAL:N | 2.29 | 0.47 |
| 1:V:14:SER:HB2 | 1:V:183:ARG:HH22 | 1.80 | 0.47 |
| 1:A:336:LYS:HE2 | 2:A:401:ADP:C5' | 2.38 | 0.47 |
| 1:B:106:THR:HB | 1:B:137:GLN:HG2 | 1.97 | 0.47 |
| 1:B:288:ASP:OD2 | 1:D:204:ALA:HB1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:134:VAL:O | 1:C:375:PHE:OXT | 2.33 | 0.47 |
| 1:C:369:ILE:HG23 | 1:C:370:VAL:N | 2.30 | 0.47 |
| 1:D:8:LEU:O | 1:D:104:LEU:N | 2.47 | 0.47 |
| 1:D:106:THR:HB | 1:D:137:GLN:HG2 | 1.97 | 0.47 |
| 1:F:147:ARG:HH21 | 1:F:147:ARG:HG3 | 1.80 | 0.47 |
| 1:G:288:ASP:OD2 | 1:I:204:ALA:HB1 | 2.14 | 0.47 |
| 1:I:173:HIS:HE1 | 1:J:268:GLY:CA | 2.28 | 0.47 |
| 1:I:335:ARG:O | 1:I:338:SER:HB3 | 2.14 | 0.47 |
| 1:J:142:LEU:HD21 | 1:J:165:ILE:CD1 | 2.38 | 0.47 |
| 1:K:288:ASP:OD2 | 1:M:204:ALA:HB1 | 2.14 | 0.47 |
| 1:K:369:ILE:HG22 | 1:K:370:VAL:N | 2.29 | 0.47 |
| 1:N:288:ASP:OD2 | 1:P:204:ALA:HB1 | 2.14 | 0.47 |
| 1:O:34:ILE:HG22 | 1:O:54:VAL:HG21 | 1.96 | 0.47 |
| 1:O:61:LYS:HG2 | 1:O:64:ILE:CG2 | 2.45 | 0.47 |
| 1:O:300:SER:HA | 1:O:335:ARG:HG2 | 1.89 | 0.47 |
| 1:P:2:GLU:OE2 | 1:P:2:GLU:HA | 2.11 | 0.47 |
| 1:P:169:TYR:CD1 | 1:R:42:GLY:HA3 | 2.50 | 0.47 |
| 1:P:288:ASP:OD1 | 1:R:208:ILE:HD12 | 2.15 | 0.47 |
| 1:R:134:VAL:O | 1:R:375:PHE:OXT | 2.33 | 0.47 |
| 1:R:236:LEU:HD22 | 1:R:251:GLY:C | 2.34 | 0.47 |
| 1:R:288:ASP:OD1 | 1:T:208:ILE:HD12 | 2.15 | 0.47 |
| 1:S:288:ASP:OD1 | 1:U:208:ILE:HD12 | 2.15 | 0.47 |
| 1:T:37:ARG:O | 1:T:66:THR:CG2 | 2.63 | 0.47 |
| 1:W:236:LEU:HD22 | 1:W:251:GLY:C | 2.34 | 0.47 |
| 1:A:61:LYS:HG2 | 1:A:64:ILE:CG2 | 2.45 | 0.47 |
| 1:A:169:TYR:CD1 | 1:C:42:GLY:HA3 | 2.50 | 0.47 |
| 1:B:8:LEU:O | 1:B:104:LEU:N | 2.47 | 0.47 |
| 1:C:34:ILE:HD13 | 1:C:67:LEU:CD1 | 2.41 | 0.47 |
| 1:C:336:LYS:HE2 | 2:C:401:ADP:C5' | 2.38 | 0.47 |
| 1:D:236:LEU:HD22 | 1:D:251:GLY:C | 2.34 | 0.47 |
| 1:D:288:ASP:OD1 | 1:F:208:ILE:HD12 | 2.15 | 0.47 |
| 1:G:8:LEU:O | 1:G:104:LEU:N | 2.47 | 0.47 |
| 1:H:34:ILE:HG23 | 1:H:68:LYS:H | 1.79 | 0.47 |
| 1:H:106:THR:HB | 1:H:137:GLN:HG2 | 1.97 | 0.47 |
| 1:H:369:ILE:HG22 | 1:H:370:VAL:N | 2.29 | 0.47 |
| 1:I:288:ASP:OD2 | 1:K:204:ALA:HB1 | 2.14 | 0.47 |
| 1:M:34:ILE:HG22 | 1:M:54:VAL:HG21 | 1.96 | 0.47 |
| 1:M:169:TYR:CD1 | 1:O:42:GLY:HA3 | 2.50 | 0.47 |
| 1:O:58:ALA:CB | 1:O:65:LEU:CD2 | 2.90 | 0.47 |
| 1:S:143:TYR:CZ | 1:S:345:ILE:CG2 | 2.98 | 0.47 |
| 1:S:143:TYR:CE2 | 1:S:346:LEU:HD13 | 2.51 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:288:ASP:OD1 | 1:V:208:ILE:HD12 | 2.15 | 0.47 |
| 1:U:14:SER:HB2 | 1:U:183:ARG:HH22 | 1.80 | 0.47 |
| 1:U:37:ARG:O | 1:U:66:THR:CG2 | 2.63 | 0.47 |
| 1:V:236:LEU:HD22 | 1:V:251:GLY:C | 2.34 | 0.47 |
| 1:A:143:TYR:CZ | 1:A:345:ILE:CG2 | 2.98 | 0.46 |
| 1:A:147:ARG:HH21 | 1:A:147:ARG:HG3 | 1.80 | 0.46 |
| 1:A:152:VAL:HG22 | 1:A:298:VAL:HB | 1.98 | 0.46 |
| 1:A:288:ASP:OD1 | 1:C:208:ILE:HD12 | 2.15 | 0.46 |
| 1:A:290:ARG:HB2 | 1:C:244:ASP:HA | 1.97 | 0.46 |
| 1:B:369:ILE:HG22 | 1:B:370:VAL:N | 2.29 | 0.46 |
| 1:D:143:TYR:CZ | 1:D:345:ILE:CG2 | 2.98 | 0.46 |
| 1:D:223:PHE:CD1 | 1:D:259:GLU:CG | 2.96 | 0.46 |
| 1:E:134:VAL:O | 1:E:375:PHE:OXT | 2.33 | 0.46 |
| 1:F:61:LYS:HG2 | 1:F:64:ILE:CG2 | 2.45 | 0.46 |
| 1:F:152:VAL:HG22 | 1:F:298:VAL:HB | 1.98 | 0.46 |
| 1:F:223:PHE:CD1 | 1:F:259:GLU:CG | 2.96 | 0.46 |
| 1:F:227:MET:HE3 | 1:F:227:MET:HA | 1.96 | 0.46 |
| 1:H:37:ARG:O | 1:H:66:THR:CG2 | 2.63 | 0.46 |
| 1:J:34:ILE:HG23 | 1:J:68:LYS:H | 1.79 | 0.46 |
| 1:K:143:TYR:CZ | 1:K:345:ILE:CG2 | 2.98 | 0.46 |
| 1:L:14:SER:HB2 | 1:L:183:ARG:HH22 | 1.80 | 0.46 |
| 1:L:143:TYR:CE2 | 1:L:346:LEU:HD13 | 2.51 | 0.46 |
| 1:L:152:VAL:HG22 | 1:L:298:VAL:HB | 1.98 | 0.46 |
| 1:M:134:VAL:O | 1:M:375:PHE:OXT | 2.33 | 0.46 |
| 1:M:143:TYR:CZ | 1:M:345:ILE:CG2 | 2.98 | 0.46 |
| 1:N:34:ILE:HD13 | 1:N:67:LEU:CD1 | 2.41 | 0.46 |
| 1:N:39:ARG:NE | 1:N:66:THR:CA | 2.69 | 0.46 |
| 1:N:152:VAL:HG22 | 1:N:298:VAL:HB | 1.98 | 0.46 |
| 1:O:143:TYR:CZ | 1:O:345:ILE:CG2 | 2.98 | 0.46 |
| 1:P:8:LEU:O | 1:P:104:LEU:N | 2.47 | 0.46 |
| 1:P:290:ARG:HB2 | 1:R:244:ASP:HA | 1.97 | 0.46 |
| 1:S:14:SER:HB2 | 1:S:183:ARG:HH22 | 1.80 | 0.46 |
| 1:T:369:ILE:HG22 | 1:T:370:VAL:N | 2.29 | 0.46 |
| 1:U:58:ALA:O | 1:U:59:GLN:C | 2.53 | 0.46 |
| 1:U:288:ASP:OD2 | 1:W:204:ALA:HB1 | 2.14 | 0.46 |
| 1:W:106:THR:HB | 1:W:137:GLN:HG2 | 1.97 | 0.46 |
| 1:W:369:ILE:HG22 | 1:W:370:VAL:N | 2.29 | 0.46 |
| 1:A:236:LEU:HD22 | 1:A:251:GLY:C | 2.34 | 0.46 |
| 1:B:14:SER:HB2 | 1:B:183:ARG:HH22 | 1.80 | 0.46 |
| 1:B:152:VAL:HG22 | 1:B:298:VAL:HB | 1.98 | 0.46 |
| 1:B:180:LEU:O | 1:B:180:LEU:HG | 2.11 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:223:PHE:CD1 | 1:B:259:GLU:CG | 2.96 | 0.46 |
| 1:D:147:ARG:HH21 | 1:D:147:ARG:HG3 | 1.80 | 0.46 |
| 1:E:143:TYR:CE2 | 1:E:346:LEU:HD13 | 2.51 | 0.46 |
| 1:E:290:ARG:HB2 | 1:G:244:ASP:HA | 1.97 | 0.46 |
| 1:F:169:TYR:CD1 | 1:H:42:GLY:HA3 | 2.50 | 0.46 |
| 1:F:374:CYS:HB2 | 1:F:375:PHE:H | 1.62 | 0.46 |
| 1:G:134:VAL:O | 1:G:375:PHE:OXT | 2.33 | 0.46 |
| 1:H:34:ILE:HG22 | 1:H:35:VAL:H | 1.78 | 0.46 |
| 1:H:39:ARG:NE | 1:H:66:THR:CA | 2.69 | 0.46 |
| 1:I:14:SER:HB2 | 1:I:183:ARG:HH22 | 1.80 | 0.46 |
| 1:J:143:TYR:CE2 | 1:J:346:LEU:HD13 | 2.50 | 0.46 |
| 1:J:287:ILE:HD12 | 1:L:208:ILE:HD13 | 1.96 | 0.46 |
| 1:K:34:ILE:HG22 | 1:K:54:VAL:HG21 | 1.96 | 0.46 |
| 1:L:2:GLU:OE2 | 1:L:2:GLU:HA | 2.10 | 0.46 |
| 1:L:37:ARG:O | 1:L:66:THR:CG2 | 2.63 | 0.46 |
| 1:N:143:TYR:CE2 | 1:N:346:LEU:HD13 | 2.51 | 0.46 |
| 1:N:169:TYR:CD1 | 1:P:42:GLY:HA3 | 2.50 | 0.46 |
| 1:N:223:PHE:CD1 | 1:N:259:GLU:CG | 2.96 | 0.46 |
| 1:N:300:SER:HA | 1:N:335:ARG:HG2 | 1.89 | 0.46 |
| 1:O:152:VAL:HG22 | 1:O:298:VAL:HB | 1.97 | 0.46 |
| 1:P:61:LYS:HG2 | 1:P:64:ILE:CG2 | 2.45 | 0.46 |
| 1:P:227:MET:HA | 1:P:227:MET:HE3 | 1.97 | 0.46 |
| 1:Q:8:LEU:O | 1:Q:104:LEU:N | 2.47 | 0.46 |
| 1:T:14:SER:HB2 | 1:T:183:ARG:HH22 | 1.80 | 0.46 |
| 1:U:106:THR:HB | 1:U:137:GLN:HG2 | 1.97 | 0.46 |
| 1:U:288:ASP:OD1 | 1:W:208:ILE:HD12 | 2.15 | 0.46 |
| 1:V:34:ILE:HG22 | 1:V:35:VAL:H | 1.78 | 0.46 |
| 1:V:58:ALA:CB | 1:V:65:LEU:CD2 | 2.90 | 0.46 |
| 1:W:61:LYS:HG2 | 1:W:64:ILE:CG2 | 2.45 | 0.46 |
| 1:C:37:ARG:O | 1:C:66:THR:CG2 | 2.63 | 0.46 |
| 1:D:169:TYR:CD1 | 1:F:42:GLY:HA3 | 2.50 | 0.46 |
| 1:E:361:GLU:HB3 | 1:E:369:ILE:CD1 | 2.14 | 0.46 |
| 1:F:73:HIC:HA | 1:F:183:ARG:NH1 | 2.18 | 0.46 |
| 1:F:369:ILE:HG22 | 1:F:370:VAL:N | 2.29 | 0.46 |
| 1:G:288:ASP:OD1 | 1:I:208:ILE:HD12 | 2.15 | 0.46 |
| 1:H:58:ALA:CB | 1:H:65:LEU:CD2 | 2.90 | 0.46 |
| 1:H:287:ILE:HB | 1:J:244:ASP:HB3 | 1.97 | 0.46 |
| 1:I:288:ASP:OD1 | 1:K:208:ILE:HD12 | 2.15 | 0.46 |
| 1:J:180:LEU:O | 1:J:180:LEU:HG | 2.11 | 0.46 |
| 1:K:134:VAL:O | 1:K:375:PHE:OXT | 2.33 | 0.46 |
| 1:L:169:TYR:CD1 | 1:N:42:GLY:HA3 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:152:VAL:HG22 | 1:M:298:VAL:HB | 1.98 | 0.46 |
| 1:M:287:ILE:HD12 | 1:O:208:ILE:HD13 | 1.96 | 0.46 |
| 1:O:288:ASP:OD1 | 1:Q:208:ILE:HD12 | 2.15 | 0.46 |
| 1:O:369:ILE:HG23 | 1:O:370:VAL:N | 2.30 | 0.46 |
| 1:P:336:LYS:HE2 | 2:P:401:ADP:C5' | 2.38 | 0.46 |
| 1:P:369:ILE:HG23 | 1:P:370:VAL:N | 2.30 | 0.46 |
| 1:Q:143:TYR:CZ | 1:Q:345:ILE:CG2 | 2.98 | 0.46 |
| 1:Q:143:TYR:CE2 | 1:Q:346:LEU:HD13 | 2.51 | 0.46 |
| 1:Q:152:VAL:HG22 | 1:Q:298:VAL:HB | 1.98 | 0.46 |
| 1:R:8:LEU:O | 1:R:104:LEU:N | 2.47 | 0.46 |
| 1:R:61:LYS:HG2 | 1:R:64:ILE:CG2 | 2.45 | 0.46 |
| 1:R:152:VAL:HG22 | 1:R:298:VAL:HB | 1.98 | 0.46 |
| 1:S:152:VAL:HG22 | 1:S:298:VAL:HB | 1.98 | 0.46 |
| 1:T:61:LYS:HG2 | 1:T:64:ILE:CG2 | 2.45 | 0.46 |
| 1:T:134:VAL:O | 1:T:375:PHE:OXT | 2.33 | 0.46 |
| 1:T:223:PHE:CD1 | 1:T:259:GLU:CG | 2.96 | 0.46 |
| 1:U:73:HIC:HA | 1:U:183:ARG:NH1 | 2.18 | 0.46 |
| 1:U:143:TYR:CE2 | 1:U:346:LEU:HD13 | 2.51 | 0.46 |
| 1:U:152:VAL:HG22 | 1:U:298:VAL:HB | 1.98 | 0.46 |
| 1:V:143:TYR:CZ | 1:V:345:ILE:CG2 | 2.98 | 0.46 |
| 1:D:37:ARG:O | 1:D:66:THR:CG2 | 2.63 | 0.46 |
| 1:D:369:ILE:HG23 | 1:D:370:VAL:N | 2.30 | 0.46 |
| 1:E:14:SER:HB2 | 1:E:183:ARG:HH22 | 1.80 | 0.46 |
| 1:E:152:VAL:HG22 | 1:E:298:VAL:HB | 1.97 | 0.46 |
| 1:G:143:TYR:CE2 | 1:G:346:LEU:HD13 | 2.51 | 0.46 |
| 1:G:361:GLU:HB3 | 1:G:369:ILE:CD1 | 2.14 | 0.46 |
| 1:H:152:VAL:HG22 | 1:H:298:VAL:HB | 1.98 | 0.46 |
| 1:I:58:ALA:CB | 1:I:65:LEU:CD2 | 2.90 | 0.46 |
| 1:J:173:HIS:HE1 | 1:K:268:GLY:CA | 2.28 | 0.46 |
| 1:J:288:ASP:OD1 | 1:L:208:ILE:HD12 | 2.15 | 0.46 |
| 1:L:290:ARG:HB2 | 1:N:244:ASP:HA | 1.97 | 0.46 |
| 1:M:34:ILE:HG22 | 1:M:35:VAL:H | 1.78 | 0.46 |
| 1:M:37:ARG:O | 1:M:66:THR:CG2 | 2.63 | 0.46 |
| 1:M:290:ARG:HB2 | 1:O:244:ASP:HA | 1.97 | 0.46 |
| 1:M:300:SER:HA | 1:M:335:ARG:HG2 | 1.89 | 0.46 |
| 1:N:37:ARG:O | 1:N:66:THR:CG2 | 2.63 | 0.46 |
| 1:N:61:LYS:HG2 | 1:N:64:ILE:CG2 | 2.45 | 0.46 |
| 1:P:143:TYR:CE2 | 1:P:346:LEU:HD13 | 2.51 | 0.46 |
| 1:P:152:VAL:HG22 | 1:P:298:VAL:HB | 1.98 | 0.46 |
| 1:Q:169:TYR:CD1 | 1:S:42:GLY:HA3 | 2.50 | 0.46 |
| 1:R:173:HIS:HE1 | 1:S:268:GLY:CA | 2.28 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:169:TYR:CD1 | 1:U:42:GLY:HA3 | 2.50 | 0.46 |
| 1:T:34:ILE:HD13 | 1:T:67:LEU:CD2 | 2.46 | 0.46 |
| 1:U:287:ILE:HD12 | 1:W:208:ILE:HD13 | 1.96 | 0.46 |
| 1:V:61:LYS:HG2 | 1:V:64:ILE:CG2 | 2.45 | 0.46 |
| 1:V:134:VAL:O | 1:V:375:PHE:OXT | 2.33 | 0.46 |
| 1:W:227:MET:HA | 1:W:227:MET:HE3 | 1.96 | 0.46 |
| 1:W:369:ILE:HG23 | 1:W:370:VAL:N | 2.30 | 0.46 |
| 1:A:227:MET:HA | 1:A:227:MET:HE3 | 1.97 | 0.46 |
| 1:B:143:TYR:CE2 | 1:B:346:LEU:HD13 | 2.51 | 0.46 |
| 1:C:143:TYR:CE2 | 1:C:346:LEU:HD13 | 2.51 | 0.46 |
| 1:D:73:HIC:HA | 1:D:183:ARG:NH1 | 2.18 | 0.46 |
| 1:D:152:VAL:HG22 | 1:D:298:VAL:HB | 1.98 | 0.46 |
| 1:F:31:PHE:HA | 1:F:32:PRO:HD3 | 1.66 | 0.46 |
| 1:F:58:ALA:CB | 1:F:65:LEU:CD2 | 2.90 | 0.46 |
| 1:F:287:ILE:HB | 1:H:244:ASP:HB3 | 1.97 | 0.46 |
| 1:G:152:VAL:HG22 | 1:G:298:VAL:HB | 1.98 | 0.46 |
| 1:G:287:ILE:HB | 1:I:244:ASP:HB3 | 1.97 | 0.46 |
| 1:G:299:MET:HE1 | 1:G:304:THR:HB | 1.98 | 0.46 |
| 1:H:169:TYR:CD1 | 1:J:42:GLY:HA3 | 2.50 | 0.46 |
| 1:I:9:VAL:HG21 | 1:I:344:SER:HA | 1.98 | 0.46 |
| 1:I:34:ILE:HG23 | 1:I:68:LYS:H | 1.79 | 0.46 |
| 1:I:106:THR:HB | 1:I:137:GLN:HG2 | 1.97 | 0.46 |
| 1:I:134:VAL:O | 1:I:375:PHE:OXT | 2.33 | 0.46 |
| 1:I:335:ARG:HA | 1:I:335:ARG:HD3 | 1.39 | 0.46 |
| 1:J:106:THR:HB | 1:J:137:GLN:HG2 | 1.97 | 0.46 |
| 1:J:169:TYR:CD1 | 1:L:42:GLY:HA3 | 2.50 | 0.46 |
| 1:J:287:ILE:HB | 1:L:244:ASP:HB3 | 1.97 | 0.46 |
| 1:K:106:THR:HB | 1:K:137:GLN:HG2 | 1.97 | 0.46 |
| 1:M:147:ARG:HH21 | 1:M:147:ARG:HG3 | 1.80 | 0.46 |
| 1:N:8:LEU:O | 1:N:104:LEU:N | 2.47 | 0.46 |
| 1:N:135:ALA:HB3 | 1:N:140:LEU:HD11 | 1.98 | 0.46 |
| 1:O:37:ARG:O | 1:O:66:THR:CG2 | 2.63 | 0.46 |
| 1:O:147:ARG:HH21 | 1:O:147:ARG:HG3 | 1.80 | 0.46 |
| 1:R:14:SER:HB2 | 1:R:183:ARG:HH22 | 1.80 | 0.46 |
| 1:R:223:PHE:CD1 | 1:R:259:GLU:CG | 2.96 | 0.46 |
| 1:S:34:ILE:CG2 | 1:S:67:LEU:HD22 | 2.28 | 0.46 |
| 1:S:37:ARG:O | 1:S:66:THR:CG2 | 2.63 | 0.46 |
| 1:S:369:ILE:HG23 | 1:S:370:VAL:N | 2.30 | 0.46 |
| 1:T:143:TYR:CZ | 1:T:345:ILE:CG2 | 2.98 | 0.46 |
| 1:T:152:VAL:HG22 | 1:T:298:VAL:HB | 1.98 | 0.46 |
| 1:V:223:PHE:CD1 | 1:V:259:GLU:CG | 2.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:152:VAL:HG22 | 1:W:298:VAL:HB | 1.98 | 0.46 |
| 1:C:58:ALA:CB | 1:C:65:LEU:CD2 | 2.90 | 0.46 |
| 1:D:135:ALA:HB3 | 1:D:140:LEU:HD11 | 1.98 | 0.46 |
| 1:F:8:LEU:O | 1:F:104:LEU:N | 2.47 | 0.46 |
| 1:I:143:TYR:CZ | 1:I:345:ILE:CG2 | 2.98 | 0.46 |
| 1:I:290:ARG:HB2 | 1:K:244:ASP:HA | 1.97 | 0.46 |
| 1:J:152:VAL:HG22 | 1:J:298:VAL:HB | 1.98 | 0.46 |
| 1:K:152:VAL:HG22 | 1:K:298:VAL:HB | 1.98 | 0.46 |
| 1:M:106:THR:HB | 1:M:137:GLN:HG2 | 1.97 | 0.46 |
| 1:M:144:ALA:HB2 | 1:M:342:GLY:N | 2.31 | 0.46 |
| 1:N:173:HIS:HE1 | 1:O:268:GLY:CA | 2.28 | 0.46 |
| 1:O:143:TYR:CE2 | 1:O:346:LEU:HD13 | 2.51 | 0.46 |
| 1:O:169:TYR:CD1 | 1:Q:42:GLY:HA3 | 2.50 | 0.46 |
| 1:P:44:MET:CG | 1:P:45:VAL:H | 2.18 | 0.46 |
| 1:Q:61:LYS:HG2 | 1:Q:64:ILE:CG2 | 2.45 | 0.46 |
| 1:S:106:THR:HB | 1:S:137:GLN:HG2 | 1.97 | 0.46 |
| 1:S:135:ALA:HB3 | 1:S:140:LEU:HD11 | 1.98 | 0.46 |
| 1:T:9:VAL:HG21 | 1:T:344:SER:HA | 1.98 | 0.46 |
| 1:W:73:HIC:HA | 1:W:183:ARG:NH1 | 2.18 | 0.46 |
| 1:A:180:LEU:O | 1:A:180:LEU:HG | 2.11 | 0.46 |
| 1:A:369:ILE:HG23 | 1:A:370:VAL:N | 2.30 | 0.46 |
| 1:B:37:ARG:O | 1:B:66:THR:CG2 | 2.63 | 0.46 |
| 1:B:135:ALA:HB3 | 1:B:140:LEU:HD11 | 1.98 | 0.46 |
| 1:B:143:TYR:CZ | 1:B:345:ILE:CG2 | 2.98 | 0.46 |
| 1:C:33:SER:O | 1:C:69:TYR:CD1 | 2.69 | 0.46 |
| 1:C:152:VAL:HG22 | 1:C:298:VAL:HB | 1.98 | 0.46 |
| 1:C:173:HIS:HE1 | 1:D:268:GLY:CA | 2.28 | 0.46 |
| 1:D:236:LEU:CD1 | 1:D:237:GLU:CG | 2.93 | 0.46 |
| 1:E:299:MET:HE1 | 1:E:304:THR:HB | 1.98 | 0.46 |
| 1:G:9:VAL:HG21 | 1:G:344:SER:HA | 1.98 | 0.46 |
| 1:G:34:ILE:HD13 | 1:G:67:LEU:CD2 | 2.46 | 0.46 |
| 1:G:34:ILE:CG2 | 1:G:67:LEU:HD22 | 2.27 | 0.46 |
| 1:H:61:LYS:HG2 | 1:H:64:ILE:CG2 | 2.45 | 0.46 |
| 1:H:361:GLU:HB3 | 1:H:369:ILE:CD1 | 2.14 | 0.46 |
| 1:I:143:TYR:CE2 | 1:I:346:LEU:HD13 | 2.50 | 0.46 |
| 1:J:369:ILE:HG23 | 1:J:370:VAL:N | 2.30 | 0.46 |
| 1:K:144:ALA:HB2 | 1:K:342:GLY:N | 2.31 | 0.46 |
| 1:K:290:ARG:HB2 | 1:M:244:ASP:HA | 1.97 | 0.46 |
| 1:K:299:MET:HE1 | 1:K:304:THR:HB | 1.98 | 0.46 |
| 1:K:369:ILE:HG23 | 1:K:370:VAL:N | 2.30 | 0.46 |
| 1:L:135:ALA:HB3 | 1:L:140:LEU:HD11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:299:MET:HE1 | 1:L:304:THR:HB | 1.98 | 0.46 |
| 1:P:14:SER:HB2 | 1:P:183:ARG:HH22 | 1.80 | 0.46 |
| 1:P:135:ALA:HB3 | 1:P:140:LEU:HD11 | 1.98 | 0.46 |
| 1:P:144:ALA:HB2 | 1:P:342:GLY:N | 2.31 | 0.46 |
| 1:Q:135:ALA:HB3 | 1:Q:140:LEU:HD11 | 1.98 | 0.46 |
| 1:R:9:VAL:HG21 | 1:R:344:SER:HA | 1.98 | 0.46 |
| 1:R:144:ALA:HB2 | 1:R:342:GLY:N | 2.31 | 0.46 |
| 1:T:290:ARG:HB2 | 1:V:244:ASP:HA | 1.97 | 0.46 |
| 1:U:335:ARG:HA | 1:U:335:ARG:HD3 | 1.39 | 0.46 |
| 1:A:34:ILE:HG22 | 1:A:35:VAL:H | 1.78 | 0.46 |
| 1:A:135:ALA:HB3 | 1:A:140:LEU:HD11 | 1.98 | 0.46 |
| 1:C:9:VAL:HG21 | 1:C:344:SER:HA | 1.98 | 0.46 |
| 1:C:61:LYS:HG2 | 1:C:64:ILE:CG2 | 2.45 | 0.46 |
| 1:D:143:TYR:CE2 | 1:D:346:LEU:HD13 | 2.51 | 0.46 |
| 1:D:287:ILE:HB | 1:F:244:ASP:HB3 | 1.97 | 0.46 |
| 1:E:39:ARG:NE | 1:E:66:THR:CA | 2.69 | 0.46 |
| 1:E:336:LYS:HE2 | 2:E:401:ADP:C5' | 2.38 | 0.46 |
| 1:E:349:LEU:HD23 | 1:E:349:LEU:HA | 1.80 | 0.46 |
| 1:F:135:ALA:HB3 | 1:F:140:LEU:HD11 | 1.98 | 0.46 |
| 1:G:14:SER:HB2 | 1:G:183:ARG:HH22 | 1.80 | 0.46 |
| 1:G:33:SER:O | 1:G:69:TYR:CD1 | 2.69 | 0.46 |
| 1:H:143:TYR:CE2 | 1:H:346:LEU:HD13 | 2.51 | 0.46 |
| 1:I:152:VAL:HG22 | 1:I:298:VAL:HB | 1.98 | 0.46 |
| 1:I:287:ILE:HB | 1:K:244:ASP:HB3 | 1.97 | 0.46 |
| 1:K:37:ARG:O | 1:K:66:THR:CG2 | 2.63 | 0.46 |
| 1:K:135:ALA:HB3 | 1:K:140:LEU:HD11 | 1.98 | 0.46 |
| 1:K:287:ILE:HB | 1:M:244:ASP:HB3 | 1.97 | 0.46 |
| 1:L:173:HIS:HE1 | 1:M:268:GLY:CA | 2.28 | 0.46 |
| 1:N:33:SER:O | 1:N:69:TYR:CD1 | 2.69 | 0.46 |
| 1:O:9:VAL:HG21 | 1:O:344:SER:HA | 1.98 | 0.46 |
| 1:P:39:ARG:NE | 1:P:66:THR:CA | 2.69 | 0.46 |
| 1:P:223:PHE:CD1 | 1:P:259:GLU:CG | 2.96 | 0.46 |
| 1:Q:180:LEU:O | 1:Q:180:LEU:HG | 2.11 | 0.46 |
| 1:Q:335:ARG:HA | 1:Q:335:ARG:HD3 | 1.39 | 0.46 |
| 1:R:33:SER:O | 1:R:69:TYR:CD1 | 2.69 | 0.46 |
| 1:S:73:HIC:HA | 1:S:183:ARG:NH1 | 2.18 | 0.46 |
| 1:T:147:ARG:HH21 | 1:T:147:ARG:HG3 | 1.80 | 0.46 |
| 1:T:287:ILE:HD12 | 1:V:208:ILE:HD13 | 1.96 | 0.46 |
| 1:V:33:SER:O | 1:V:69:TYR:CD1 | 2.69 | 0.46 |
| 1:W:33:SER:O | 1:W:69:TYR:CD1 | 2.69 | 0.46 |
| 1:W:143:TYR:CE2 | 1:W:346:LEU:HD13 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:106:THR:HB | 1:A:137:GLN:HG2 | 1.98 | 0.46 |
| 1:B:369:ILE:HG22 | 1:B:370:VAL:H | 1.81 | 0.46 |
| 1:C:147:ARG:HH21 | 1:C:147:ARG:HG3 | 1.80 | 0.46 |
| 1:D:144:ALA:HB2 | 1:D:342:GLY:N | 2.31 | 0.46 |
| 1:E:135:ALA:HB3 | 1:E:140:LEU:HD11 | 1.98 | 0.46 |
| 1:F:34:ILE:HG22 | 1:F:35:VAL:H | 1.78 | 0.46 |
| 1:G:135:ALA:HB3 | 1:G:140:LEU:HD11 | 1.98 | 0.46 |
| 1:H:73:HIC:HA | 1:H:183:ARG:NH1 | 2.18 | 0.46 |
| 1:H:369:ILE:HG23 | 1:H:370:VAL:N | 2.30 | 0.46 |
| 1:J:135:ALA:HB3 | 1:J:140:LEU:HD11 | 1.98 | 0.46 |
| 1:K:34:ILE:HD13 | 1:K:67:LEU:CD2 | 2.46 | 0.46 |
| 1:K:227:MET:HA | 1:K:227:MET:HE3 | 1.98 | 0.46 |
| 1:L:287:ILE:HB | 1:N:244:ASP:HB3 | 1.97 | 0.46 |
| 1:N:144:ALA:HB2 | 1:N:342:GLY:N | 2.31 | 0.46 |
| 1:O:7:ALA:HB1 | 1:O:347:ALA:HB1 | 1.98 | 0.46 |
| 1:Q:287:ILE:HD12 | 1:S:208:ILE:HD13 | 1.96 | 0.46 |
| 1:Q:361:GLU:HB3 | 1:Q:369:ILE:CD1 | 2.14 | 0.46 |
| 1:R:34:ILE:N | 1:R:54:VAL:HG11 | 2.31 | 0.46 |
| 1:R:44:MET:CG | 1:R:45:VAL:H | 2.18 | 0.46 |
| 1:R:135:ALA:HB3 | 1:R:140:LEU:HD11 | 1.98 | 0.46 |
| 1:T:43:VAL:C | 1:T:44:MET:HG2 | 2.37 | 0.46 |
| 1:T:135:ALA:HB3 | 1:T:140:LEU:HD11 | 1.98 | 0.46 |
| 1:U:61:LYS:HG2 | 1:U:64:ILE:CG2 | 2.45 | 0.46 |
| 1:U:135:ALA:HB3 | 1:U:140:LEU:HD11 | 1.98 | 0.46 |
| 1:U:369:ILE:HG22 | 1:U:370:VAL:H | 1.81 | 0.46 |
| 1:V:37:ARG:O | 1:V:66:THR:CG2 | 2.63 | 0.46 |
| 1:V:38:PRO:HD3 | 1:V:49:GLN:HE22 | 1.81 | 0.46 |
| 1:V:143:TYR:CE2 | 1:V:346:LEU:HD13 | 2.51 | 0.46 |
| 1:V:152:VAL:HG22 | 1:V:298:VAL:HB | 1.97 | 0.46 |
| 1:V:369:ILE:HG23 | 1:V:370:VAL:N | 2.30 | 0.46 |
| 1:W:37:ARG:O | 1:W:66:THR:CG2 | 2.63 | 0.46 |
| 1:B:290:ARG:HB2 | 1:D:244:ASP:HA | 1.97 | 0.46 |
| 1:C:106:THR:HB | 1:C:137:GLN:HG2 | 1.97 | 0.46 |
| 1:C:135:ALA:HB3 | 1:C:140:LEU:HD11 | 1.98 | 0.46 |
| 1:C:290:ARG:HB2 | 1:E:244:ASP:HA | 1.97 | 0.46 |
| 1:E:106:THR:HB | 1:E:137:GLN:HG2 | 1.97 | 0.46 |
| 1:G:38:PRO:HD3 | 1:G:49:GLN:HE22 | 1.81 | 0.46 |
| 1:G:106:THR:HB | 1:G:137:GLN:HG2 | 1.98 | 0.46 |
| 1:H:38:PRO:HD3 | 1:H:49:GLN:HE22 | 1.81 | 0.46 |
| 1:I:144:ALA:HB2 | 1:I:342:GLY:N | 2.31 | 0.46 |
| 1:J:58:ALA:CB | 1:J:65:LEU:CD2 | 2.90 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:61:LYS:HG2 | 1:J:64:ILE:CG2 | 2.45 | 0.46 |
| 1:K:33:SER:O | 1:K:69:TYR:CD1 | 2.69 | 0.46 |
| 1:L:61:LYS:HG2 | 1:L:64:ILE:CG2 | 2.45 | 0.46 |
| 1:M:135:ALA:HB3 | 1:M:140:LEU:HD11 | 1.98 | 0.46 |
| 1:O:38:PRO:HD3 | 1:O:49:GLN:HE22 | 1.81 | 0.46 |
| 1:O:106:THR:HB | 1:O:137:GLN:HG2 | 1.97 | 0.46 |
| 1:O:135:ALA:HB3 | 1:O:140:LEU:HD11 | 1.98 | 0.46 |
| 1:R:43:VAL:C | 1:R:44:MET:HG2 | 2.37 | 0.46 |
| 1:S:369:ILE:HG22 | 1:S:370:VAL:H | 1.81 | 0.46 |
| 1:T:33:SER:O | 1:T:69:TYR:CD1 | 2.69 | 0.46 |
| 1:T:144:ALA:HB2 | 1:T:342:GLY:N | 2.31 | 0.46 |
| 1:U:33:SER:O | 1:U:69:TYR:CD1 | 2.69 | 0.46 |
| 1:U:43:VAL:C | 1:U:44:MET:HG2 | 2.37 | 0.46 |
| 1:U:169:TYR:CD1 | 1:W:42:GLY:HA3 | 2.50 | 0.46 |
| 1:V:106:THR:HB | 1:V:137:GLN:HG2 | 1.97 | 0.46 |
| 1:V:335:ARG:HA | 1:V:335:ARG:HD3 | 1.39 | 0.46 |
| 1:A:8:LEU:O | 1:A:104:LEU:N | 2.47 | 0.45 |
| 1:A:38:PRO:HD3 | 1:A:49:GLN:HE22 | 1.81 | 0.45 |
| 1:B:144:ALA:HB2 | 1:B:342:GLY:N | 2.31 | 0.45 |
| 1:B:169:TYR:CD1 | 1:D:42:GLY:HA3 | 2.50 | 0.45 |
| 1:D:349:LEU:HD23 | 1:D:349:LEU:HA | 1.80 | 0.45 |
| 1:E:144:ALA:HB2 | 1:E:342:GLY:N | 2.31 | 0.45 |
| 1:H:135:ALA:HB3 | 1:H:140:LEU:HD11 | 1.98 | 0.45 |
| 1:I:33:SER:O | 1:I:69:TYR:CD1 | 2.69 | 0.45 |
| 1:J:38:PRO:HD3 | 1:J:49:GLN:HE22 | 1.81 | 0.45 |
| 1:K:300:SER:HA | 1:K:335:ARG:HG2 | 1.89 | 0.45 |
| 1:M:7:ALA:HB1 | 1:M:347:ALA:HB1 | 1.98 | 0.45 |
| 1:M:9:VAL:HG21 | 1:M:344:SER:HA | 1.98 | 0.45 |
| 1:M:33:SER:O | 1:M:69:TYR:CD1 | 2.69 | 0.45 |
| 1:N:14:SER:HB2 | 1:N:183:ARG:HH22 | 1.80 | 0.45 |
| 1:N:44:MET:CG | 1:N:45:VAL:H | 2.18 | 0.45 |
| 1:O:144:ALA:HB2 | 1:O:342:GLY:N | 2.31 | 0.45 |
| 1:P:34:ILE:HD13 | 1:P:67:LEU:CD2 | 2.46 | 0.45 |
| 1:Q:7:ALA:HB1 | 1:Q:347:ALA:HB1 | 1.98 | 0.45 |
| 1:S:7:ALA:HB1 | 1:S:347:ALA:HB1 | 1.98 | 0.45 |
| 1:S:287:ILE:HB | 1:U:244:ASP:HB3 | 1.97 | 0.45 |
| 1:V:43:VAL:C | 1:V:44:MET:HG2 | 2.37 | 0.45 |
| 1:V:144:ALA:HB2 | 1:V:342:GLY:N | 2.31 | 0.45 |
| 1:W:7:ALA:HB1 | 1:W:347:ALA:HB1 | 1.98 | 0.45 |
| 1:W:34:ILE:N | 1:W:54:VAL:HG11 | 2.31 | 0.45 |
| 1:W:38:PRO:HD3 | 1:W:49:GLN:HE22 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:43:VAL:C | 1:W:44:MET:HG2 | 2.37 | 0.45 |
| 1:W:135:ALA:HB3 | 1:W:140:LEU:HD11 | 1.98 | 0.45 |
| 1:W:299:MET:HE1 | 1:W:304:THR:HB | 1.98 | 0.45 |
| 1:W:369:ILE:HG22 | 1:W:370:VAL:H | 1.81 | 0.45 |
| 1:A:43:VAL:C | 1:A:44:MET:HG2 | 2.37 | 0.45 |
| 1:A:143:TYR:CE2 | 1:A:346:LEU:HD13 | 2.51 | 0.45 |
| 1:A:287:ILE:HB | 1:C:244:ASP:HB3 | 1.97 | 0.45 |
| 1:C:34:ILE:HD13 | 1:C:67:LEU:CD2 | 2.46 | 0.45 |
| 1:C:43:VAL:C | 1:C:44:MET:HG2 | 2.37 | 0.45 |
| 1:E:133:TYR:CE2 | 1:E:375:PHE:HB2 | 2.51 | 0.45 |
| 1:F:143:TYR:CE2 | 1:F:346:LEU:HD13 | 2.51 | 0.45 |
| 1:F:144:ALA:HB2 | 1:F:342:GLY:N | 2.31 | 0.45 |
| 1:G:144:ALA:HB2 | 1:G:342:GLY:N | 2.31 | 0.45 |
| 1:G:369:ILE:HG23 | 1:G:370:VAL:N | 2.30 | 0.45 |
| 1:I:135:ALA:HB3 | 1:I:140:LEU:HD11 | 1.98 | 0.45 |
| 1:I:369:ILE:HG22 | 1:I:370:VAL:H | 1.81 | 0.45 |
| 1:J:8:LEU:O | 1:J:104:LEU:N | 2.47 | 0.45 |
| 1:J:33:SER:O | 1:J:69:TYR:CD1 | 2.69 | 0.45 |
| 1:J:34:ILE:N | 1:J:54:VAL:HG11 | 2.31 | 0.45 |
| 1:K:7:ALA:HB1 | 1:K:347:ALA:HB1 | 1.98 | 0.45 |
| 1:K:143:TYR:CE2 | 1:K:346:LEU:HD13 | 2.50 | 0.45 |
| 1:L:8:LEU:O | 1:L:104:LEU:N | 2.47 | 0.45 |
| 1:N:9:VAL:HG21 | 1:N:344:SER:HA | 1.98 | 0.45 |
| 1:N:133:TYR:CE2 | 1:N:375:PHE:HB2 | 2.51 | 0.45 |
| 1:P:7:ALA:HB1 | 1:P:347:ALA:HB1 | 1.98 | 0.45 |
| 1:P:38:PRO:HD3 | 1:P:49:GLN:HE22 | 1.81 | 0.45 |
| 1:Q:33:SER:O | 1:Q:69:TYR:CD1 | 2.69 | 0.45 |
| 1:Q:106:THR:HB | 1:Q:137:GLN:HG2 | 1.97 | 0.45 |
| 1:R:7:ALA:HB1 | 1:R:347:ALA:HB1 | 1.98 | 0.45 |
| 1:R:143:TYR:CE2 | 1:R:346:LEU:HD13 | 2.51 | 0.45 |
| 1:R:287:ILE:HB | 1:T:244:ASP:HB3 | 1.97 | 0.45 |
| 1:S:33:SER:O | 1:S:69:TYR:CD1 | 2.69 | 0.45 |
| 1:T:143:TYR:CE2 | 1:T:346:LEU:HD13 | 2.51 | 0.45 |
| 1:T:180:LEU:CD1 | 1:T:181:ALA:N | 2.78 | 0.45 |
| 1:T:287:ILE:HB | 1:V:244:ASP:HB3 | 1.97 | 0.45 |
| 1:U:7:ALA:HB1 | 1:U:347:ALA:HB1 | 1.98 | 0.45 |
| 1:U:8:LEU:O | 1:U:104:LEU:N | 2.47 | 0.45 |
| 1:U:34:ILE:N | 1:U:54:VAL:HG11 | 2.31 | 0.45 |
| 1:U:116:ARG:NH1 | 1:U:375:PHE:HA | 2.32 | 0.45 |
| 1:U:180:LEU:O | 1:U:180:LEU:HG | 2.11 | 0.45 |
| 1:U:287:ILE:HB | 1:W:244:ASP:HB3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:147:ARG:HH21 | 1:V:147:ARG:HG3 | 1.80 | 0.45 |
| 1:W:144:ALA:HB2 | 1:W:342:GLY:N | 2.31 | 0.45 |
| 1:A:7:ALA:HB1 | 1:A:347:ALA:HB1 | 1.98 | 0.45 |
| 1:A:9:VAL:HG21 | 1:A:344:SER:HA | 1.98 | 0.45 |
| 1:B:287:ILE:HB | 1:D:244:ASP:HB3 | 1.97 | 0.45 |
| 1:D:335:ARG:HA | 1:D:335:ARG:HD3 | 1.39 | 0.45 |
| 1:D:369:ILE:HG22 | 1:D:370:VAL:H | 1.81 | 0.45 |
| 1:E:173:HIS:HE1 | 1:F:268:GLY:CA | 2.28 | 0.45 |
| 1:F:37:ARG:O | 1:F:66:THR:CG2 | 2.63 | 0.45 |
| 1:F:180:LEU:O | 1:F:180:LEU:HG | 2.11 | 0.45 |
| 1:I:164:PRO:CG | 1:I:174:ALA:CB | 2.95 | 0.45 |
| 1:I:287:ILE:HG22 | 1:I:290:ARG:NH1 | 2.32 | 0.45 |
| 1:J:290:ARG:HB2 | 1:L:244:ASP:HA | 1.97 | 0.45 |
| 1:K:173:HIS:HE1 | 1:L:268:GLY:CA | 2.28 | 0.45 |
| 1:K:287:ILE:HG22 | 1:K:290:ARG:NH1 | 2.31 | 0.45 |
| 1:L:33:SER:O | 1:L:69:TYR:CD1 | 2.69 | 0.45 |
| 1:L:58:ALA:CB | 1:L:65:LEU:CD2 | 2.90 | 0.45 |
| 1:M:287:ILE:HB | 1:O:244:ASP:HB3 | 1.97 | 0.45 |
| 1:N:7:ALA:HB1 | 1:N:347:ALA:HB1 | 1.98 | 0.45 |
| 1:N:34:ILE:N | 1:N:54:VAL:HG11 | 2.31 | 0.45 |
| 1:N:290:ARG:HB2 | 1:P:244:ASP:HA | 1.97 | 0.45 |
| 1:O:33:SER:O | 1:O:69:TYR:CD1 | 2.69 | 0.45 |
| 1:O:299:MET:HE1 | 1:O:304:THR:HB | 1.98 | 0.45 |
| 1:P:33:SER:O | 1:P:69:TYR:CD1 | 2.69 | 0.45 |
| 1:P:43:VAL:C | 1:P:44:MET:HG2 | 2.37 | 0.45 |
| 1:Q:37:ARG:O | 1:Q:66:THR:CG2 | 2.63 | 0.45 |
| 1:Q:38:PRO:HD3 | 1:Q:49:GLN:HE22 | 1.81 | 0.45 |
| 1:Q:287:ILE:HB | 1:S:244:ASP:HB3 | 1.97 | 0.45 |
| 1:R:180:LEU:CD1 | 1:R:181:ALA:N | 2.78 | 0.45 |
| 1:R:287:ILE:HG22 | 1:R:290:ARG:NH1 | 2.32 | 0.45 |
| 1:R:336:LYS:HE2 | 2:R:401:ADP:C5' | 2.38 | 0.45 |
| 1:S:8:LEU:O | 1:S:104:LEU:N | 2.47 | 0.45 |
| 1:S:290:ARG:HB2 | 1:U:244:ASP:HA | 1.97 | 0.45 |
| 1:V:135:ALA:HB3 | 1:V:140:LEU:HD11 | 1.98 | 0.45 |
| 1:V:164:PRO:CG | 1:V:174:ALA:CB | 2.95 | 0.45 |
| 1:W:8:LEU:O | 1:W:104:LEU:N | 2.47 | 0.45 |
| 1:W:374:CYS:HB2 | 1:W:375:PHE:H | 1.62 | 0.45 |
| 1:A:44:MET:CG | 1:A:45:VAL:N | 2.75 | 0.45 |
| 1:B:9:VAL:HG21 | 1:B:344:SER:HA | 1.98 | 0.45 |
| 1:C:44:MET:CG | 1:C:45:VAL:N | 2.75 | 0.45 |
| 1:C:180:LEU:CD1 | 1:C:181:ALA:N | 2.78 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:43:VAL:C | 1:E:44:MET:HG2 | 2.37 | 0.45 |
| 1:E:180:LEU:CD1 | 1:E:181:ALA:N | 2.78 | 0.45 |
| 1:E:287:ILE:HB | 1:G:244:ASP:HB3 | 1.98 | 0.45 |
| 1:F:34:ILE:N | 1:F:54:VAL:HG11 | 2.31 | 0.45 |
| 1:G:164:PRO:CG | 1:G:174:ALA:CB | 2.95 | 0.45 |
| 1:I:34:ILE:N | 1:I:54:VAL:HG11 | 2.31 | 0.45 |
| 1:J:38:PRO:CG | 1:J:49:GLN:NE2 | 2.79 | 0.45 |
| 1:J:133:TYR:HH | 1:J:375:PHE:HB2 | 1.80 | 0.45 |
| 1:K:164:PRO:CG | 1:K:174:ALA:CB | 2.95 | 0.45 |
| 1:L:106:THR:HB | 1:L:137:GLN:HG2 | 1.97 | 0.45 |
| 1:M:369:ILE:HG23 | 1:M:370:VAL:N | 2.30 | 0.45 |
| 1:N:357:ILE:HD12 | 1:N:357:ILE:HA | 1.79 | 0.45 |
| 1:Q:236:LEU:CD1 | 1:Q:237:GLU:CG | 2.93 | 0.45 |
| 1:S:287:ILE:HD12 | 1:U:208:ILE:HD13 | 1.96 | 0.45 |
| 1:T:7:ALA:HB1 | 1:T:347:ALA:HB1 | 1.98 | 0.45 |
| 1:W:236:LEU:CD1 | 1:W:237:GLU:CG | 2.93 | 0.45 |
| 1:W:336:LYS:HE2 | 2:W:401:ADP:C5' | 2.38 | 0.45 |
| 1:B:38:PRO:HD3 | 1:B:49:GLN:HE22 | 1.81 | 0.45 |
| 1:C:116:ARG:NH1 | 1:C:375:PHE:HA | 2.32 | 0.45 |
| 1:D:9:VAL:HG21 | 1:D:344:SER:HA | 1.98 | 0.45 |
| 1:E:37:ARG:O | 1:E:66:THR:CG2 | 2.63 | 0.45 |
| 1:E:44:MET:CG | 1:E:45:VAL:N | 2.76 | 0.45 |
| 1:E:116:ARG:NH1 | 1:E:375:PHE:HA | 2.32 | 0.45 |
| 1:F:43:VAL:C | 1:F:44:MET:HG2 | 2.37 | 0.45 |
| 1:F:290:ARG:HB2 | 1:H:244:ASP:HA | 1.97 | 0.45 |
| 1:F:369:ILE:HG23 | 1:F:370:VAL:N | 2.30 | 0.45 |
| 1:G:369:ILE:HG22 | 1:G:370:VAL:H | 1.81 | 0.45 |
| 1:H:31:PHE:HA | 1:H:32:PRO:HD3 | 1.66 | 0.45 |
| 1:I:38:PRO:HD3 | 1:I:49:GLN:HE22 | 1.81 | 0.45 |
| 1:J:43:VAL:C | 1:J:44:MET:HG2 | 2.37 | 0.45 |
| 1:K:34:ILE:N | 1:K:54:VAL:HG11 | 2.31 | 0.45 |
| 1:K:369:ILE:HG22 | 1:K:370:VAL:H | 1.81 | 0.45 |
| 1:L:7:ALA:HB1 | 1:L:347:ALA:HB1 | 1.98 | 0.45 |
| 1:L:236:LEU:CD1 | 1:L:237:GLU:CG | 2.93 | 0.45 |
| 1:L:369:ILE:HG22 | 1:L:370:VAL:H | 1.82 | 0.45 |
| 1:M:164:PRO:CG | 1:M:174:ALA:CB | 2.95 | 0.45 |
| 1:N:369:ILE:HG22 | 1:N:370:VAL:H | 1.82 | 0.45 |
| 1:O:34:ILE:HD13 | 1:O:67:LEU:CD2 | 2.46 | 0.45 |
| 1:O:287:ILE:HB | 1:Q:244:ASP:HB3 | 1.97 | 0.45 |
| 1:P:34:ILE:N | 1:P:54:VAL:HG11 | 2.31 | 0.45 |
| 1:Q:290:ARG:HB2 | 1:S:244:ASP:HA | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:116:ARG:NH1 | 1:S:375:PHE:HA | 2.32 | 0.45 |
| 1:S:300:SER:HA | 1:S:335:ARG:NE | 2.32 | 0.45 |
| 1:T:38:PRO:HD3 | 1:T:49:GLN:HE22 | 1.81 | 0.45 |
| 1:T:335:ARG:HA | 1:T:335:ARG:HD3 | 1.39 | 0.45 |
| 1:V:7:ALA:HB1 | 1:V:347:ALA:HB1 | 1.98 | 0.45 |
| 1:W:58:ALA:CB | 1:W:65:LEU:CD2 | 2.90 | 0.45 |
| 1:B:73:HIC:HA | 1:B:183:ARG:NH1 | 2.18 | 0.45 |
| 1:B:164:PRO:CG | 1:B:174:ALA:CB | 2.95 | 0.45 |
| 1:B:287:ILE:HG22 | 1:B:290:ARG:NH1 | 2.32 | 0.45 |
| 1:C:287:ILE:HG22 | 1:C:290:ARG:NH1 | 2.32 | 0.45 |
| 1:D:290:ARG:HB2 | 1:F:244:ASP:HA | 1.97 | 0.45 |
| 1:E:34:ILE:N | 1:E:54:VAL:HG11 | 2.31 | 0.45 |
| 1:G:61:LYS:HG2 | 1:G:64:ILE:CG2 | 2.45 | 0.45 |
| 1:G:287:ILE:HG22 | 1:G:290:ARG:NH1 | 2.32 | 0.45 |
| 1:H:33:SER:O | 1:H:69:TYR:CD1 | 2.69 | 0.45 |
| 1:H:34:ILE:N | 1:H:54:VAL:HG11 | 2.31 | 0.45 |
| 1:H:38:PRO:CG | 1:H:49:GLN:NE2 | 2.79 | 0.45 |
| 1:H:43:VAL:C | 1:H:44:MET:HG2 | 2.37 | 0.45 |
| 1:H:144:ALA:HB2 | 1:H:342:GLY:N | 2.31 | 0.45 |
| 1:H:236:LEU:CD1 | 1:H:237:GLU:CG | 2.93 | 0.45 |
| 1:H:287:ILE:HD12 | 1:J:208:ILE:HD13 | 1.96 | 0.45 |
| 1:I:287:ILE:HD12 | 1:K:208:ILE:HD13 | 1.96 | 0.45 |
| 1:I:362:TYR:CE1 | 1:I:367:PRO:CB | 2.99 | 0.45 |
| 1:J:164:PRO:CG | 1:J:174:ALA:CB | 2.95 | 0.45 |
| 1:J:369:ILE:HG22 | 1:J:370:VAL:H | 1.81 | 0.45 |
| 1:K:9:VAL:HG21 | 1:K:344:SER:HA | 1.98 | 0.45 |
| 1:L:43:VAL:C | 1:L:44:MET:HG2 | 2.37 | 0.45 |
| 1:L:116:ARG:NH1 | 1:L:375:PHE:HA | 2.32 | 0.45 |
| 1:L:144:ALA:HB2 | 1:L:342:GLY:N | 2.31 | 0.45 |
| 1:L:164:PRO:CG | 1:L:174:ALA:CB | 2.95 | 0.45 |
| 1:M:38:PRO:HD3 | 1:M:49:GLN:HE22 | 1.81 | 0.45 |
| 1:N:287:ILE:HB | 1:P:244:ASP:HB3 | 1.97 | 0.45 |
| 1:P:287:ILE:HG22 | 1:P:290:ARG:NH1 | 2.32 | 0.45 |
| 1:Q:300:SER:HA | 1:Q:335:ARG:NE | 2.32 | 0.45 |
| 1:Q:369:ILE:HG22 | 1:Q:370:VAL:H | 1.81 | 0.45 |
| 1:S:144:ALA:HB2 | 1:S:342:GLY:N | 2.31 | 0.45 |
| 1:T:39:ARG:NE | 1:T:66:THR:CA | 2.69 | 0.45 |
| 1:T:106:THR:HB | 1:T:137:GLN:HG2 | 1.97 | 0.45 |
| 1:T:287:ILE:HG22 | 1:T:290:ARG:NH1 | 2.32 | 0.45 |
| 1:U:300:SER:HA | 1:U:335:ARG:NE | 2.32 | 0.45 |
| 1:V:180:LEU:O | 1:V:180:LEU:HG | 2.11 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:34:ILE:N | 1:A:54:VAL:HG11 | 2.31 | 0.45 |
| 1:A:164:PRO:CG | 1:A:174:ALA:CB | 2.95 | 0.45 |
| 1:B:227:MET:HA | 1:B:227:MET:HE3 | 1.99 | 0.45 |
| 1:C:287:ILE:HB | 1:E:244:ASP:HB3 | 1.97 | 0.45 |
| 1:D:164:PRO:CG | 1:D:174:ALA:CB | 2.95 | 0.45 |
| 1:D:287:ILE:HD12 | 1:F:208:ILE:HD13 | 1.96 | 0.45 |
| 1:E:38:PRO:HD3 | 1:E:49:GLN:HE22 | 1.81 | 0.45 |
| 1:E:147:ARG:HH21 | 1:E:147:ARG:HG3 | 1.80 | 0.45 |
| 1:G:233:SER:HB3 | 1:G:236:LEU:HG | 1.99 | 0.45 |
| 1:G:335:ARG:HA | 1:G:335:ARG:HD3 | 1.39 | 0.45 |
| 1:H:167:GLU:OE1 | 1:J:61:LYS:CD | 2.65 | 0.45 |
| 1:I:233:SER:HB3 | 1:I:236:LEU:HG | 1.99 | 0.45 |
| 1:J:116:ARG:NH1 | 1:J:375:PHE:HA | 2.32 | 0.45 |
| 1:K:38:PRO:CG | 1:K:49:GLN:NE2 | 2.79 | 0.45 |
| 1:K:180:LEU:O | 1:K:180:LEU:HG | 2.11 | 0.45 |
| 1:N:38:PRO:HD3 | 1:N:49:GLN:HE22 | 1.81 | 0.45 |
| 1:N:164:PRO:CG | 1:N:174:ALA:CB | 2.95 | 0.45 |
| 1:N:362:TYR:CE1 | 1:N:367:PRO:CB | 2.99 | 0.45 |
| 1:P:287:ILE:HB | 1:R:244:ASP:HB3 | 1.97 | 0.45 |
| 1:Q:144:ALA:HB2 | 1:Q:342:GLY:N | 2.31 | 0.45 |
| 1:R:324:THR:HG23 | 1:T:241:GLU:OE2 | 2.17 | 0.45 |
| 1:S:34:ILE:N | 1:S:54:VAL:HG11 | 2.31 | 0.45 |
| 1:S:43:VAL:C | 1:S:44:MET:HG2 | 2.37 | 0.45 |
| 1:T:58:ALA:CB | 1:T:65:LEU:CD2 | 2.90 | 0.45 |
| 1:T:164:PRO:CG | 1:T:174:ALA:CB | 2.95 | 0.45 |
| 1:T:167:GLU:OE1 | 1:V:61:LYS:CD | 2.65 | 0.45 |
| 1:T:324:THR:HG23 | 1:V:241:GLU:OE2 | 2.16 | 0.45 |
| 1:U:7:ALA:HB3 | 1:U:347:ALA:HB1 | 1.99 | 0.45 |
| 1:U:290:ARG:HB2 | 1:W:244:ASP:HA | 1.97 | 0.45 |
| 1:V:34:ILE:N | 1:V:54:VAL:HG11 | 2.31 | 0.45 |
| 1:V:116:ARG:NH1 | 1:V:375:PHE:HA | 2.32 | 0.45 |
| 1:V:300:SER:HA | 1:V:335:ARG:NE | 2.32 | 0.45 |
| 1:W:164:PRO:CG | 1:W:174:ALA:CB | 2.95 | 0.45 |
| 1:W:287:ILE:HG22 | 1:W:290:ARG:NH1 | 2.32 | 0.45 |
| 1:A:31:PHE:HA | 1:A:32:PRO:HD3 | 1.66 | 0.45 |
| 1:A:33:SER:O | 1:A:69:TYR:CD1 | 2.69 | 0.45 |
| 1:A:144:ALA:HB2 | 1:A:342:GLY:N | 2.31 | 0.45 |
| 1:A:167:GLU:OE1 | 1:C:61:LYS:CD | 2.65 | 0.45 |
| 1:B:34:ILE:HD13 | 1:B:67:LEU:CD2 | 2.46 | 0.45 |
| 1:C:7:ALA:HB1 | 1:C:347:ALA:HB1 | 1.98 | 0.45 |
| 1:D:34:ILE:HG22 | 1:D:35:VAL:H | 1.78 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:35:VAL:H | 1:D:68:LYS:H | 1.65 | 0.45 |
| 1:E:61:LYS:HG2 | 1:E:64:ILE:CG2 | 2.45 | 0.45 |
| 1:E:164:PRO:CG | 1:E:174:ALA:CB | 2.95 | 0.45 |
| 1:E:324:THR:HG23 | 1:G:241:GLU:OE2 | 2.16 | 0.45 |
| 1:G:43:VAL:C | 1:G:44:MET:HG2 | 2.37 | 0.45 |
| 1:G:44:MET:CG | 1:G:45:VAL:N | 2.75 | 0.45 |
| 1:G:362:TYR:CE1 | 1:G:367:PRO:CB | 2.99 | 0.45 |
| 1:H:8:LEU:O | 1:H:104:LEU:N | 2.47 | 0.45 |
| 1:H:290:ARG:HB2 | 1:J:244:ASP:HA | 1.97 | 0.45 |
| 1:N:116:ARG:NH1 | 1:N:375:PHE:HA | 2.32 | 0.45 |
| 1:O:164:PRO:CG | 1:O:174:ALA:CB | 2.95 | 0.45 |
| 1:P:133:TYR:CE2 | 1:P:375:PHE:HB2 | 2.51 | 0.45 |
| 1:P:173:HIS:HE1 | 1:Q:268:GLY:CA | 2.28 | 0.45 |
| 1:S:7:ALA:HB3 | 1:S:347:ALA:HB1 | 1.99 | 0.45 |
| 1:S:9:VAL:HG21 | 1:S:344:SER:HA | 1.98 | 0.45 |
| 1:S:133:TYR:CE2 | 1:S:375:PHE:HB2 | 2.51 | 0.45 |
| 1:S:299:MET:HE1 | 1:S:304:THR:HB | 1.98 | 0.45 |
| 1:T:173:HIS:HE1 | 1:U:268:GLY:CA | 2.28 | 0.45 |
| 1:U:144:ALA:HB2 | 1:U:342:GLY:N | 2.31 | 0.45 |
| 1:U:324:THR:HG23 | 1:W:241:GLU:OE2 | 2.16 | 0.45 |
| 1:W:116:ARG:NH1 | 1:W:375:PHE:HA | 2.32 | 0.45 |
| 1:A:116:ARG:NH1 | 1:A:375:PHE:HA | 2.32 | 0.45 |
| 1:A:173:HIS:HE1 | 1:B:268:GLY:CA | 2.28 | 0.45 |
| 1:A:287:ILE:HG22 | 1:A:290:ARG:NH1 | 2.32 | 0.45 |
| 1:B:7:ALA:HB3 | 1:B:347:ALA:HB1 | 1.99 | 0.45 |
| 1:C:44:MET:CG | 1:C:45:VAL:H | 2.18 | 0.45 |
| 1:D:33:SER:O | 1:D:69:TYR:CD1 | 2.69 | 0.45 |
| 1:D:43:VAL:C | 1:D:44:MET:HG2 | 2.37 | 0.45 |
| 1:E:33:SER:O | 1:E:69:TYR:CD1 | 2.69 | 0.45 |
| 1:E:227:MET:HA | 1:E:227:MET:HE3 | 1.99 | 0.45 |
| 1:E:233:SER:HB3 | 1:E:236:LEU:HG | 1.99 | 0.45 |
| 1:E:287:ILE:HG22 | 1:E:290:ARG:NH1 | 2.32 | 0.45 |
| 1:F:38:PRO:CG | 1:F:49:GLN:NE2 | 2.79 | 0.45 |
| 1:F:369:ILE:HG22 | 1:F:370:VAL:H | 1.81 | 0.45 |
| 1:G:34:ILE:N | 1:G:54:VAL:HG11 | 2.31 | 0.45 |
| 1:G:116:ARG:NH1 | 1:G:375:PHE:HA | 2.32 | 0.45 |
| 1:G:133:TYR:CE2 | 1:G:375:PHE:HB2 | 2.51 | 0.45 |
| 1:H:6:THR:O | 1:H:102:PRO:HD2 | 2.17 | 0.45 |
| 1:H:9:VAL:HG21 | 1:H:344:SER:HA | 1.98 | 0.45 |
| 1:I:7:ALA:HB1 | 1:I:347:ALA:HB1 | 1.98 | 0.45 |
| 1:I:180:LEU:CD1 | 1:I:181:ALA:N | 2.78 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:167:GLU:OE1 | 1:L:61:LYS:CD | 2.65 | 0.45 |
| 1:K:324:THR:HG23 | 1:M:241:GLU:OE2 | 2.16 | 0.45 |
| 1:N:43:VAL:C | 1:N:44:MET:HG2 | 2.37 | 0.45 |
| 1:O:290:ARG:HB2 | 1:Q:244:ASP:HA | 1.97 | 0.45 |
| 1:O:300:SER:HA | 1:O:335:ARG:NE | 2.32 | 0.45 |
| 1:P:167:GLU:OE1 | 1:R:61:LYS:CD | 2.65 | 0.45 |
| 1:P:369:ILE:HG22 | 1:P:370:VAL:H | 1.81 | 0.45 |
| 1:Q:7:ALA:HB3 | 1:Q:347:ALA:HB1 | 1.99 | 0.45 |
| 1:Q:116:ARG:NH1 | 1:Q:375:PHE:HA | 2.32 | 0.45 |
| 1:Q:133:TYR:CE2 | 1:Q:375:PHE:HB2 | 2.51 | 0.45 |
| 1:Q:287:ILE:HG22 | 1:Q:290:ARG:NH1 | 2.31 | 0.45 |
| 1:R:287:ILE:HD12 | 1:T:208:ILE:HD13 | 1.96 | 0.45 |
| 1:S:34:ILE:HD13 | 1:S:67:LEU:CD2 | 2.46 | 0.45 |
| 1:S:61:LYS:HG2 | 1:S:64:ILE:CG2 | 2.45 | 0.45 |
| 1:S:287:ILE:HG22 | 1:S:290:ARG:NH1 | 2.32 | 0.45 |
| 1:T:34:ILE:N | 1:T:54:VAL:HG11 | 2.31 | 0.45 |
| 1:T:116:ARG:NH1 | 1:T:375:PHE:HA | 2.32 | 0.45 |
| 1:U:287:ILE:HG22 | 1:U:290:ARG:NH1 | 2.32 | 0.45 |
| 1:V:7:ALA:HB3 | 1:V:347:ALA:HB1 | 1.99 | 0.45 |
| 1:V:9:VAL:HG21 | 1:V:344:SER:HA | 1.98 | 0.45 |
| 1:W:7:ALA:HB3 | 1:W:347:ALA:HB1 | 1.99 | 0.45 |
| 1:B:7:ALA:HB1 | 1:B:347:ALA:HB1 | 1.98 | 0.45 |
| 1:B:38:PRO:CG | 1:B:49:GLN:NE2 | 2.79 | 0.45 |
| 1:C:34:ILE:N | 1:C:54:VAL:HG11 | 2.31 | 0.45 |
| 1:C:144:ALA:HB2 | 1:C:342:GLY:N | 2.31 | 0.45 |
| 1:C:300:SER:HA | 1:C:335:ARG:NE | 2.32 | 0.45 |
| 1:D:38:PRO:CG | 1:D:49:GLN:NE2 | 2.79 | 0.45 |
| 1:D:287:ILE:HG22 | 1:D:290:ARG:NH1 | 2.32 | 0.45 |
| 1:E:300:SER:HA | 1:E:335:ARG:NE | 2.32 | 0.45 |
| 1:E:369:ILE:HG22 | 1:E:370:VAL:H | 1.82 | 0.45 |
| 1:F:6:THR:O | 1:F:102:PRO:HD2 | 2.17 | 0.45 |
| 1:F:33:SER:O | 1:F:69:TYR:CD1 | 2.69 | 0.45 |
| 1:F:38:PRO:HD3 | 1:F:49:GLN:HE22 | 1.81 | 0.45 |
| 1:F:164:PRO:CG | 1:F:174:ALA:CB | 2.95 | 0.45 |
| 1:J:7:ALA:HB1 | 1:J:347:ALA:HB1 | 1.98 | 0.45 |
| 1:J:110:LEU:CD1 | 1:J:177:ARG:NH1 | 2.80 | 0.45 |
| 1:J:144:ALA:HB2 | 1:J:342:GLY:N | 2.31 | 0.45 |
| 1:J:300:SER:HA | 1:J:335:ARG:NE | 2.32 | 0.45 |
| 1:K:31:PHE:HA | 1:K:32:PRO:HD3 | 1.65 | 0.45 |
| 1:K:287:ILE:HD12 | 1:M:208:ILE:HD13 | 1.96 | 0.45 |
| 1:L:34:ILE:N | 1:L:54:VAL:HG11 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:300:SER:HA | 1:L:335:ARG:NE | 2.32 | 0.45 |
| 1:L:374:CYS:HB2 | 1:L:375:PHE:H | 1.62 | 0.45 |
| 1:M:35:VAL:H | 1:M:68:LYS:H | 1.65 | 0.45 |
| 1:M:300:SER:HA | 1:M:335:ARG:NE | 2.32 | 0.45 |
| 1:N:106:THR:HB | 1:N:137:GLN:HG2 | 1.97 | 0.45 |
| 1:N:233:SER:HB3 | 1:N:236:LEU:HG | 1.99 | 0.45 |
| 1:N:287:ILE:HG22 | 1:N:290:ARG:NH1 | 2.32 | 0.45 |
| 1:N:300:SER:HA | 1:N:335:ARG:NE | 2.32 | 0.45 |
| 1:O:7:ALA:HB3 | 1:O:347:ALA:HB1 | 1.99 | 0.45 |
| 1:O:44:MET:CG | 1:O:45:VAL:H | 2.18 | 0.45 |
| 1:O:167:GLU:OE1 | 1:Q:61:LYS:CD | 2.65 | 0.45 |
| 1:Q:34:ILE:N | 1:Q:54:VAL:HG11 | 2.31 | 0.45 |
| 1:Q:167:GLU:OE1 | 1:S:61:LYS:CD | 2.65 | 0.45 |
| 1:Q:369:ILE:HG23 | 1:Q:370:VAL:N | 2.30 | 0.45 |
| 1:R:167:GLU:OE1 | 1:T:61:LYS:CD | 2.65 | 0.45 |
| 1:S:324:THR:HG23 | 1:U:241:GLU:OE2 | 2.16 | 0.45 |
| 1:U:31:PHE:HA | 1:U:32:PRO:HD3 | 1.66 | 0.45 |
| 1:U:133:TYR:CE2 | 1:U:375:PHE:HB2 | 2.51 | 0.45 |
| 1:U:369:ILE:HG23 | 1:U:370:VAL:N | 2.30 | 0.45 |
| 1:V:287:ILE:HG22 | 1:V:290:ARG:NH1 | 2.32 | 0.45 |
| 1:B:43:VAL:C | 1:B:44:MET:HG2 | 2.37 | 0.44 |
| 1:B:116:ARG:NH1 | 1:B:375:PHE:HA | 2.32 | 0.44 |
| 1:B:300:SER:HA | 1:B:335:ARG:NE | 2.32 | 0.44 |
| 1:B:369:ILE:HG23 | 1:B:370:VAL:N | 2.30 | 0.44 |
| 1:C:164:PRO:CG | 1:C:174:ALA:CB | 2.95 | 0.44 |
| 1:E:9:VAL:HG21 | 1:E:344:SER:HA | 1.98 | 0.44 |
| 1:F:34:ILE:HD13 | 1:F:67:LEU:CD2 | 2.46 | 0.44 |
| 1:F:35:VAL:H | 1:F:68:LYS:H | 1.65 | 0.44 |
| 1:F:167:GLU:OE1 | 1:H:61:LYS:CD | 2.65 | 0.44 |
| 1:F:287:ILE:HG22 | 1:F:290:ARG:NH1 | 2.32 | 0.44 |
| 1:H:164:PRO:CG | 1:H:174:ALA:CB | 2.95 | 0.44 |
| 1:H:300:SER:HA | 1:H:335:ARG:NE | 2.32 | 0.44 |
| 1:I:167:GLU:OE1 | 1:K:61:LYS:CD | 2.65 | 0.44 |
| 1:I:300:SER:HA | 1:I:335:ARG:HG2 | 1.89 | 0.44 |
| 1:K:167:GLU:OE1 | 1:M:61:LYS:CD | 2.65 | 0.44 |
| 1:K:233:SER:HB3 | 1:K:236:LEU:HG | 1.99 | 0.44 |
| 1:L:9:VAL:HG21 | 1:L:344:SER:HA | 1.98 | 0.44 |
| 1:L:180:LEU:O | 1:L:180:LEU:HG | 2.11 | 0.44 |
| 1:M:34:ILE:N | 1:M:54:VAL:HG11 | 2.31 | 0.44 |
| 1:M:143:TYR:CE2 | 1:M:346:LEU:HD13 | 2.51 | 0.44 |
| 1:M:167:GLU:OE1 | 1:O:61:LYS:CD | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:287:ILE:HG22 | 1:M:290:ARG:NH1 | 2.31 | 0.44 |
| 1:M:369:ILE:HG22 | 1:M:370:VAL:H | 1.81 | 0.44 |
| 1:N:167:GLU:OE1 | 1:P:61:LYS:CD | 2.65 | 0.44 |
| 1:O:34:ILE:N | 1:O:54:VAL:HG11 | 2.31 | 0.44 |
| 1:O:35:VAL:H | 1:O:68:LYS:H | 1.65 | 0.44 |
| 1:P:164:PRO:CG | 1:P:174:ALA:CB | 2.95 | 0.44 |
| 1:P:233:SER:HB3 | 1:P:236:LEU:HG | 1.99 | 0.44 |
| 1:Q:34:ILE:O | 1:Q:54:VAL:HB | 2.18 | 0.44 |
| 1:Q:43:VAL:C | 1:Q:44:MET:HG2 | 2.37 | 0.44 |
| 1:Q:164:PRO:CG | 1:Q:174:ALA:CB | 2.95 | 0.44 |
| 1:R:58:ALA:CB | 1:R:65:LEU:CD2 | 2.90 | 0.44 |
| 1:T:7:ALA:HB3 | 1:T:347:ALA:HB1 | 1.99 | 0.44 |
| 1:T:34:ILE:HG22 | 1:T:35:VAL:H | 1.78 | 0.44 |
| 1:T:38:PRO:CG | 1:T:49:GLN:NE2 | 2.79 | 0.44 |
| 1:U:38:PRO:HD3 | 1:U:49:GLN:HE22 | 1.81 | 0.44 |
| 1:U:164:PRO:CG | 1:U:174:ALA:CB | 2.95 | 0.44 |
| 1:U:167:GLU:OE1 | 1:W:61:LYS:CD | 2.65 | 0.44 |
| 1:V:180:LEU:CD1 | 1:V:181:ALA:N | 2.78 | 0.44 |
| 1:A:44:MET:CG | 1:A:45:VAL:H | 2.18 | 0.44 |
| 1:A:58:ALA:CB | 1:A:65:LEU:CD2 | 2.90 | 0.44 |
| 1:A:110:LEU:CD1 | 1:A:177:ARG:NH1 | 2.80 | 0.44 |
| 1:C:38:PRO:HD3 | 1:C:49:GLN:HE22 | 1.82 | 0.44 |
| 1:C:167:GLU:OE1 | 1:E:61:LYS:CD | 2.65 | 0.44 |
| 1:C:233:SER:HB3 | 1:C:236:LEU:HG | 1.99 | 0.44 |
| 1:D:7:ALA:HB3 | 1:D:347:ALA:HB1 | 1.99 | 0.44 |
| 1:D:116:ARG:NH1 | 1:D:375:PHE:HA | 2.32 | 0.44 |
| 1:H:287:ILE:HG22 | 1:H:290:ARG:NH1 | 2.32 | 0.44 |
| 1:J:6:THR:O | 1:J:102:PRO:HD2 | 2.17 | 0.44 |
| 1:J:287:ILE:HG22 | 1:J:290:ARG:NH1 | 2.32 | 0.44 |
| 1:K:180:LEU:CD1 | 1:K:181:ALA:N | 2.78 | 0.44 |
| 1:L:110:LEU:CD1 | 1:L:177:ARG:NH1 | 2.80 | 0.44 |
| 1:M:7:ALA:HB3 | 1:M:347:ALA:HB1 | 1.99 | 0.44 |
| 1:O:43:VAL:C | 1:O:44:MET:HG2 | 2.37 | 0.44 |
| 1:O:133:TYR:CE2 | 1:O:375:PHE:HB2 | 2.51 | 0.44 |
| 1:Q:73:HIC:HA | 1:Q:183:ARG:NH1 | 2.18 | 0.44 |
| 1:R:38:PRO:HD3 | 1:R:49:GLN:HE22 | 1.81 | 0.44 |
| 1:R:106:THR:HB | 1:R:137:GLN:HG2 | 1.97 | 0.44 |
| 1:R:164:PRO:CG | 1:R:174:ALA:CB | 2.95 | 0.44 |
| 1:R:357:ILE:HD12 | 1:R:357:ILE:HA | 1.79 | 0.44 |
| 1:S:38:PRO:HD3 | 1:S:49:GLN:HE22 | 1.82 | 0.44 |
| 1:S:167:GLU:OE1 | 1:U:61:LYS:CD | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:300:SER:HA | 1:T:335:ARG:NE | 2.32 | 0.44 |
| 1:V:110:LEU:CD1 | 1:V:177:ARG:NH1 | 2.80 | 0.44 |
| 1:A:148:THR:CG2 | 1:A:149:THR:N | 2.81 | 0.44 |
| 1:B:35:VAL:H | 1:B:68:LYS:H | 1.65 | 0.44 |
| 1:B:349:LEU:HD23 | 1:B:349:LEU:HA | 1.80 | 0.44 |
| 1:C:369:ILE:HG22 | 1:C:370:VAL:H | 1.81 | 0.44 |
| 1:F:7:ALA:HB3 | 1:F:347:ALA:HB1 | 1.99 | 0.44 |
| 1:G:167:GLU:OE1 | 1:I:61:LYS:CD | 2.65 | 0.44 |
| 1:H:116:ARG:NH1 | 1:H:375:PHE:HA | 2.32 | 0.44 |
| 1:I:324:THR:HG23 | 1:K:241:GLU:OE2 | 2.17 | 0.44 |
| 1:J:34:ILE:HD13 | 1:J:67:LEU:CD2 | 2.46 | 0.44 |
| 1:J:73:HIC:HA | 1:J:183:ARG:NH1 | 2.18 | 0.44 |
| 1:L:233:SER:HB3 | 1:L:236:LEU:HG | 1.99 | 0.44 |
| 1:M:38:PRO:CG | 1:M:49:GLN:NE2 | 2.79 | 0.44 |
| 1:O:116:ARG:NH1 | 1:O:375:PHE:HA | 2.32 | 0.44 |
| 1:P:106:THR:HB | 1:P:137:GLN:HG2 | 1.97 | 0.44 |
| 1:P:116:ARG:NH1 | 1:P:375:PHE:HA | 2.32 | 0.44 |
| 1:R:300:SER:HA | 1:R:335:ARG:NE | 2.32 | 0.44 |
| 1:U:9:VAL:HG21 | 1:U:344:SER:HA | 1.98 | 0.44 |
| 1:U:151:ILE:O | 1:U:297:ASN:HA | 2.17 | 0.44 |
| 1:V:34:ILE:O | 1:V:54:VAL:HB | 2.18 | 0.44 |
| 1:W:6:THR:O | 1:W:102:PRO:HD2 | 2.17 | 0.44 |
| 1:W:300:SER:HA | 1:W:335:ARG:NE | 2.32 | 0.44 |
| 1:A:34:ILE:O | 1:A:54:VAL:HB | 2.18 | 0.44 |
| 1:A:170:ALA:O | 1:A:172:PRO:HD3 | 2.18 | 0.44 |
| 1:C:148:THR:CG2 | 1:C:149:THR:N | 2.81 | 0.44 |
| 1:C:298:VAL:CG1 | 1:C:335:ARG:NH1 | 2.81 | 0.44 |
| 1:D:7:ALA:HB1 | 1:D:347:ALA:HB1 | 1.98 | 0.44 |
| 1:D:38:PRO:HD3 | 1:D:49:GLN:HE22 | 1.81 | 0.44 |
| 1:G:34:ILE:O | 1:G:54:VAL:HB | 2.18 | 0.44 |
| 1:G:180:LEU:CD1 | 1:G:181:ALA:N | 2.78 | 0.44 |
| 1:G:227:MET:HA | 1:G:227:MET:HE3 | 2.00 | 0.44 |
| 1:G:287:ILE:HD12 | 1:I:208:ILE:HD13 | 1.96 | 0.44 |
| 1:G:300:SER:HA | 1:G:335:ARG:NE | 2.32 | 0.44 |
| 1:G:357:ILE:HD12 | 1:G:357:ILE:HA | 1.79 | 0.44 |
| 1:H:369:ILE:HG22 | 1:H:370:VAL:H | 1.81 | 0.44 |
| 1:I:116:ARG:NH1 | 1:I:375:PHE:HA | 2.32 | 0.44 |
| 1:J:9:VAL:HG21 | 1:J:344:SER:HA | 1.98 | 0.44 |
| 1:J:31:PHE:HA | 1:J:32:PRO:HD3 | 1.66 | 0.44 |
| 1:J:170:ALA:O | 1:J:172:PRO:HD3 | 2.18 | 0.44 |
| 1:K:34:ILE:O | 1:K:54:VAL:HB | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:362:TYR:CE1 | 1:K:367:PRO:CB | 2.99 | 0.44 |
| 1:L:34:ILE:HD13 | 1:L:67:LEU:CD2 | 2.46 | 0.44 |
| 1:L:38:PRO:HD3 | 1:L:49:GLN:HE22 | 1.81 | 0.44 |
| 1:L:287:ILE:HG22 | 1:L:290:ARG:NH1 | 2.31 | 0.44 |
| 1:M:34:ILE:O | 1:M:54:VAL:HB | 2.18 | 0.44 |
| 1:N:34:ILE:O | 1:N:54:VAL:HB | 2.18 | 0.44 |
| 1:O:148:THR:CG2 | 1:O:149:THR:N | 2.81 | 0.44 |
| 1:O:287:ILE:HG22 | 1:O:290:ARG:NH1 | 2.32 | 0.44 |
| 1:O:369:ILE:HG22 | 1:O:370:VAL:H | 1.81 | 0.44 |
| 1:P:9:VAL:HG21 | 1:P:344:SER:HA | 1.98 | 0.44 |
| 1:P:300:SER:HA | 1:P:335:ARG:NE | 2.32 | 0.44 |
| 1:P:357:ILE:HD12 | 1:P:357:ILE:HA | 1.79 | 0.44 |
| 1:R:7:ALA:HB3 | 1:R:347:ALA:HB1 | 1.99 | 0.44 |
| 1:R:233:SER:HB3 | 1:R:236:LEU:HG | 1.99 | 0.44 |
| 1:T:6:THR:O | 1:T:102:PRO:HD2 | 2.17 | 0.44 |
| 1:T:31:PHE:HA | 1:T:32:PRO:HD3 | 1.66 | 0.44 |
| 1:V:151:ILE:O | 1:V:297:ASN:HA | 2.18 | 0.44 |
| 1:V:298:VAL:CG1 | 1:V:335:ARG:NH1 | 2.81 | 0.44 |
| 1:W:34:ILE:O | 1:W:54:VAL:HB | 2.18 | 0.44 |
| 1:W:133:TYR:CE2 | 1:W:375:PHE:HB2 | 2.51 | 0.44 |
| 1:W:151:ILE:O | 1:W:297:ASN:HA | 2.17 | 0.44 |
| 1:A:6:THR:O | 1:A:102:PRO:HD2 | 2.17 | 0.44 |
| 1:A:300:SER:HA | 1:A:335:ARG:NE | 2.32 | 0.44 |
| 1:B:33:SER:O | 1:B:69:TYR:CD1 | 2.69 | 0.44 |
| 1:B:34:ILE:O | 1:B:54:VAL:HB | 2.18 | 0.44 |
| 1:B:34:ILE:N | 1:B:54:VAL:HG11 | 2.31 | 0.44 |
| 1:B:61:LYS:HG2 | 1:B:64:ILE:CG2 | 2.45 | 0.44 |
| 1:B:167:GLU:OE1 | 1:D:61:LYS:CD | 2.65 | 0.44 |
| 1:B:298:VAL:CG1 | 1:B:335:ARG:NH1 | 2.81 | 0.44 |
| 1:D:6:THR:O | 1:D:102:PRO:HD2 | 2.17 | 0.44 |
| 1:D:233:SER:HB3 | 1:D:236:LEU:HG | 1.99 | 0.44 |
| 1:D:298:VAL:CG1 | 1:D:335:ARG:NH1 | 2.81 | 0.44 |
| 1:D:300:SER:HA | 1:D:335:ARG:NE | 2.32 | 0.44 |
| 1:E:34:ILE:O | 1:E:54:VAL:HB | 2.18 | 0.44 |
| 1:E:44:MET:CG | 1:E:45:VAL:H | 2.18 | 0.44 |
| 1:E:148:THR:CG2 | 1:E:149:THR:N | 2.81 | 0.44 |
| 1:E:298:VAL:CG1 | 1:E:335:ARG:NH1 | 2.81 | 0.44 |
| 1:F:34:ILE:O | 1:F:54:VAL:HB | 2.18 | 0.44 |
| 1:F:298:VAL:CG1 | 1:F:335:ARG:NH1 | 2.81 | 0.44 |
| 1:F:335:ARG:HA | 1:F:335:ARG:HD3 | 1.39 | 0.44 |
| 1:G:151:ILE:O | 1:G:297:ASN:HA | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:180:LEU:O | 1:G:180:LEU:HG | 2.11 | 0.44 |
| 1:H:7:ALA:HB1 | 1:H:347:ALA:HB1 | 1.98 | 0.44 |
| 1:H:298:VAL:CG1 | 1:H:335:ARG:NH1 | 2.81 | 0.44 |
| 1:J:34:ILE:O | 1:J:54:VAL:HB | 2.18 | 0.44 |
| 1:K:300:SER:HA | 1:K:335:ARG:NE | 2.32 | 0.44 |
| 1:L:369:ILE:HG23 | 1:L:370:VAL:N | 2.30 | 0.44 |
| 1:M:43:VAL:C | 1:M:44:MET:HG2 | 2.37 | 0.44 |
| 1:M:374:CYS:HB2 | 1:M:375:PHE:H | 1.61 | 0.44 |
| 1:N:34:ILE:CG2 | 1:N:67:LEU:HD22 | 2.28 | 0.44 |
| 1:N:110:LEU:CD1 | 1:N:177:ARG:NH1 | 2.80 | 0.44 |
| 1:O:287:ILE:HD12 | 1:Q:208:ILE:HD13 | 1.96 | 0.44 |
| 1:Q:9:VAL:HG21 | 1:Q:344:SER:HA | 1.98 | 0.44 |
| 1:Q:148:THR:CG2 | 1:Q:149:THR:N | 2.81 | 0.44 |
| 1:Q:233:SER:HB3 | 1:Q:236:LEU:HG | 1.99 | 0.44 |
| 1:R:369:ILE:HG22 | 1:R:370:VAL:H | 1.81 | 0.44 |
| 1:S:164:PRO:CG | 1:S:174:ALA:CB | 2.95 | 0.44 |
| 1:S:233:SER:HB3 | 1:S:236:LEU:HG | 1.99 | 0.44 |
| 1:S:335:ARG:HA | 1:S:335:ARG:HD3 | 1.39 | 0.44 |
| 1:U:6:THR:O | 1:U:102:PRO:HD2 | 2.17 | 0.44 |
| 1:U:170:ALA:O | 1:U:172:PRO:HD3 | 2.18 | 0.44 |
| 1:V:38:PRO:CG | 1:V:49:GLN:NE2 | 2.79 | 0.44 |
| 1:W:34:ILE:HD13 | 1:W:67:LEU:CD2 | 2.46 | 0.44 |
| 1:A:180:LEU:CD1 | 1:A:181:ALA:N | 2.78 | 0.44 |
| 1:B:170:ALA:O | 1:B:172:PRO:HD3 | 2.18 | 0.44 |
| 1:D:34:ILE:HD13 | 1:D:67:LEU:CD2 | 2.46 | 0.44 |
| 1:D:34:ILE:N | 1:D:54:VAL:HG11 | 2.31 | 0.44 |
| 1:D:148:THR:CG2 | 1:D:149:THR:N | 2.81 | 0.44 |
| 1:D:167:GLU:OE1 | 1:F:61:LYS:CD | 2.65 | 0.44 |
| 1:E:7:ALA:HB1 | 1:E:347:ALA:HB1 | 1.98 | 0.44 |
| 1:E:167:GLU:OE1 | 1:G:61:LYS:CD | 2.65 | 0.44 |
| 1:F:9:VAL:HG21 | 1:F:344:SER:HA | 1.98 | 0.44 |
| 1:F:148:THR:CG2 | 1:F:149:THR:N | 2.81 | 0.44 |
| 1:F:233:SER:HB3 | 1:F:236:LEU:HG | 1.99 | 0.44 |
| 1:F:300:SER:HA | 1:F:335:ARG:NE | 2.32 | 0.44 |
| 1:G:6:THR:O | 1:G:102:PRO:HD2 | 2.17 | 0.44 |
| 1:G:7:ALA:HB1 | 1:G:347:ALA:HB1 | 1.98 | 0.44 |
| 1:H:34:ILE:O | 1:H:54:VAL:HB | 2.18 | 0.44 |
| 1:H:44:MET:CG | 1:H:45:VAL:N | 2.76 | 0.44 |
| 1:I:6:THR:O | 1:I:102:PRO:HD2 | 2.17 | 0.44 |
| 1:I:43:VAL:C | 1:I:44:MET:HG2 | 2.37 | 0.44 |
| 1:J:298:VAL:CG1 | 1:J:335:ARG:NH1 | 2.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:362:TYR:CE1 | 1:J:367:PRO:CB | 2.99 | 0.44 |
| 1:K:7:ALA:HB3 | 1:K:347:ALA:HB1 | 1.99 | 0.44 |
| 1:K:34:ILE:HG22 | 1:K:35:VAL:H | 1.78 | 0.44 |
| 1:K:38:PRO:HD3 | 1:K:49:GLN:HE22 | 1.81 | 0.44 |
| 1:L:147:ARG:HH21 | 1:L:147:ARG:HG3 | 1.80 | 0.44 |
| 1:L:170:ALA:O | 1:L:172:PRO:HD3 | 2.18 | 0.44 |
| 1:M:170:ALA:O | 1:M:172:PRO:HD3 | 2.18 | 0.44 |
| 1:M:324:THR:HG23 | 1:O:241:GLU:OE2 | 2.16 | 0.44 |
| 1:O:180:LEU:O | 1:O:180:LEU:HG | 2.11 | 0.44 |
| 1:P:180:LEU:CD1 | 1:P:181:ALA:N | 2.78 | 0.44 |
| 1:Q:324:THR:HG23 | 1:S:241:GLU:OE2 | 2.17 | 0.44 |
| 1:R:369:ILE:HG23 | 1:R:370:VAL:N | 2.30 | 0.44 |
| 1:S:6:THR:O | 1:S:102:PRO:HD2 | 2.17 | 0.44 |
| 1:S:151:ILE:O | 1:S:297:ASN:HA | 2.18 | 0.44 |
| 1:T:110:LEU:CD1 | 1:T:177:ARG:NH1 | 2.80 | 0.44 |
| 1:V:6:THR:O | 1:V:102:PRO:HD2 | 2.17 | 0.44 |
| 1:V:369:ILE:HG22 | 1:V:370:VAL:H | 1.81 | 0.44 |
| 1:W:35:VAL:H | 1:W:68:LYS:H | 1.65 | 0.44 |
| 1:W:39:ARG:NE | 1:W:66:THR:CA | 2.69 | 0.44 |
| 1:A:7:ALA:HB3 | 1:A:347:ALA:HB1 | 1.99 | 0.44 |
| 1:C:110:LEU:CD1 | 1:C:177:ARG:NH1 | 2.80 | 0.44 |
| 1:C:170:ALA:O | 1:C:172:PRO:HD3 | 2.18 | 0.44 |
| 1:G:324:THR:HG23 | 1:I:241:GLU:OE2 | 2.16 | 0.44 |
| 1:H:7:ALA:HB3 | 1:H:347:ALA:HB1 | 1.99 | 0.44 |
| 1:I:369:ILE:HG23 | 1:I:370:VAL:N | 2.30 | 0.44 |
| 1:K:35:VAL:H | 1:K:68:LYS:H | 1.65 | 0.44 |
| 1:K:151:ILE:O | 1:K:297:ASN:HA | 2.18 | 0.44 |
| 1:M:357:ILE:HD12 | 1:M:357:ILE:HA | 1.79 | 0.44 |
| 1:N:180:LEU:CD1 | 1:N:181:ALA:N | 2.78 | 0.44 |
| 1:O:6:THR:O | 1:O:102:PRO:HD2 | 2.17 | 0.44 |
| 1:P:34:ILE:O | 1:P:54:VAL:HB | 2.18 | 0.44 |
| 1:Q:6:THR:O | 1:Q:102:PRO:HD2 | 2.17 | 0.44 |
| 1:Q:170:ALA:O | 1:Q:172:PRO:HD3 | 2.18 | 0.44 |
| 1:R:116:ARG:NH1 | 1:R:375:PHE:HA | 2.32 | 0.44 |
| 1:S:8:LEU:CB | 1:S:103:THR:HG23 | 2.48 | 0.44 |
| 1:S:34:ILE:O | 1:S:54:VAL:HB | 2.18 | 0.44 |
| 1:T:298:VAL:CG1 | 1:T:335:ARG:NH1 | 2.81 | 0.44 |
| 1:U:35:VAL:H | 1:U:68:LYS:H | 1.65 | 0.44 |
| 1:W:9:VAL:HG21 | 1:W:344:SER:HA | 1.98 | 0.44 |
| 1:W:362:TYR:CE1 | 1:W:367:PRO:CB | 2.99 | 0.44 |
| 1:A:298:VAL:CG1 | 1:A:335:ARG:NH1 | 2.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:369:ILE:HG22 | 1:A:370:VAL:H | 1.81 | 0.44 |
| 1:C:349:LEU:HD23 | 1:C:349:LEU:HA | 1.79 | 0.44 |
| 1:F:7:ALA:HB1 | 1:F:347:ALA:HB1 | 1.98 | 0.44 |
| 1:F:287:ILE:HD12 | 1:H:208:ILE:HD13 | 1.96 | 0.44 |
| 1:G:298:VAL:CG1 | 1:G:335:ARG:NH1 | 2.81 | 0.44 |
| 1:H:227:MET:HA | 1:H:227:MET:HE3 | 1.99 | 0.44 |
| 1:I:44:MET:CG | 1:I:45:VAL:N | 2.76 | 0.44 |
| 1:I:170:ALA:O | 1:I:172:PRO:HD3 | 2.18 | 0.44 |
| 1:L:6:THR:O | 1:L:102:PRO:HD2 | 2.17 | 0.44 |
| 1:L:167:GLU:OE1 | 1:N:61:LYS:CD | 2.65 | 0.44 |
| 1:M:6:THR:O | 1:M:102:PRO:HD2 | 2.17 | 0.44 |
| 1:M:116:ARG:NH1 | 1:M:375:PHE:HA | 2.32 | 0.44 |
| 1:M:233:SER:HB3 | 1:M:236:LEU:HG | 1.99 | 0.44 |
| 1:P:110:LEU:CD1 | 1:P:177:ARG:NH1 | 2.80 | 0.44 |
| 1:Q:8:LEU:CB | 1:Q:103:THR:HG23 | 2.48 | 0.44 |
| 1:Q:35:VAL:H | 1:Q:68:LYS:H | 1.65 | 0.44 |
| 1:R:6:THR:O | 1:R:102:PRO:HD2 | 2.17 | 0.44 |
| 1:R:110:LEU:CD1 | 1:R:177:ARG:NH1 | 2.80 | 0.44 |
| 1:R:133:TYR:CE2 | 1:R:375:PHE:HB2 | 2.51 | 0.44 |
| 1:R:151:ILE:O | 1:R:297:ASN:HA | 2.17 | 0.44 |
| 1:T:233:SER:HB3 | 1:T:236:LEU:HG | 1.99 | 0.44 |
| 1:U:233:SER:HB3 | 1:U:236:LEU:HG | 1.99 | 0.44 |
| 1:U:236:LEU:CD1 | 1:U:237:GLU:CG | 2.94 | 0.44 |
| 1:V:8:LEU:CB | 1:V:103:THR:HG23 | 2.48 | 0.44 |
| 1:A:34:ILE:CG2 | 1:A:67:LEU:CB | 2.96 | 0.44 |
| 1:A:223:PHE:CD1 | 1:A:259:GLU:CG | 2.96 | 0.44 |
| 1:B:236:LEU:HD11 | 1:B:237:GLU:HG2 | 1.96 | 0.44 |
| 1:C:7:ALA:HB3 | 1:C:347:ALA:HB1 | 1.99 | 0.44 |
| 1:E:6:THR:O | 1:E:102:PRO:HD2 | 2.17 | 0.44 |
| 1:F:116:ARG:NH1 | 1:F:375:PHE:HA | 2.32 | 0.44 |
| 1:G:8:LEU:CB | 1:G:103:THR:HG23 | 2.48 | 0.44 |
| 1:G:64:ILE:CG2 | 1:G:65:LEU:N | 2.81 | 0.44 |
| 1:G:148:THR:CG2 | 1:G:149:THR:N | 2.81 | 0.44 |
| 1:H:233:SER:HB3 | 1:H:236:LEU:HG | 1.99 | 0.44 |
| 1:I:151:ILE:O | 1:I:297:ASN:HA | 2.18 | 0.44 |
| 1:K:6:THR:O | 1:K:102:PRO:HD2 | 2.17 | 0.44 |
| 1:L:64:ILE:CG2 | 1:L:65:LEU:N | 2.81 | 0.44 |
| 1:L:298:VAL:CG1 | 1:L:335:ARG:NH1 | 2.81 | 0.44 |
| 1:M:110:LEU:CD1 | 1:M:177:ARG:NH1 | 2.80 | 0.44 |
| 1:M:148:THR:CG2 | 1:M:149:THR:N | 2.81 | 0.44 |
| 1:O:38:PRO:CG | 1:O:49:GLN:NE2 | 2.79 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:73:HIC:HA | 1:O:183:ARG:NH1 | 2.18 | 0.44 |
| 1:O:236:LEU:HD11 | 1:O:237:GLU:HG2 | 1.96 | 0.44 |
| 1:P:7:ALA:HB3 | 1:P:347:ALA:HB1 | 1.99 | 0.44 |
| 1:P:58:ALA:CB | 1:P:65:LEU:CD2 | 2.90 | 0.44 |
| 1:R:34:ILE:HD13 | 1:R:67:LEU:CD2 | 2.46 | 0.44 |
| 1:R:34:ILE:O | 1:R:54:VAL:HB | 2.18 | 0.44 |
| 1:R:170:ALA:O | 1:R:172:PRO:HD3 | 2.18 | 0.44 |
| 1:T:170:ALA:O | 1:T:172:PRO:HD3 | 2.18 | 0.44 |
| 1:V:34:ILE:HD13 | 1:V:67:LEU:CD2 | 2.46 | 0.44 |
| 1:A:64:ILE:CG2 | 1:A:65:LEU:N | 2.81 | 0.43 |
| 1:B:233:SER:HB3 | 1:B:236:LEU:HG | 1.99 | 0.43 |
| 1:C:6:THR:O | 1:C:102:PRO:HD2 | 2.17 | 0.43 |
| 1:C:34:ILE:CG2 | 1:C:67:LEU:CB | 2.96 | 0.43 |
| 1:D:151:ILE:O | 1:D:297:ASN:HA | 2.18 | 0.43 |
| 1:E:8:LEU:CB | 1:E:103:THR:HG23 | 2.48 | 0.43 |
| 1:E:110:LEU:CD1 | 1:E:177:ARG:NH1 | 2.80 | 0.43 |
| 1:E:151:ILE:O | 1:E:297:ASN:HA | 2.18 | 0.43 |
| 1:F:151:ILE:O | 1:F:297:ASN:HA | 2.17 | 0.43 |
| 1:H:151:ILE:O | 1:H:297:ASN:HA | 2.18 | 0.43 |
| 1:I:300:SER:HA | 1:I:335:ARG:NE | 2.32 | 0.43 |
| 1:J:233:SER:HB3 | 1:J:236:LEU:HG | 1.99 | 0.43 |
| 1:K:43:VAL:C | 1:K:44:MET:HG2 | 2.37 | 0.43 |
| 1:N:7:ALA:HB3 | 1:N:347:ALA:HB1 | 1.99 | 0.43 |
| 1:N:151:ILE:O | 1:N:297:ASN:HA | 2.18 | 0.43 |
| 1:N:298:VAL:CG1 | 1:N:335:ARG:NH1 | 2.81 | 0.43 |
| 1:O:110:LEU:CD1 | 1:O:177:ARG:NH1 | 2.80 | 0.43 |
| 1:P:34:ILE:CG2 | 1:P:67:LEU:CB | 2.96 | 0.43 |
| 1:Q:34:ILE:HD13 | 1:Q:67:LEU:CD2 | 2.46 | 0.43 |
| 1:R:34:ILE:CG2 | 1:R:67:LEU:CB | 2.96 | 0.43 |
| 1:T:151:ILE:O | 1:T:297:ASN:HA | 2.17 | 0.43 |
| 1:V:35:VAL:H | 1:V:68:LYS:H | 1.65 | 0.43 |
| 1:W:233:SER:HB3 | 1:W:236:LEU:HG | 1.99 | 0.43 |
| 1:A:34:ILE:HD13 | 1:A:67:LEU:CD2 | 2.46 | 0.43 |
| 1:B:8:LEU:CB | 1:B:103:THR:HG23 | 2.48 | 0.43 |
| 1:B:151:ILE:O | 1:B:297:ASN:HA | 2.18 | 0.43 |
| 1:B:299:MET:O | 1:B:332:PRO:HD2 | 2.18 | 0.43 |
| 1:D:170:ALA:O | 1:D:172:PRO:HD3 | 2.18 | 0.43 |
| 1:F:170:ALA:O | 1:F:172:PRO:HD3 | 2.18 | 0.43 |
| 1:G:170:ALA:O | 1:G:172:PRO:HD3 | 2.18 | 0.43 |
| 1:H:324:THR:HG23 | 1:J:241:GLU:OE2 | 2.17 | 0.43 |
| 1:I:7:ALA:HB3 | 1:I:347:ALA:HB1 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:324:THR:HG23 | 1:L:241:GLU:OE2 | 2.16 | 0.43 |
| 1:J:349:LEU:HD23 | 1:J:349:LEU:HA | 1.80 | 0.43 |
| 1:K:116:ARG:NH1 | 1:K:375:PHE:HA | 2.32 | 0.43 |
| 1:L:69:TYR:CD2 | 1:L:69:TYR:N | 2.87 | 0.43 |
| 1:L:73:HIC:HA | 1:L:183:ARG:NH1 | 2.18 | 0.43 |
| 1:L:151:ILE:O | 1:L:297:ASN:HA | 2.18 | 0.43 |
| 1:L:180:LEU:CD1 | 1:L:181:ALA:N | 2.78 | 0.43 |
| 1:L:362:TYR:CE1 | 1:L:367:PRO:CB | 2.99 | 0.43 |
| 1:M:299:MET:O | 1:M:332:PRO:HD2 | 2.18 | 0.43 |
| 1:N:69:TYR:CD2 | 1:N:69:TYR:N | 2.86 | 0.43 |
| 1:N:227:MET:HE3 | 1:N:227:MET:HA | 2.00 | 0.43 |
| 1:O:233:SER:HB3 | 1:O:236:LEU:HG | 1.99 | 0.43 |
| 1:O:298:VAL:CG1 | 1:O:335:ARG:NH1 | 2.81 | 0.43 |
| 1:P:64:ILE:CG2 | 1:P:65:LEU:N | 2.81 | 0.43 |
| 1:Q:69:TYR:N | 1:Q:69:TYR:CD2 | 2.86 | 0.43 |
| 1:R:64:ILE:CG2 | 1:R:65:LEU:N | 2.81 | 0.43 |
| 1:S:69:TYR:CD2 | 1:S:69:TYR:N | 2.87 | 0.43 |
| 1:S:147:ARG:HH21 | 1:S:147:ARG:HG3 | 1.80 | 0.43 |
| 1:S:170:ALA:O | 1:S:172:PRO:HD3 | 2.18 | 0.43 |
| 1:U:64:ILE:CG2 | 1:U:65:LEU:N | 2.81 | 0.43 |
| 1:U:69:TYR:CD2 | 1:U:69:TYR:N | 2.87 | 0.43 |
| 1:V:233:SER:HB3 | 1:V:236:LEU:HG | 1.99 | 0.43 |
| 1:V:236:LEU:HD11 | 1:V:237:GLU:HG2 | 1.96 | 0.43 |
| 1:W:180:LEU:O | 1:W:180:LEU:HG | 2.11 | 0.43 |
| 1:A:233:SER:HB3 | 1:A:236:LEU:HG | 1.99 | 0.43 |
| 1:E:7:ALA:HB3 | 1:E:347:ALA:HB1 | 1.99 | 0.43 |
| 1:F:324:THR:HG23 | 1:H:241:GLU:OE2 | 2.16 | 0.43 |
| 1:G:147:ARG:HH21 | 1:G:147:ARG:HG3 | 1.80 | 0.43 |
| 1:H:35:VAL:H | 1:H:68:LYS:H | 1.65 | 0.43 |
| 1:H:148:THR:CG2 | 1:H:149:THR:N | 2.81 | 0.43 |
| 1:H:170:ALA:O | 1:H:172:PRO:HD3 | 2.18 | 0.43 |
| 1:H:362:TYR:CE1 | 1:H:367:PRO:CB | 2.99 | 0.43 |
| 1:I:73:HIC:HA | 1:I:183:ARG:NH1 | 2.18 | 0.43 |
| 1:I:133:TYR:CE2 | 1:I:375:PHE:HB2 | 2.51 | 0.43 |
| 1:I:299:MET:HE1 | 1:I:304:THR:HB | 2.01 | 0.43 |
| 1:J:8:LEU:CB | 1:J:103:THR:HG23 | 2.48 | 0.43 |
| 1:J:44:MET:CG | 1:J:45:VAL:N | 2.76 | 0.43 |
| 1:J:69:TYR:CD2 | 1:J:69:TYR:N | 2.86 | 0.43 |
| 1:K:110:LEU:CD1 | 1:K:177:ARG:NH1 | 2.80 | 0.43 |
| 1:K:172:PRO:HA | 1:K:175:ILE:CD1 | 2.49 | 0.43 |
| 1:L:324:THR:HG23 | 1:N:241:GLU:OE2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:6:THR:O | 1:N:102:PRO:HD2 | 2.17 | 0.43 |
| 1:N:34:ILE:CG2 | 1:N:67:LEU:CB | 2.96 | 0.43 |
| 1:N:58:ALA:CB | 1:N:65:LEU:CD2 | 2.90 | 0.43 |
| 1:N:170:ALA:O | 1:N:172:PRO:HD3 | 2.18 | 0.43 |
| 1:O:34:ILE:O | 1:O:54:VAL:HB | 2.18 | 0.43 |
| 1:Q:38:PRO:CG | 1:Q:49:GLN:NE2 | 2.79 | 0.43 |
| 1:Q:298:VAL:CG1 | 1:Q:335:ARG:NH1 | 2.81 | 0.43 |
| 1:R:31:PHE:HA | 1:R:32:PRO:HD3 | 1.65 | 0.43 |
| 1:R:172:PRO:HA | 1:R:175:ILE:CD1 | 2.49 | 0.43 |
| 1:R:298:VAL:CG1 | 1:R:335:ARG:NH1 | 2.81 | 0.43 |
| 1:S:148:THR:CG2 | 1:S:149:THR:N | 2.81 | 0.43 |
| 1:S:149:THR:HG23 | 1:S:150:GLY:N | 2.34 | 0.43 |
| 1:T:8:LEU:CB | 1:T:103:THR:HG23 | 2.48 | 0.43 |
| 1:T:172:PRO:HA | 1:T:175:ILE:CD1 | 2.49 | 0.43 |
| 1:U:8:LEU:CB | 1:U:103:THR:HG23 | 2.48 | 0.43 |
| 1:W:38:PRO:CG | 1:W:49:GLN:NE2 | 2.79 | 0.43 |
| 1:W:64:ILE:CG2 | 1:W:65:LEU:N | 2.81 | 0.43 |
| 1:W:69:TYR:CD2 | 1:W:69:TYR:N | 2.87 | 0.43 |
| 1:B:6:THR:O | 1:B:102:PRO:HD2 | 2.17 | 0.43 |
| 1:B:34:ILE:CG2 | 1:B:67:LEU:CB | 2.96 | 0.43 |
| 1:B:172:PRO:HA | 1:B:175:ILE:CD1 | 2.49 | 0.43 |
| 1:C:8:LEU:CB | 1:C:103:THR:HG23 | 2.48 | 0.43 |
| 1:D:324:THR:HG23 | 1:F:241:GLU:OE2 | 2.16 | 0.43 |
| 1:F:64:ILE:CG2 | 1:F:65:LEU:N | 2.81 | 0.43 |
| 1:F:149:THR:HG23 | 1:F:150:GLY:N | 2.34 | 0.43 |
| 1:F:236:LEU:CD1 | 1:F:237:GLU:CG | 2.94 | 0.43 |
| 1:G:7:ALA:HB3 | 1:G:347:ALA:HB1 | 1.99 | 0.43 |
| 1:H:8:LEU:CB | 1:H:103:THR:HG23 | 2.48 | 0.43 |
| 1:H:149:THR:HG23 | 1:H:150:GLY:N | 2.34 | 0.43 |
| 1:I:39:ARG:NE | 1:I:66:THR:CA | 2.69 | 0.43 |
| 1:I:148:THR:CG2 | 1:I:149:THR:N | 2.81 | 0.43 |
| 1:I:172:PRO:HA | 1:I:175:ILE:CD1 | 2.49 | 0.43 |
| 1:I:299:MET:O | 1:I:332:PRO:HD2 | 2.18 | 0.43 |
| 1:I:374:CYS:HB2 | 1:I:375:PHE:H | 1.61 | 0.43 |
| 1:J:64:ILE:CG2 | 1:J:65:LEU:N | 2.81 | 0.43 |
| 1:L:8:LEU:CB | 1:L:103:THR:HG23 | 2.48 | 0.43 |
| 1:M:236:LEU:HD11 | 1:M:237:GLU:HG2 | 1.96 | 0.43 |
| 1:M:298:VAL:CG1 | 1:M:335:ARG:NH1 | 2.81 | 0.43 |
| 1:N:324:THR:HG23 | 1:P:241:GLU:OE2 | 2.16 | 0.43 |
| 1:O:151:ILE:O | 1:O:297:ASN:HA | 2.18 | 0.43 |
| 1:Q:149:THR:HG23 | 1:Q:150:GLY:N | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:151:ILE:O | 1:Q:297:ASN:HA | 2.18 | 0.43 |
| 1:Q:236:LEU:HD11 | 1:Q:237:GLU:HG2 | 1.97 | 0.43 |
| 1:S:38:PRO:CG | 1:S:49:GLN:NE2 | 2.79 | 0.43 |
| 1:T:34:ILE:CG2 | 1:T:67:LEU:CB | 2.96 | 0.43 |
| 1:U:38:PRO:CG | 1:U:49:GLN:NE2 | 2.79 | 0.43 |
| 1:V:64:ILE:CG2 | 1:V:65:LEU:N | 2.81 | 0.43 |
| 1:V:172:PRO:HA | 1:V:175:ILE:CD1 | 2.49 | 0.43 |
| 1:W:170:ALA:O | 1:W:172:PRO:HD3 | 2.18 | 0.43 |
| 1:W:298:VAL:CG1 | 1:W:335:ARG:NH1 | 2.81 | 0.43 |
| 1:W:357:ILE:HD12 | 1:W:357:ILE:HA | 1.79 | 0.43 |
| 1:B:34:ILE:HG22 | 1:B:35:VAL:H | 1.78 | 0.43 |
| 1:B:299:MET:HE1 | 1:B:309:ILE:HD13 | 2.00 | 0.43 |
| 1:C:136:ILE:O | 1:C:139:VAL:HB | 2.19 | 0.43 |
| 1:D:34:ILE:O | 1:D:54:VAL:HB | 2.18 | 0.43 |
| 1:D:167:GLU:CD | 1:F:61:LYS:CE | 2.85 | 0.43 |
| 1:E:136:ILE:O | 1:E:139:VAL:HB | 2.19 | 0.43 |
| 1:E:374:CYS:HB2 | 1:E:375:PHE:H | 1.62 | 0.43 |
| 1:G:299:MET:O | 1:G:332:PRO:HD2 | 2.18 | 0.43 |
| 1:I:8:LEU:CB | 1:I:103:THR:HG23 | 2.48 | 0.43 |
| 1:I:298:VAL:CG1 | 1:I:335:ARG:NH1 | 2.81 | 0.43 |
| 1:J:7:ALA:HB3 | 1:J:347:ALA:HB1 | 1.99 | 0.43 |
| 1:J:107:GLU:O | 1:J:137:GLN:HG3 | 2.19 | 0.43 |
| 1:J:151:ILE:O | 1:J:297:ASN:HA | 2.18 | 0.43 |
| 1:K:298:VAL:CG1 | 1:K:335:ARG:NH1 | 2.81 | 0.43 |
| 1:M:151:ILE:O | 1:M:297:ASN:HA | 2.18 | 0.43 |
| 1:M:172:PRO:HA | 1:M:175:ILE:CD1 | 2.49 | 0.43 |
| 1:N:148:THR:CG2 | 1:N:149:THR:N | 2.81 | 0.43 |
| 1:P:6:THR:O | 1:P:102:PRO:HD2 | 2.17 | 0.43 |
| 1:R:136:ILE:O | 1:R:139:VAL:HB | 2.19 | 0.43 |
| 1:R:180:LEU:O | 1:R:180:LEU:HG | 2.11 | 0.43 |
| 1:T:369:ILE:HG22 | 1:T:370:VAL:H | 1.81 | 0.43 |
| 1:U:34:ILE:HD13 | 1:U:67:LEU:CD2 | 2.46 | 0.43 |
| 1:V:149:THR:HG23 | 1:V:150:GLY:N | 2.34 | 0.43 |
| 1:W:148:THR:CG2 | 1:W:149:THR:N | 2.81 | 0.43 |
| 1:A:69:TYR:N | 1:A:69:TYR:CD2 | 2.86 | 0.43 |
| 1:A:104:LEU:HD13 | 1:A:347:ALA:HB2 | 2.01 | 0.43 |
| 1:A:167:GLU:CD | 1:C:61:LYS:CE | 2.85 | 0.43 |
| 1:A:172:PRO:HA | 1:A:175:ILE:CD1 | 2.49 | 0.43 |
| 1:A:357:ILE:HD12 | 1:A:357:ILE:HA | 1.78 | 0.43 |
| 1:B:324:THR:HG23 | 1:D:241:GLU:OE2 | 2.16 | 0.43 |
| 1:C:69:TYR:CD2 | 1:C:69:TYR:N | 2.87 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:151:ILE:O | 1:C:297:ASN:HA | 2.18 | 0.43 |
| 1:C:183:ARG:HE | 1:C:183:ARG:HB3 | 1.59 | 0.43 |
| 1:E:64:ILE:CG2 | 1:E:65:LEU:N | 2.81 | 0.43 |
| 1:E:172:PRO:HA | 1:E:175:ILE:CD1 | 2.49 | 0.43 |
| 1:H:69:TYR:CD2 | 1:H:69:TYR:N | 2.86 | 0.43 |
| 1:I:167:GLU:CD | 1:K:61:LYS:CE | 2.85 | 0.43 |
| 1:K:170:ALA:O | 1:K:172:PRO:HD3 | 2.18 | 0.43 |
| 1:K:299:MET:O | 1:K:332:PRO:HD2 | 2.18 | 0.43 |
| 1:L:7:ALA:HB3 | 1:L:347:ALA:HB1 | 1.99 | 0.43 |
| 1:L:35:VAL:H | 1:L:68:LYS:H | 1.65 | 0.43 |
| 1:L:39:ARG:NE | 1:L:66:THR:CA | 2.69 | 0.43 |
| 1:L:148:THR:CG2 | 1:L:149:THR:N | 2.81 | 0.43 |
| 1:L:299:MET:O | 1:L:332:PRO:HD2 | 2.18 | 0.43 |
| 1:M:180:LEU:CD1 | 1:M:181:ALA:N | 2.78 | 0.43 |
| 1:O:31:PHE:HA | 1:O:32:PRO:HD3 | 1.65 | 0.43 |
| 1:O:69:TYR:CD2 | 1:O:69:TYR:N | 2.86 | 0.43 |
| 1:O:149:THR:HG23 | 1:O:150:GLY:N | 2.34 | 0.43 |
| 1:P:104:LEU:HD13 | 1:P:347:ALA:HB2 | 2.01 | 0.43 |
| 1:P:107:GLU:O | 1:P:137:GLN:HG3 | 2.19 | 0.43 |
| 1:P:136:ILE:O | 1:P:139:VAL:HB | 2.19 | 0.43 |
| 1:P:298:VAL:CG1 | 1:P:335:ARG:NH1 | 2.81 | 0.43 |
| 1:P:324:THR:HG23 | 1:R:241:GLU:OE2 | 2.16 | 0.43 |
| 1:Q:110:LEU:CD1 | 1:Q:177:ARG:NH1 | 2.80 | 0.43 |
| 1:Q:299:MET:O | 1:Q:332:PRO:HD2 | 2.18 | 0.43 |
| 1:S:298:VAL:CG1 | 1:S:335:ARG:NH1 | 2.81 | 0.43 |
| 1:T:34:ILE:O | 1:T:54:VAL:HB | 2.18 | 0.43 |
| 1:T:136:ILE:O | 1:T:139:VAL:HB | 2.19 | 0.43 |
| 1:T:149:THR:HG23 | 1:T:150:GLY:N | 2.34 | 0.43 |
| 1:U:298:VAL:CG1 | 1:U:335:ARG:NH1 | 2.81 | 0.43 |
| 1:A:136:ILE:O | 1:A:139:VAL:HB | 2.19 | 0.43 |
| 1:C:34:ILE:O | 1:C:54:VAL:HB | 2.17 | 0.43 |
| 1:C:35:VAL:H | 1:C:68:LYS:H | 1.65 | 0.43 |
| 1:C:172:PRO:HA | 1:C:175:ILE:CD1 | 2.49 | 0.43 |
| 1:D:65:LEU:HD13 | 1:D:67:LEU:HD23 | 2.01 | 0.43 |
| 1:D:149:THR:HG23 | 1:D:150:GLY:N | 2.34 | 0.43 |
| 1:D:172:PRO:HA | 1:D:175:ILE:CD1 | 2.49 | 0.43 |
| 1:E:287:ILE:HD12 | 1:G:208:ILE:HD13 | 1.96 | 0.43 |
| 1:L:44:MET:CG | 1:L:45:VAL:N | 2.76 | 0.43 |
| 1:L:104:LEU:HD13 | 1:L:347:ALA:HB2 | 2.01 | 0.43 |
| 1:N:8:LEU:CB | 1:N:103:THR:HG23 | 2.48 | 0.43 |
| 1:N:104:LEU:HD13 | 1:N:347:ALA:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:65:LEU:HD13 | 1:O:67:LEU:HD23 | 2.01 | 0.43 |
| 1:O:170:ALA:O | 1:O:172:PRO:HD3 | 2.18 | 0.43 |
| 1:O:324:THR:HG23 | 1:Q:241:GLU:OE2 | 2.17 | 0.43 |
| 1:P:35:VAL:H | 1:P:68:LYS:H | 1.65 | 0.43 |
| 1:P:151:ILE:O | 1:P:297:ASN:HA | 2.18 | 0.43 |
| 1:P:170:ALA:O | 1:P:172:PRO:HD3 | 2.18 | 0.43 |
| 1:Q:65:LEU:HD13 | 1:Q:67:LEU:HD23 | 2.01 | 0.43 |
| 1:Q:171:LEU:HA | 1:Q:172:PRO:HD3 | 1.79 | 0.43 |
| 1:S:65:LEU:HD13 | 1:S:67:LEU:HD23 | 2.01 | 0.43 |
| 1:S:227:MET:HA | 1:S:227:MET:HE3 | 2.00 | 0.43 |
| 1:V:149:THR:CG2 | 1:V:150:GLY:N | 2.82 | 0.43 |
| 1:A:35:VAL:H | 1:A:68:LYS:H | 1.65 | 0.43 |
| 1:A:151:ILE:O | 1:A:297:ASN:HA | 2.17 | 0.43 |
| 1:A:374:CYS:HB2 | 1:A:375:PHE:H | 1.61 | 0.43 |
| 1:B:69:TYR:CD2 | 1:B:69:TYR:N | 2.86 | 0.43 |
| 1:C:178:LEU:HG | 1:C:180:LEU:H | 1.84 | 0.43 |
| 1:C:335:ARG:HD3 | 1:C:335:ARG:HA | 1.39 | 0.43 |
| 1:D:8:LEU:CB | 1:D:103:THR:HG23 | 2.48 | 0.43 |
| 1:D:64:ILE:CG2 | 1:D:65:LEU:N | 2.81 | 0.43 |
| 1:E:357:ILE:HD12 | 1:E:357:ILE:HA | 1.79 | 0.43 |
| 1:F:65:LEU:HD13 | 1:F:67:LEU:HD23 | 2.01 | 0.43 |
| 1:G:136:ILE:O | 1:G:139:VAL:HB | 2.19 | 0.43 |
| 1:H:104:LEU:HD13 | 1:H:347:ALA:HB2 | 2.01 | 0.43 |
| 1:I:34:ILE:HD13 | 1:I:67:LEU:CD2 | 2.46 | 0.43 |
| 1:I:64:ILE:CG2 | 1:I:65:LEU:N | 2.81 | 0.43 |
| 1:I:72:GLU:O | 1:I:183:ARG:NH2 | 2.52 | 0.43 |
| 1:J:171:LEU:HA | 1:J:172:PRO:HD3 | 1.79 | 0.43 |
| 1:N:136:ILE:O | 1:N:139:VAL:HB | 2.19 | 0.43 |
| 1:N:299:MET:O | 1:N:332:PRO:HD2 | 2.18 | 0.43 |
| 1:P:69:TYR:CD2 | 1:P:69:TYR:N | 2.87 | 0.43 |
| 1:P:148:THR:CG2 | 1:P:149:THR:N | 2.81 | 0.43 |
| 1:P:287:ILE:HD12 | 1:R:208:ILE:HD13 | 1.96 | 0.43 |
| 1:R:149:THR:HG23 | 1:R:150:GLY:N | 2.34 | 0.43 |
| 1:U:34:ILE:O | 1:U:54:VAL:HB | 2.18 | 0.43 |
| 1:U:44:MET:CG | 1:U:45:VAL:H | 2.18 | 0.43 |
| 1:U:104:LEU:HD13 | 1:U:347:ALA:HB2 | 2.01 | 0.43 |
| 1:U:107:GLU:O | 1:U:137:GLN:HG3 | 2.19 | 0.43 |
| 1:V:299:MET:O | 1:V:332:PRO:HD2 | 2.18 | 0.43 |
| 1:W:104:LEU:HD13 | 1:W:347:ALA:HB2 | 2.01 | 0.43 |
| 1:A:107:GLU:O | 1:A:137:GLN:HG3 | 2.19 | 0.43 |
| 1:B:34:ILE:CG2 | 1:B:67:LEU:HD22 | 2.28 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:65:LEU:HD13 | 1:B:67:LEU:HD23 | 2.01 | 0.43 |
| 1:C:104:LEU:HD13 | 1:C:347:ALA:HB2 | 2.01 | 0.43 |
| 1:D:180:LEU:O | 1:D:180:LEU:HG | 2.11 | 0.43 |
| 1:D:236:LEU:HD11 | 1:D:237:GLU:HG2 | 1.96 | 0.43 |
| 1:E:34:ILE:HD13 | 1:E:67:LEU:CD2 | 2.46 | 0.43 |
| 1:E:69:TYR:CD2 | 1:E:69:TYR:N | 2.87 | 0.43 |
| 1:E:104:LEU:HD13 | 1:E:347:ALA:HB2 | 2.01 | 0.43 |
| 1:G:104:LEU:HD13 | 1:G:347:ALA:HB2 | 2.01 | 0.43 |
| 1:G:172:PRO:HA | 1:G:175:ILE:CD1 | 2.49 | 0.43 |
| 1:H:64:ILE:CG2 | 1:H:65:LEU:N | 2.81 | 0.43 |
| 1:I:34:ILE:O | 1:I:54:VAL:HB | 2.18 | 0.43 |
| 1:I:105:LEU:HD11 | 1:I:123:MET:HG3 | 2.01 | 0.43 |
| 1:I:110:LEU:CD1 | 1:I:177:ARG:NH1 | 2.80 | 0.43 |
| 1:I:136:ILE:O | 1:I:139:VAL:HB | 2.19 | 0.43 |
| 1:J:104:LEU:HD13 | 1:J:347:ALA:HB2 | 2.01 | 0.43 |
| 1:J:148:THR:CG2 | 1:J:149:THR:N | 2.81 | 0.43 |
| 1:J:236:LEU:CD1 | 1:J:237:GLU:CG | 2.93 | 0.43 |
| 1:J:299:MET:O | 1:J:332:PRO:HD2 | 2.18 | 0.43 |
| 1:L:34:ILE:O | 1:L:54:VAL:HB | 2.18 | 0.43 |
| 1:L:167:GLU:CD | 1:N:61:LYS:CE | 2.85 | 0.43 |
| 1:M:2:GLU:HB3 | 1:M:3:ASP:H | 1.66 | 0.43 |
| 1:M:72:GLU:O | 1:M:183:ARG:NH2 | 2.52 | 0.43 |
| 1:M:362:TYR:CE1 | 1:M:367:PRO:CB | 2.99 | 0.43 |
| 1:N:35:VAL:H | 1:N:68:LYS:H | 1.65 | 0.43 |
| 1:N:105:LEU:HD11 | 1:N:123:MET:HG3 | 2.01 | 0.43 |
| 1:N:107:GLU:O | 1:N:137:GLN:HG3 | 2.19 | 0.43 |
| 1:O:64:ILE:CG2 | 1:O:65:LEU:N | 2.81 | 0.43 |
| 1:O:172:PRO:HA | 1:O:175:ILE:CD1 | 2.49 | 0.43 |
| 1:P:149:THR:HG23 | 1:P:150:GLY:N | 2.34 | 0.43 |
| 1:Q:183:ARG:HE | 1:Q:183:ARG:HB3 | 1.58 | 0.43 |
| 1:R:39:ARG:NE | 1:R:66:THR:CA | 2.69 | 0.43 |
| 1:R:104:LEU:HD13 | 1:R:347:ALA:HB2 | 2.01 | 0.43 |
| 1:S:34:ILE:CG2 | 1:S:67:LEU:CB | 2.96 | 0.43 |
| 1:S:35:VAL:H | 1:S:68:LYS:H | 1.65 | 0.43 |
| 1:S:180:LEU:O | 1:S:180:LEU:HG | 2.11 | 0.43 |
| 1:V:105:LEU:HD11 | 1:V:123:MET:HG3 | 2.01 | 0.43 |
| 1:V:107:GLU:O | 1:V:137:GLN:HG3 | 2.19 | 0.43 |
| 1:A:8:LEU:CB | 1:A:103:THR:HG23 | 2.48 | 0.43 |
| 1:B:178:LEU:HG | 1:B:180:LEU:H | 1.84 | 0.43 |
| 1:C:324:THR:HG23 | 1:E:241:GLU:OE2 | 2.16 | 0.43 |
| 1:D:299:MET:O | 1:D:332:PRO:HD2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:35:VAL:H | 1:E:68:LYS:H | 1.65 | 0.43 |
| 1:E:107:GLU:O | 1:E:137:GLN:HG3 | 2.19 | 0.43 |
| 1:F:69:TYR:CD2 | 1:F:69:TYR:N | 2.86 | 0.43 |
| 1:F:104:LEU:HD13 | 1:F:347:ALA:HB2 | 2.01 | 0.43 |
| 1:G:149:THR:CG2 | 1:G:150:GLY:N | 2.82 | 0.43 |
| 1:G:173:HIS:HE1 | 1:H:268:GLY:CA | 2.28 | 0.43 |
| 1:H:106:THR:HG22 | 1:H:140:LEU:HD11 | 2.01 | 0.43 |
| 1:H:299:MET:HE1 | 1:H:304:THR:HB | 2.01 | 0.43 |
| 1:I:104:LEU:HD13 | 1:I:347:ALA:HB2 | 2.01 | 0.43 |
| 1:K:148:THR:CG2 | 1:K:149:THR:N | 2.81 | 0.43 |
| 1:K:236:LEU:HD11 | 1:K:237:GLU:HG2 | 1.96 | 0.43 |
| 1:M:64:ILE:CG2 | 1:M:65:LEU:N | 2.81 | 0.43 |
| 1:M:149:THR:HG23 | 1:M:150:GLY:N | 2.34 | 0.43 |
| 1:Q:178:LEU:HG | 1:Q:180:LEU:H | 1.84 | 0.43 |
| 1:R:35:VAL:H | 1:R:68:LYS:H | 1.65 | 0.43 |
| 1:S:107:GLU:O | 1:S:137:GLN:HG3 | 2.19 | 0.43 |
| 1:T:105:LEU:HD11 | 1:T:123:MET:HG3 | 2.01 | 0.43 |
| 1:T:299:MET:O | 1:T:332:PRO:HD2 | 2.18 | 0.43 |
| 1:V:104:LEU:HD13 | 1:V:347:ALA:HB2 | 2.01 | 0.43 |
| 1:V:136:ILE:O | 1:V:139:VAL:HB | 2.19 | 0.43 |
| 1:A:105:LEU:HD11 | 1:A:123:MET:HG3 | 2.01 | 0.42 |
| 1:B:107:GLU:O | 1:B:137:GLN:HG3 | 2.19 | 0.42 |
| 1:B:148:THR:CG2 | 1:B:149:THR:N | 2.81 | 0.42 |
| 1:B:149:THR:CG2 | 1:B:150:GLY:N | 2.82 | 0.42 |
| 1:B:173:HIS:HE1 | 1:C:268:GLY:CA | 2.28 | 0.42 |
| 1:B:362:TYR:CE1 | 1:B:367:PRO:CB | 2.99 | 0.42 |
| 1:C:105:LEU:HD11 | 1:C:123:MET:HG3 | 2.01 | 0.42 |
| 1:D:110:LEU:CD1 | 1:D:177:ARG:HH11 | 2.32 | 0.42 |
| 1:E:72:GLU:O | 1:E:183:ARG:NH2 | 2.52 | 0.42 |
| 1:E:170:ALA:O | 1:E:172:PRO:HD3 | 2.18 | 0.42 |
| 1:F:106:THR:HG22 | 1:F:140:LEU:HD11 | 2.01 | 0.42 |
| 1:F:172:PRO:HA | 1:F:175:ILE:CD1 | 2.49 | 0.42 |
| 1:G:105:LEU:HD11 | 1:G:123:MET:HG3 | 2.01 | 0.42 |
| 1:H:65:LEU:HD13 | 1:H:67:LEU:HD23 | 2.01 | 0.42 |
| 1:H:180:LEU:O | 1:H:180:LEU:HG | 2.11 | 0.42 |
| 1:K:2:GLU:HB3 | 1:K:3:ASP:H | 1.66 | 0.42 |
| 1:K:8:LEU:CB | 1:K:103:THR:HG23 | 2.48 | 0.42 |
| 1:K:105:LEU:HD11 | 1:K:123:MET:HG3 | 2.01 | 0.42 |
| 1:L:136:ILE:O | 1:L:139:VAL:HB | 2.19 | 0.42 |
| 1:M:73:HIC:HA | 1:M:183:ARG:NH1 | 2.18 | 0.42 |
| 1:N:8:LEU:N | 1:N:102:PRO:O | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:8:LEU:CB | 1:P:103:THR:HG23 | 2.48 | 0.42 |
| 1:P:105:LEU:HD11 | 1:P:123:MET:HG3 | 2.01 | 0.42 |
| 1:R:178:LEU:HG | 1:R:180:LEU:H | 1.84 | 0.42 |
| 1:S:299:MET:O | 1:S:332:PRO:HD2 | 2.18 | 0.42 |
| 1:T:72:GLU:O | 1:T:183:ARG:NH2 | 2.52 | 0.42 |
| 1:T:104:LEU:HD13 | 1:T:347:ALA:HB2 | 2.01 | 0.42 |
| 1:V:180:LEU:HD12 | 1:V:181:ALA:CA | 2.50 | 0.42 |
| 1:B:133:TYR:CE2 | 1:B:375:PHE:HB2 | 2.51 | 0.42 |
| 1:B:167:GLU:OE1 | 1:D:61:LYS:HE2 | 2.20 | 0.42 |
| 1:B:287:ILE:HD12 | 1:D:208:ILE:HD13 | 1.96 | 0.42 |
| 1:B:357:ILE:HD12 | 1:B:357:ILE:HA | 1.79 | 0.42 |
| 1:C:167:GLU:OE1 | 1:E:61:LYS:HE2 | 2.19 | 0.42 |
| 1:C:357:ILE:HD12 | 1:C:357:ILE:HA | 1.79 | 0.42 |
| 1:D:107:GLU:O | 1:D:137:GLN:HG3 | 2.19 | 0.42 |
| 1:E:167:GLU:OE1 | 1:G:61:LYS:HE2 | 2.20 | 0.42 |
| 1:E:178:LEU:HG | 1:E:180:LEU:H | 1.84 | 0.42 |
| 1:F:136:ILE:O | 1:F:139:VAL:HB | 2.19 | 0.42 |
| 1:F:299:MET:O | 1:F:332:PRO:HD2 | 2.18 | 0.42 |
| 1:G:34:ILE:CG2 | 1:G:67:LEU:CB | 2.96 | 0.42 |
| 1:G:35:VAL:H | 1:G:68:LYS:H | 1.65 | 0.42 |
| 1:G:69:TYR:N | 1:G:69:TYR:CD2 | 2.87 | 0.42 |
| 1:G:167:GLU:OE1 | 1:I:61:LYS:HE2 | 2.20 | 0.42 |
| 1:H:107:GLU:O | 1:H:137:GLN:HG3 | 2.19 | 0.42 |
| 1:H:136:ILE:O | 1:H:139:VAL:HB | 2.19 | 0.42 |
| 1:H:172:PRO:HA | 1:H:175:ILE:CD1 | 2.49 | 0.42 |
| 1:I:2:GLU:HB3 | 1:I:3:ASP:H | 1.66 | 0.42 |
| 1:I:167:GLU:OE1 | 1:K:64:ILE:HD13 | 2.19 | 0.42 |
| 1:J:135:ALA:CB | 1:J:140:LEU:HD21 | 2.49 | 0.42 |
| 1:J:167:GLU:OE1 | 1:L:64:ILE:HD13 | 2.19 | 0.42 |
| 1:J:172:PRO:HA | 1:J:175:ILE:CD1 | 2.49 | 0.42 |
| 1:K:72:GLU:O | 1:K:183:ARG:NH2 | 2.52 | 0.42 |
| 1:L:34:ILE:HG23 | 1:L:67:LEU:HB3 | 2.02 | 0.42 |
| 1:L:167:GLU:OE1 | 1:N:64:ILE:HD13 | 2.19 | 0.42 |
| 1:L:172:PRO:HA | 1:L:175:ILE:CD1 | 2.49 | 0.42 |
| 1:M:105:LEU:HD11 | 1:M:123:MET:HG3 | 2.01 | 0.42 |
| 1:N:172:PRO:HA | 1:N:175:ILE:CD1 | 2.49 | 0.42 |
| 1:O:136:ILE:O | 1:O:139:VAL:HB | 2.19 | 0.42 |
| 1:O:299:MET:O | 1:O:332:PRO:HD2 | 2.18 | 0.42 |
| 1:O:349:LEU:HD23 | 1:O:349:LEU:HA | 1.80 | 0.42 |
| 1:P:106:THR:HG22 | 1:P:140:LEU:HD11 | 2.01 | 0.42 |
| 1:P:172:PRO:HA | 1:P:175:ILE:CD1 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:299:MET:O | 1:P:332:PRO:HD2 | 2.18 | 0.42 |
| 1:Q:149:THR:CG2 | 1:Q:150:GLY:N | 2.82 | 0.42 |
| 1:Q:362:TYR:CE1 | 1:Q:367:PRO:CB | 2.99 | 0.42 |
| 1:R:72:GLU:O | 1:R:183:ARG:NH2 | 2.52 | 0.42 |
| 1:S:64:ILE:CG2 | 1:S:65:LEU:N | 2.81 | 0.42 |
| 1:S:104:LEU:HD13 | 1:S:347:ALA:HB2 | 2.01 | 0.42 |
| 1:S:106:THR:HG22 | 1:S:140:LEU:HD11 | 2.01 | 0.42 |
| 1:S:110:LEU:CD1 | 1:S:177:ARG:NH1 | 2.80 | 0.42 |
| 1:T:35:VAL:H | 1:T:68:LYS:H | 1.65 | 0.42 |
| 1:T:64:ILE:CG2 | 1:T:65:LEU:N | 2.81 | 0.42 |
| 1:T:180:LEU:HD12 | 1:T:181:ALA:CA | 2.50 | 0.42 |
| 1:U:65:LEU:HD13 | 1:U:67:LEU:HD23 | 2.01 | 0.42 |
| 1:U:149:THR:HG23 | 1:U:150:GLY:N | 2.34 | 0.42 |
| 1:U:180:LEU:HD12 | 1:U:181:ALA:CA | 2.49 | 0.42 |
| 1:U:299:MET:HE1 | 1:U:304:THR:HB | 2.01 | 0.42 |
| 1:U:299:MET:O | 1:U:332:PRO:HD2 | 2.18 | 0.42 |
| 1:V:2:GLU:HB3 | 1:V:3:ASP:H | 1.66 | 0.42 |
| 1:V:170:ALA:O | 1:V:172:PRO:HD3 | 2.18 | 0.42 |
| 1:W:8:LEU:CB | 1:W:103:THR:HG23 | 2.48 | 0.42 |
| 1:W:34:ILE:CG2 | 1:W:67:LEU:CB | 2.96 | 0.42 |
| 1:A:299:MET:O | 1:A:332:PRO:HD2 | 2.18 | 0.42 |
| 1:B:72:GLU:O | 1:B:183:ARG:NH2 | 2.52 | 0.42 |
| 1:B:105:LEU:HD11 | 1:B:123:MET:HG3 | 2.01 | 0.42 |
| 1:B:121:GLN:HG3 | 1:B:362:TYR:OH | 2.20 | 0.42 |
| 1:B:374:CYS:HB2 | 1:B:375:PHE:H | 1.61 | 0.42 |
| 1:D:69:TYR:CD2 | 1:D:69:TYR:N | 2.87 | 0.42 |
| 1:D:167:GLU:OE1 | 1:F:61:LYS:HE2 | 2.20 | 0.42 |
| 1:E:299:MET:O | 1:E:332:PRO:HD2 | 2.18 | 0.42 |
| 1:G:121:GLN:HG3 | 1:G:362:TYR:OH | 2.20 | 0.42 |
| 1:G:149:THR:HG23 | 1:G:150:GLY:N | 2.34 | 0.42 |
| 1:H:34:ILE:HD13 | 1:H:67:LEU:CD2 | 2.46 | 0.42 |
| 1:I:34:ILE:CG2 | 1:I:67:LEU:CB | 2.96 | 0.42 |
| 1:J:35:VAL:H | 1:J:68:LYS:H | 1.65 | 0.42 |
| 1:J:105:LEU:HD11 | 1:J:123:MET:HG3 | 2.01 | 0.42 |
| 1:K:149:THR:CG2 | 1:K:150:GLY:N | 2.82 | 0.42 |
| 1:K:149:THR:HG23 | 1:K:150:GLY:N | 2.34 | 0.42 |
| 1:L:34:ILE:CG2 | 1:L:67:LEU:CB | 2.96 | 0.42 |
| 1:L:105:LEU:HD11 | 1:L:123:MET:HG3 | 2.01 | 0.42 |
| 1:L:135:ALA:CB | 1:L:140:LEU:HD21 | 2.49 | 0.42 |
| 1:M:65:LEU:HD13 | 1:M:67:LEU:HD23 | 2.01 | 0.42 |
| 1:M:167:GLU:OE1 | 1:O:64:ILE:HD13 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:73:HIC:HA | 1:N:183:ARG:NH1 | 2.18 | 0.42 |
| 1:N:149:THR:HG23 | 1:N:150:GLY:N | 2.34 | 0.42 |
| 1:O:178:LEU:HG | 1:O:180:LEU:H | 1.84 | 0.42 |
| 1:P:299:MET:HE1 | 1:P:309:ILE:HD13 | 2.00 | 0.42 |
| 1:Q:64:ILE:CG2 | 1:Q:65:LEU:N | 2.81 | 0.42 |
| 1:Q:173:HIS:HE1 | 1:R:268:GLY:CA | 2.28 | 0.42 |
| 1:R:148:THR:CG2 | 1:R:149:THR:N | 2.81 | 0.42 |
| 1:R:180:LEU:HD12 | 1:R:181:ALA:CA | 2.49 | 0.42 |
| 1:S:34:ILE:HG23 | 1:S:67:LEU:HB3 | 2.02 | 0.42 |
| 1:S:136:ILE:O | 1:S:139:VAL:HB | 2.19 | 0.42 |
| 1:S:167:GLU:CD | 1:U:61:LYS:CE | 2.85 | 0.42 |
| 1:S:362:TYR:CE1 | 1:S:367:PRO:CB | 2.99 | 0.42 |
| 1:T:107:GLU:O | 1:T:137:GLN:HG3 | 2.19 | 0.42 |
| 1:T:133:TYR:CE2 | 1:T:375:PHE:HB2 | 2.51 | 0.42 |
| 1:U:34:ILE:HG23 | 1:U:67:LEU:HB3 | 2.02 | 0.42 |
| 1:U:72:GLU:O | 1:U:183:ARG:NH2 | 2.52 | 0.42 |
| 1:U:110:LEU:CD1 | 1:U:177:ARG:HH11 | 2.32 | 0.42 |
| 1:U:136:ILE:O | 1:U:139:VAL:HB | 2.19 | 0.42 |
| 1:U:167:GLU:OE1 | 1:W:64:ILE:HD13 | 2.19 | 0.42 |
| 1:V:69:TYR:CD2 | 1:V:69:TYR:N | 2.86 | 0.42 |
| 1:V:72:GLU:O | 1:V:183:ARG:NH2 | 2.52 | 0.42 |
| 1:W:49:GLN:HG3 | 1:W:50:LYS:N | 2.21 | 0.42 |
| 1:W:105:LEU:HD11 | 1:W:123:MET:HG3 | 2.01 | 0.42 |
| 1:W:107:GLU:O | 1:W:137:GLN:HG3 | 2.19 | 0.42 |
| 1:W:180:LEU:HD12 | 1:W:181:ALA:CA | 2.50 | 0.42 |
| 1:W:299:MET:O | 1:W:332:PRO:HD2 | 2.18 | 0.42 |
| 1:A:180:LEU:HD12 | 1:A:181:ALA:CA | 2.50 | 0.42 |
| 1:B:136:ILE:O | 1:B:139:VAL:HB | 2.19 | 0.42 |
| 1:B:149:THR:HG23 | 1:B:150:GLY:N | 2.34 | 0.42 |
| 1:B:180:LEU:CD1 | 1:B:181:ALA:N | 2.78 | 0.42 |
| 1:C:72:GLU:O | 1:C:183:ARG:NH2 | 2.52 | 0.42 |
| 1:D:121:GLN:HG3 | 1:D:362:TYR:OH | 2.20 | 0.42 |
| 1:E:105:LEU:HD11 | 1:E:123:MET:HG3 | 2.01 | 0.42 |
| 1:F:121:GLN:HG3 | 1:F:362:TYR:OH | 2.20 | 0.42 |
| 1:F:167:GLU:OE1 | 1:H:61:LYS:HE2 | 2.20 | 0.42 |
| 1:G:65:LEU:HD13 | 1:G:67:LEU:HD23 | 2.01 | 0.42 |
| 1:G:110:LEU:CD1 | 1:G:177:ARG:NH1 | 2.80 | 0.42 |
| 1:H:105:LEU:HD11 | 1:H:123:MET:HG3 | 2.01 | 0.42 |
| 1:I:69:TYR:N | 1:I:69:TYR:CD2 | 2.86 | 0.42 |
| 1:I:121:GLN:HG3 | 1:I:362:TYR:OH | 2.20 | 0.42 |
| 1:I:149:THR:HG23 | 1:I:150:GLY:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:178:LEU:HG | 1:I:180:LEU:H | 1.84 | 0.42 |
| 1:J:34:ILE:HG23 | 1:J:67:LEU:HB3 | 2.02 | 0.42 |
| 1:J:72:GLU:O | 1:J:183:ARG:NH2 | 2.52 | 0.42 |
| 1:J:180:LEU:CD1 | 1:J:181:ALA:N | 2.78 | 0.42 |
| 1:M:335:ARG:HA | 1:M:335:ARG:HD3 | 1.39 | 0.42 |
| 1:N:300:SER:HA | 1:N:335:ARG:CD | 2.50 | 0.42 |
| 1:O:34:ILE:HG23 | 1:O:67:LEU:HB3 | 2.01 | 0.42 |
| 1:O:105:LEU:HD11 | 1:O:123:MET:HG3 | 2.01 | 0.42 |
| 1:O:362:TYR:CE1 | 1:O:367:PRO:CB | 2.99 | 0.42 |
| 1:Q:34:ILE:HG23 | 1:Q:67:LEU:HB3 | 2.02 | 0.42 |
| 1:Q:106:THR:HG22 | 1:Q:140:LEU:HD11 | 2.01 | 0.42 |
| 1:R:69:TYR:CD2 | 1:R:69:TYR:N | 2.87 | 0.42 |
| 1:R:105:LEU:HD11 | 1:R:123:MET:HG3 | 2.01 | 0.42 |
| 1:R:106:THR:HG22 | 1:R:140:LEU:HD11 | 2.01 | 0.42 |
| 1:S:180:LEU:HD12 | 1:S:181:ALA:CA | 2.49 | 0.42 |
| 1:S:236:LEU:HD11 | 1:S:237:GLU:HG2 | 1.96 | 0.42 |
| 1:T:178:LEU:HG | 1:T:180:LEU:H | 1.84 | 0.42 |
| 1:U:105:LEU:HD11 | 1:U:123:MET:HG3 | 2.01 | 0.42 |
| 1:U:106:THR:HG22 | 1:U:140:LEU:HD11 | 2.01 | 0.42 |
| 1:U:178:LEU:HG | 1:U:180:LEU:H | 1.84 | 0.42 |
| 1:U:357:ILE:HD12 | 1:U:357:ILE:HA | 1.79 | 0.42 |
| 1:A:167:GLU:OE1 | 1:C:61:LYS:HE2 | 2.20 | 0.42 |
| 1:B:8:LEU:N | 1:B:102:PRO:O | 2.48 | 0.42 |
| 1:C:34:ILE:HG23 | 1:C:67:LEU:HB3 | 2.01 | 0.42 |
| 1:C:149:THR:CG2 | 1:C:150:GLY:N | 2.82 | 0.42 |
| 1:C:180:LEU:HD12 | 1:C:181:ALA:CA | 2.50 | 0.42 |
| 1:D:34:ILE:CG2 | 1:D:67:LEU:CB | 2.96 | 0.42 |
| 1:D:104:LEU:HD13 | 1:D:347:ALA:HB2 | 2.01 | 0.42 |
| 1:E:121:GLN:HG3 | 1:E:362:TYR:OH | 2.20 | 0.42 |
| 1:F:72:GLU:O | 1:F:183:ARG:NH2 | 2.52 | 0.42 |
| 1:F:362:TYR:CE1 | 1:F:367:PRO:CB | 2.99 | 0.42 |
| 1:G:2:GLU:HB3 | 1:G:3:ASP:H | 1.66 | 0.42 |
| 1:G:167:GLU:OE1 | 1:I:64:ILE:HD13 | 2.19 | 0.42 |
| 1:H:110:LEU:CD1 | 1:H:177:ARG:HH11 | 2.32 | 0.42 |
| 1:H:135:ALA:CB | 1:H:140:LEU:HD21 | 2.49 | 0.42 |
| 1:J:106:THR:HG22 | 1:J:140:LEU:HD11 | 2.01 | 0.42 |
| 1:J:178:LEU:HG | 1:J:180:LEU:H | 1.84 | 0.42 |
| 1:K:64:ILE:CG2 | 1:K:65:LEU:N | 2.81 | 0.42 |
| 1:K:121:GLN:HG3 | 1:K:362:TYR:OH | 2.20 | 0.42 |
| 1:K:136:ILE:O | 1:K:139:VAL:HB | 2.19 | 0.42 |
| 1:K:178:LEU:HG | 1:K:180:LEU:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:107:GLU:O | 1:L:137:GLN:HG3 | 2.19 | 0.42 |
| 1:M:34:ILE:HD13 | 1:M:67:LEU:CD2 | 2.46 | 0.42 |
| 1:M:136:ILE:O | 1:M:139:VAL:HB | 2.19 | 0.42 |
| 1:N:178:LEU:HG | 1:N:180:LEU:H | 1.84 | 0.42 |
| 1:O:110:LEU:CD1 | 1:O:177:ARG:HH11 | 2.32 | 0.42 |
| 1:O:121:GLN:HG3 | 1:O:362:TYR:OH | 2.20 | 0.42 |
| 1:P:180:LEU:HD12 | 1:P:181:ALA:CA | 2.50 | 0.42 |
| 1:P:300:SER:HA | 1:P:335:ARG:CD | 2.50 | 0.42 |
| 1:Q:172:PRO:HA | 1:Q:175:ILE:CD1 | 2.49 | 0.42 |
| 1:R:121:GLN:HG3 | 1:R:362:TYR:OH | 2.20 | 0.42 |
| 1:S:105:LEU:HD11 | 1:S:123:MET:HG3 | 2.01 | 0.42 |
| 1:S:135:ALA:CB | 1:S:140:LEU:HD21 | 2.49 | 0.42 |
| 1:S:357:ILE:CG2 | 1:S:358:THR:N | 2.83 | 0.42 |
| 1:W:34:ILE:HG23 | 1:W:67:LEU:HB3 | 2.02 | 0.42 |
| 1:W:65:LEU:HD13 | 1:W:67:LEU:HD23 | 2.01 | 0.42 |
| 1:W:172:PRO:HA | 1:W:175:ILE:CD1 | 2.49 | 0.42 |
| 1:A:65:LEU:HD13 | 1:A:67:LEU:HD23 | 2.01 | 0.42 |
| 1:B:167:GLU:OE1 | 1:D:64:ILE:HD13 | 2.19 | 0.42 |
| 1:C:149:THR:HG23 | 1:C:150:GLY:N | 2.34 | 0.42 |
| 1:D:106:THR:HG22 | 1:D:140:LEU:HD11 | 2.01 | 0.42 |
| 1:E:149:THR:HG23 | 1:E:150:GLY:N | 2.34 | 0.42 |
| 1:E:180:LEU:HD12 | 1:E:181:ALA:CA | 2.50 | 0.42 |
| 1:F:8:LEU:CB | 1:F:103:THR:HG23 | 2.48 | 0.42 |
| 1:F:167:GLU:OE1 | 1:H:64:ILE:HD13 | 2.19 | 0.42 |
| 1:F:178:LEU:HG | 1:F:180:LEU:H | 1.84 | 0.42 |
| 1:G:72:GLU:O | 1:G:183:ARG:NH2 | 2.52 | 0.42 |
| 1:H:178:LEU:HG | 1:H:180:LEU:H | 1.84 | 0.42 |
| 1:I:35:VAL:H | 1:I:68:LYS:H | 1.65 | 0.42 |
| 1:I:167:GLU:OE1 | 1:K:61:LYS:HE2 | 2.20 | 0.42 |
| 1:J:65:LEU:HD13 | 1:J:67:LEU:HD23 | 2.01 | 0.42 |
| 1:J:110:LEU:CD1 | 1:J:177:ARG:HH11 | 2.32 | 0.42 |
| 1:J:136:ILE:O | 1:J:139:VAL:HB | 2.19 | 0.42 |
| 1:K:44:MET:CG | 1:K:45:VAL:N | 2.76 | 0.42 |
| 1:K:69:TYR:CD2 | 1:K:69:TYR:N | 2.86 | 0.42 |
| 1:K:104:LEU:HD13 | 1:K:347:ALA:HB2 | 2.01 | 0.42 |
| 1:M:31:PHE:HA | 1:M:32:PRO:HD3 | 1.65 | 0.42 |
| 1:N:34:ILE:HG23 | 1:N:67:LEU:HB3 | 2.02 | 0.42 |
| 1:N:64:ILE:CG2 | 1:N:65:LEU:N | 2.81 | 0.42 |
| 1:N:72:GLU:O | 1:N:183:ARG:NH2 | 2.52 | 0.42 |
| 1:N:106:THR:HG22 | 1:N:140:LEU:HD11 | 2.01 | 0.42 |
| 1:N:135:ALA:CB | 1:N:140:LEU:HD21 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:167:GLU:OE1 | 1:P:64:ILE:HD13 | 2.19 | 0.42 |
| 1:N:180:LEU:HD12 | 1:N:181:ALA:CA | 2.50 | 0.42 |
| 1:N:374:CYS:HB2 | 1:N:375:PHE:H | 1.61 | 0.42 |
| 1:O:104:LEU:HD13 | 1:O:347:ALA:HB2 | 2.01 | 0.42 |
| 1:O:167:GLU:CD | 1:Q:61:LYS:CE | 2.85 | 0.42 |
| 1:P:72:GLU:O | 1:P:183:ARG:NH2 | 2.52 | 0.42 |
| 1:Q:72:GLU:O | 1:Q:183:ARG:NH2 | 2.52 | 0.42 |
| 1:Q:105:LEU:HD11 | 1:Q:123:MET:HG3 | 2.01 | 0.42 |
| 1:Q:110:LEU:CD1 | 1:Q:177:ARG:HH11 | 2.32 | 0.42 |
| 1:R:299:MET:O | 1:R:332:PRO:HD2 | 2.18 | 0.42 |
| 1:S:172:PRO:HA | 1:S:175:ILE:CD1 | 2.49 | 0.42 |
| 1:S:178:LEU:HG | 1:S:180:LEU:H | 1.84 | 0.42 |
| 1:T:65:LEU:HD13 | 1:T:67:LEU:HD23 | 2.01 | 0.42 |
| 1:T:121:GLN:HG3 | 1:T:362:TYR:OH | 2.20 | 0.42 |
| 1:U:172:PRO:HA | 1:U:175:ILE:CD1 | 2.49 | 0.42 |
| 1:U:362:TYR:CE1 | 1:U:367:PRO:CB | 2.99 | 0.42 |
| 1:V:34:ILE:HG23 | 1:V:67:LEU:HB3 | 2.01 | 0.42 |
| 1:W:178:LEU:HG | 1:W:180:LEU:H | 1.84 | 0.42 |
| 1:A:324:THR:HG23 | 1:C:241:GLU:OE2 | 2.16 | 0.42 |
| 1:B:104:LEU:HD13 | 1:B:347:ALA:HB2 | 2.01 | 0.42 |
| 1:B:180:LEU:HD12 | 1:B:181:ALA:CA | 2.50 | 0.42 |
| 1:D:105:LEU:HD11 | 1:D:123:MET:HG3 | 2.01 | 0.42 |
| 1:D:178:LEU:HG | 1:D:180:LEU:H | 1.84 | 0.42 |
| 1:D:357:ILE:CG2 | 1:D:358:THR:N | 2.83 | 0.42 |
| 1:E:34:ILE:CG2 | 1:E:67:LEU:CB | 2.96 | 0.42 |
| 1:E:34:ILE:HG23 | 1:E:67:LEU:HB3 | 2.02 | 0.42 |
| 1:E:167:GLU:OE1 | 1:G:64:ILE:HD13 | 2.19 | 0.42 |
| 1:F:105:LEU:HD11 | 1:F:123:MET:HG3 | 2.01 | 0.42 |
| 1:F:107:GLU:O | 1:F:137:GLN:HG3 | 2.19 | 0.42 |
| 1:H:121:GLN:HG3 | 1:H:362:TYR:OH | 2.20 | 0.42 |
| 1:H:167:GLU:OE1 | 1:J:61:LYS:HE2 | 2.20 | 0.42 |
| 1:K:34:ILE:CG2 | 1:K:67:LEU:CB | 2.96 | 0.42 |
| 1:L:149:THR:HG23 | 1:L:150:GLY:N | 2.34 | 0.42 |
| 1:L:178:LEU:HG | 1:L:180:LEU:H | 1.84 | 0.42 |
| 1:L:180:LEU:HD12 | 1:L:181:ALA:CA | 2.49 | 0.42 |
| 1:M:121:GLN:HG3 | 1:M:362:TYR:OH | 2.20 | 0.42 |
| 1:M:173:HIS:HE1 | 1:N:268:GLY:CA | 2.28 | 0.42 |
| 1:M:357:ILE:CG2 | 1:M:358:THR:N | 2.83 | 0.42 |
| 1:N:65:LEU:HD13 | 1:N:67:LEU:HD23 | 2.01 | 0.42 |
| 1:N:335:ARG:HA | 1:N:335:ARG:HD3 | 1.39 | 0.42 |
| 1:P:121:GLN:HG3 | 1:P:362:TYR:OH | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:104:LEU:HD13 | 1:Q:347:ALA:HB2 | 2.01 | 0.42 |
| 1:Q:121:GLN:HG3 | 1:Q:362:TYR:OH | 2.20 | 0.42 |
| 1:Q:180:LEU:HD12 | 1:Q:181:ALA:CA | 2.50 | 0.42 |
| 1:R:8:LEU:CB | 1:R:103:THR:HG23 | 2.48 | 0.42 |
| 1:R:300:SER:HA | 1:R:335:ARG:CD | 2.49 | 0.42 |
| 1:S:110:LEU:CD1 | 1:S:177:ARG:HH11 | 2.32 | 0.42 |
| 1:S:167:GLU:OE1 | 1:U:64:ILE:HD13 | 2.19 | 0.42 |
| 1:T:148:THR:CG2 | 1:T:149:THR:N | 2.81 | 0.42 |
| 1:T:167:GLU:OE1 | 1:V:64:ILE:HD13 | 2.19 | 0.42 |
| 1:U:167:GLU:OE1 | 1:W:61:LYS:HE2 | 2.20 | 0.42 |
| 1:V:374:CYS:HB2 | 1:V:375:PHE:H | 1.61 | 0.42 |
| 1:W:136:ILE:O | 1:W:139:VAL:HB | 2.19 | 0.42 |
| 1:A:72:GLU:O | 1:A:183:ARG:NH2 | 2.52 | 0.42 |
| 1:B:64:ILE:CG2 | 1:B:65:LEU:N | 2.81 | 0.42 |
| 1:C:106:THR:HG22 | 1:C:140:LEU:HD11 | 2.01 | 0.42 |
| 1:C:107:GLU:O | 1:C:137:GLN:HG3 | 2.19 | 0.42 |
| 1:C:299:MET:O | 1:C:332:PRO:HD2 | 2.18 | 0.42 |
| 1:D:362:TYR:CE1 | 1:D:367:PRO:CB | 2.99 | 0.42 |
| 1:E:65:LEU:HD13 | 1:E:67:LEU:HD23 | 2.01 | 0.42 |
| 1:E:106:THR:HG22 | 1:E:140:LEU:HD11 | 2.01 | 0.42 |
| 1:F:110:LEU:CD1 | 1:F:177:ARG:HH11 | 2.32 | 0.42 |
| 1:G:73:HIC:HA | 1:G:183:ARG:NH1 | 2.18 | 0.42 |
| 1:G:107:GLU:O | 1:G:137:GLN:HG3 | 2.19 | 0.42 |
| 1:G:180:LEU:HD12 | 1:G:181:ALA:CA | 2.50 | 0.42 |
| 1:I:349:LEU:HD23 | 1:I:349:LEU:HA | 1.80 | 0.42 |
| 1:J:35:VAL:C | 1:J:54:VAL:CG2 | 2.88 | 0.42 |
| 1:K:133:TYR:CE2 | 1:K:375:PHE:HB2 | 2.51 | 0.42 |
| 1:K:167:GLU:OE1 | 1:M:64:ILE:HD13 | 2.19 | 0.42 |
| 1:L:35:VAL:C | 1:L:54:VAL:CG2 | 2.88 | 0.42 |
| 1:L:227:MET:HA | 1:L:227:MET:HE3 | 2.01 | 0.42 |
| 1:M:34:ILE:HG23 | 1:M:67:LEU:HB3 | 2.02 | 0.42 |
| 1:M:104:LEU:HD13 | 1:M:347:ALA:HB2 | 2.01 | 0.42 |
| 1:O:35:VAL:C | 1:O:54:VAL:CG2 | 2.88 | 0.42 |
| 1:O:167:GLU:OE1 | 1:Q:64:ILE:HD13 | 2.19 | 0.42 |
| 1:O:171:LEU:HA | 1:O:172:PRO:HD3 | 1.79 | 0.42 |
| 1:P:65:LEU:HD13 | 1:P:67:LEU:HD23 | 2.01 | 0.42 |
| 1:Q:35:VAL:C | 1:Q:54:VAL:CG2 | 2.88 | 0.42 |
| 1:Q:135:ALA:CB | 1:Q:140:LEU:HD21 | 2.49 | 0.42 |
| 1:R:35:VAL:C | 1:R:54:VAL:CG2 | 2.88 | 0.42 |
| 1:S:35:VAL:C | 1:S:54:VAL:CG2 | 2.88 | 0.42 |
| 1:T:35:VAL:C | 1:T:54:VAL:CG2 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:135:ALA:CB | 1:U:140:LEU:HD21 | 2.49 | 0.42 |
| 1:U:148:THR:CG2 | 1:U:149:THR:N | 2.81 | 0.42 |
| 1:V:121:GLN:HG3 | 1:V:362:TYR:OH | 2.20 | 0.42 |
| 1:W:149:THR:HG23 | 1:W:150:GLY:N | 2.34 | 0.42 |
| 1:A:178:LEU:HG | 1:A:180:LEU:H | 1.84 | 0.42 |
| 1:C:103:THR:O | 1:C:132:MET:HA | 2.20 | 0.42 |
| 1:C:180:LEU:O | 1:C:180:LEU:HG | 2.11 | 0.42 |
| 1:D:136:ILE:O | 1:D:139:VAL:HB | 2.19 | 0.42 |
| 1:E:140:LEU:HB3 | 1:E:343:GLY:N | 2.35 | 0.42 |
| 1:F:44:MET:CG | 1:F:45:VAL:H | 2.18 | 0.42 |
| 1:G:34:ILE:HG23 | 1:G:67:LEU:HB3 | 2.02 | 0.42 |
| 1:G:236:LEU:CD1 | 1:G:237:GLU:CG | 2.93 | 0.42 |
| 1:H:34:ILE:HG23 | 1:H:67:LEU:HB3 | 2.02 | 0.42 |
| 1:H:167:GLU:OE1 | 1:J:64:ILE:HD13 | 2.19 | 0.42 |
| 1:I:135:ALA:CB | 1:I:140:LEU:HD21 | 2.49 | 0.42 |
| 1:I:236:LEU:HD11 | 1:I:237:GLU:HG2 | 1.96 | 0.42 |
| 1:K:65:LEU:HD13 | 1:K:67:LEU:HD23 | 2.01 | 0.42 |
| 1:L:103:THR:O | 1:L:132:MET:HA | 2.20 | 0.42 |
| 1:N:35:VAL:C | 1:N:54:VAL:CG2 | 2.88 | 0.42 |
| 1:O:72:GLU:O | 1:O:183:ARG:NH2 | 2.52 | 0.42 |
| 1:O:106:THR:HG22 | 1:O:140:LEU:HD11 | 2.01 | 0.42 |
| 1:O:107:GLU:O | 1:O:137:GLN:HG3 | 2.19 | 0.42 |
| 1:O:180:LEU:HD12 | 1:O:181:ALA:CA | 2.49 | 0.42 |
| 1:Q:107:GLU:O | 1:Q:137:GLN:HG3 | 2.19 | 0.42 |
| 1:Q:136:ILE:O | 1:Q:139:VAL:HB | 2.19 | 0.42 |
| 1:Q:167:GLU:OE1 | 1:S:64:ILE:HD13 | 2.19 | 0.42 |
| 1:R:107:GLU:O | 1:R:137:GLN:HG3 | 2.19 | 0.42 |
| 1:S:121:GLN:HG3 | 1:S:362:TYR:OH | 2.20 | 0.42 |
| 1:S:167:GLU:OE1 | 1:U:61:LYS:HE2 | 2.20 | 0.42 |
| 1:T:69:TYR:CD2 | 1:T:69:TYR:N | 2.86 | 0.42 |
| 1:U:34:ILE:CG2 | 1:U:67:LEU:CB | 2.96 | 0.42 |
| 1:U:110:LEU:CD1 | 1:U:177:ARG:NH1 | 2.80 | 0.42 |
| 1:V:35:VAL:C | 1:V:54:VAL:CG2 | 2.88 | 0.42 |
| 1:V:65:LEU:HD13 | 1:V:67:LEU:HD23 | 2.01 | 0.42 |
| 1:V:148:THR:CG2 | 1:V:149:THR:N | 2.81 | 0.42 |
| 1:A:34:ILE:HG23 | 1:A:67:LEU:HB3 | 2.01 | 0.42 |
| 1:C:38:PRO:CG | 1:C:49:GLN:NE2 | 2.79 | 0.42 |
| 1:D:180:LEU:HD12 | 1:D:181:ALA:CA | 2.50 | 0.42 |
| 1:E:103:THR:O | 1:E:132:MET:HA | 2.20 | 0.42 |
| 1:G:135:ALA:CB | 1:G:140:LEU:HD21 | 2.49 | 0.42 |
| 1:H:35:VAL:C | 1:H:54:VAL:CG2 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:149:THR:HG23 | 1:J:150:GLY:N | 2.34 | 0.42 |
| 1:J:167:GLU:OE1 | 1:L:61:LYS:HE2 | 2.20 | 0.42 |
| 1:K:167:GLU:OE1 | 1:M:61:LYS:HE2 | 2.20 | 0.42 |
| 1:M:69:TYR:CD2 | 1:M:69:TYR:N | 2.87 | 0.42 |
| 1:N:103:THR:O | 1:N:132:MET:HA | 2.20 | 0.42 |
| 1:N:110:LEU:CD1 | 1:N:177:ARG:HH11 | 2.32 | 0.42 |
| 1:O:173:HIS:HE1 | 1:P:268:GLY:CA | 2.28 | 0.42 |
| 1:P:149:THR:CG2 | 1:P:150:GLY:N | 2.82 | 0.42 |
| 1:Q:140:LEU:HB3 | 1:Q:343:GLY:N | 2.35 | 0.42 |
| 1:R:167:GLU:OE1 | 1:T:64:ILE:HD13 | 2.19 | 0.42 |
| 1:T:106:THR:HG22 | 1:T:140:LEU:HD11 | 2.01 | 0.42 |
| 1:U:35:VAL:C | 1:U:54:VAL:CG2 | 2.88 | 0.42 |
| 1:V:103:THR:O | 1:V:132:MET:HA | 2.20 | 0.42 |
| 1:V:183:ARG:HE | 1:V:183:ARG:HB3 | 1.59 | 0.42 |
| 1:V:357:ILE:CG2 | 1:V:358:THR:N | 2.83 | 0.42 |
| 1:W:72:GLU:O | 1:W:183:ARG:NH2 | 2.52 | 0.42 |
| 1:A:73:HIC:HA | 1:A:183:ARG:NH1 | 2.18 | 0.41 |
| 1:A:103:THR:O | 1:A:132:MET:HA | 2.20 | 0.41 |
| 1:A:135:ALA:CB | 1:A:140:LEU:HD21 | 2.49 | 0.41 |
| 1:A:349:LEU:HD23 | 1:A:349:LEU:HA | 1.80 | 0.41 |
| 1:B:135:ALA:CB | 1:B:140:LEU:HD21 | 2.49 | 0.41 |
| 1:B:140:LEU:HB3 | 1:B:343:GLY:N | 2.35 | 0.41 |
| 1:C:65:LEU:HD13 | 1:C:67:LEU:HD23 | 2.01 | 0.41 |
| 1:C:135:ALA:CB | 1:C:140:LEU:HD21 | 2.50 | 0.41 |
| 1:D:72:GLU:O | 1:D:183:ARG:NH2 | 2.52 | 0.41 |
| 1:D:133:TYR:CE2 | 1:D:375:PHE:HB2 | 2.51 | 0.41 |
| 1:F:173:HIS:HE1 | 1:G:268:GLY:CA | 2.28 | 0.41 |
| 1:G:106:THR:HG22 | 1:G:140:LEU:HD11 | 2.01 | 0.41 |
| 1:G:140:LEU:HB3 | 1:G:343:GLY:N | 2.35 | 0.41 |
| 1:H:121:GLN:HA | 1:H:362:TYR:CZ | 2.55 | 0.41 |
| 1:H:173:HIS:HE1 | 1:I:268:GLY:CA | 2.28 | 0.41 |
| 1:H:299:MET:O | 1:H:332:PRO:HD2 | 2.18 | 0.41 |
| 1:J:103:THR:O | 1:J:132:MET:HA | 2.20 | 0.41 |
| 1:J:180:LEU:HD12 | 1:J:181:ALA:CA | 2.50 | 0.41 |
| 1:K:107:GLU:O | 1:K:137:GLN:HG3 | 2.19 | 0.41 |
| 1:L:65:LEU:HD13 | 1:L:67:LEU:HD23 | 2.01 | 0.41 |
| 1:L:72:GLU:O | 1:L:183:ARG:NH2 | 2.52 | 0.41 |
| 1:M:34:ILE:CG2 | 1:M:67:LEU:CB | 2.96 | 0.41 |
| 1:M:107:GLU:O | 1:M:137:GLN:HG3 | 2.19 | 0.41 |
| 1:N:34:ILE:HD13 | 1:N:67:LEU:CD2 | 2.46 | 0.41 |
| 1:O:2:GLU:HB3 | 1:O:3:ASP:H | 1.66 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:103:THR:O | 1:O:132:MET:HA | 2.20 | 0.41 |
| 1:P:35:VAL:C | 1:P:54:VAL:CG2 | 2.88 | 0.41 |
| 1:P:178:LEU:HG | 1:P:180:LEU:H | 1.84 | 0.41 |
| 1:Q:103:THR:O | 1:Q:132:MET:HA | 2.20 | 0.41 |
| 1:Q:121:GLN:HA | 1:Q:362:TYR:CZ | 2.55 | 0.41 |
| 1:R:103:THR:O | 1:R:132:MET:HA | 2.20 | 0.41 |
| 1:T:208:ILE:CG2 | 1:T:209:VAL:N | 2.83 | 0.41 |
| 1:W:121:GLN:HA | 1:W:362:TYR:CZ | 2.55 | 0.41 |
| 1:A:38:PRO:CG | 1:A:49:GLN:NE2 | 2.79 | 0.41 |
| 1:A:149:THR:HG23 | 1:A:150:GLY:N | 2.34 | 0.41 |
| 1:B:106:THR:HG22 | 1:B:140:LEU:HD11 | 2.01 | 0.41 |
| 1:B:121:GLN:HA | 1:B:362:TYR:CZ | 2.55 | 0.41 |
| 1:C:39:ARG:NE | 1:C:66:THR:CA | 2.69 | 0.41 |
| 1:C:121:GLN:HG3 | 1:C:362:TYR:OH | 2.20 | 0.41 |
| 1:C:140:LEU:HB3 | 1:C:343:GLY:N | 2.36 | 0.41 |
| 1:D:180:LEU:CD1 | 1:D:181:ALA:N | 2.78 | 0.41 |
| 1:E:189:LEU:HA | 1:E:192:ILE:HG12 | 2.02 | 0.41 |
| 1:F:135:ALA:CB | 1:F:140:LEU:HD21 | 2.49 | 0.41 |
| 1:F:180:LEU:HD12 | 1:F:181:ALA:CA | 2.49 | 0.41 |
| 1:G:103:THR:O | 1:G:132:MET:HA | 2.20 | 0.41 |
| 1:H:140:LEU:HB3 | 1:H:343:GLY:N | 2.35 | 0.41 |
| 1:I:180:LEU:HD12 | 1:I:181:ALA:CA | 2.50 | 0.41 |
| 1:J:140:LEU:HB3 | 1:J:343:GLY:N | 2.35 | 0.41 |
| 1:K:135:ALA:CB | 1:K:140:LEU:HD21 | 2.49 | 0.41 |
| 1:L:47:MET:HB3 | 1:L:48:GLY:H | 1.61 | 0.41 |
| 1:M:8:LEU:CB | 1:M:103:THR:HG23 | 2.48 | 0.41 |
| 1:M:35:VAL:C | 1:M:54:VAL:CG2 | 2.88 | 0.41 |
| 1:M:103:THR:O | 1:M:132:MET:HA | 2.20 | 0.41 |
| 1:M:140:LEU:HB3 | 1:M:343:GLY:N | 2.35 | 0.41 |
| 1:M:180:LEU:HD12 | 1:M:181:ALA:CA | 2.50 | 0.41 |
| 1:P:34:ILE:HG23 | 1:P:67:LEU:HB3 | 2.02 | 0.41 |
| 1:R:65:LEU:HD13 | 1:R:67:LEU:HD23 | 2.01 | 0.41 |
| 1:R:121:GLN:HA | 1:R:362:TYR:CZ | 2.55 | 0.41 |
| 1:S:140:LEU:HB3 | 1:S:343:GLY:N | 2.35 | 0.41 |
| 1:S:173:HIS:HE1 | 1:T:268:GLY:CA | 2.28 | 0.41 |
| 1:T:121:GLN:HA | 1:T:362:TYR:CZ | 2.56 | 0.41 |
| 1:U:39:ARG:NE | 1:U:66:THR:CA | 2.69 | 0.41 |
| 1:U:180:LEU:CD1 | 1:U:181:ALA:N | 2.78 | 0.41 |
| 1:V:121:GLN:HA | 1:V:362:TYR:CZ | 2.55 | 0.41 |
| 1:V:357:ILE:HD12 | 1:V:357:ILE:HA | 1.79 | 0.41 |
| 1:V:362:TYR:CE1 | 1:V:367:PRO:CB | 2.99 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:106:THR:HG22 | 1:W:140:LEU:HD11 | 2.01 | 0.41 |
| 1:W:180:LEU:CD1 | 1:W:181:ALA:N | 2.78 | 0.41 |
| 1:A:140:LEU:HB3 | 1:A:343:GLY:N | 2.35 | 0.41 |
| 1:A:167:GLU:OE1 | 1:C:64:ILE:HD13 | 2.19 | 0.41 |
| 1:C:64:ILE:CG2 | 1:C:65:LEU:N | 2.81 | 0.41 |
| 1:C:167:GLU:OE1 | 1:E:64:ILE:HD13 | 2.19 | 0.41 |
| 1:D:173:HIS:HE1 | 1:E:268:GLY:CA | 2.28 | 0.41 |
| 1:E:135:ALA:CB | 1:E:140:LEU:HD21 | 2.49 | 0.41 |
| 1:E:357:ILE:CG2 | 1:E:358:THR:N | 2.82 | 0.41 |
| 1:F:35:VAL:C | 1:F:54:VAL:CG2 | 2.88 | 0.41 |
| 1:F:140:LEU:HB3 | 1:F:343:GLY:N | 2.35 | 0.41 |
| 1:H:103:THR:O | 1:H:132:MET:HA | 2.20 | 0.41 |
| 1:I:65:LEU:HD13 | 1:I:67:LEU:HD23 | 2.01 | 0.41 |
| 1:I:208:ILE:CG2 | 1:I:209:VAL:N | 2.83 | 0.41 |
| 1:J:34:ILE:CG2 | 1:J:67:LEU:CB | 2.96 | 0.41 |
| 1:K:35:VAL:C | 1:K:54:VAL:CG2 | 2.88 | 0.41 |
| 1:K:110:LEU:CD1 | 1:K:177:ARG:HH11 | 2.32 | 0.41 |
| 1:K:140:LEU:HB3 | 1:K:343:GLY:N | 2.35 | 0.41 |
| 1:L:106:THR:HG22 | 1:L:140:LEU:HD11 | 2.01 | 0.41 |
| 1:L:140:LEU:HB3 | 1:L:343:GLY:N | 2.35 | 0.41 |
| 1:L:167:GLU:OE1 | 1:N:61:LYS:HE2 | 2.20 | 0.41 |
| 1:N:121:GLN:HG3 | 1:N:362:TYR:OH | 2.20 | 0.41 |
| 1:N:167:GLU:OE1 | 1:P:61:LYS:HE2 | 2.19 | 0.41 |
| 1:N:357:ILE:CG2 | 1:N:358:THR:N | 2.82 | 0.41 |
| 1:O:149:THR:CG2 | 1:O:150:GLY:N | 2.82 | 0.41 |
| 1:O:180:LEU:CD1 | 1:O:181:ALA:N | 2.78 | 0.41 |
| 1:P:103:THR:O | 1:P:132:MET:HA | 2.20 | 0.41 |
| 1:P:121:GLN:HA | 1:P:362:TYR:CZ | 2.55 | 0.41 |
| 1:Q:180:LEU:CD1 | 1:Q:181:ALA:N | 2.78 | 0.41 |
| 1:Q:335:ARG:O | 1:Q:338:SER:CB | 2.69 | 0.41 |
| 1:R:189:LEU:HA | 1:R:192:ILE:HG12 | 2.03 | 0.41 |
| 1:S:180:LEU:CD1 | 1:S:181:ALA:N | 2.78 | 0.41 |
| 1:U:299:MET:HE1 | 1:U:309:ILE:HD13 | 2.02 | 0.41 |
| 1:V:106:THR:HG22 | 1:V:140:LEU:HD11 | 2.01 | 0.41 |
| 1:V:140:LEU:HB3 | 1:V:343:GLY:N | 2.35 | 0.41 |
| 1:V:173:HIS:HE1 | 1:W:268:GLY:CA | 2.28 | 0.41 |
| 1:W:35:VAL:C | 1:W:54:VAL:CG2 | 2.88 | 0.41 |
| 1:A:47:MET:HB3 | 1:A:48:GLY:H | 1.61 | 0.41 |
| 1:A:149:THR:CG2 | 1:A:150:GLY:N | 2.82 | 0.41 |
| 1:A:300:SER:HA | 1:A:335:ARG:CD | 2.50 | 0.41 |
| 1:B:39:ARG:NE | 1:B:66:THR:CA | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:335:ARG:O | 1:B:338:SER:CB | 2.69 | 0.41 |
| 1:H:72:GLU:O | 1:H:183:ARG:NH2 | 2.52 | 0.41 |
| 1:H:300:SER:HA | 1:H:335:ARG:CD | 2.50 | 0.41 |
| 1:I:35:VAL:C | 1:I:54:VAL:CG2 | 2.88 | 0.41 |
| 1:I:103:THR:O | 1:I:132:MET:HA | 2.20 | 0.41 |
| 1:I:106:THR:HG22 | 1:I:140:LEU:HD11 | 2.01 | 0.41 |
| 1:I:107:GLU:O | 1:I:137:GLN:HG3 | 2.19 | 0.41 |
| 1:I:140:LEU:HB3 | 1:I:343:GLY:N | 2.35 | 0.41 |
| 1:J:47:MET:HB3 | 1:J:48:GLY:H | 1.61 | 0.41 |
| 1:K:73:HIC:HA | 1:K:183:ARG:NH1 | 2.18 | 0.41 |
| 1:K:171:LEU:HA | 1:K:172:PRO:HD3 | 1.79 | 0.41 |
| 1:K:180:LEU:HD12 | 1:K:181:ALA:CA | 2.49 | 0.41 |
| 1:M:106:THR:HG22 | 1:M:140:LEU:HD11 | 2.01 | 0.41 |
| 1:N:349:LEU:HD23 | 1:N:349:LEU:HA | 1.80 | 0.41 |
| 1:O:135:ALA:CB | 1:O:140:LEU:HD21 | 2.49 | 0.41 |
| 1:T:149:THR:CG2 | 1:T:150:GLY:N | 2.82 | 0.41 |
| 1:T:189:LEU:HA | 1:T:192:ILE:HG12 | 2.03 | 0.41 |
| 1:T:300:SER:HA | 1:T:335:ARG:CD | 2.50 | 0.41 |
| 1:U:335:ARG:O | 1:U:338:SER:CB | 2.69 | 0.41 |
| 1:V:135:ALA:CB | 1:V:140:LEU:HD21 | 2.49 | 0.41 |
| 1:W:44:MET:CG | 1:W:45:VAL:N | 2.75 | 0.41 |
| 1:W:110:LEU:CD1 | 1:W:177:ARG:NH1 | 2.80 | 0.41 |
| 1:A:106:THR:HG22 | 1:A:140:LEU:HD11 | 2.01 | 0.41 |
| 1:A:121:GLN:HG3 | 1:A:362:TYR:OH | 2.20 | 0.41 |
| 1:A:189:LEU:HA | 1:A:192:ILE:HG12 | 2.02 | 0.41 |
| 1:B:2:GLU:HB3 | 1:B:3:ASP:H | 1.66 | 0.41 |
| 1:C:110:LEU:CD1 | 1:C:177:ARG:HH11 | 2.32 | 0.41 |
| 1:D:39:ARG:NE | 1:D:66:THR:CA | 2.69 | 0.41 |
| 1:E:167:GLU:CD | 1:G:61:LYS:CE | 2.85 | 0.41 |
| 1:F:34:ILE:HG23 | 1:F:67:LEU:HB3 | 2.01 | 0.41 |
| 1:F:335:ARG:O | 1:F:338:SER:CB | 2.69 | 0.41 |
| 1:G:35:VAL:C | 1:G:54:VAL:CG2 | 2.88 | 0.41 |
| 1:H:224:GLU:OE1 | 1:H:224:GLU:N | 2.51 | 0.41 |
| 1:I:34:ILE:HG23 | 1:I:67:LEU:HB3 | 2.01 | 0.41 |
| 1:J:149:THR:CG2 | 1:J:150:GLY:N | 2.82 | 0.41 |
| 1:M:167:GLU:OE1 | 1:O:61:LYS:HE2 | 2.20 | 0.41 |
| 1:M:236:LEU:HD12 | 1:M:237:GLU:CA | 2.51 | 0.41 |
| 1:O:183:ARG:HE | 1:O:183:ARG:HB3 | 1.58 | 0.41 |
| 1:P:167:GLU:CD | 1:R:61:LYS:CE | 2.85 | 0.41 |
| 1:P:167:GLU:OE1 | 1:R:64:ILE:HD13 | 2.19 | 0.41 |
| 1:P:189:LEU:HA | 1:P:192:ILE:HG12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:335:ARG:HA | 1:P:335:ARG:HD3 | 1.39 | 0.41 |
| 1:Q:8:LEU:N | 1:Q:102:PRO:O | 2.48 | 0.41 |
| 1:S:103:THR:O | 1:S:132:MET:HA | 2.20 | 0.41 |
| 1:T:103:THR:O | 1:T:132:MET:HA | 2.20 | 0.41 |
| 1:T:140:LEU:HB3 | 1:T:343:GLY:N | 2.35 | 0.41 |
| 1:T:153:LEU:HD23 | 1:T:299:MET:HE2 | 2.03 | 0.41 |
| 1:U:103:THR:O | 1:U:132:MET:HA | 2.20 | 0.41 |
| 1:U:121:GLN:HG3 | 1:U:362:TYR:OH | 2.20 | 0.41 |
| 1:W:8:LEU:N | 1:W:102:PRO:O | 2.48 | 0.41 |
| 1:W:135:ALA:CB | 1:W:140:LEU:HD21 | 2.49 | 0.41 |
| 1:W:140:LEU:HB3 | 1:W:343:GLY:N | 2.35 | 0.41 |
| 1:W:236:LEU:HD12 | 1:W:237:GLU:CA | 2.51 | 0.41 |
| 1:A:133:TYR:CE2 | 1:A:375:PHE:HB2 | 2.51 | 0.41 |
| 1:B:236:LEU:HD12 | 1:B:237:GLU:CA | 2.51 | 0.41 |
| 1:C:189:LEU:HA | 1:C:192:ILE:HG12 | 2.03 | 0.41 |
| 1:D:35:VAL:C | 1:D:54:VAL:CG2 | 2.88 | 0.41 |
| 1:D:121:GLN:HA | 1:D:362:TYR:CZ | 2.55 | 0.41 |
| 1:D:140:LEU:HB3 | 1:D:343:GLY:N | 2.35 | 0.41 |
| 1:E:38:PRO:CG | 1:E:49:GLN:NE2 | 2.79 | 0.41 |
| 1:E:49:GLN:HG3 | 1:E:50:LYS:N | 2.20 | 0.41 |
| 1:F:224:GLU:OE1 | 1:F:224:GLU:N | 2.51 | 0.41 |
| 1:F:236:LEU:HD12 | 1:F:237:GLU:CA | 2.51 | 0.41 |
| 1:G:189:LEU:HA | 1:G:192:ILE:HG12 | 2.03 | 0.41 |
| 1:G:357:ILE:CG2 | 1:G:358:THR:N | 2.82 | 0.41 |
| 1:H:149:THR:CG2 | 1:H:150:GLY:N | 2.82 | 0.41 |
| 1:H:180:LEU:HD12 | 1:H:181:ALA:CA | 2.50 | 0.41 |
| 1:H:299:MET:HE1 | 1:H:309:ILE:HD13 | 2.03 | 0.41 |
| 1:H:335:ARG:O | 1:H:338:SER:CB | 2.69 | 0.41 |
| 1:H:349:LEU:HD23 | 1:H:349:LEU:HA | 1.80 | 0.41 |
| 1:J:121:GLN:HA | 1:J:362:TYR:CZ | 2.55 | 0.41 |
| 1:J:121:GLN:HG3 | 1:J:362:TYR:OH | 2.20 | 0.41 |
| 1:J:335:ARG:O | 1:J:338:SER:CB | 2.69 | 0.41 |
| 1:K:34:ILE:HG23 | 1:K:67:LEU:HB3 | 2.02 | 0.41 |
| 1:K:103:THR:O | 1:K:132:MET:HA | 2.20 | 0.41 |
| 1:K:374:CYS:HB2 | 1:K:375:PHE:H | 1.62 | 0.41 |
| 1:L:189:LEU:HA | 1:L:192:ILE:HG12 | 2.02 | 0.41 |
| 1:L:236:LEU:HD12 | 1:L:237:GLU:CA | 2.51 | 0.41 |
| 1:N:189:LEU:HA | 1:N:192:ILE:HG12 | 2.02 | 0.41 |
| 1:P:167:GLU:OE1 | 1:R:61:LYS:HE2 | 2.20 | 0.41 |
| 1:Q:31:PHE:HA | 1:Q:32:PRO:HD3 | 1.66 | 0.41 |
| 1:Q:236:LEU:HD12 | 1:Q:237:GLU:CA | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:8:LEU:N | 1:S:102:PRO:O | 2.48 | 0.41 |
| 1:S:72:GLU:O | 1:S:183:ARG:NH2 | 2.52 | 0.41 |
| 1:T:34:ILE:HG23 | 1:T:67:LEU:HB3 | 2.02 | 0.41 |
| 1:T:110:LEU:CD1 | 1:T:177:ARG:HH11 | 2.32 | 0.41 |
| 1:T:357:ILE:CG2 | 1:T:358:THR:N | 2.83 | 0.41 |
| 1:V:178:LEU:HG | 1:V:180:LEU:H | 1.84 | 0.41 |
| 1:V:349:LEU:HD23 | 1:V:349:LEU:HA | 1.80 | 0.41 |
| 1:A:35:VAL:C | 1:A:54:VAL:CG2 | 2.88 | 0.41 |
| 1:A:110:LEU:CD1 | 1:A:177:ARG:HH11 | 2.32 | 0.41 |
| 1:A:121:GLN:HA | 1:A:362:TYR:CZ | 2.55 | 0.41 |
| 1:B:35:VAL:C | 1:B:54:VAL:CG2 | 2.88 | 0.41 |
| 1:B:110:LEU:CD1 | 1:B:177:ARG:HH11 | 2.32 | 0.41 |
| 1:C:31:PHE:HA | 1:C:32:PRO:HD3 | 1.66 | 0.41 |
| 1:E:35:VAL:C | 1:E:54:VAL:CG2 | 2.88 | 0.41 |
| 1:F:110:LEU:CD1 | 1:F:177:ARG:NH1 | 2.80 | 0.41 |
| 1:G:236:LEU:HD12 | 1:G:237:GLU:CA | 2.51 | 0.41 |
| 1:I:299:MET:HE1 | 1:I:309:ILE:HD13 | 2.03 | 0.41 |
| 1:I:335:ARG:O | 1:I:338:SER:CB | 2.69 | 0.41 |
| 1:J:227:MET:HE3 | 1:J:227:MET:HA | 2.02 | 0.41 |
| 1:K:106:THR:HG22 | 1:K:140:LEU:HD11 | 2.01 | 0.41 |
| 1:L:335:ARG:O | 1:L:338:SER:CB | 2.69 | 0.41 |
| 1:M:135:ALA:CB | 1:M:140:LEU:HD21 | 2.49 | 0.41 |
| 1:N:121:GLN:HA | 1:N:362:TYR:CZ | 2.55 | 0.41 |
| 1:N:140:LEU:HB3 | 1:N:343:GLY:N | 2.35 | 0.41 |
| 1:N:335:ARG:O | 1:N:338:SER:CB | 2.69 | 0.41 |
| 1:O:34:ILE:CG2 | 1:O:67:LEU:CB | 2.96 | 0.41 |
| 1:P:73:HIC:HA | 1:P:183:ARG:NH1 | 2.18 | 0.41 |
| 1:P:374:CYS:HB2 | 1:P:375:PHE:H | 1.62 | 0.41 |
| 1:R:236:LEU:HD12 | 1:R:237:GLU:CA | 2.51 | 0.41 |
| 1:W:110:LEU:CD1 | 1:W:177:ARG:HH11 | 2.32 | 0.41 |
| 1:C:287:ILE:HD12 | 1:E:208:ILE:HD13 | 1.96 | 0.41 |
| 1:E:73:HIC:HA | 1:E:183:ARG:NH1 | 2.18 | 0.41 |
| 1:F:103:THR:O | 1:F:132:MET:HA | 2.20 | 0.41 |
| 1:F:121:GLN:HA | 1:F:362:TYR:CZ | 2.55 | 0.41 |
| 1:F:180:LEU:CD1 | 1:F:181:ALA:N | 2.78 | 0.41 |
| 1:G:8:LEU:CD1 | 1:G:90:PHE:CD1 | 3.04 | 0.41 |
| 1:G:110:LEU:CD1 | 1:G:177:ARG:HH11 | 2.32 | 0.41 |
| 1:H:49:GLN:HG3 | 1:H:50:LYS:N | 2.20 | 0.41 |
| 1:H:180:LEU:CD1 | 1:H:181:ALA:N | 2.78 | 0.41 |
| 1:I:236:LEU:HD12 | 1:I:237:GLU:CA | 2.51 | 0.41 |
| 1:J:8:LEU:N | 1:J:102:PRO:O | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:110:LEU:CD1 | 1:L:177:ARG:HH11 | 2.32 | 0.41 |
| 1:M:178:LEU:HG | 1:M:180:LEU:H | 1.84 | 0.41 |
| 1:O:121:GLN:HA | 1:O:362:TYR:CZ | 2.55 | 0.41 |
| 1:P:335:ARG:O | 1:P:338:SER:CB | 2.69 | 0.41 |
| 1:R:110:LEU:CD1 | 1:R:177:ARG:HH11 | 2.32 | 0.41 |
| 1:S:121:GLN:HA | 1:S:362:TYR:CZ | 2.56 | 0.41 |
| 1:S:236:LEU:HD12 | 1:S:237:GLU:CA | 2.51 | 0.41 |
| 1:T:2:GLU:HB3 | 1:T:3:ASP:H | 1.66 | 0.41 |
| 1:U:121:GLN:HA | 1:U:362:TYR:CZ | 2.56 | 0.41 |
| 1:U:357:ILE:CG2 | 1:U:358:THR:N | 2.83 | 0.41 |
| 1:V:110:LEU:CD1 | 1:V:177:ARG:HH11 | 2.32 | 0.41 |
| 1:W:164:PRO:CG | 1:W:174:ALA:HB3 | 2.51 | 0.41 |
| 1:A:43:VAL:O | 1:A:44:MET:CE | 2.69 | 0.41 |
| 1:A:236:LEU:HD12 | 1:A:237:GLU:CA | 2.51 | 0.41 |
| 1:C:35:VAL:C | 1:C:54:VAL:CG2 | 2.88 | 0.41 |
| 1:C:224:GLU:OE1 | 1:C:224:GLU:N | 2.51 | 0.41 |
| 1:C:335:ARG:O | 1:C:338:SER:CB | 2.69 | 0.41 |
| 1:D:34:ILE:HG23 | 1:D:67:LEU:HB3 | 2.01 | 0.41 |
| 1:D:103:THR:O | 1:D:132:MET:HA | 2.20 | 0.41 |
| 1:D:335:ARG:O | 1:D:338:SER:CB | 2.69 | 0.41 |
| 1:E:43:VAL:O | 1:E:44:MET:CE | 2.69 | 0.41 |
| 1:E:335:ARG:O | 1:E:338:SER:CB | 2.69 | 0.41 |
| 1:F:43:VAL:O | 1:F:44:MET:CE | 2.69 | 0.41 |
| 1:F:133:TYR:CE2 | 1:F:375:PHE:HB2 | 2.51 | 0.41 |
| 1:G:164:PRO:HG2 | 1:G:174:ALA:CB | 2.51 | 0.41 |
| 1:G:178:LEU:HG | 1:G:180:LEU:H | 1.85 | 0.41 |
| 1:H:8:LEU:N | 1:H:102:PRO:O | 2.48 | 0.41 |
| 1:H:43:VAL:O | 1:H:44:MET:CE | 2.69 | 0.41 |
| 1:H:236:LEU:HD12 | 1:H:237:GLU:CA | 2.51 | 0.41 |
| 1:I:8:LEU:CD1 | 1:I:90:PHE:CD1 | 3.04 | 0.41 |
| 1:I:34:ILE:CG2 | 1:I:68:LYS:N | 2.84 | 0.41 |
| 1:J:43:VAL:O | 1:J:44:MET:CE | 2.69 | 0.41 |
| 1:J:183:ARG:HE | 1:J:183:ARG:HB3 | 1.58 | 0.41 |
| 1:J:236:LEU:HD12 | 1:J:237:GLU:CA | 2.51 | 0.41 |
| 1:K:34:ILE:CG2 | 1:K:68:LYS:N | 2.84 | 0.41 |
| 1:K:121:GLN:HA | 1:K:362:TYR:CZ | 2.55 | 0.41 |
| 1:K:335:ARG:O | 1:K:338:SER:CB | 2.69 | 0.41 |
| 1:L:43:VAL:O | 1:L:44:MET:CE | 2.69 | 0.41 |
| 1:L:121:GLN:HG3 | 1:L:362:TYR:OH | 2.20 | 0.41 |
| 1:L:332:PRO:HA | 1:L:333:PRO:HD3 | 1.95 | 0.41 |
| 1:M:34:ILE:CG2 | 1:M:68:LYS:N | 2.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:110:LEU:CD1 | 1:M:177:ARG:HH11 | 2.32 | 0.41 |
| 1:N:43:VAL:O | 1:N:44:MET:CE | 2.69 | 0.41 |
| 1:N:164:PRO:HG2 | 1:N:174:ALA:CB | 2.51 | 0.41 |
| 1:O:167:GLU:OE1 | 1:Q:61:LYS:HE2 | 2.20 | 0.41 |
| 1:O:335:ARG:O | 1:O:338:SER:CB | 2.69 | 0.41 |
| 1:O:357:ILE:CG2 | 1:O:358:THR:N | 2.83 | 0.41 |
| 1:P:43:VAL:O | 1:P:44:MET:CE | 2.69 | 0.41 |
| 1:P:164:PRO:HG2 | 1:P:174:ALA:CB | 2.51 | 0.41 |
| 1:P:299:MET:HE1 | 1:P:304:THR:HB | 2.03 | 0.41 |
| 1:Q:8:LEU:CD1 | 1:Q:90:PHE:CD1 | 3.04 | 0.41 |
| 1:Q:34:ILE:CG2 | 1:Q:67:LEU:CB | 2.96 | 0.41 |
| 1:R:8:LEU:CD1 | 1:R:90:PHE:CD1 | 3.04 | 0.41 |
| 1:R:43:VAL:O | 1:R:44:MET:CE | 2.69 | 0.41 |
| 1:R:140:LEU:HB3 | 1:R:343:GLY:N | 2.35 | 0.41 |
| 1:R:167:GLU:OE1 | 1:T:61:LYS:HE2 | 2.20 | 0.41 |
| 1:S:164:PRO:HG2 | 1:S:174:ALA:CB | 2.51 | 0.41 |
| 1:S:335:ARG:O | 1:S:338:SER:CB | 2.69 | 0.41 |
| 1:T:43:VAL:O | 1:T:44:MET:CE | 2.69 | 0.41 |
| 1:T:135:ALA:CB | 1:T:140:LEU:HD21 | 2.49 | 0.41 |
| 1:T:236:LEU:HD12 | 1:T:237:GLU:CA | 2.51 | 0.41 |
| 1:T:335:ARG:O | 1:T:338:SER:CB | 2.69 | 0.41 |
| 1:U:43:VAL:O | 1:U:44:MET:CE | 2.69 | 0.41 |
| 1:U:140:LEU:HB3 | 1:U:343:GLY:N | 2.35 | 0.41 |
| 1:U:164:PRO:HG2 | 1:U:174:ALA:CB | 2.51 | 0.41 |
| 1:U:164:PRO:CG | 1:U:174:ALA:HB3 | 2.51 | 0.41 |
| 1:U:169:TYR:CE2 | 1:W:40:HIS:HB2 | 2.56 | 0.41 |
| 1:U:171:LEU:HA | 1:U:172:PRO:HD3 | 1.79 | 0.41 |
| 1:U:173:HIS:HE1 | 1:V:268:GLY:CA | 2.28 | 0.41 |
| 1:U:236:LEU:HD12 | 1:U:237:GLU:CA | 2.51 | 0.41 |
| 1:V:34:ILE:CG2 | 1:V:67:LEU:CB | 2.96 | 0.41 |
| 1:V:189:LEU:HA | 1:V:192:ILE:HG12 | 2.02 | 0.41 |
| 1:W:43:VAL:O | 1:W:44:MET:CE | 2.69 | 0.41 |
| 1:W:103:THR:O | 1:W:132:MET:HA | 2.20 | 0.41 |
| 1:W:121:GLN:HG3 | 1:W:362:TYR:OH | 2.20 | 0.41 |
| 1:W:149:THR:CG2 | 1:W:150:GLY:N | 2.82 | 0.41 |
| 1:W:164:PRO:HG2 | 1:W:174:ALA:CB | 2.51 | 0.41 |
| 1:W:223:PHE:CZ | 1:W:266:PHE:CZ | 3.09 | 0.41 |
| 1:W:335:ARG:O | 1:W:338:SER:CB | 2.69 | 0.41 |
| 1:D:43:VAL:O | 1:D:44:MET:CE | 2.69 | 0.41 |
| 1:D:110:LEU:CD1 | 1:D:177:ARG:NH1 | 2.80 | 0.41 |
| 1:D:153:LEU:HD23 | 1:D:299:MET:HE2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:164:PRO:HG2 | 1:D:174:ALA:CB | 2.51 | 0.41 |
| 1:D:224:GLU:OE1 | 1:D:224:GLU:N | 2.51 | 0.41 |
| 1:E:31:PHE:HA | 1:E:32:PRO:HD3 | 1.65 | 0.41 |
| 1:E:50:LYS:CG | 1:E:53:TYR:CE2 | 3.03 | 0.41 |
| 1:E:149:THR:CG2 | 1:E:150:GLY:N | 2.82 | 0.41 |
| 1:F:357:ILE:CG2 | 1:F:358:THR:N | 2.82 | 0.41 |
| 1:G:43:VAL:O | 1:G:44:MET:CE | 2.69 | 0.41 |
| 1:I:164:PRO:HG2 | 1:I:174:ALA:CB | 2.51 | 0.41 |
| 1:I:189:LEU:HA | 1:I:192:ILE:HG12 | 2.02 | 0.41 |
| 1:J:189:LEU:HA | 1:J:192:ILE:HG12 | 2.03 | 0.41 |
| 1:K:335:ARG:HA | 1:K:335:ARG:HD3 | 1.39 | 0.41 |
| 1:M:121:GLN:HA | 1:M:362:TYR:CZ | 2.55 | 0.41 |
| 1:M:171:LEU:HA | 1:M:172:PRO:HD3 | 1.79 | 0.41 |
| 1:N:47:MET:HB3 | 1:N:48:GLY:H | 1.61 | 0.41 |
| 1:N:224:GLU:OE1 | 1:N:224:GLU:N | 2.51 | 0.41 |
| 1:O:34:ILE:CG2 | 1:O:68:LYS:N | 2.84 | 0.41 |
| 1:O:143:TYR:CE2 | 1:Q:45:VAL:CG2 | 3.04 | 0.41 |
| 1:Q:227:MET:HE3 | 1:Q:227:MET:HA | 2.03 | 0.41 |
| 1:R:34:ILE:HG23 | 1:R:67:LEU:HB3 | 2.02 | 0.41 |
| 1:R:50:LYS:CG | 1:R:53:TYR:CE2 | 3.03 | 0.41 |
| 1:S:149:THR:CG2 | 1:S:150:GLY:N | 2.82 | 0.41 |
| 1:A:164:PRO:CG | 1:A:174:ALA:HB3 | 2.51 | 0.40 |
| 1:A:335:ARG:HD3 | 1:A:335:ARG:HA | 1.39 | 0.40 |
| 1:A:357:ILE:CG2 | 1:A:358:THR:N | 2.83 | 0.40 |
| 1:B:34:ILE:CG2 | 1:B:68:LYS:N | 2.84 | 0.40 |
| 1:D:50:LYS:CG | 1:D:53:TYR:CE2 | 3.03 | 0.40 |
| 1:D:135:ALA:CB | 1:D:140:LEU:HD21 | 2.49 | 0.40 |
| 1:D:164:PRO:CG | 1:D:174:ALA:HB3 | 2.51 | 0.40 |
| 1:D:167:GLU:OE1 | 1:F:64:ILE:HD13 | 2.19 | 0.40 |
| 1:D:374:CYS:HB2 | 1:D:375:PHE:H | 1.61 | 0.40 |
| 1:E:2:GLU:HB3 | 1:E:3:ASP:H | 1.66 | 0.40 |
| 1:E:110:LEU:CD1 | 1:E:177:ARG:HH11 | 2.32 | 0.40 |
| 1:F:39:ARG:NE | 1:F:66:THR:CA | 2.69 | 0.40 |
| 1:F:164:PRO:CG | 1:F:174:ALA:HB3 | 2.51 | 0.40 |
| 1:G:34:ILE:CG2 | 1:G:68:LYS:N | 2.84 | 0.40 |
| 1:I:121:GLN:HA | 1:I:362:TYR:CZ | 2.56 | 0.40 |
| 1:J:332:PRO:HA | 1:J:333:PRO:HD3 | 1.95 | 0.40 |
| 1:K:236:LEU:HD12 | 1:K:237:GLU:CA | 2.51 | 0.40 |
| 1:M:335:ARG:O | 1:M:338:SER:CB | 2.69 | 0.40 |
| 1:N:143:TYR:CE2 | 1:P:45:VAL:CG2 | 3.04 | 0.40 |
| 1:N:223:PHE:CZ | 1:N:266:PHE:CZ | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:287:ILE:HD12 | 1:P:208:ILE:HD13 | 1.96 | 0.40 |
| 1:O:8:LEU:CD1 | 1:O:90:PHE:CD1 | 3.04 | 0.40 |
| 1:O:142:LEU:CD1 | 1:O:165:ILE:HD11 | 2.47 | 0.40 |
| 1:P:38:PRO:CG | 1:P:49:GLN:NE2 | 2.79 | 0.40 |
| 1:P:143:TYR:CE2 | 1:R:45:VAL:CG2 | 3.04 | 0.40 |
| 1:P:164:PRO:CG | 1:P:174:ALA:HB3 | 2.51 | 0.40 |
| 1:P:357:ILE:CG2 | 1:P:358:THR:N | 2.82 | 0.40 |
| 1:Q:50:LYS:CG | 1:Q:53:TYR:CE2 | 3.03 | 0.40 |
| 1:R:164:PRO:HG2 | 1:R:174:ALA:CB | 2.51 | 0.40 |
| 1:R:164:PRO:CG | 1:R:174:ALA:HB3 | 2.51 | 0.40 |
| 1:S:164:PRO:CG | 1:S:174:ALA:HB3 | 2.51 | 0.40 |
| 1:S:374:CYS:HB2 | 1:S:375:PHE:H | 1.62 | 0.40 |
| 1:T:236:LEU:CD1 | 1:T:237:GLU:CG | 2.93 | 0.40 |
| 1:T:362:TYR:CE1 | 1:T:367:PRO:CB | 2.99 | 0.40 |
| 1:U:223:PHE:CZ | 1:U:266:PHE:CZ | 3.09 | 0.40 |
| 1:V:335:ARG:O | 1:V:338:SER:CB | 2.69 | 0.40 |
| 1:B:103:THR:O | 1:B:132:MET:HA | 2.20 | 0.40 |
| 1:B:164:PRO:HG2 | 1:B:174:ALA:CB | 2.51 | 0.40 |
| 1:B:175:ILE:H | 1:B:175:ILE:HG13 | 1.71 | 0.40 |
| 1:C:43:VAL:O | 1:C:44:MET:CE | 2.69 | 0.40 |
| 1:D:34:ILE:CG2 | 1:D:68:LYS:N | 2.84 | 0.40 |
| 1:D:113:LYS:HB3 | 1:D:371:HIS:CD2 | 2.57 | 0.40 |
| 1:E:164:PRO:HG2 | 1:E:174:ALA:CB | 2.51 | 0.40 |
| 1:F:8:LEU:CD1 | 1:F:90:PHE:CD1 | 3.04 | 0.40 |
| 1:F:8:LEU:N | 1:F:102:PRO:O | 2.48 | 0.40 |
| 1:F:164:PRO:HG2 | 1:F:174:ALA:CB | 2.51 | 0.40 |
| 1:H:374:CYS:HB2 | 1:H:375:PHE:H | 1.62 | 0.40 |
| 1:I:236:LEU:CD1 | 1:I:237:GLU:CG | 2.93 | 0.40 |
| 1:L:31:PHE:HA | 1:L:32:PRO:HD3 | 1.66 | 0.40 |
| 1:L:164:PRO:HG2 | 1:L:174:ALA:CB | 2.51 | 0.40 |
| 1:M:133:TYR:CE2 | 1:M:375:PHE:HB2 | 2.51 | 0.40 |
| 1:N:164:PRO:CG | 1:N:174:ALA:HB3 | 2.51 | 0.40 |
| 1:N:180:LEU:O | 1:N:180:LEU:HG | 2.11 | 0.40 |
| 1:O:8:LEU:CB | 1:O:103:THR:HG23 | 2.48 | 0.40 |
| 1:Q:143:TYR:CE2 | 1:S:45:VAL:CG2 | 3.04 | 0.40 |
| 1:R:38:PRO:CG | 1:R:49:GLN:NE2 | 2.79 | 0.40 |
| 1:R:143:TYR:CE2 | 1:T:45:VAL:CG2 | 3.04 | 0.40 |
| 1:S:223:PHE:CZ | 1:S:266:PHE:CZ | 3.09 | 0.40 |
| 1:V:43:VAL:O | 1:V:44:MET:CE | 2.69 | 0.40 |
| 1:V:133:TYR:CE2 | 1:V:375:PHE:HB2 | 2.51 | 0.40 |
| 1:V:236:LEU:HD12 | 1:V:237:GLU:CA | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:300:SER:HA | 1:V:335:ARG:CD | 2.50 | 0.40 |
| 1:W:189:LEU:HA | 1:W:192:ILE:HG12 | 2.03 | 0.40 |
| 1:B:8:LEU:CD1 | 1:B:90:PHE:CD1 | 3.04 | 0.40 |
| 1:B:143:TYR:CE2 | 1:D:45:VAL:CG2 | 3.04 | 0.40 |
| 1:B:171:LEU:HA | 1:B:172:PRO:HD3 | 1.79 | 0.40 |
| 1:C:121:GLN:HA | 1:C:362:TYR:CZ | 2.55 | 0.40 |
| 1:C:173:HIS:CE1 | 1:D:268:GLY:N | 2.90 | 0.40 |
| 1:C:300:SER:HA | 1:C:335:ARG:CD | 2.50 | 0.40 |
| 1:G:164:PRO:CG | 1:G:174:ALA:HB3 | 2.51 | 0.40 |
| 1:I:113:LYS:HB3 | 1:I:371:HIS:CD2 | 2.57 | 0.40 |
| 1:J:300:SER:HA | 1:J:335:ARG:CD | 2.50 | 0.40 |
| 1:K:8:LEU:CD1 | 1:K:90:PHE:CD1 | 3.04 | 0.40 |
| 1:K:357:ILE:HD12 | 1:K:357:ILE:HA | 1.79 | 0.40 |
| 1:L:121:GLN:HA | 1:L:362:TYR:CZ | 2.55 | 0.40 |
| 1:M:236:LEU:CD1 | 1:M:237:GLU:CG | 2.93 | 0.40 |
| 1:N:38:PRO:CG | 1:N:49:GLN:NE2 | 2.79 | 0.40 |
| 1:O:43:VAL:O | 1:O:44:MET:CE | 2.69 | 0.40 |
| 1:O:140:LEU:HB3 | 1:O:343:GLY:N | 2.35 | 0.40 |
| 1:O:189:LEU:HA | 1:O:192:ILE:HG12 | 2.02 | 0.40 |
| 1:P:65:LEU:C | 1:P:65:LEU:CD1 | 2.90 | 0.40 |
| 1:P:140:LEU:HB3 | 1:P:343:GLY:N | 2.35 | 0.40 |
| 1:Q:34:ILE:CG2 | 1:Q:68:LYS:N | 2.84 | 0.40 |
| 1:Q:43:VAL:O | 1:Q:44:MET:CE | 2.69 | 0.40 |
| 1:Q:189:LEU:HA | 1:Q:192:ILE:HG12 | 2.02 | 0.40 |
| 1:Q:223:PHE:CZ | 1:Q:266:PHE:CZ | 3.09 | 0.40 |
| 1:T:8:LEU:CD1 | 1:T:90:PHE:CD1 | 3.04 | 0.40 |
| 1:T:113:LYS:HB3 | 1:T:371:HIS:CD2 | 2.57 | 0.40 |
| 1:T:143:TYR:CE2 | 1:V:45:VAL:CG2 | 3.04 | 0.40 |
| 1:A:143:TYR:CE2 | 1:C:45:VAL:CG2 | 3.04 | 0.40 |
| 1:A:332:PRO:HA | 1:A:333:PRO:HD3 | 1.95 | 0.40 |
| 1:B:183:ARG:HE | 1:B:183:ARG:HB3 | 1.58 | 0.40 |
| 1:B:224:GLU:OE1 | 1:B:224:GLU:N | 2.51 | 0.40 |
| 1:B:335:ARG:HA | 1:B:335:ARG:HD3 | 1.39 | 0.40 |
| 1:C:73:HIC:HA | 1:C:183:ARG:NH1 | 2.18 | 0.40 |
| 1:C:143:TYR:CE2 | 1:E:45:VAL:CG2 | 3.04 | 0.40 |
| 1:D:157:ASP:H | 2:D:401:ADP:PB | 2.45 | 0.40 |
| 1:D:173:HIS:CE1 | 1:E:268:GLY:N | 2.90 | 0.40 |
| 1:E:8:LEU:CD1 | 1:E:90:PHE:CD1 | 3.04 | 0.40 |
| 1:E:8:LEU:N | 1:E:102:PRO:O | 2.48 | 0.40 |
| 1:E:34:ILE:CG2 | 1:E:68:LYS:N | 2.84 | 0.40 |
| 1:E:121:GLN:HA | 1:E:362:TYR:CZ | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:173:HIS:CE1 | 1:F:268:GLY:N | 2.90 | 0.40 |
| 1:F:34:ILE:CG2 | 1:F:67:LEU:CB | 2.96 | 0.40 |
| 1:F:65:LEU:C | 1:F:65:LEU:CD1 | 2.90 | 0.40 |
| 1:F:149:THR:CG2 | 1:F:150:GLY:N | 2.82 | 0.40 |
| 1:F:173:HIS:CE1 | 1:G:268:GLY:N | 2.90 | 0.40 |
| 1:G:121:GLN:HA | 1:G:362:TYR:CZ | 2.55 | 0.40 |
| 1:H:34:ILE:CG2 | 1:H:67:LEU:CB | 2.96 | 0.40 |
| 1:H:110:LEU:CD1 | 1:H:177:ARG:NH1 | 2.80 | 0.40 |
| 1:H:164:PRO:CG | 1:H:174:ALA:HB3 | 2.51 | 0.40 |
| 1:J:164:PRO:CG | 1:J:174:ALA:HB3 | 2.51 | 0.40 |
| 1:K:164:PRO:HG2 | 1:K:174:ALA:CB | 2.51 | 0.40 |
| 1:K:189:LEU:HA | 1:K:192:ILE:HG12 | 2.03 | 0.40 |
| 1:L:143:TYR:CE2 | 1:N:45:VAL:CG2 | 3.04 | 0.40 |
| 1:L:164:PRO:CG | 1:L:174:ALA:HB3 | 2.51 | 0.40 |
| 1:M:43:VAL:O | 1:M:44:MET:CE | 2.69 | 0.40 |
| 1:M:113:LYS:HB3 | 1:M:371:HIS:CD2 | 2.57 | 0.40 |
| 1:M:143:TYR:CE2 | 1:O:45:VAL:CG2 | 3.04 | 0.40 |
| 1:O:236:LEU:HD12 | 1:O:237:GLU:CA | 2.51 | 0.40 |
| 1:P:236:LEU:HD12 | 1:P:237:GLU:CA | 2.51 | 0.40 |
| 1:Q:167:GLU:OE1 | 1:S:61:LYS:HE2 | 2.19 | 0.40 |
| 1:R:135:ALA:CB | 1:R:140:LEU:HD21 | 2.50 | 0.40 |
| 1:S:357:ILE:HD12 | 1:S:357:ILE:HA | 1.79 | 0.40 |
| 1:T:34:ILE:CG2 | 1:T:68:LYS:N | 2.84 | 0.40 |
| 1:U:8:LEU:N | 1:U:102:PRO:O | 2.48 | 0.40 |
| 1:W:332:PRO:HA | 1:W:333:PRO:HD3 | 1.95 | 0.40 |
| 1:W:357:ILE:CG2 | 1:W:358:THR:N | 2.82 | 0.40 |
| 1:A:8:LEU:CD1 | 1:A:90:PHE:CD1 | 3.04 | 0.40 |
| 1:A:335:ARG:O | 1:A:338:SER:CB | 2.69 | 0.40 |
| 1:B:157:ASP:H | 2:B:401:ADP:PB | 2.45 | 0.40 |
| 1:C:35:VAL:CG1 | 1:C:35:VAL:O | 2.70 | 0.40 |
| 1:E:143:TYR:CE2 | 1:G:45:VAL:CG2 | 3.04 | 0.40 |
| 1:F:34:ILE:CG2 | 1:F:68:LYS:N | 2.84 | 0.40 |
| 1:G:38:PRO:CG | 1:G:49:GLN:NE2 | 2.79 | 0.40 |
| 1:G:335:ARG:O | 1:G:338:SER:CB | 2.69 | 0.40 |
| 1:H:47:MET:HB3 | 1:H:48:GLY:H | 1.61 | 0.40 |
| 1:H:143:TYR:CE2 | 1:J:45:VAL:CG2 | 3.04 | 0.40 |
| 1:H:164:PRO:HG2 | 1:H:174:ALA:CB | 2.51 | 0.40 |
| 1:H:169:TYR:CE2 | 1:J:40:HIS:HB2 | 2.56 | 0.40 |
| 1:H:208:ILE:CG2 | 1:H:209:VAL:N | 2.83 | 0.40 |
| 1:J:164:PRO:HG2 | 1:J:174:ALA:CB | 2.51 | 0.40 |
| 1:J:169:TYR:CE2 | 1:L:40:HIS:HB2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:157:ASP:H | 2:K:401:ADP:PB | 2.45 | 0.40 |
| 1:M:189:LEU:HA | 1:M:192:ILE:HG12 | 2.02 | 0.40 |
| 1:N:149:THR:CG2 | 1:N:150:GLY:N | 2.82 | 0.40 |
| 1:O:113:LYS:HB3 | 1:O:371:HIS:CD2 | 2.57 | 0.40 |
| 1:O:223:PHE:CZ | 1:O:266:PHE:CZ | 3.08 | 0.40 |
| 1:P:173:HIS:CE1 | 1:Q:268:GLY:N | 2.90 | 0.40 |
| 1:Q:35:VAL:CG1 | 1:Q:35:VAL:O | 2.70 | 0.40 |
| 1:Q:175:ILE:H | 1:Q:175:ILE:HG13 | 1.71 | 0.40 |
| 1:R:2:GLU:HB3 | 1:R:3:ASP:H | 1.66 | 0.40 |
| 1:R:335:ARG:O | 1:R:338:SER:CB | 2.69 | 0.40 |
| 1:S:8:LEU:CD1 | 1:S:90:PHE:CD1 | 3.04 | 0.40 |
| 1:S:169:TYR:CE2 | 1:U:40:HIS:HB2 | 2.56 | 0.40 |
| 1:T:44:MET:CG | 1:T:45:VAL:H | 2.18 | 0.40 |
| 1:T:167:GLU:OE1 | 1:V:61:LYS:HE2 | 2.20 | 0.40 |
| 1:U:173:HIS:CE1 | 1:V:268:GLY:N | 2.90 | 0.40 |
| 1:V:31:PHE:HA | 1:V:32:PRO:HD3 | 1.66 | 0.40 |
| 1:V:164:PRO:CG | 1:V:174:ALA:HB3 | 2.51 | 0.40 |
| 1:W:47:MET:HB3 | 1:W:48:GLY:H | 1.61 | 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 | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 26 |
| 1 | B | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 26 |
| 1 | C | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 26 |
| 1 | D | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 26 |
| 1 | E | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 26 |
| 1 | F | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | G | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | H | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | I | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | J | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | K | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | L | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | M | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | N | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | O | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | P | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | Q | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | R | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | S | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | T | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | U | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | V | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| 1 | W | 372/375 (99%) | 329 (88%) | 31 (8%) | 12 (3%) | 4 | 26 |
| All | All | 8556/8625 (99%) | 7567 (88%) | 713 (8%) | 276 (3%) | 7 | 26 |

All (276) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3 | ASP |
| 1 | A | 41 | GLN |
| 1 | A | 44 | MET |
| 1 | B | 3 | ASP |
| 1 | B | 41 | GLN |
| 1 | B | 44 | MET |
| 1 | C | 3 | ASP |
| 1 | C | 41 | GLN |
| 1 | C | 44 | MET |
| 1 | D | 3 | ASP |
| 1 | D | 41 | GLN |
| 1 | D | 44 | MET |
| 1 | E | 3 | ASP |
| 1 | E | 41 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 44 | MET |
| 1 | F | 3 | ASP |
| 1 | F | 41 | GLN |
| 1 | F | 44 | MET |
| 1 | G | 3 | ASP |
| 1 | G | 41 | GLN |
| 1 | G | 44 | MET |
| 1 | H | 3 | ASP |
| 1 | H | 41 | GLN |
| 1 | H | 44 | MET |
| 1 | I | 3 | ASP |
| 1 | I | 41 | GLN |
| 1 | I | 44 | MET |
| 1 | J | 3 | ASP |
| 1 | J | 41 | GLN |
| 1 | J | 44 | MET |
| 1 | K | 3 | ASP |
| 1 | K | 41 | GLN |
| 1 | K | 44 | MET |
| 1 | L | 3 | ASP |
| 1 | L | 41 | GLN |
| 1 | L | 44 | MET |
| 1 | M | 3 | ASP |
| 1 | M | 41 | GLN |
| 1 | M | 44 | MET |
| 1 | N | 3 | ASP |
| 1 | N | 41 | GLN |
| 1 | N | 44 | MET |
| 1 | O | 3 | ASP |
| 1 | O | 41 | GLN |
| 1 | O | 44 | MET |
| 1 | P | 3 | ASP |
| 1 | P | 41 | GLN |
| 1 | P | 44 | MET |
| 1 | Q | 3 | ASP |
| 1 | Q | 41 | GLN |
| 1 | Q | 44 | MET |
| 1 | R | 3 | ASP |
| 1 | R | 41 | GLN |
| 1 | R | 44 | MET |
| 1 | S | 3 | ASP |
| 1 | S | 41 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 44 | MET |
| 1 | T | 3 | ASP |
| 1 | T | 41 | GLN |
| 1 | T | 44 | MET |
| 1 | U | 3 | ASP |
| 1 | U | 41 | GLN |
| 1 | U | 44 | MET |
| 1 | V | 3 | ASP |
| 1 | V | 41 | GLN |
| 1 | V | 44 | MET |
| 1 | W | 3 | ASP |
| 1 | W | 41 | GLN |
| 1 | W | 44 | MET |
| 1 | A | 4 | GLU |
| 1 | A | 55 | GLY |
| 1 | A | 374 | CYS |
| 1 | B | 4 | GLU |
| 1 | B | 55 | GLY |
| 1 | B | 374 | CYS |
| 1 | C | 4 | GLU |
| 1 | C | 55 | GLY |
| 1 | C | 374 | CYS |
| 1 | D | 4 | GLU |
| 1 | D | 55 | GLY |
| 1 | D | 374 | CYS |
| 1 | E | 4 | GLU |
| 1 | E | 55 | GLY |
| 1 | E | 374 | CYS |
| 1 | F | 4 | GLU |
| 1 | F | 55 | GLY |
| 1 | F | 374 | CYS |
| 1 | G | 4 | GLU |
| 1 | G | 55 | GLY |
| 1 | G | 374 | CYS |
| 1 | H | 4 | GLU |
| 1 | H | 55 | GLY |
| 1 | H | 374 | CYS |
| 1 | I | 4 | GLU |
| 1 | I | 55 | GLY |
| 1 | I | 374 | CYS |
| 1 | J | 4 | GLU |
| 1 | J | 55 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 374 | CYS |
| 1 | K | 4 | GLU |
| 1 | K | 55 | GLY |
| 1 | K | 374 | CYS |
| 1 | L | 4 | GLU |
| 1 | L | 55 | GLY |
| 1 | L | 374 | CYS |
| 1 | M | 4 | GLU |
| 1 | M | 55 | GLY |
| 1 | M | 374 | CYS |
| 1 | N | 4 | GLU |
| 1 | N | 55 | GLY |
| 1 | N | 374 | CYS |
| 1 | O | 4 | GLU |
| 1 | O | 55 | GLY |
| 1 | O | 374 | CYS |
| 1 | P | 4 | GLU |
| 1 | P | 55 | GLY |
| 1 | P | 374 | CYS |
| 1 | Q | 4 | GLU |
| 1 | Q | 55 | GLY |
| 1 | Q | 374 | CYS |
| 1 | R | 4 | GLU |
| 1 | R | 55 | GLY |
| 1 | R | 374 | CYS |
| 1 | S | 4 | GLU |
| 1 | S | 55 | GLY |
| 1 | S | 374 | CYS |
| 1 | T | 4 | GLU |
| 1 | T | 55 | GLY |
| 1 | T | 374 | CYS |
| 1 | U | 4 | GLU |
| 1 | U | 55 | GLY |
| 1 | U | 374 | CYS |
| 1 | V | 4 | GLU |
| 1 | V | 55 | GLY |
| 1 | V | 374 | CYS |
| 1 | W | 4 | GLU |
| 1 | W | 55 | GLY |
| 1 | W | 374 | CYS |
| 1 | A | 2 | GLU |
| 1 | B | 2 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 2 | GLU |
| 1 | D | 2 | GLU |
| 1 | E | 2 | GLU |
| 1 | F | 2 | GLU |
| 1 | G | 2 | GLU |
| 1 | H | 2 | GLU |
| 1 | I | 2 | GLU |
| 1 | J | 2 | GLU |
| 1 | K | 2 | GLU |
| 1 | L | 2 | GLU |
| 1 | M | 2 | GLU |
| 1 | N | 2 | GLU |
| 1 | O | 2 | GLU |
| 1 | P | 2 | GLU |
| 1 | Q | 2 | GLU |
| 1 | R | 2 | GLU |
| 1 | S | 2 | GLU |
| 1 | T | 2 | GLU |
| 1 | U | 2 | GLU |
| 1 | V | 2 | GLU |
| 1 | W | 2 | GLU |
| 1 | A | 43 | VAL |
| 1 | A | 54 | VAL |
| 1 | B | 43 | VAL |
| 1 | B | 54 | VAL |
| 1 | C | 43 | VAL |
| 1 | C | 54 | VAL |
| 1 | D | 43 | VAL |
| 1 | D | 54 | VAL |
| 1 | E | 43 | VAL |
| 1 | E | 54 | VAL |
| 1 | F | 43 | VAL |
| 1 | F | 54 | VAL |
| 1 | G | 43 | VAL |
| 1 | G | 54 | VAL |
| 1 | H | 43 | VAL |
| 1 | H | 54 | VAL |
| 1 | I | 43 | VAL |
| 1 | I | 54 | VAL |
| 1 | J | 43 | VAL |
| 1 | J | 54 | VAL |
| 1 | K | 43 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 54 | VAL |
| 1 | L | 43 | VAL |
| 1 | L | 54 | VAL |
| 1 | M | 43 | VAL |
| 1 | M | 54 | VAL |
| 1 | N | 43 | VAL |
| 1 | N | 54 | VAL |
| 1 | O | 43 | VAL |
| 1 | O | 54 | VAL |
| 1 | P | 43 | VAL |
| 1 | P | 54 | VAL |
| 1 | Q | 43 | VAL |
| 1 | Q | 54 | VAL |
| 1 | R | 43 | VAL |
| 1 | R | 54 | VAL |
| 1 | S | 43 | VAL |
| 1 | S | 54 | VAL |
| 1 | T | 43 | VAL |
| 1 | T | 54 | VAL |
| 1 | U | 43 | VAL |
| 1 | U | 54 | VAL |
| 1 | V | 43 | VAL |
| 1 | V | 54 | VAL |
| 1 | W | 43 | VAL |
| 1 | W | 54 | VAL |
| 1 | A | 58 | ALA |
| 1 | B | 58 | ALA |
| 1 | C | 58 | ALA |
| 1 | E | 58 | ALA |
| 1 | F | 58 | ALA |
| 1 | H | 58 | ALA |
| 1 | M | 58 | ALA |
| 1 | N | 58 | ALA |
| 1 | S | 58 | ALA |
| 1 | T | 58 | ALA |
| 1 | U | 58 | ALA |
| 1 | D | 58 | ALA |
| 1 | G | 58 | ALA |
| 1 | I | 58 | ALA |
| 1 | J | 58 | ALA |
| 1 | K | 58 | ALA |
| 1 | L | 58 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 58 | ALA |
| 1 | P | 58 | ALA |
| 1 | Q | 58 | ALA |
| 1 | R | 58 | ALA |
| 1 | V | 58 | ALA |
| 1 | W | 58 | ALA |
| 1 | A | 45 | VAL |
| 1 | B | 45 | VAL |
| 1 | E | 45 | VAL |
| 1 | F | 45 | VAL |
| 1 | G | 45 | VAL |
| 1 | H | 45 | VAL |
| 1 | I | 45 | VAL |
| 1 | J | 45 | VAL |
| 1 | K | 45 | VAL |
| 1 | M | 45 | VAL |
| 1 | N | 45 | VAL |
| 1 | O | 45 | VAL |
| 1 | P | 45 | VAL |
| 1 | R | 45 | VAL |
| 1 | S | 45 | VAL |
| 1 | T | 45 | VAL |
| 1 | U | 45 | VAL |
| 1 | V | 45 | VAL |
| 1 | W | 45 | VAL |
| 1 | C | 45 | VAL |
| 1 | D | 45 | VAL |
| 1 | L | 45 | VAL |
| 1 | Q | 45 | VAL |
| 1 | A | 370 | VAL |
| 1 | B | 370 | VAL |
| 1 | C | 370 | VAL |
| 1 | D | 370 | VAL |
| 1 | E | 370 | VAL |
| 1 | F | 370 | VAL |
| 1 | G | 370 | VAL |
| 1 | H | 370 | VAL |
| 1 | I | 370 | VAL |
| 1 | J | 370 | VAL |
| 1 | K | 370 | VAL |
| 1 | L | 370 | VAL |
| 1 | M | 370 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 370 | VAL |
| 1 | O | 370 | VAL |
| 1 | P | 370 | VAL |
| 1 | Q | 370 | VAL |
| 1 | R | 370 | VAL |
| 1 | S | 370 | VAL |
| 1 | T | 370 | VAL |
| 1 | U | 370 | VAL |
| 1 | V | 370 | VAL |
| 1 | W | 370 | VAL |

### 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 | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | B | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | C | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | D | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | E | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | F | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | G | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | H | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | I | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | J | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | K | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | L | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | M | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | N | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | O | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |
| 1 | P | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | Q | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 | 21 |
| 1 | R | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 | 21 |
| 1 | S | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 | 21 |
| 1 | T | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 | 21 |
| 1 | U | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 | 21 |
| 1 | V | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 | 21 |
| 1 | W | 317/317 (100%) | 280 (88%) | 37 (12%) | 5 | 21 |
| All | All | 7291/7291 (100%) | 6440 (88%) | 851 (12%) | 9 | 21 |

All (851) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 8 | LEU |
| 1 | A | 33 | SER |
| 1 | A | 35 | VAL |
| 1 | A | 37 | ARG |
| 1 | A | 45 | VAL |
| 1 | A | 49 | GLN |
| 1 | A | 51 | ASP |
| 1 | A | 56 | ASP |
| 1 | A | 57 | GLU |
| 1 | A | 66 | THR |
| 1 | A | 68 | LYS |
| 1 | A | 113 | LYS |
| 1 | A | 132 | MET |
| 1 | A | 141 | SER |
| 1 | A | 143 | TYR |
| 1 | A | 145 | SER |
| 1 | A | 147 | ARG |
| 1 | A | 148 | THR |
| 1 | A | 149 | THR |
| 1 | A | 167 | GLU |
| 1 | A | 171 | LEU |
| 1 | A | 176 | MET |
| 1 | A | 179 | ASP |
| 1 | A | 180 | LEU |
| 1 | A | 183 | ARG |
| 1 | A | 208 | ILE |
| 1 | A | 232 | SER |
| 1 | A | 236 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 244 | ASP |
| 1 | A | 269 | MET |
| 1 | A | 286 | ASP |
| 1 | A | 335 | ARG |
| 1 | A | 350 | SER |
| 1 | A | 357 | ILE |
| 1 | A | 370 | VAL |
| 1 | A | 372 | ARG |
| 1 | A | 373 | LYS |
| 1 | B | 8 | LEU |
| 1 | B | 33 | SER |
| 1 | B | 35 | VAL |
| 1 | B | 37 | ARG |
| 1 | B | 45 | VAL |
| 1 | B | 49 | GLN |
| 1 | B | 51 | ASP |
| 1 | B | 56 | ASP |
| 1 | B | 57 | GLU |
| 1 | B | 66 | THR |
| 1 | B | 68 | LYS |
| 1 | B | 113 | LYS |
| 1 | B | 132 | MET |
| 1 | B | 141 | SER |
| 1 | B | 143 | TYR |
| 1 | B | 145 | SER |
| 1 | B | 147 | ARG |
| 1 | B | 148 | THR |
| 1 | B | 149 | THR |
| 1 | B | 167 | GLU |
| 1 | B | 171 | LEU |
| 1 | B | 176 | MET |
| 1 | B | 179 | ASP |
| 1 | B | 180 | LEU |
| 1 | B | 183 | ARG |
| 1 | B | 208 | ILE |
| 1 | B | 232 | SER |
| 1 | B | 236 | LEU |
| 1 | B | 244 | ASP |
| 1 | B | 269 | MET |
| 1 | B | 286 | ASP |
| 1 | B | 335 | ARG |
| 1 | B | 350 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 357 | ILE |
| 1 | B | 370 | VAL |
| 1 | B | 372 | ARG |
| 1 | B | 373 | LYS |
| 1 | C | 8 | LEU |
| 1 | C | 33 | SER |
| 1 | C | 35 | VAL |
| 1 | C | 37 | ARG |
| 1 | C | 45 | VAL |
| 1 | C | 49 | GLN |
| 1 | C | 51 | ASP |
| 1 | C | 56 | ASP |
| 1 | C | 57 | GLU |
| 1 | C | 66 | THR |
| 1 | C | 68 | LYS |
| 1 | C | 113 | LYS |
| 1 | C | 132 | MET |
| 1 | C | 141 | SER |
| 1 | C | 143 | TYR |
| 1 | C | 145 | SER |
| 1 | C | 147 | ARG |
| 1 | C | 148 | THR |
| 1 | C | 149 | THR |
| 1 | C | 167 | GLU |
| 1 | C | 171 | LEU |
| 1 | C | 176 | MET |
| 1 | C | 179 | ASP |
| 1 | C | 180 | LEU |
| 1 | C | 183 | ARG |
| 1 | C | 208 | ILE |
| 1 | C | 232 | SER |
| 1 | C | 236 | LEU |
| 1 | C | 244 | ASP |
| 1 | C | 269 | MET |
| 1 | C | 286 | ASP |
| 1 | C | 335 | ARG |
| 1 | C | 350 | SER |
| 1 | C | 357 | ILE |
| 1 | C | 370 | VAL |
| 1 | C | 372 | ARG |
| 1 | C | 373 | LYS |
| 1 | D | 8 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 33 | SER |
| 1 | D | 35 | VAL |
| 1 | D | 37 | ARG |
| 1 | D | 45 | VAL |
| 1 | D | 49 | GLN |
| 1 | D | 51 | ASP |
| 1 | D | 56 | ASP |
| 1 | D | 57 | GLU |
| 1 | D | 66 | THR |
| 1 | D | 68 | LYS |
| 1 | D | 113 | LYS |
| 1 | D | 132 | MET |
| 1 | D | 141 | SER |
| 1 | D | 143 | TYR |
| 1 | D | 145 | SER |
| 1 | D | 147 | ARG |
| 1 | D | 148 | THR |
| 1 | D | 149 | THR |
| 1 | D | 167 | GLU |
| 1 | D | 171 | LEU |
| 1 | D | 176 | MET |
| 1 | D | 179 | ASP |
| 1 | D | 180 | LEU |
| 1 | D | 183 | ARG |
| 1 | D | 208 | ILE |
| 1 | D | 232 | SER |
| 1 | D | 236 | LEU |
| 1 | D | 244 | ASP |
| 1 | D | 269 | MET |
| 1 | D | 286 | ASP |
| 1 | D | 335 | ARG |
| 1 | D | 350 | SER |
| 1 | D | 357 | ILE |
| 1 | D | 370 | VAL |
| 1 | D | 372 | ARG |
| 1 | D | 373 | LYS |
| 1 | E | 8 | LEU |
| 1 | E | 33 | SER |
| 1 | E | 35 | VAL |
| 1 | E | 37 | ARG |
| 1 | E | 45 | VAL |
| 1 | E | 49 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 51 | ASP |
| 1 | E | 56 | ASP |
| 1 | E | 57 | GLU |
| 1 | E | 66 | THR |
| 1 | E | 68 | LYS |
| 1 | E | 113 | LYS |
| 1 | E | 132 | MET |
| 1 | E | 141 | SER |
| 1 | E | 143 | TYR |
| 1 | E | 145 | SER |
| 1 | E | 147 | ARG |
| 1 | E | 148 | THR |
| 1 | E | 149 | THR |
| 1 | E | 167 | GLU |
| 1 | E | 171 | LEU |
| 1 | E | 176 | MET |
| 1 | E | 179 | ASP |
| 1 | E | 180 | LEU |
| 1 | E | 183 | ARG |
| 1 | E | 208 | ILE |
| 1 | E | 232 | SER |
| 1 | E | 236 | LEU |
| 1 | E | 244 | ASP |
| 1 | E | 269 | MET |
| 1 | E | 286 | ASP |
| 1 | E | 335 | ARG |
| 1 | E | 350 | SER |
| 1 | E | 357 | ILE |
| 1 | E | 370 | VAL |
| 1 | E | 372 | ARG |
| 1 | E | 373 | LYS |
| 1 | F | 8 | LEU |
| 1 | F | 33 | SER |
| 1 | F | 35 | VAL |
| 1 | F | 37 | ARG |
| 1 | F | 45 | VAL |
| 1 | F | 49 | GLN |
| 1 | F | 51 | ASP |
| 1 | F | 56 | ASP |
| 1 | F | 57 | GLU |
| 1 | F | 66 | THR |
| 1 | F | 68 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 113 | LYS |
| 1 | F | 132 | MET |
| 1 | F | 141 | SER |
| 1 | F | 143 | TYR |
| 1 | F | 145 | SER |
| 1 | F | 147 | ARG |
| 1 | F | 148 | THR |
| 1 | F | 149 | THR |
| 1 | F | 167 | GLU |
| 1 | F | 171 | LEU |
| 1 | F | 176 | MET |
| 1 | F | 179 | ASP |
| 1 | F | 180 | LEU |
| 1 | F | 183 | ARG |
| 1 | F | 208 | ILE |
| 1 | F | 232 | SER |
| 1 | F | 236 | LEU |
| 1 | F | 244 | ASP |
| 1 | F | 269 | MET |
| 1 | F | 286 | ASP |
| 1 | F | 335 | ARG |
| 1 | F | 350 | SER |
| 1 | F | 357 | ILE |
| 1 | F | 370 | VAL |
| 1 | F | 372 | ARG |
| 1 | F | 373 | LYS |
| 1 | G | 8 | LEU |
| 1 | G | 33 | SER |
| 1 | G | 35 | VAL |
| 1 | G | 37 | ARG |
| 1 | G | 45 | VAL |
| 1 | G | 49 | GLN |
| 1 | G | 51 | ASP |
| 1 | G | 56 | ASP |
| 1 | G | 57 | GLU |
| 1 | G | 66 | THR |
| 1 | G | 68 | LYS |
| 1 | G | 113 | LYS |
| 1 | G | 132 | MET |
| 1 | G | 141 | SER |
| 1 | G | 143 | TYR |
| 1 | G | 145 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 147 | ARG |
| 1 | G | 148 | THR |
| 1 | G | 149 | THR |
| 1 | G | 167 | GLU |
| 1 | G | 171 | LEU |
| 1 | G | 176 | MET |
| 1 | G | 179 | ASP |
| 1 | G | 180 | LEU |
| 1 | G | 183 | ARG |
| 1 | G | 208 | ILE |
| 1 | G | 232 | SER |
| 1 | G | 236 | LEU |
| 1 | G | 244 | ASP |
| 1 | G | 269 | MET |
| 1 | G | 286 | ASP |
| 1 | G | 335 | ARG |
| 1 | G | 350 | SER |
| 1 | G | 357 | ILE |
| 1 | G | 370 | VAL |
| 1 | G | 372 | ARG |
| 1 | G | 373 | LYS |
| 1 | H | 8 | LEU |
| 1 | H | 33 | SER |
| 1 | H | 35 | VAL |
| 1 | H | 37 | ARG |
| 1 | H | 45 | VAL |
| 1 | H | 49 | GLN |
| 1 | H | 51 | ASP |
| 1 | H | 56 | ASP |
| 1 | H | 57 | GLU |
| 1 | H | 66 | THR |
| 1 | H | 68 | LYS |
| 1 | H | 113 | LYS |
| 1 | H | 132 | MET |
| 1 | H | 141 | SER |
| 1 | H | 143 | TYR |
| 1 | H | 145 | SER |
| 1 | H | 147 | ARG |
| 1 | H | 148 | THR |
| 1 | H | 149 | THR |
| 1 | H | 167 | GLU |
| 1 | H | 171 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 176 | MET |
| 1 | H | 179 | ASP |
| 1 | H | 180 | LEU |
| 1 | H | 183 | ARG |
| 1 | H | 208 | ILE |
| 1 | H | 232 | SER |
| 1 | H | 236 | LEU |
| 1 | H | 244 | ASP |
| 1 | H | 269 | MET |
| 1 | H | 286 | ASP |
| 1 | H | 335 | ARG |
| 1 | H | 350 | SER |
| 1 | H | 357 | ILE |
| 1 | H | 370 | VAL |
| 1 | H | 372 | ARG |
| 1 | H | 373 | LYS |
| 1 | I | 8 | LEU |
| 1 | I | 33 | SER |
| 1 | I | 35 | VAL |
| 1 | I | 37 | ARG |
| 1 | I | 45 | VAL |
| 1 | I | 49 | GLN |
| 1 | I | 51 | ASP |
| 1 | I | 56 | ASP |
| 1 | I | 57 | GLU |
| 1 | I | 66 | THR |
| 1 | I | 68 | LYS |
| 1 | I | 113 | LYS |
| 1 | I | 132 | MET |
| 1 | I | 141 | SER |
| 1 | I | 143 | TYR |
| 1 | I | 145 | SER |
| 1 | I | 147 | ARG |
| 1 | I | 148 | THR |
| 1 | I | 149 | THR |
| 1 | I | 167 | GLU |
| 1 | I | 171 | LEU |
| 1 | I | 176 | MET |
| 1 | I | 179 | ASP |
| 1 | I | 180 | LEU |
| 1 | I | 183 | ARG |
| 1 | I | 208 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 232 | SER |
| 1 | I | 236 | LEU |
| 1 | I | 244 | ASP |
| 1 | I | 269 | MET |
| 1 | I | 286 | ASP |
| 1 | I | 335 | ARG |
| 1 | I | 350 | SER |
| 1 | I | 357 | ILE |
| 1 | I | 370 | VAL |
| 1 | I | 372 | ARG |
| 1 | I | 373 | LYS |
| 1 | J | 8 | LEU |
| 1 | J | 33 | SER |
| 1 | J | 35 | VAL |
| 1 | J | 37 | ARG |
| 1 | J | 45 | VAL |
| 1 | J | 49 | GLN |
| 1 | J | 51 | ASP |
| 1 | J | 56 | ASP |
| 1 | J | 57 | GLU |
| 1 | J | 66 | THR |
| 1 | J | 68 | LYS |
| 1 | J | 113 | LYS |
| 1 | J | 132 | MET |
| 1 | J | 141 | SER |
| 1 | J | 143 | TYR |
| 1 | J | 145 | SER |
| 1 | J | 147 | ARG |
| 1 | J | 148 | THR |
| 1 | J | 149 | THR |
| 1 | J | 167 | GLU |
| 1 | J | 171 | LEU |
| 1 | J | 176 | MET |
| 1 | J | 179 | ASP |
| 1 | J | 180 | LEU |
| 1 | J | 183 | ARG |
| 1 | J | 208 | ILE |
| 1 | J | 232 | SER |
| 1 | J | 236 | LEU |
| 1 | J | 244 | ASP |
| 1 | J | 269 | MET |
| 1 | J | 286 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 335 | ARG |
| 1 | J | 350 | SER |
| 1 | J | 357 | ILE |
| 1 | J | 370 | VAL |
| 1 | J | 372 | ARG |
| 1 | J | 373 | LYS |
| 1 | K | 8 | LEU |
| 1 | K | 33 | SER |
| 1 | K | 35 | VAL |
| 1 | K | 37 | ARG |
| 1 | K | 45 | VAL |
| 1 | K | 49 | GLN |
| 1 | K | 51 | ASP |
| 1 | K | 56 | ASP |
| 1 | K | 57 | GLU |
| 1 | K | 66 | THR |
| 1 | K | 68 | LYS |
| 1 | K | 113 | LYS |
| 1 | K | 132 | MET |
| 1 | K | 141 | SER |
| 1 | K | 143 | TYR |
| 1 | K | 145 | SER |
| 1 | K | 147 | ARG |
| 1 | K | 148 | THR |
| 1 | K | 149 | THR |
| 1 | K | 167 | GLU |
| 1 | K | 171 | LEU |
| 1 | K | 176 | MET |
| 1 | K | 179 | ASP |
| 1 | K | 180 | LEU |
| 1 | K | 183 | ARG |
| 1 | K | 208 | ILE |
| 1 | K | 232 | SER |
| 1 | K | 236 | LEU |
| 1 | K | 244 | ASP |
| 1 | K | 269 | MET |
| 1 | K | 286 | ASP |
| 1 | K | 335 | ARG |
| 1 | K | 350 | SER |
| 1 | K | 357 | ILE |
| 1 | K | 370 | VAL |
| 1 | K | 372 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 373 | LYS |
| 1 | L | 8 | LEU |
| 1 | L | 33 | SER |
| 1 | L | 35 | VAL |
| 1 | L | 37 | ARG |
| 1 | L | 45 | VAL |
| 1 | L | 49 | GLN |
| 1 | L | 51 | ASP |
| 1 | L | 56 | ASP |
| 1 | L | 57 | GLU |
| 1 | L | 66 | THR |
| 1 | L | 68 | LYS |
| 1 | L | 113 | LYS |
| 1 | L | 132 | MET |
| 1 | L | 141 | SER |
| 1 | L | 143 | TYR |
| 1 | L | 145 | SER |
| 1 | L | 147 | ARG |
| 1 | L | 148 | THR |
| 1 | L | 149 | THR |
| 1 | L | 167 | GLU |
| 1 | L | 171 | LEU |
| 1 | L | 176 | MET |
| 1 | L | 179 | ASP |
| 1 | L | 180 | LEU |
| 1 | L | 183 | ARG |
| 1 | L | 208 | ILE |
| 1 | L | 232 | SER |
| 1 | L | 236 | LEU |
| 1 | L | 244 | ASP |
| 1 | L | 269 | MET |
| 1 | L | 286 | ASP |
| 1 | L | 335 | ARG |
| 1 | L | 350 | SER |
| 1 | L | 357 | ILE |
| 1 | L | 370 | VAL |
| 1 | L | 372 | ARG |
| 1 | L | 373 | LYS |
| 1 | M | 8 | LEU |
| 1 | M | 33 | SER |
| 1 | M | 35 | VAL |
| 1 | M | 37 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 45 | VAL |
| 1 | M | 49 | GLN |
| 1 | M | 51 | ASP |
| 1 | M | 56 | ASP |
| 1 | M | 57 | GLU |
| 1 | M | 66 | THR |
| 1 | M | 68 | LYS |
| 1 | M | 113 | LYS |
| 1 | M | 132 | MET |
| 1 | M | 141 | SER |
| 1 | M | 143 | TYR |
| 1 | M | 145 | SER |
| 1 | M | 147 | ARG |
| 1 | M | 148 | THR |
| 1 | M | 149 | THR |
| 1 | M | 167 | GLU |
| 1 | M | 171 | LEU |
| 1 | M | 176 | MET |
| 1 | M | 179 | ASP |
| 1 | M | 180 | LEU |
| 1 | M | 183 | ARG |
| 1 | M | 208 | ILE |
| 1 | M | 232 | SER |
| 1 | M | 236 | LEU |
| 1 | M | 244 | ASP |
| 1 | M | 269 | MET |
| 1 | M | 286 | ASP |
| 1 | M | 335 | ARG |
| 1 | M | 350 | SER |
| 1 | M | 357 | ILE |
| 1 | M | 370 | VAL |
| 1 | M | 372 | ARG |
| 1 | M | 373 | LYS |
| 1 | N | 8 | LEU |
| 1 | N | 33 | SER |
| 1 | N | 35 | VAL |
| 1 | N | 37 | ARG |
| 1 | N | 45 | VAL |
| 1 | N | 49 | GLN |
| 1 | N | 51 | ASP |
| 1 | N | 56 | ASP |
| 1 | N | 57 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 66 | THR |
| 1 | N | 68 | LYS |
| 1 | N | 113 | LYS |
| 1 | N | 132 | MET |
| 1 | N | 141 | SER |
| 1 | N | 143 | TYR |
| 1 | N | 145 | SER |
| 1 | N | 147 | ARG |
| 1 | N | 148 | THR |
| 1 | N | 149 | THR |
| 1 | N | 167 | GLU |
| 1 | N | 171 | LEU |
| 1 | N | 176 | MET |
| 1 | N | 179 | ASP |
| 1 | N | 180 | LEU |
| 1 | N | 183 | ARG |
| 1 | N | 208 | ILE |
| 1 | N | 232 | SER |
| 1 | N | 236 | LEU |
| 1 | N | 244 | ASP |
| 1 | N | 269 | MET |
| 1 | N | 286 | ASP |
| 1 | N | 335 | ARG |
| 1 | N | 350 | SER |
| 1 | N | 357 | ILE |
| 1 | N | 370 | VAL |
| 1 | N | 372 | ARG |
| 1 | N | 373 | LYS |
| 1 | O | 8 | LEU |
| 1 | O | 33 | SER |
| 1 | O | 35 | VAL |
| 1 | O | 37 | ARG |
| 1 | O | 45 | VAL |
| 1 | O | 49 | GLN |
| 1 | O | 51 | ASP |
| 1 | O | 56 | ASP |
| 1 | O | 57 | GLU |
| 1 | O | 66 | THR |
| 1 | O | 68 | LYS |
| 1 | O | 113 | LYS |
| 1 | O | 132 | MET |
| 1 | O | 141 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 143 | TYR |
| 1 | O | 145 | SER |
| 1 | O | 147 | ARG |
| 1 | O | 148 | THR |
| 1 | O | 149 | THR |
| 1 | O | 167 | GLU |
| 1 | O | 171 | LEU |
| 1 | O | 176 | MET |
| 1 | O | 179 | ASP |
| 1 | O | 180 | LEU |
| 1 | O | 183 | ARG |
| 1 | O | 208 | ILE |
| 1 | O | 232 | SER |
| 1 | O | 236 | LEU |
| 1 | O | 244 | ASP |
| 1 | O | 269 | MET |
| 1 | O | 286 | ASP |
| 1 | O | 335 | ARG |
| 1 | O | 350 | SER |
| 1 | O | 357 | ILE |
| 1 | O | 370 | VAL |
| 1 | O | 372 | ARG |
| 1 | O | 373 | LYS |
| 1 | P | 8 | LEU |
| 1 | P | 33 | SER |
| 1 | P | 35 | VAL |
| 1 | P | 37 | ARG |
| 1 | P | 45 | VAL |
| 1 | P | 49 | GLN |
| 1 | P | 51 | ASP |
| 1 | P | 56 | ASP |
| 1 | P | 57 | GLU |
| 1 | P | 66 | THR |
| 1 | P | 68 | LYS |
| 1 | P | 113 | LYS |
| 1 | P | 132 | MET |
| 1 | P | 141 | SER |
| 1 | P | 143 | TYR |
| 1 | P | 145 | SER |
| 1 | P | 147 | ARG |
| 1 | P | 148 | THR |
| 1 | P | 149 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 167 | GLU |
| 1 | P | 171 | LEU |
| 1 | P | 176 | MET |
| 1 | P | 179 | ASP |
| 1 | P | 180 | LEU |
| 1 | P | 183 | ARG |
| 1 | P | 208 | ILE |
| 1 | P | 232 | SER |
| 1 | P | 236 | LEU |
| 1 | P | 244 | ASP |
| 1 | P | 269 | MET |
| 1 | P | 286 | ASP |
| 1 | P | 335 | ARG |
| 1 | P | 350 | SER |
| 1 | P | 357 | ILE |
| 1 | P | 370 | VAL |
| 1 | P | 372 | ARG |
| 1 | P | 373 | LYS |
| 1 | Q | 8 | LEU |
| 1 | Q | 33 | SER |
| 1 | Q | 35 | VAL |
| 1 | Q | 37 | ARG |
| 1 | Q | 45 | VAL |
| 1 | Q | 49 | GLN |
| 1 | Q | 51 | ASP |
| 1 | Q | 56 | ASP |
| 1 | Q | 57 | GLU |
| 1 | Q | 66 | THR |
| 1 | Q | 68 | LYS |
| 1 | Q | 113 | LYS |
| 1 | Q | 132 | MET |
| 1 | Q | 141 | SER |
| 1 | Q | 143 | TYR |
| 1 | Q | 145 | SER |
| 1 | Q | 147 | ARG |
| 1 | Q | 148 | THR |
| 1 | Q | 149 | THR |
| 1 | Q | 167 | GLU |
| 1 | Q | 171 | LEU |
| 1 | Q | 176 | MET |
| 1 | Q | 179 | ASP |
| 1 | Q | 180 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Q | 183 | ARG |
| 1 | Q | 208 | ILE |
| 1 | Q | 232 | SER |
| 1 | Q | 236 | LEU |
| 1 | Q | 244 | ASP |
| 1 | Q | 269 | MET |
| 1 | Q | 286 | ASP |
| 1 | Q | 335 | ARG |
| 1 | Q | 350 | SER |
| 1 | Q | 357 | ILE |
| 1 | Q | 370 | VAL |
| 1 | Q | 372 | ARG |
| 1 | Q | 373 | LYS |
| 1 | R | 8 | LEU |
| 1 | R | 33 | SER |
| 1 | R | 35 | VAL |
| 1 | R | 37 | ARG |
| 1 | R | 45 | VAL |
| 1 | R | 49 | GLN |
| 1 | R | 51 | ASP |
| 1 | R | 56 | ASP |
| 1 | R | 57 | GLU |
| 1 | R | 66 | THR |
| 1 | R | 68 | LYS |
| 1 | R | 113 | LYS |
| 1 | R | 132 | MET |
| 1 | R | 141 | SER |
| 1 | R | 143 | TYR |
| 1 | R | 145 | SER |
| 1 | R | 147 | ARG |
| 1 | R | 148 | THR |
| 1 | R | 149 | THR |
| 1 | R | 167 | GLU |
| 1 | R | 171 | LEU |
| 1 | R | 176 | MET |
| 1 | R | 179 | ASP |
| 1 | R | 180 | LEU |
| 1 | R | 183 | ARG |
| 1 | R | 208 | ILE |
| 1 | R | 232 | SER |
| 1 | R | 236 | LEU |
| 1 | R | 244 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | R | 269 | MET |
| 1 | R | 286 | ASP |
| 1 | R | 335 | ARG |
| 1 | R | 350 | SER |
| 1 | R | 357 | ILE |
| 1 | R | 370 | VAL |
| 1 | R | 372 | ARG |
| 1 | R | 373 | LYS |
| 1 | S | 8 | LEU |
| 1 | S | 33 | SER |
| 1 | S | 35 | VAL |
| 1 | S | 37 | ARG |
| 1 | S | 45 | VAL |
| 1 | S | 49 | GLN |
| 1 | S | 51 | ASP |
| 1 | S | 56 | ASP |
| 1 | S | 57 | GLU |
| 1 | S | 66 | THR |
| 1 | S | 68 | LYS |
| 1 | S | 113 | LYS |
| 1 | S | 132 | MET |
| 1 | S | 141 | SER |
| 1 | S | 143 | TYR |
| 1 | S | 145 | SER |
| 1 | S | 147 | ARG |
| 1 | S | 148 | THR |
| 1 | S | 149 | THR |
| 1 | S | 167 | GLU |
| 1 | S | 171 | LEU |
| 1 | S | 176 | MET |
| 1 | S | 179 | ASP |
| 1 | S | 180 | LEU |
| 1 | S | 183 | ARG |
| 1 | S | 208 | ILE |
| 1 | S | 232 | SER |
| 1 | S | 236 | LEU |
| 1 | S | 244 | ASP |
| 1 | S | 269 | MET |
| 1 | S | 286 | ASP |
| 1 | S | 335 | ARG |
| 1 | S | 350 | SER |
| 1 | S | 357 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 370 | VAL |
| 1 | S | 372 | ARG |
| 1 | S | 373 | LYS |
| 1 | T | 8 | LEU |
| 1 | T | 33 | SER |
| 1 | T | 35 | VAL |
| 1 | T | 37 | ARG |
| 1 | T | 45 | VAL |
| 1 | T | 49 | GLN |
| 1 | T | 51 | ASP |
| 1 | T | 56 | ASP |
| 1 | T | 57 | GLU |
| 1 | T | 66 | THR |
| 1 | T | 68 | LYS |
| 1 | T | 113 | LYS |
| 1 | T | 132 | MET |
| 1 | T | 141 | SER |
| 1 | T | 143 | TYR |
| 1 | T | 145 | SER |
| 1 | T | 147 | ARG |
| 1 | T | 148 | THR |
| 1 | T | 149 | THR |
| 1 | T | 167 | GLU |
| 1 | T | 171 | LEU |
| 1 | T | 176 | MET |
| 1 | T | 179 | ASP |
| 1 | T | 180 | LEU |
| 1 | T | 183 | ARG |
| 1 | T | 208 | ILE |
| 1 | T | 232 | SER |
| 1 | T | 236 | LEU |
| 1 | T | 244 | ASP |
| 1 | T | 269 | MET |
| 1 | T | 286 | ASP |
| 1 | T | 335 | ARG |
| 1 | T | 350 | SER |
| 1 | T | 357 | ILE |
| 1 | T | 370 | VAL |
| 1 | T | 372 | ARG |
| 1 | T | 373 | LYS |
| 1 | U | 8 | LEU |
| 1 | U | 33 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | U | 35 | VAL |
| 1 | U | 37 | ARG |
| 1 | U | 45 | VAL |
| 1 | U | 49 | GLN |
| 1 | U | 51 | ASP |
| 1 | U | 56 | ASP |
| 1 | U | 57 | GLU |
| 1 | U | 66 | THR |
| 1 | U | 68 | LYS |
| 1 | U | 113 | LYS |
| 1 | U | 132 | MET |
| 1 | U | 141 | SER |
| 1 | U | 143 | TYR |
| 1 | U | 145 | SER |
| 1 | U | 147 | ARG |
| 1 | U | 148 | THR |
| 1 | U | 149 | THR |
| 1 | U | 167 | GLU |
| 1 | U | 171 | LEU |
| 1 | U | 176 | MET |
| 1 | U | 179 | ASP |
| 1 | U | 180 | LEU |
| 1 | U | 183 | ARG |
| 1 | U | 208 | ILE |
| 1 | U | 232 | SER |
| 1 | U | 236 | LEU |
| 1 | U | 244 | ASP |
| 1 | U | 269 | MET |
| 1 | U | 286 | ASP |
| 1 | U | 335 | ARG |
| 1 | U | 350 | SER |
| 1 | U | 357 | ILE |
| 1 | U | 370 | VAL |
| 1 | U | 372 | ARG |
| 1 | U | 373 | LYS |
| 1 | V | 8 | LEU |
| 1 | V | 33 | SER |
| 1 | V | 35 | VAL |
| 1 | V | 37 | ARG |
| 1 | V | 45 | VAL |
| 1 | V | 49 | GLN |
| 1 | V | 51 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | V | 56 | ASP |
| 1 | V | 57 | GLU |
| 1 | V | 66 | THR |
| 1 | V | 68 | LYS |
| 1 | V | 113 | LYS |
| 1 | V | 132 | MET |
| 1 | V | 141 | SER |
| 1 | V | 143 | TYR |
| 1 | V | 145 | SER |
| 1 | V | 147 | ARG |
| 1 | V | 148 | THR |
| 1 | V | 149 | THR |
| 1 | V | 167 | GLU |
| 1 | V | 171 | LEU |
| 1 | V | 176 | MET |
| 1 | V | 179 | ASP |
| 1 | V | 180 | LEU |
| 1 | V | 183 | ARG |
| 1 | V | 208 | ILE |
| 1 | V | 232 | SER |
| 1 | V | 236 | LEU |
| 1 | V | 244 | ASP |
| 1 | V | 269 | MET |
| 1 | V | 286 | ASP |
| 1 | V | 335 | ARG |
| 1 | V | 350 | SER |
| 1 | V | 357 | ILE |
| 1 | V | 370 | VAL |
| 1 | V | 372 | ARG |
| 1 | V | 373 | LYS |
| 1 | W | 8 | LEU |
| 1 | W | 33 | SER |
| 1 | W | 35 | VAL |
| 1 | W | 37 | ARG |
| 1 | W | 45 | VAL |
| 1 | W | 49 | GLN |
| 1 | W | 51 | ASP |
| 1 | W | 56 | ASP |
| 1 | W | 57 | GLU |
| 1 | W | 66 | THR |
| 1 | W | 68 | LYS |
| 1 | W | 113 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | W | 132 | MET |
| 1 | W | 141 | SER |
| 1 | W | 143 | TYR |
| 1 | W | 145 | SER |
| 1 | W | 147 | ARG |
| 1 | W | 148 | THR |
| 1 | W | 149 | THR |
| 1 | W | 167 | GLU |
| 1 | W | 171 | LEU |
| 1 | W | 176 | MET |
| 1 | W | 179 | ASP |
| 1 | W | 180 | LEU |
| 1 | W | 183 | ARG |
| 1 | W | 208 | ILE |
| 1 | W | 232 | SER |
| 1 | W | 236 | LEU |
| 1 | W | 244 | ASP |
| 1 | W | 269 | MET |
| 1 | W | 286 | ASP |
| 1 | W | 335 | ARG |
| 1 | W | 350 | SER |
| 1 | W | 357 | ILE |
| 1 | W | 370 | VAL |
| 1 | W | 372 | ARG |
| 1 | W | 373 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 49 | GLN |
| 1 | A | 59 | GLN |
| 1 | A | 92 | ASN |
| 1 | A | 121 | GLN |
| 1 | A | 173 | HIS |
| 1 | A | 353 | GLN |
| 1 | B | 49 | GLN |
| 1 | B | 59 | GLN |
| 1 | B | 92 | ASN |
| 1 | B | 121 | GLN |
| 1 | B | 173 | HIS |
| 1 | B | 353 | GLN |
| 1 | C | 49 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 59 | GLN |
| 1 | C | 92 | ASN |
| 1 | C | 121 | GLN |
| 1 | C | 173 | HIS |
| 1 | C | 353 | GLN |
| 1 | D | 49 | GLN |
| 1 | D | 59 | GLN |
| 1 | D | 92 | ASN |
| 1 | D | 121 | GLN |
| 1 | D | 353 | GLN |
| 1 | E | 49 | GLN |
| 1 | E | 59 | GLN |
| 1 | E | 92 | ASN |
| 1 | E | 121 | GLN |
| 1 | E | 173 | HIS |
| 1 | E | 353 | GLN |
| 1 | F | 49 | GLN |
| 1 | F | 59 | GLN |
| 1 | F | 92 | ASN |
| 1 | F | 121 | GLN |
| 1 | F | 173 | HIS |
| 1 | F | 353 | GLN |
| 1 | G | 49 | GLN |
| 1 | G | 59 | GLN |
| 1 | G | 92 | ASN |
| 1 | G | 121 | GLN |
| 1 | G | 173 | HIS |
| 1 | G | 353 | GLN |
| 1 | H | 49 | GLN |
| 1 | H | 59 | GLN |
| 1 | H | 92 | ASN |
| 1 | H | 121 | GLN |
| 1 | H | 173 | HIS |
| 1 | H | 353 | GLN |
| 1 | I | 49 | GLN |
| 1 | I | 59 | GLN |
| 1 | I | 92 | ASN |
| 1 | I | 121 | GLN |
| 1 | I | 173 | HIS |
| 1 | I | 353 | GLN |
| 1 | J | 49 | GLN |
| 1 | J | 59 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 92 | ASN |
| 1 | J | 121 | GLN |
| 1 | J | 173 | HIS |
| 1 | J | 353 | GLN |
| 1 | K | 49 | GLN |
| 1 | K | 59 | GLN |
| 1 | K | 92 | ASN |
| 1 | K | 121 | GLN |
| 1 | K | 173 | HIS |
| 1 | K | 353 | GLN |
| 1 | L | 49 | GLN |
| 1 | L | 59 | GLN |
| 1 | L | 92 | ASN |
| 1 | L | 121 | GLN |
| 1 | L | 173 | HIS |
| 1 | L | 353 | GLN |
| 1 | M | 49 | GLN |
| 1 | M | 59 | GLN |
| 1 | M | 92 | ASN |
| 1 | M | 121 | GLN |
| 1 | M | 173 | HIS |
| 1 | M | 353 | GLN |
| 1 | N | 49 | GLN |
| 1 | N | 59 | GLN |
| 1 | N | 92 | ASN |
| 1 | N | 121 | GLN |
| 1 | N | 173 | HIS |
| 1 | N | 353 | GLN |
| 1 | O | 49 | GLN |
| 1 | O | 59 | GLN |
| 1 | O | 92 | ASN |
| 1 | O | 121 | GLN |
| 1 | O | 173 | HIS |
| 1 | O | 353 | GLN |
| 1 | P | 49 | GLN |
| 1 | P | 59 | GLN |
| 1 | P | 92 | ASN |
| 1 | P | 121 | GLN |
| 1 | P | 173 | HIS |
| 1 | P | 353 | GLN |
| 1 | Q | 49 | GLN |
| 1 | Q | 59 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Q | 92 | ASN |
| 1 | Q | 121 | GLN |
| 1 | Q | 173 | HIS |
| 1 | Q | 353 | GLN |
| 1 | R | 49 | GLN |
| 1 | R | 59 | GLN |
| 1 | R | 92 | ASN |
| 1 | R | 121 | GLN |
| 1 | R | 173 | HIS |
| 1 | R | 353 | GLN |
| 1 | S | 49 | GLN |
| 1 | S | 59 | GLN |
| 1 | S | 92 | ASN |
| 1 | S | 121 | GLN |
| 1 | S | 173 | HIS |
| 1 | S | 353 | GLN |
| 1 | T | 49 | GLN |
| 1 | T | 59 | GLN |
| 1 | T | 92 | ASN |
| 1 | T | 121 | GLN |
| 1 | T | 173 | HIS |
| 1 | T | 353 | GLN |
| 1 | U | 49 | GLN |
| 1 | U | 59 | GLN |
| 1 | U | 92 | ASN |
| 1 | U | 121 | GLN |
| 1 | U | 173 | HIS |
| 1 | U | 353 | GLN |
| 1 | V | 49 | GLN |
| 1 | V | 59 | GLN |
| 1 | V | 92 | ASN |
| 1 | V | 121 | GLN |
| 1 | V | 173 | HIS |
| 1 | V | 353 | GLN |
| 1 | W | 49 | GLN |
| 1 | W | 59 | GLN |
| 1 | W | 92 | ASN |
| 1 | W | 121 | GLN |
| 1 | W | 353 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

23 non-standard protein/DNA/RNA residues 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 | $\#\|Z\| > 2$ |
| 1 | HIC | H | 73 | 1 | 8,11,12 | 1.06 | 0 | 6,14,16 | 1.19 | 1 (16%) |
| 1 | HIC | D | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.19 | 1 (16%) |
| 1 | HIC | K | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.20 | 1 (16%) |
| 1 | HIC | I | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.18 | 1 (16%) |
| 1 | HIC | G | 73 | 1 | 8,11,12 | 1.03 | 0 | 6,14,16 | 1.16 | 1 (16%) |
| 1 | HIC | S | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.20 | 1 (16%) |
| 1 | HIC | J | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.20 | 1 (16%) |
| 1 | HIC | B | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.19 | 1 (16%) |
| 1 | HIC | Q | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.19 | 1 (16%) |
| 1 | HIC | U | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.20 | 1 (16%) |
| 1 | HIC | R | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.20 | 1 (16%) |
| 1 | HIC | F | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.19 | 1 (16%) |
| 1 | HIC | C | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.17 | 1 (16%) |
| 1 | HIC | W | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.21 | 1 (16%) |
| 1 | HIC | P | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.18 | 1 (16%) |
| 1 | HIC | O | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.18 | 1 (16%) |
| 1 | HIC | E | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.20 | 1 (16%) |
| 1 | HIC | T | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.17 | 1 (16%) |
| 1 | HIC | L | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.18 | 1 (16%) |
| 1 | HIC | N | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.18 | 1 (16%) |
| 1 | HIC | A | 73 | 1 | 8,11,12 | 1.03 | 0 | 6,14,16 | 1.18 | 1 (16%) |
| 1 | HIC | V | 73 | 1 | 8,11,12 | 1.04 | 0 | 6,14,16 | 1.19 | 1 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 1 | HIC | M | 73 | 1 | 8,11,12 | 1.05 | 0 | 6,14,16 | 1.20 | 1 (16%) |

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 |
|---|---|---|---|---|---|---|---|
| 1 | HIC | H | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | D | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | K | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | I | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | G | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | S | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | J | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | B | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | Q | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | U | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | R | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | F | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | C | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | W | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | P | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | O | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | E | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | T | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | L | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | N | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | A | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | V | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |
| 1 | HIC | M | 73 | 1 | - | 2/5/6/8 | 0/1/1/1 |

There are no bond length outliers.

All (23) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | W | 73 | HIC | CG-CD2-NE2 | 2.28 | 110.25 | 107.78 |
| 1 | R | 73 | HIC | CG-CD2-NE2 | 2.25 | 110.22 | 107.78 |
| 1 | K | 73 | HIC | CG-CD2-NE2 | 2.25 | 110.22 | 107.78 |
| 1 | J | 73 | HIC | CG-CD2-NE2 | 2.25 | 110.22 | 107.78 |
| 1 | E | 73 | HIC | CG-CD2-NE2 | 2.25 | 110.21 | 107.78 |
| 1 | M | 73 | HIC | CG-CD2-NE2 | 2.24 | 110.21 | 107.78 |
| 1 | S | 73 | HIC | CG-CD2-NE2 | 2.24 | 110.21 | 107.78 |
| 1 | U | 73 | HIC | CG-CD2-NE2 | 2.24 | 110.21 | 107.78 |
| 1 | Q | 73 | HIC | CG-CD2-NE2 | 2.24 | 110.20 | 107.78 |
| 1 | H | 73 | HIC | CG-CD2-NE2 | 2.24 | 110.20 | 107.78 |
| 1 | F | 73 | HIC | CG-CD2-NE2 | 2.23 | 110.19 | 107.78 |
| 1 | D | 73 | HIC | CG-CD2-NE2 | 2.23 | 110.19 | 107.78 |
| 1 | B | 73 | HIC | CG-CD2-NE2 | 2.22 | 110.19 | 107.78 |
| 1 | N | 73 | HIC | CG-CD2-NE2 | 2.22 | 110.19 | 107.78 |
| 1 | V | 73 | HIC | CG-CD2-NE2 | 2.22 | 110.19 | 107.78 |
| 1 | I | 73 | HIC | CG-CD2-NE2 | 2.21 | 110.17 | 107.78 |
| 1 | L | 73 | HIC | CG-CD2-NE2 | 2.21 | 110.17 | 107.78 |
| 1 | P | 73 | HIC | CG-CD2-NE2 | 2.20 | 110.16 | 107.78 |
| 1 | O | 73 | HIC | CG-CD2-NE2 | 2.20 | 110.16 | 107.78 |
| 1 | A | 73 | HIC | CG-CD2-NE2 | 2.20 | 110.16 | 107.78 |
| 1 | T | 73 | HIC | CG-CD2-NE2 | 2.20 | 110.16 | 107.78 |
| 1 | C | 73 | HIC | CG-CD2-NE2 | 2.19 | 110.15 | 107.78 |
| 1 | G | 73 | HIC | CG-CD2-NE2 | 2.17 | 110.13 | 107.78 |

There are no chirality outliers.

All (46) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | A | 73 | HIC | O-C-CA-CB |
| 1 | A | 73 | HIC | CA-CB-CG-ND1 |
| 1 | B | 73 | HIC | O-C-CA-CB |
| 1 | B | 73 | HIC | CA-CB-CG-ND1 |
| 1 | C | 73 | HIC | O-C-CA-CB |
| 1 | C | 73 | HIC | CA-CB-CG-ND1 |
| 1 | D | 73 | HIC | O-C-CA-CB |
| 1 | D | 73 | HIC | CA-CB-CG-ND1 |
| 1 | E | 73 | HIC | O-C-CA-CB |
| 1 | E | 73 | HIC | CA-CB-CG-ND1 |
| 1 | F | 73 | HIC | O-C-CA-CB |
| 1 | F | 73 | HIC | CA-CB-CG-ND1 |
| 1 | G | 73 | HIC | O-C-CA-CB |
| 1 | G | 73 | HIC | CA-CB-CG-ND1 |
| 1 | H | 73 | HIC | O-C-CA-CB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | H | 73 | HIC | CA-CB-CG-ND1 |
| 1 | I | 73 | HIC | O-C-CA-CB |
| 1 | I | 73 | HIC | CA-CB-CG-ND1 |
| 1 | J | 73 | HIC | O-C-CA-CB |
| 1 | J | 73 | HIC | CA-CB-CG-ND1 |
| 1 | K | 73 | HIC | O-C-CA-CB |
| 1 | K | 73 | HIC | CA-CB-CG-ND1 |
| 1 | L | 73 | HIC | O-C-CA-CB |
| 1 | L | 73 | HIC | CA-CB-CG-ND1 |
| 1 | M | 73 | HIC | O-C-CA-CB |
| 1 | M | 73 | HIC | CA-CB-CG-ND1 |
| 1 | N | 73 | HIC | O-C-CA-CB |
| 1 | N | 73 | HIC | CA-CB-CG-ND1 |
| 1 | O | 73 | HIC | O-C-CA-CB |
| 1 | O | 73 | HIC | CA-CB-CG-ND1 |
| 1 | P | 73 | HIC | O-C-CA-CB |
| 1 | P | 73 | HIC | CA-CB-CG-ND1 |
| 1 | Q | 73 | HIC | O-C-CA-CB |
| 1 | Q | 73 | HIC | CA-CB-CG-ND1 |
| 1 | R | 73 | HIC | O-C-CA-CB |
| 1 | R | 73 | HIC | CA-CB-CG-ND1 |
| 1 | S | 73 | HIC | O-C-CA-CB |
| 1 | S | 73 | HIC | CA-CB-CG-ND1 |
| 1 | T | 73 | HIC | O-C-CA-CB |
| 1 | T | 73 | HIC | CA-CB-CG-ND1 |
| 1 | U | 73 | HIC | O-C-CA-CB |
| 1 | U | 73 | HIC | CA-CB-CG-ND1 |
| 1 | V | 73 | HIC | O-C-CA-CB |
| 1 | V | 73 | HIC | CA-CB-CG-ND1 |
| 1 | W | 73 | HIC | O-C-CA-CB |
| 1 | W | 73 | HIC | CA-CB-CG-ND1 |

There are no ring outliers.

23 monomers are involved in 43 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | H | 73 | HIC | 2 | 0 |
| 1 | D | 73 | HIC | 2 | 0 |
| 1 | K | 73 | HIC | 2 | 0 |
| 1 | I | 73 | HIC | 2 | 0 |
| 1 | G | 73 | HIC | 2 | 0 |
| 1 | S | 73 | HIC | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | J | 73 | HIC | 2 | 0 |
| 1 | B | 73 | HIC | 2 | 0 |
| 1 | Q | 73 | HIC | 2 | 0 |
| 1 | U | 73 | HIC | 2 | 0 |
| 1 | R | 73 | HIC | 1 | 0 |
| 1 | F | 73 | HIC | 2 | 0 |
| 1 | C | 73 | HIC | 2 | 0 |
| 1 | W | 73 | HIC | 2 | 0 |
| 1 | P | 73 | HIC | 2 | 0 |
| 1 | O | 73 | HIC | 2 | 0 |
| 1 | E | 73 | HIC | 2 | 0 |
| 1 | T | 73 | HIC | 1 | 0 |
| 1 | L | 73 | HIC | 2 | 0 |
| 1 | N | 73 | HIC | 2 | 0 |
| 1 | A | 73 | HIC | 2 | 0 |
| 1 | V | 73 | HIC | 1 | 0 |
| 1 | M | 73 | HIC | 2 | 0 |

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

23 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 | $\#\|Z\| > 2$ |
| 2 | ADP | L | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | S | 401 | - | 24,29,29 | 1.19 | 2 (8%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | U | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | I | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | E | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.40 | 4 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | ADP | R | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | D | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | G | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.39 | 4 (13%) |
| 2 | ADP | J | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | C | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | F | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | A | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | W | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | T | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | M | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | H | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | K | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.41 | 4 (13%) |
| 2 | ADP | Q | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | V | 401 | - | 24,29,29 | 1.19 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | B | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | P | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | N | 401 | - | 24,29,29 | 1.20 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 2 | ADP | O | 401 | - | 24,29,29 | 1.20 | 2 (8%) | 29,45,45 | 1.40 | 4 (13%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | ADP | L | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | S | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | U | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | I | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | E | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | R | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | D | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | G | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | J | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | C | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | F | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | A | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | W | 401 | - | - | 0/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | ADP | T | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | M | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | H | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | K | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | Q | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | V | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | B | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | P | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | N | 401 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | O | 401 | - | - | 0/12/32/32 | 0/3/3/3 |

All (35) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | P | 401 | ADP | C2-N1 | 2.99 | 1.39 | 1.33 |
| 2 | U | 401 | ADP | C2-N1 | 2.99 | 1.39 | 1.33 |
| 2 | C | 401 | ADP | C2-N1 | 2.99 | 1.39 | 1.33 |
| 2 | D | 401 | ADP | C2-N1 | 2.98 | 1.39 | 1.33 |
| 2 | M | 401 | ADP | C2-N1 | 2.98 | 1.39 | 1.33 |
| 2 | V | 401 | ADP | C2-N1 | 2.98 | 1.39 | 1.33 |
| 2 | G | 401 | ADP | C2-N1 | 2.98 | 1.39 | 1.33 |
| 2 | F | 401 | ADP | C2-N1 | 2.97 | 1.39 | 1.33 |
| 2 | E | 401 | ADP | C2-N1 | 2.96 | 1.39 | 1.33 |
| 2 | O | 401 | ADP | C2-N1 | 2.96 | 1.39 | 1.33 |
| 2 | B | 401 | ADP | C2-N1 | 2.96 | 1.39 | 1.33 |
| 2 | A | 401 | ADP | C2-N1 | 2.95 | 1.39 | 1.33 |
| 2 | T | 401 | ADP | C2-N1 | 2.95 | 1.39 | 1.33 |
| 2 | K | 401 | ADP | C2-N1 | 2.95 | 1.39 | 1.33 |
| 2 | J | 401 | ADP | C2-N1 | 2.95 | 1.39 | 1.33 |
| 2 | N | 401 | ADP | C2-N1 | 2.95 | 1.39 | 1.33 |
| 2 | W | 401 | ADP | C2-N1 | 2.95 | 1.39 | 1.33 |
| 2 | H | 401 | ADP | C2-N1 | 2.94 | 1.39 | 1.33 |
| 2 | R | 401 | ADP | C2-N1 | 2.94 | 1.39 | 1.33 |
| 2 | L | 401 | ADP | C2-N1 | 2.94 | 1.39 | 1.33 |
| 2 | I | 401 | ADP | C2-N1 | 2.94 | 1.39 | 1.33 |
| 2 | Q | 401 | ADP | C2-N1 | 2.93 | 1.39 | 1.33 |
| 2 | S | 401 | ADP | C2-N1 | 2.92 | 1.39 | 1.33 |
| 2 | L | 401 | ADP | C2'-C1' | -2.06 | 1.50 | 1.53 |
| 2 | H | 401 | ADP | C2'-C1' | -2.05 | 1.50 | 1.53 |
| 2 | T | 401 | ADP | C2'-C1' | -2.03 | 1.50 | 1.53 |
| 2 | G | 401 | ADP | C2'-C1' | -2.03 | 1.50 | 1.53 |
| 2 | O | 401 | ADP | C2'-C1' | -2.03 | 1.50 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 401 | ADP | C2'-C1' | -2.03 | 1.50 | 1.53 |
| 2 | S | 401 | ADP | C2'-C1' | -2.02 | 1.50 | 1.53 |
| 2 | F | 401 | ADP | C2'-C1' | -2.01 | 1.50 | 1.53 |
| 2 | M | 401 | ADP | C8-N7 | -2.01 | 1.31 | 1.34 |
| 2 | E | 401 | ADP | C2'-C1' | -2.01 | 1.50 | 1.53 |
| 2 | A | 401 | ADP | C2'-C1' | -2.01 | 1.50 | 1.53 |
| 2 | C | 401 | ADP | C2'-C1' | -2.00 | 1.50 | 1.53 |

All (92) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | S | 401 | ADP | C4-C5-N7 | 3.95 | 113.52 | 109.40 |
| 2 | C | 401 | ADP | C4-C5-N7 | 3.93 | 113.50 | 109.40 |
| 2 | W | 401 | ADP | C4-C5-N7 | 3.93 | 113.49 | 109.40 |
| 2 | A | 401 | ADP | C4-C5-N7 | 3.92 | 113.49 | 109.40 |
| 2 | F | 401 | ADP | C4-C5-N7 | 3.92 | 113.48 | 109.40 |
| 2 | O | 401 | ADP | C4-C5-N7 | 3.91 | 113.48 | 109.40 |
| 2 | H | 401 | ADP | C4-C5-N7 | 3.91 | 113.47 | 109.40 |
| 2 | I | 401 | ADP | C4-C5-N7 | 3.91 | 113.47 | 109.40 |
| 2 | K | 401 | ADP | C4-C5-N7 | 3.90 | 113.47 | 109.40 |
| 2 | N | 401 | ADP | C4-C5-N7 | 3.90 | 113.46 | 109.40 |
| 2 | B | 401 | ADP | C4-C5-N7 | 3.89 | 113.46 | 109.40 |
| 2 | Q | 401 | ADP | C4-C5-N7 | 3.89 | 113.46 | 109.40 |
| 2 | U | 401 | ADP | C4-C5-N7 | 3.89 | 113.46 | 109.40 |
| 2 | G | 401 | ADP | C4-C5-N7 | 3.89 | 113.45 | 109.40 |
| 2 | T | 401 | ADP | C4-C5-N7 | 3.89 | 113.45 | 109.40 |
| 2 | V | 401 | ADP | C4-C5-N7 | 3.89 | 113.45 | 109.40 |
| 2 | D | 401 | ADP | C4-C5-N7 | 3.89 | 113.45 | 109.40 |
| 2 | R | 401 | ADP | C4-C5-N7 | 3.89 | 113.45 | 109.40 |
| 2 | P | 401 | ADP | C4-C5-N7 | 3.88 | 113.44 | 109.40 |
| 2 | J | 401 | ADP | C4-C5-N7 | 3.87 | 113.44 | 109.40 |
| 2 | M | 401 | ADP | C4-C5-N7 | 3.87 | 113.44 | 109.40 |
| 2 | L | 401 | ADP | C4-C5-N7 | 3.87 | 113.43 | 109.40 |
| 2 | E | 401 | ADP | C4-C5-N7 | 3.86 | 113.42 | 109.40 |
| 2 | W | 401 | ADP | C2-N1-C6 | 2.20 | 122.52 | 118.75 |
| 2 | C | 401 | ADP | N3-C2-N1 | -2.20 | 125.24 | 128.68 |
| 2 | L | 401 | ADP | C2-N1-C6 | 2.20 | 122.51 | 118.75 |
| 2 | K | 401 | ADP | N3-C2-N1 | -2.20 | 125.25 | 128.68 |
| 2 | C | 401 | ADP | C2-N1-C6 | 2.19 | 122.51 | 118.75 |
| 2 | A | 401 | ADP | C2-N1-C6 | 2.19 | 122.50 | 118.75 |
| 2 | D | 401 | ADP | N3-C2-N1 | -2.19 | 125.25 | 128.68 |
| 2 | P | 401 | ADP | N3-C2-N1 | -2.19 | 125.25 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | D | 401 | ADP | C2-N1-C6 | 2.19 | 122.50 | 118.75 |
| 2 | K | 401 | ADP | C2-N1-C6 | 2.19 | 122.50 | 118.75 |
| 2 | E | 401 | ADP | C2-N1-C6 | 2.19 | 122.50 | 118.75 |
| 2 | H | 401 | ADP | C2-N1-C6 | 2.19 | 122.50 | 118.75 |
| 2 | T | 401 | ADP | C2-N1-C6 | 2.19 | 122.49 | 118.75 |
| 2 | A | 401 | ADP | N3-C2-N1 | -2.18 | 125.27 | 128.68 |
| 2 | P | 401 | ADP | C2-N1-C6 | 2.18 | 122.48 | 118.75 |
| 2 | V | 401 | ADP | N3-C2-N1 | -2.18 | 125.27 | 128.68 |
| 2 | M | 401 | ADP | C2-N1-C6 | 2.18 | 122.48 | 118.75 |
| 2 | V | 401 | ADP | C2-N1-C6 | 2.18 | 122.48 | 118.75 |
| 2 | L | 401 | ADP | N3-C2-N1 | -2.18 | 125.28 | 128.68 |
| 2 | M | 401 | ADP | N3-C2-N1 | -2.18 | 125.28 | 128.68 |
| 2 | B | 401 | ADP | C2-N1-C6 | 2.17 | 122.47 | 118.75 |
| 2 | N | 401 | ADP | C2-N1-C6 | 2.17 | 122.47 | 118.75 |
| 2 | R | 401 | ADP | N3-C2-N1 | -2.17 | 125.28 | 128.68 |
| 2 | F | 401 | ADP | C2-N1-C6 | 2.17 | 122.47 | 118.75 |
| 2 | O | 401 | ADP | N3-C2-N1 | -2.17 | 125.28 | 128.68 |
| 2 | R | 401 | ADP | C2-N1-C6 | 2.17 | 122.47 | 118.75 |
| 2 | T | 401 | ADP | N3-C2-N1 | -2.17 | 125.28 | 128.68 |
| 2 | B | 401 | ADP | N3-C2-N1 | -2.17 | 125.28 | 128.68 |
| 2 | H | 401 | ADP | N3-C2-N1 | -2.17 | 125.29 | 128.68 |
| 2 | W | 401 | ADP | N3-C2-N1 | -2.17 | 125.29 | 128.68 |
| 2 | E | 401 | ADP | N3-C2-N1 | -2.17 | 125.29 | 128.68 |
| 2 | O | 401 | ADP | C2-N1-C6 | 2.17 | 122.46 | 118.75 |
| 2 | F | 401 | ADP | N3-C2-N1 | -2.16 | 125.30 | 128.68 |
| 2 | U | 401 | ADP | N3-C2-N1 | -2.16 | 125.30 | 128.68 |
| 2 | S | 401 | ADP | C2-N1-C6 | 2.16 | 122.45 | 118.75 |
| 2 | J | 401 | ADP | C2-N1-C6 | 2.16 | 122.45 | 118.75 |
| 2 | Q | 401 | ADP | N3-C2-N1 | -2.16 | 125.31 | 128.68 |
| 2 | I | 401 | ADP | C2-N1-C6 | 2.16 | 122.44 | 118.75 |
| 2 | Q | 401 | ADP | C2-N1-C6 | 2.16 | 122.44 | 118.75 |
| 2 | U | 401 | ADP | C2-N1-C6 | 2.16 | 122.44 | 118.75 |
| 2 | I | 401 | ADP | N3-C2-N1 | -2.15 | 125.31 | 128.68 |
| 2 | N | 401 | ADP | N3-C2-N1 | -2.15 | 125.32 | 128.68 |
| 2 | G | 401 | ADP | N3-C2-N1 | -2.15 | 125.32 | 128.68 |
| 2 | J | 401 | ADP | N3-C2-N1 | -2.14 | 125.34 | 128.68 |
| 2 | G | 401 | ADP | C2-N1-C6 | 2.13 | 122.40 | 118.75 |
| 2 | S | 401 | ADP | N3-C2-N1 | -2.13 | 125.35 | 128.68 |
| 2 | V | 401 | ADP | O3B-PB-O2B | 2.10 | 115.68 | 107.64 |
| 2 | T | 401 | ADP | O3B-PB-O2B | 2.10 | 115.67 | 107.64 |
| 2 | D | 401 | ADP | O3B-PB-O2B | 2.10 | 115.66 | 107.64 |
| 2 | S | 401 | ADP | O3B-PB-O2B | 2.10 | 115.66 | 107.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | M | 401 | ADP | O3B-PB-O2B | 2.10 | 115.66 | 107.64 |
| 2 | W | 401 | ADP | O3B-PB-O2B | 2.10 | 115.65 | 107.64 |
| 2 | Q | 401 | ADP | O3B-PB-O2B | 2.10 | 115.65 | 107.64 |
| 2 | F | 401 | ADP | O3B-PB-O2B | 2.10 | 115.65 | 107.64 |
| 2 | N | 401 | ADP | O3B-PB-O2B | 2.09 | 115.64 | 107.64 |
| 2 | J | 401 | ADP | O3B-PB-O2B | 2.09 | 115.63 | 107.64 |
| 2 | C | 401 | ADP | O3B-PB-O2B | 2.09 | 115.63 | 107.64 |
| 2 | I | 401 | ADP | O3B-PB-O2B | 2.09 | 115.63 | 107.64 |
| 2 | U | 401 | ADP | O3B-PB-O2B | 2.09 | 115.63 | 107.64 |
| 2 | A | 401 | ADP | O3B-PB-O2B | 2.09 | 115.63 | 107.64 |
| 2 | H | 401 | ADP | O3B-PB-O2B | 2.09 | 115.62 | 107.64 |
| 2 | B | 401 | ADP | O3B-PB-O2B | 2.09 | 115.62 | 107.64 |
| 2 | L | 401 | ADP | O3B-PB-O2B | 2.09 | 115.62 | 107.64 |
| 2 | P | 401 | ADP | O3B-PB-O2B | 2.09 | 115.62 | 107.64 |
| 2 | E | 401 | ADP | O3B-PB-O2B | 2.09 | 115.61 | 107.64 |
| 2 | O | 401 | ADP | O3B-PB-O2B | 2.09 | 115.61 | 107.64 |
| 2 | K | 401 | ADP | O3B-PB-O2B | 2.08 | 115.59 | 107.64 |
| 2 | G | 401 | ADP | O3B-PB-O2B | 2.08 | 115.59 | 107.64 |
| 2 | R | 401 | ADP | O3B-PB-O2B | 2.07 | 115.57 | 107.64 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 95 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | L | 401 | ADP | 4 | 0 |
| 2 | S | 401 | ADP | 4 | 0 |
| 2 | U | 401 | ADP | 4 | 0 |
| 2 | I | 401 | ADP | 4 | 0 |
| 2 | E | 401 | ADP | 4 | 0 |
| 2 | R | 401 | ADP | 4 | 0 |
| 2 | D | 401 | ADP | 5 | 0 |
| 2 | G | 401 | ADP | 4 | 0 |
| 2 | J | 401 | ADP | 4 | 0 |
| 2 | C | 401 | ADP | 4 | 0 |
| 2 | F | 401 | ADP | 4 | 0 |
| 2 | A | 401 | ADP | 4 | 0 |
| 2 | W | 401 | ADP | 4 | 0 |
| 2 | T | 401 | ADP | 4 | 0 |
| 2 | M | 401 | ADP | 4 | 0 |

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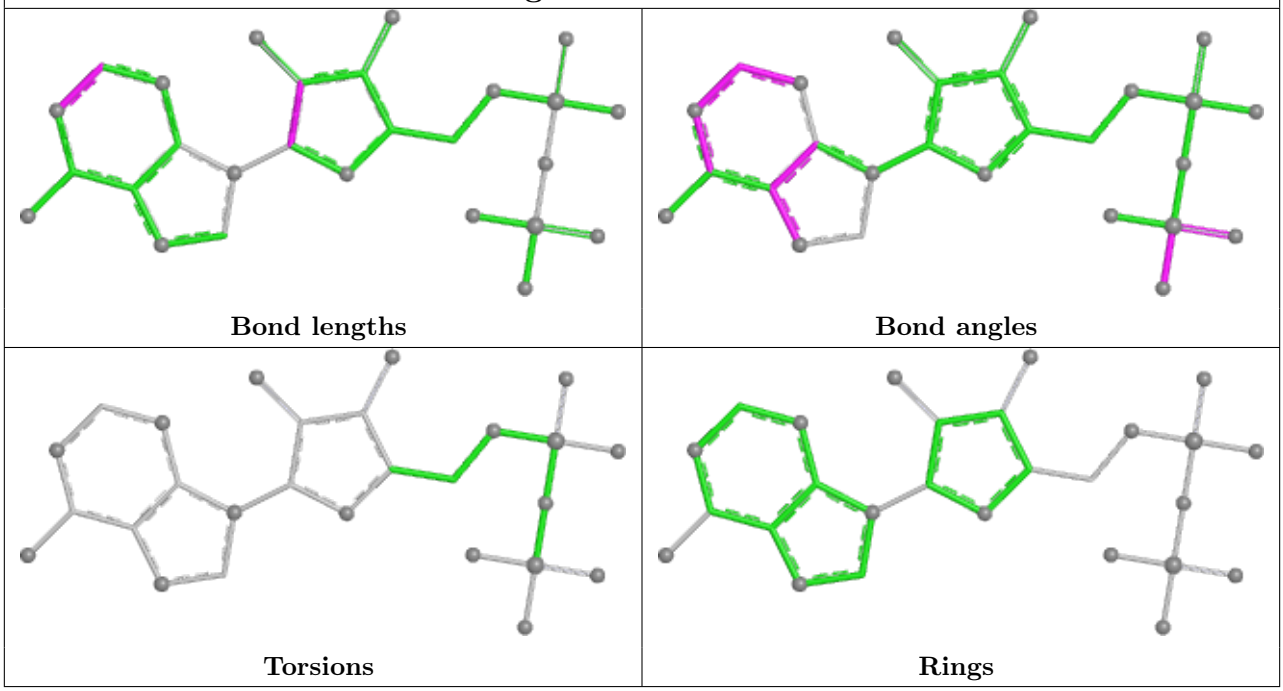
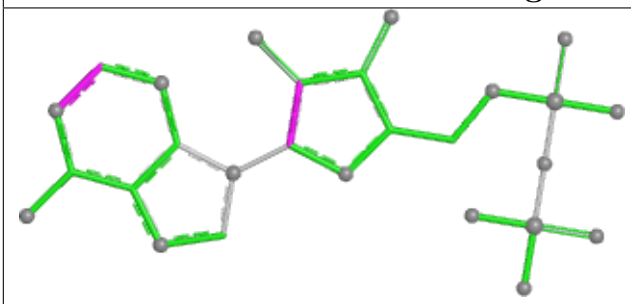
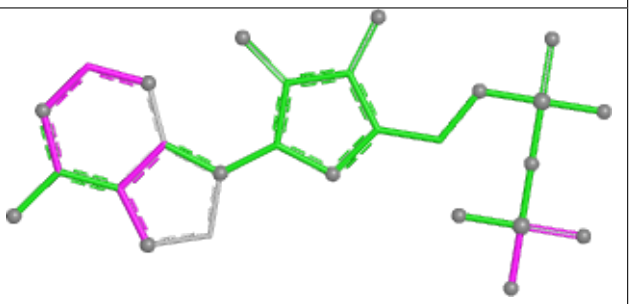
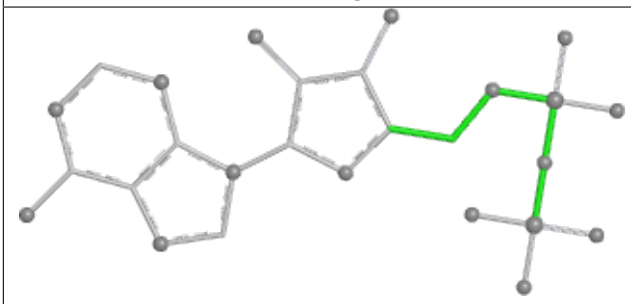
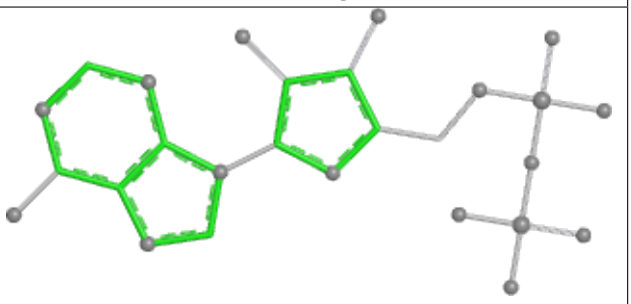
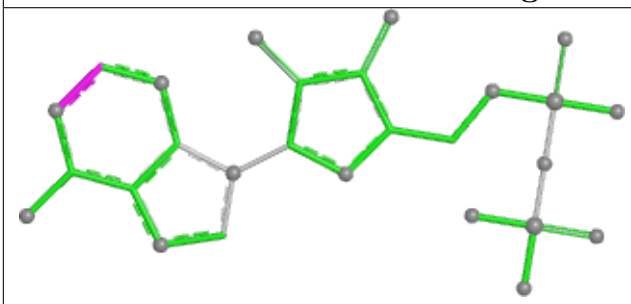
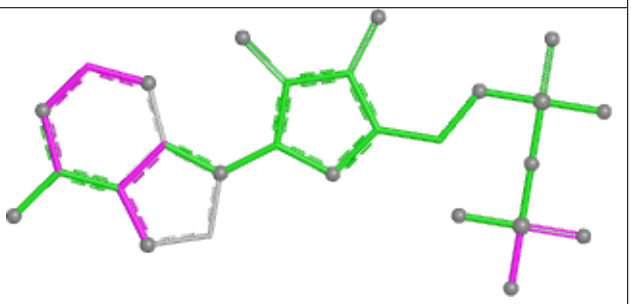
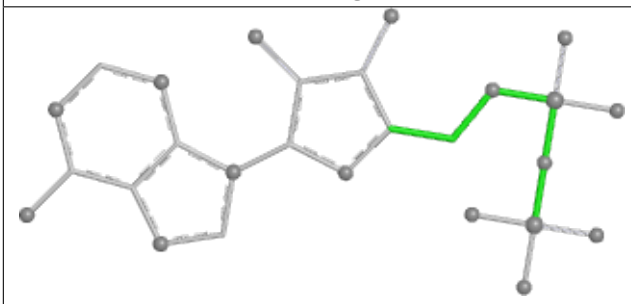
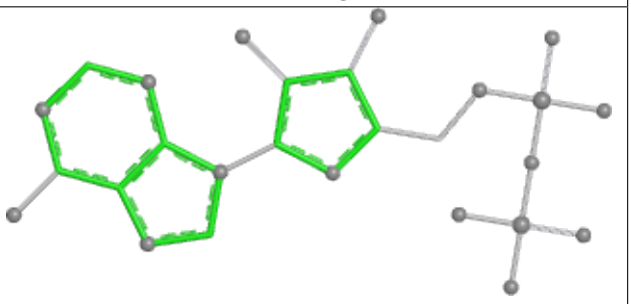
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | H | 401 | ADP | 4 | 0 |
| 2 | K | 401 | ADP | 5 | 0 |
| 2 | Q | 401 | ADP | 4 | 0 |
| 2 | V | 401 | ADP | 4 | 0 |
| 2 | B | 401 | ADP | 5 | 0 |
| 2 | P | 401 | ADP | 4 | 0 |
| 2 | N | 401 | ADP | 4 | 0 |
| 2 | O | 401 | ADP | 4 | 0 |

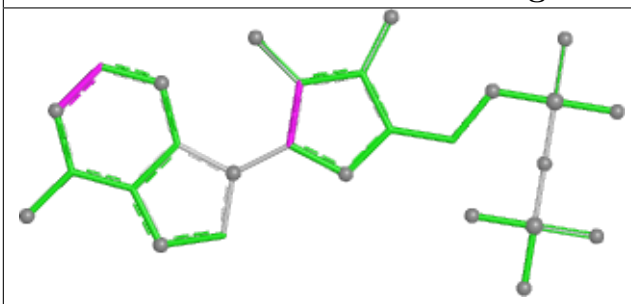
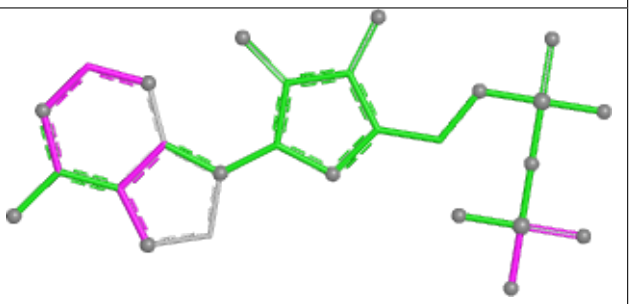
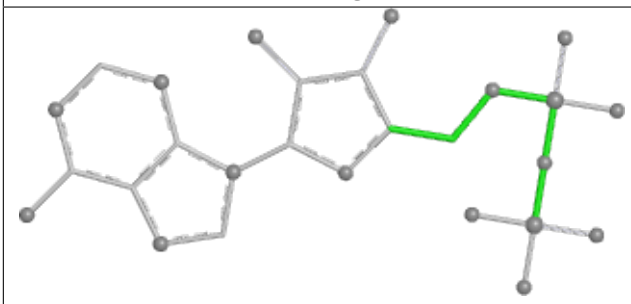
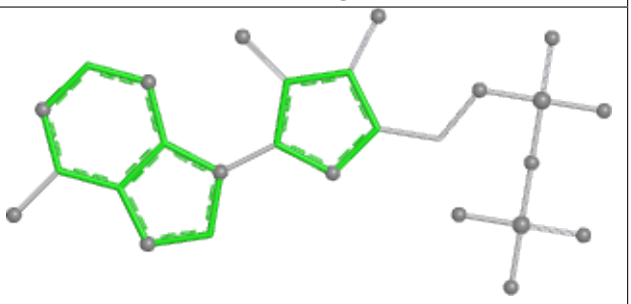
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADP L 401**



| Ligand ADP S 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP U 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP I 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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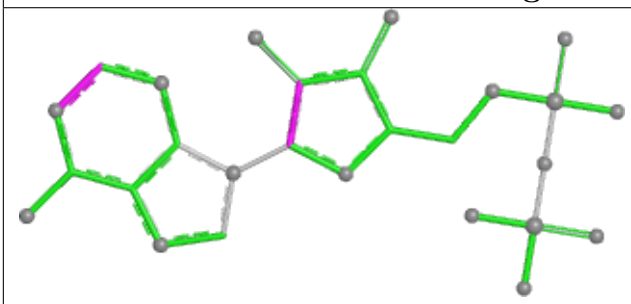
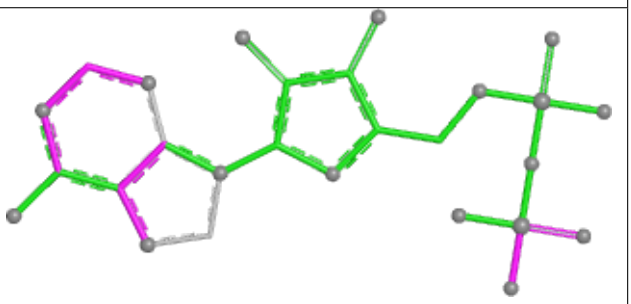
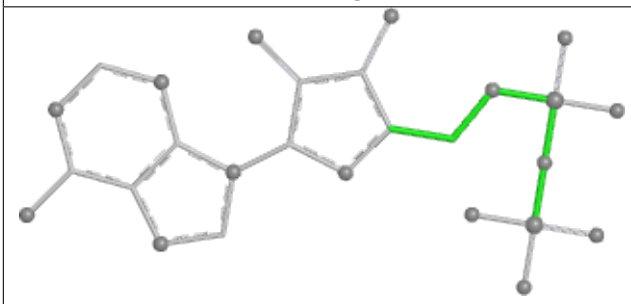
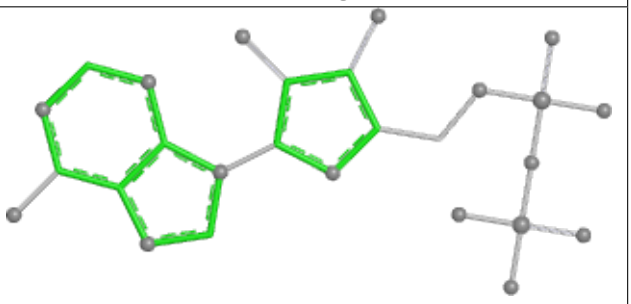
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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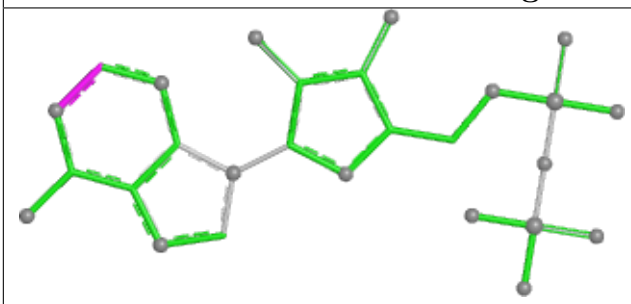
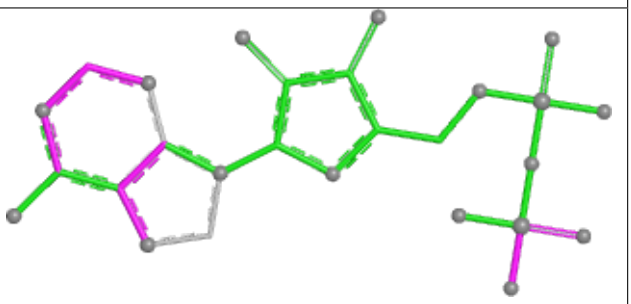
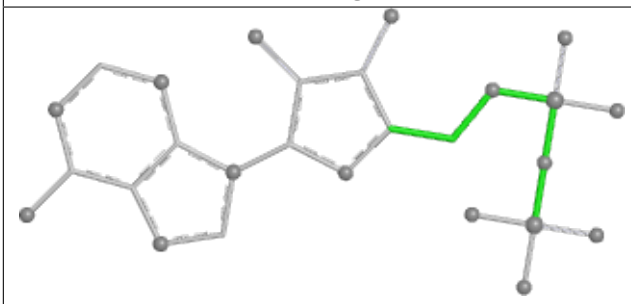
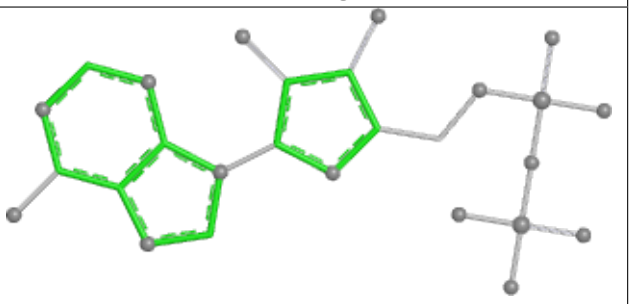
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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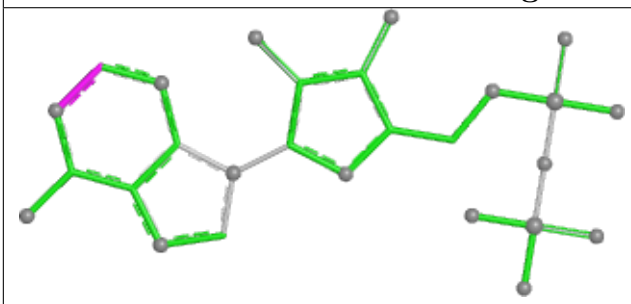
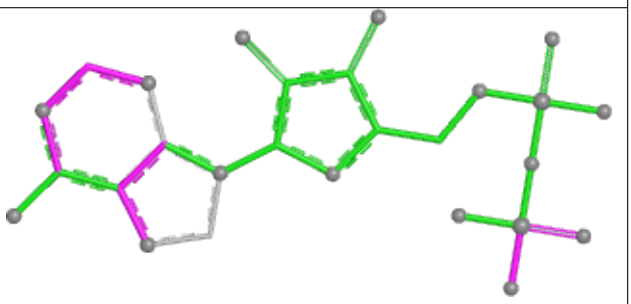
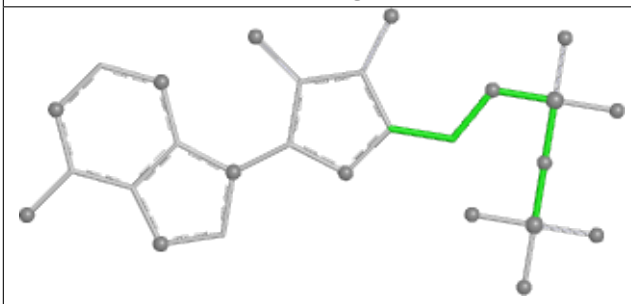
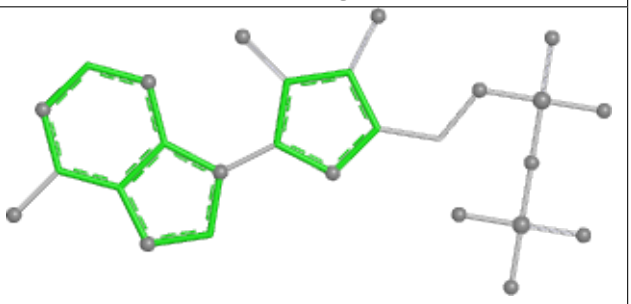
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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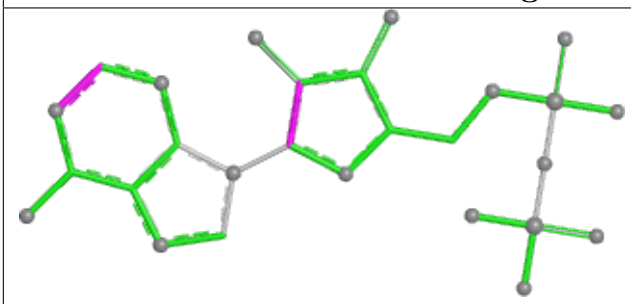
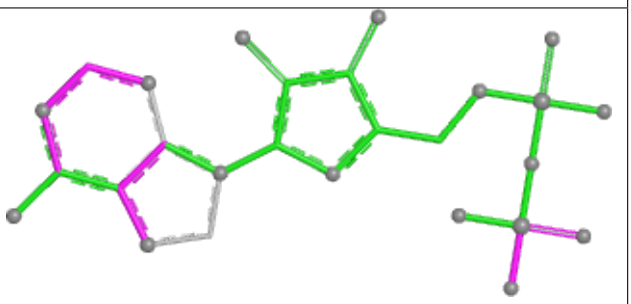
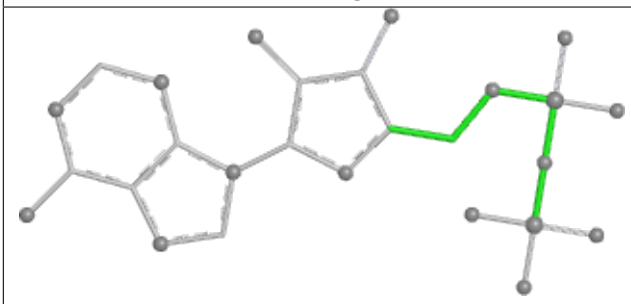
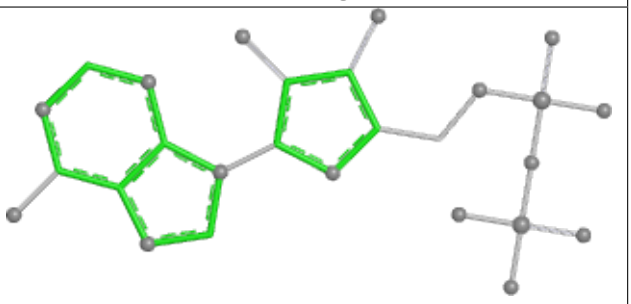
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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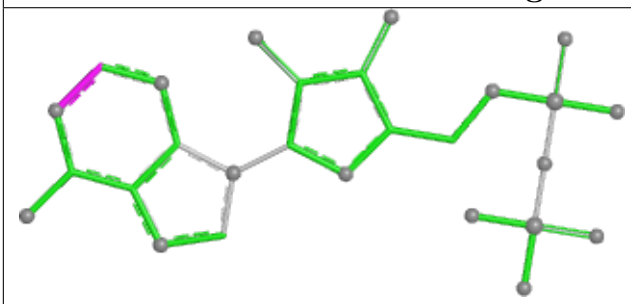
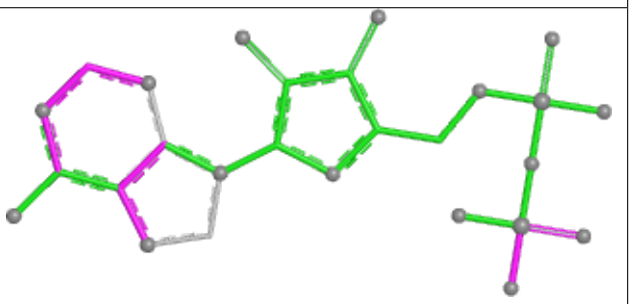
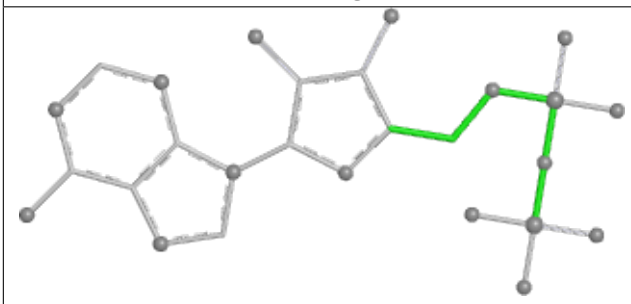
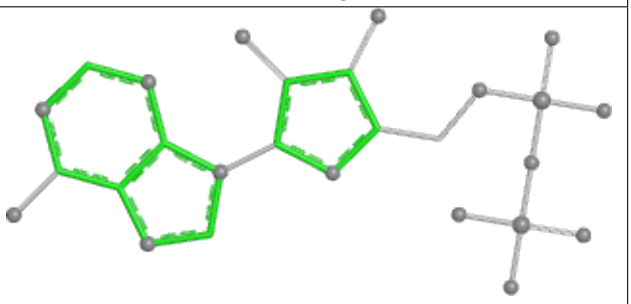
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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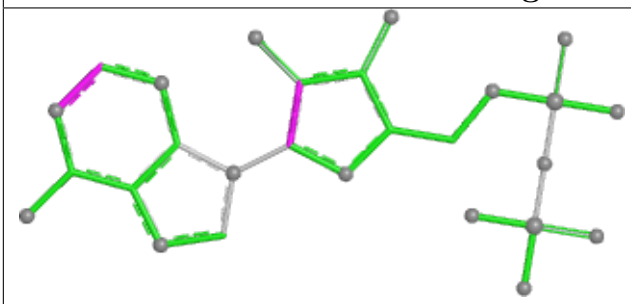
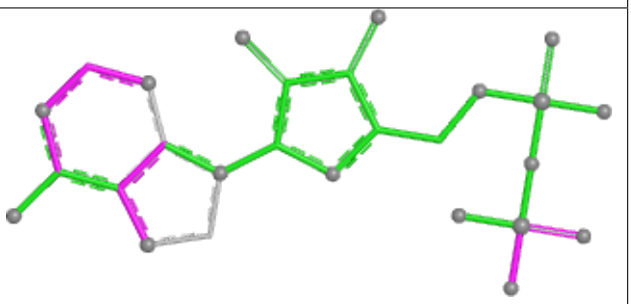
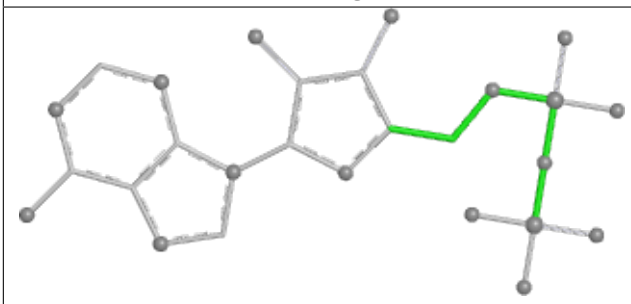
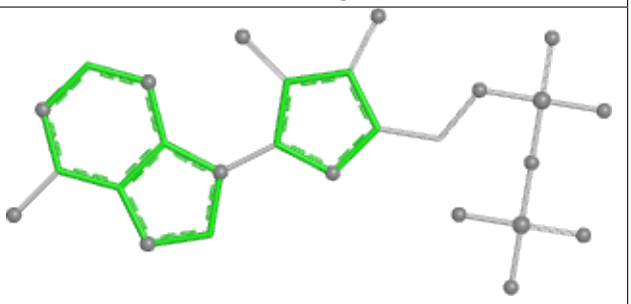
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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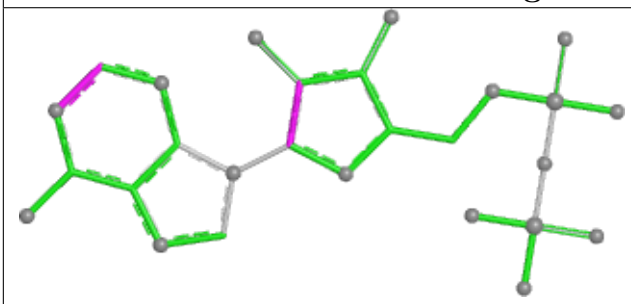
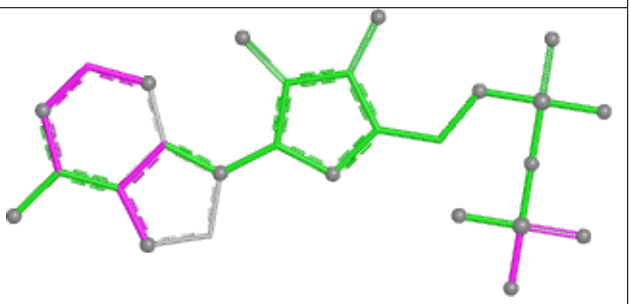
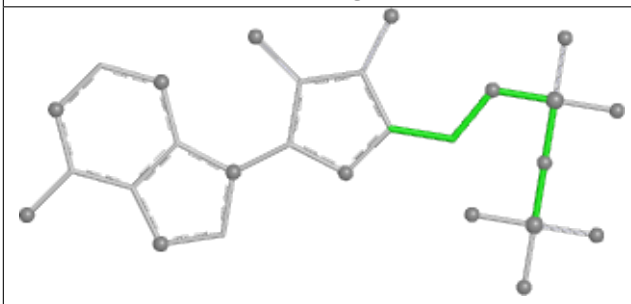
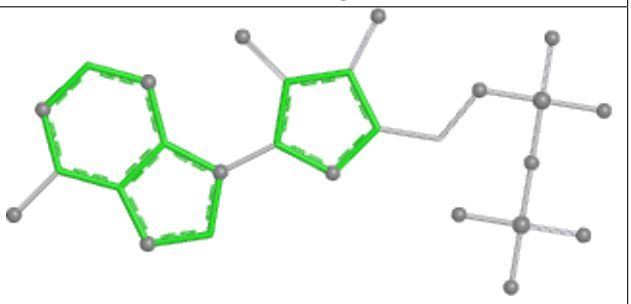
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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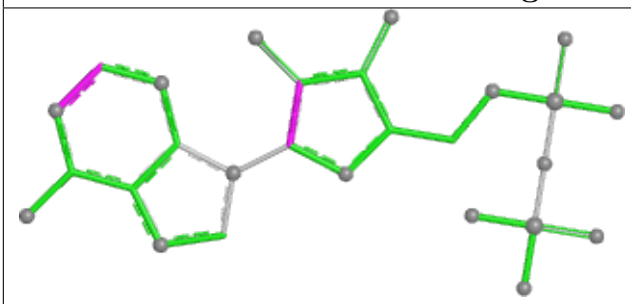
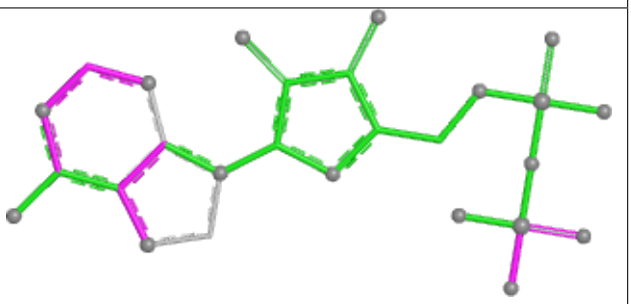
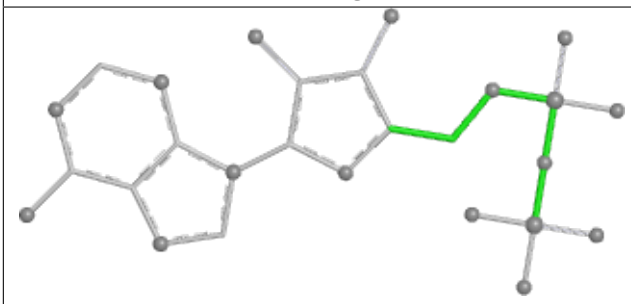
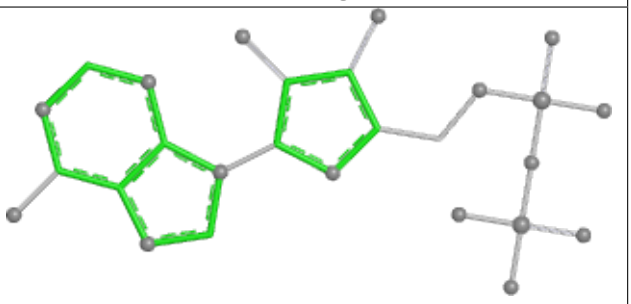
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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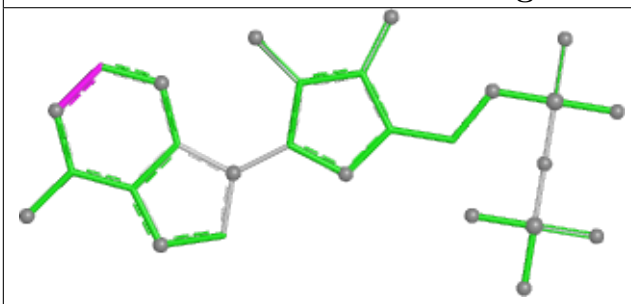
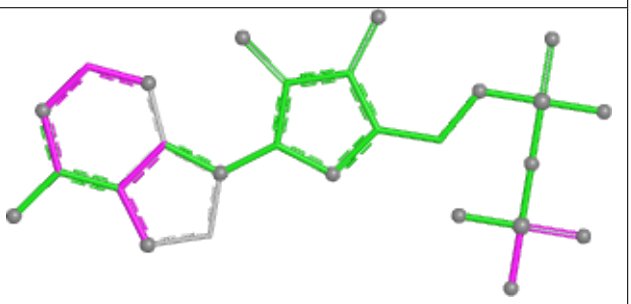
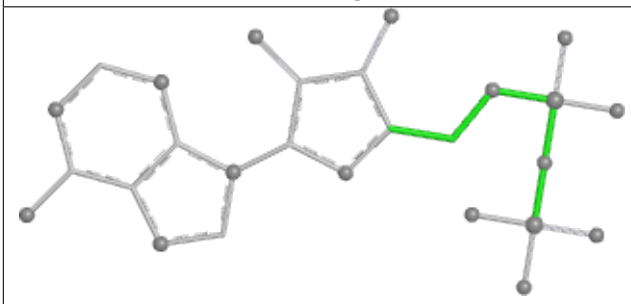
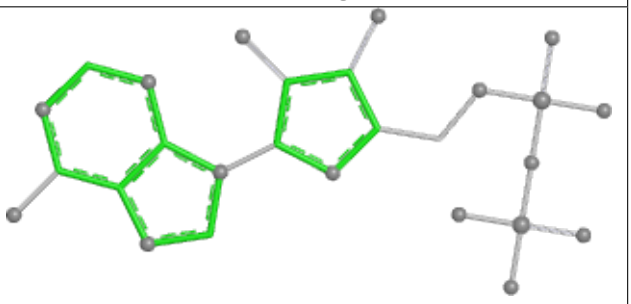
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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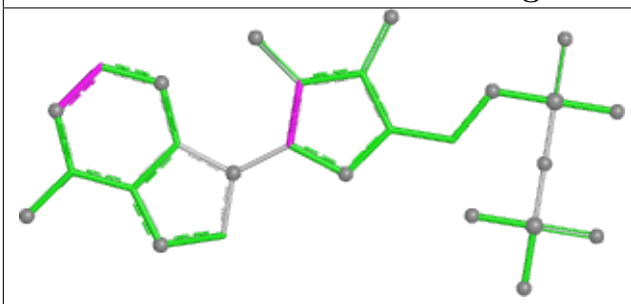
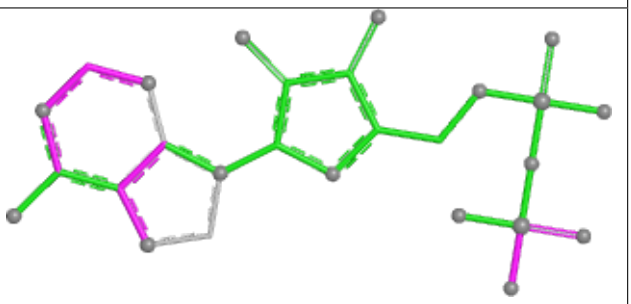
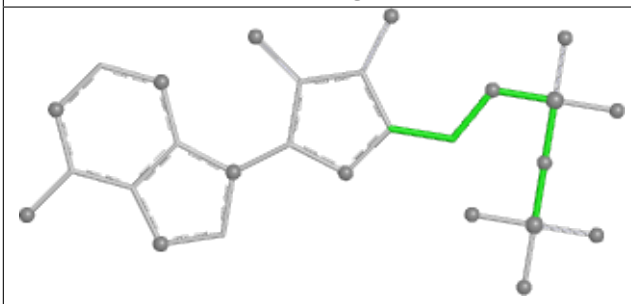
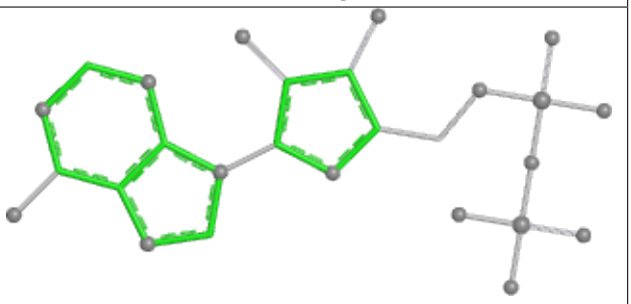
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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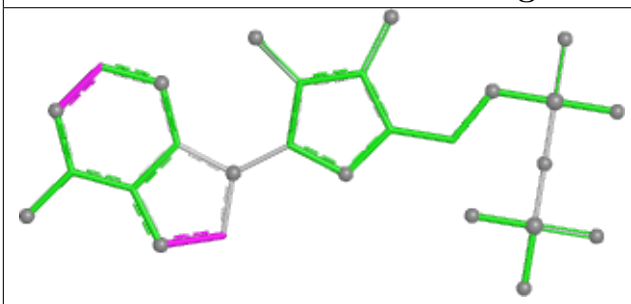
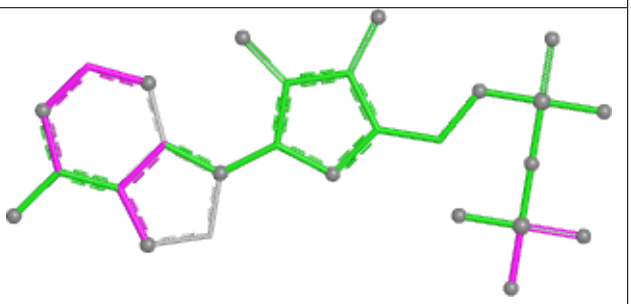
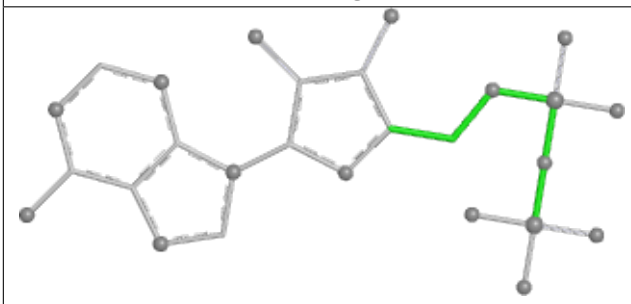
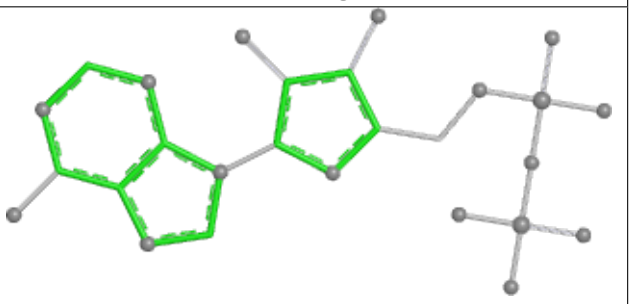
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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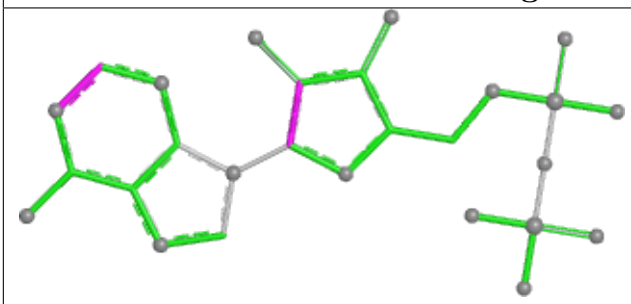
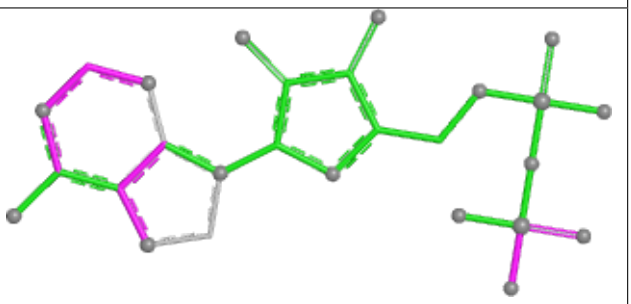
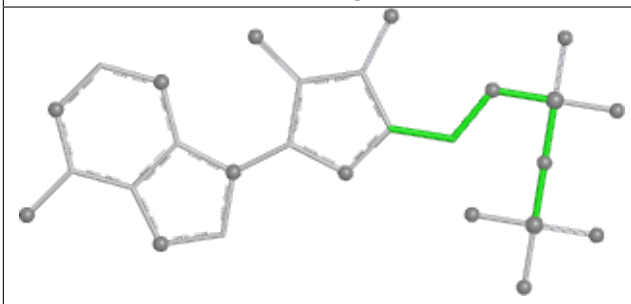
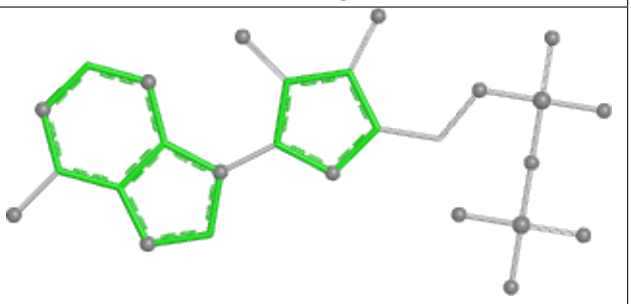
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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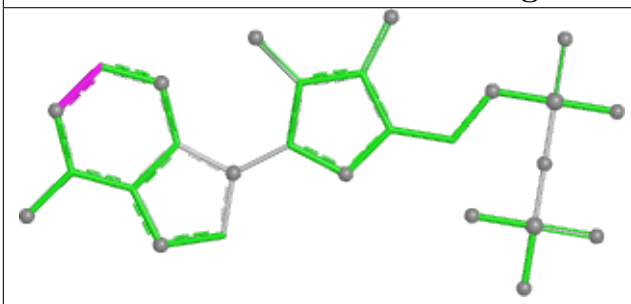
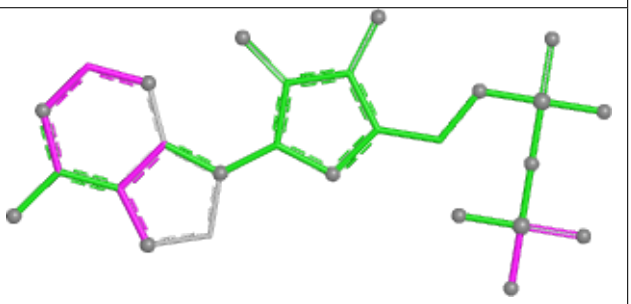
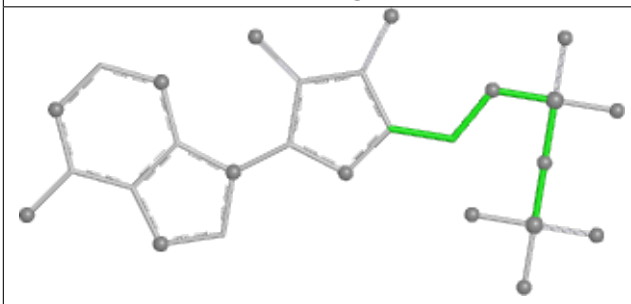
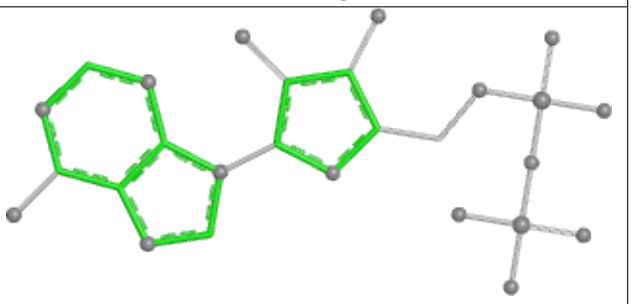
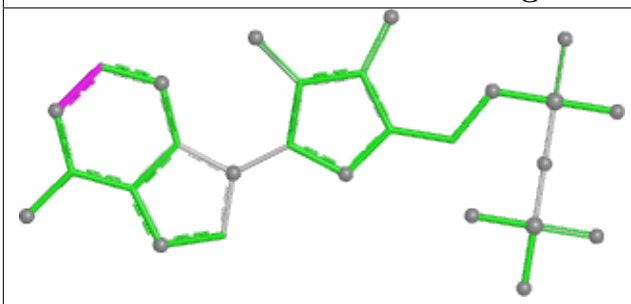
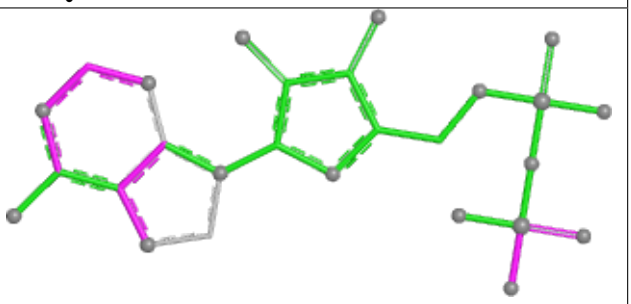
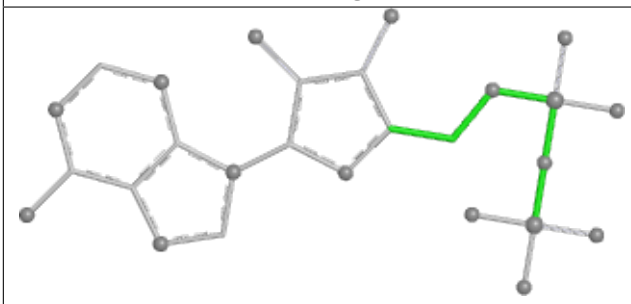
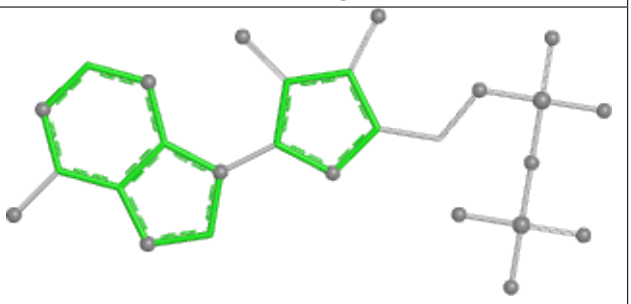
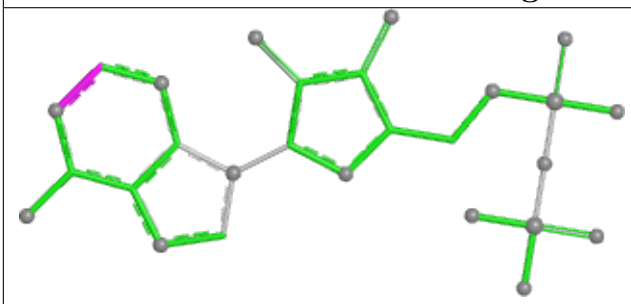
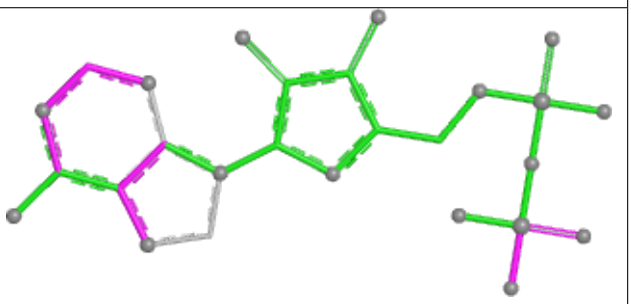
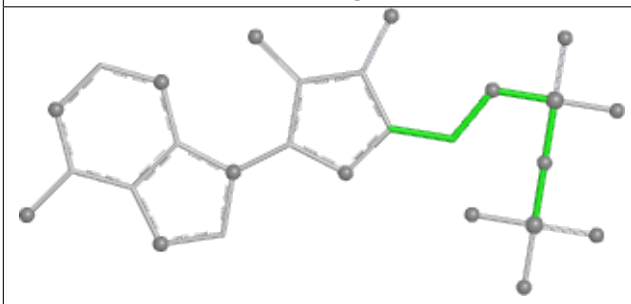
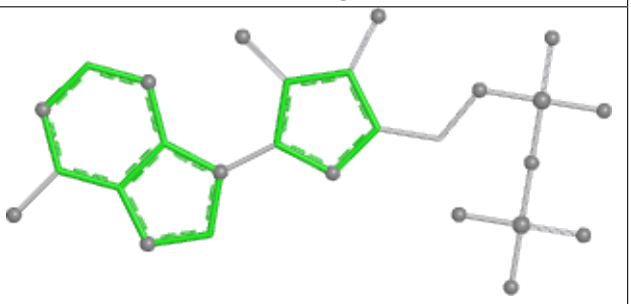
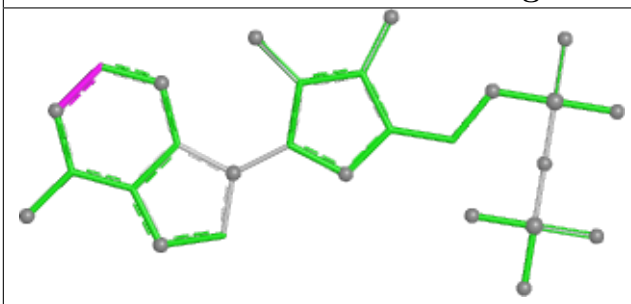
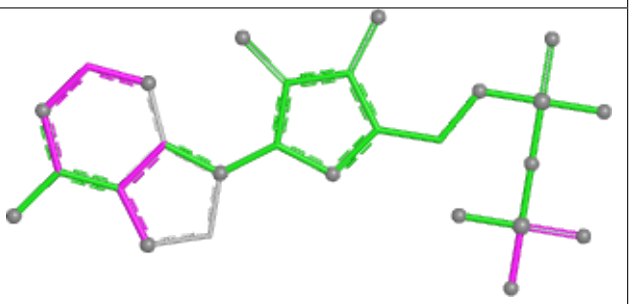
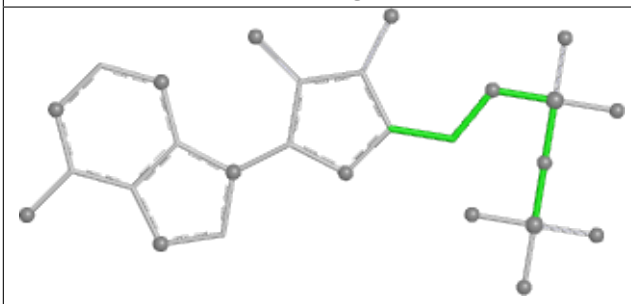
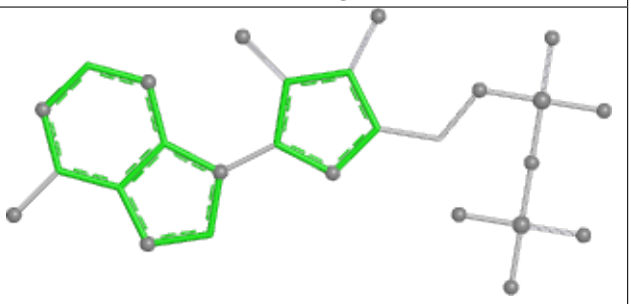
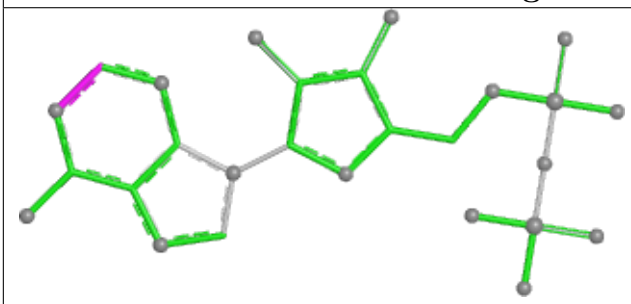
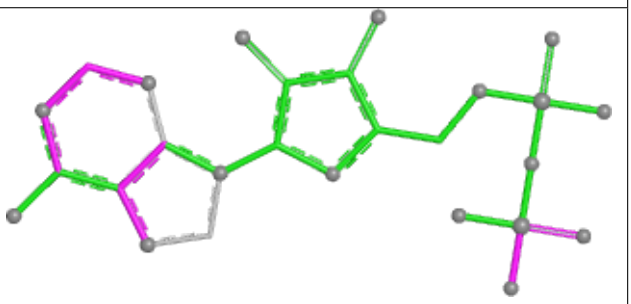
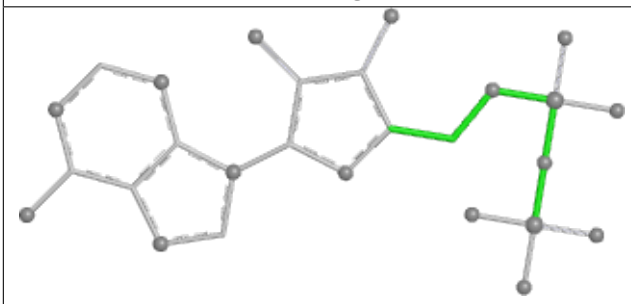
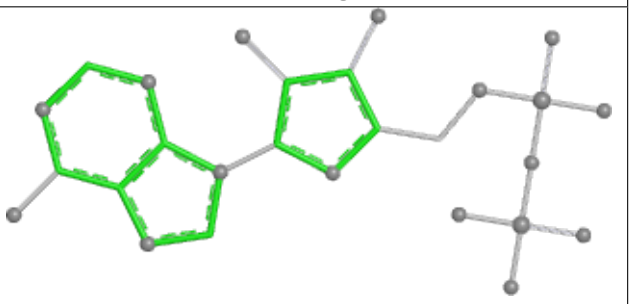
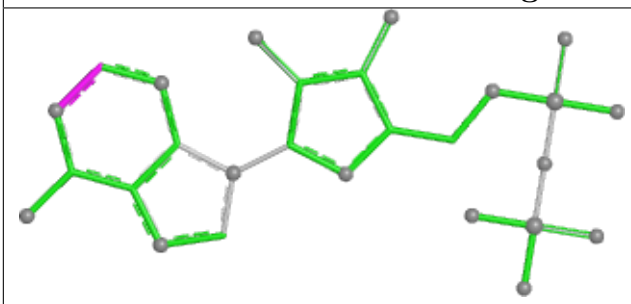
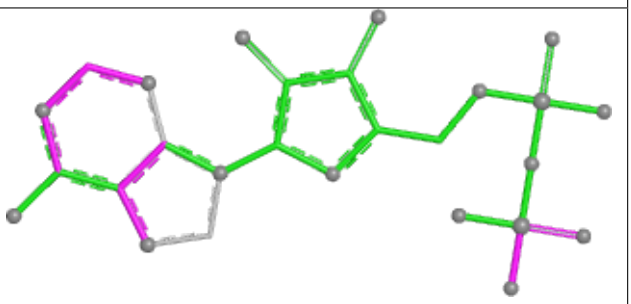
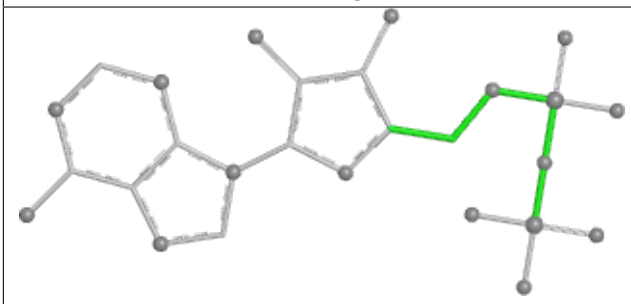
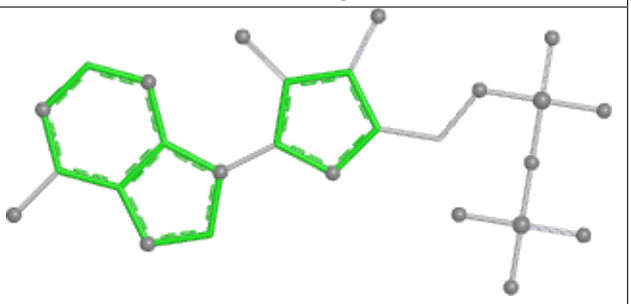
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

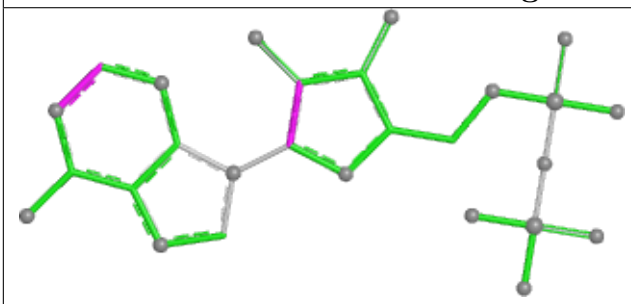
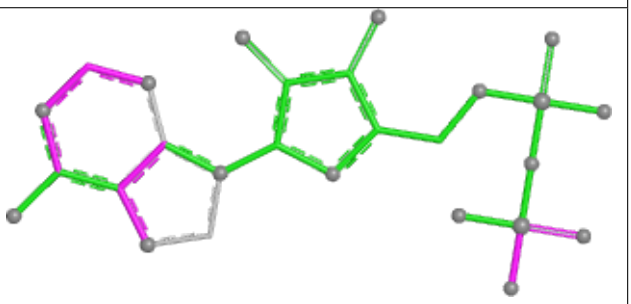
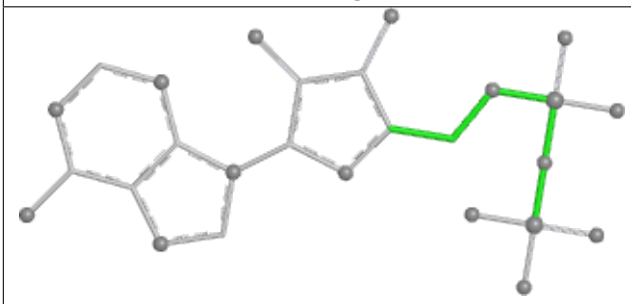
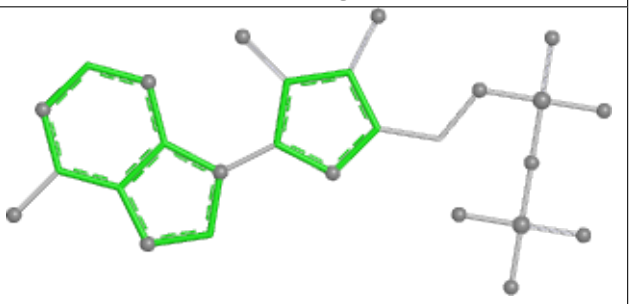
| Ligand ADP Q 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP V 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP B 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP P 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP N 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP O 401 | |
|---|---|
|  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.

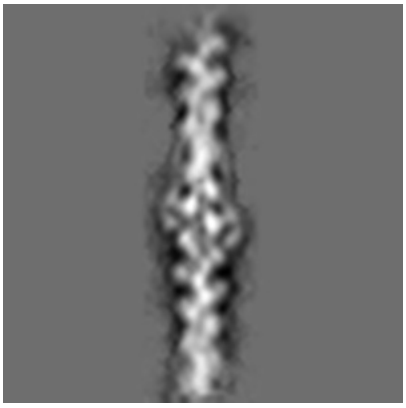
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3576. These allow visual inspection of the internal detail of the map and identification of artifacts.

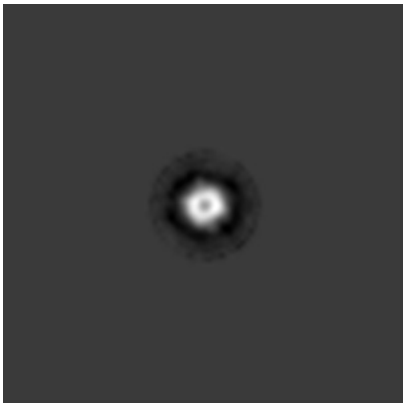
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

### 6.1.1 Primary map


X

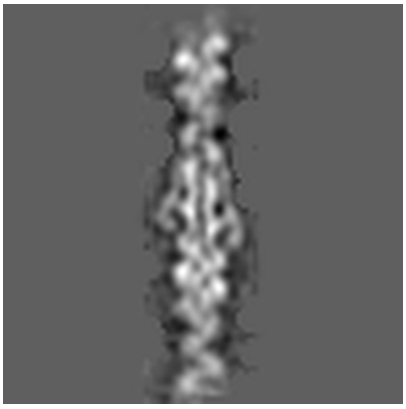
Y

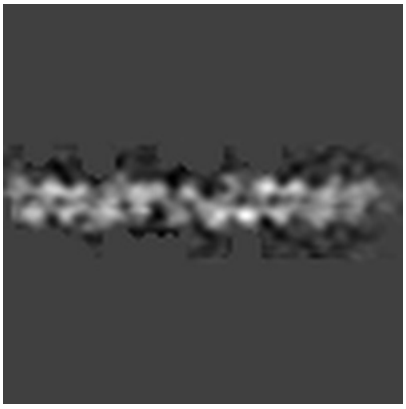

Z

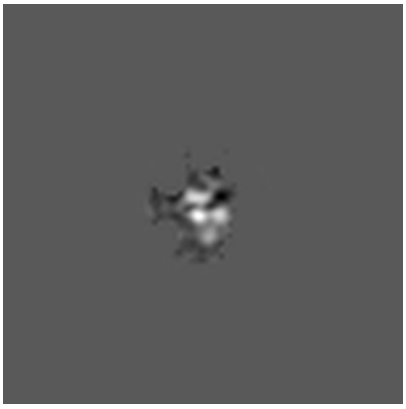
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

### 6.2.1 Primary map


X Index: 48

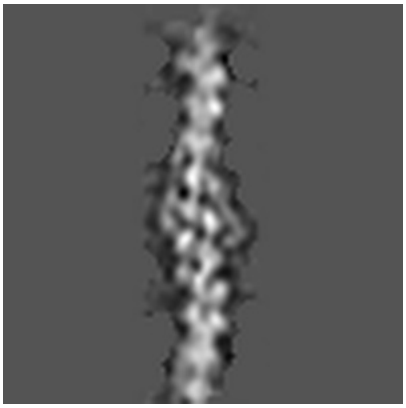

Y Index: 48


Z Index: 48

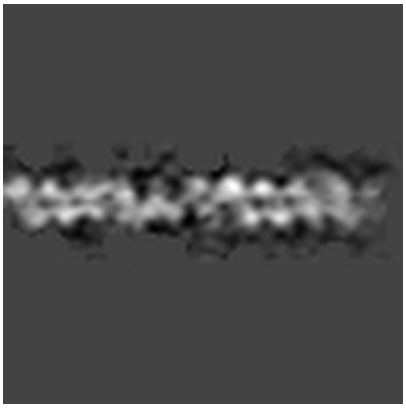
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

### 6.3.1 Primary map



X Index: 50



Y Index: 46

Z Index: 35

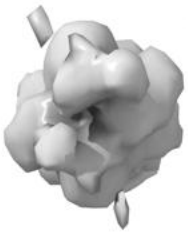
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

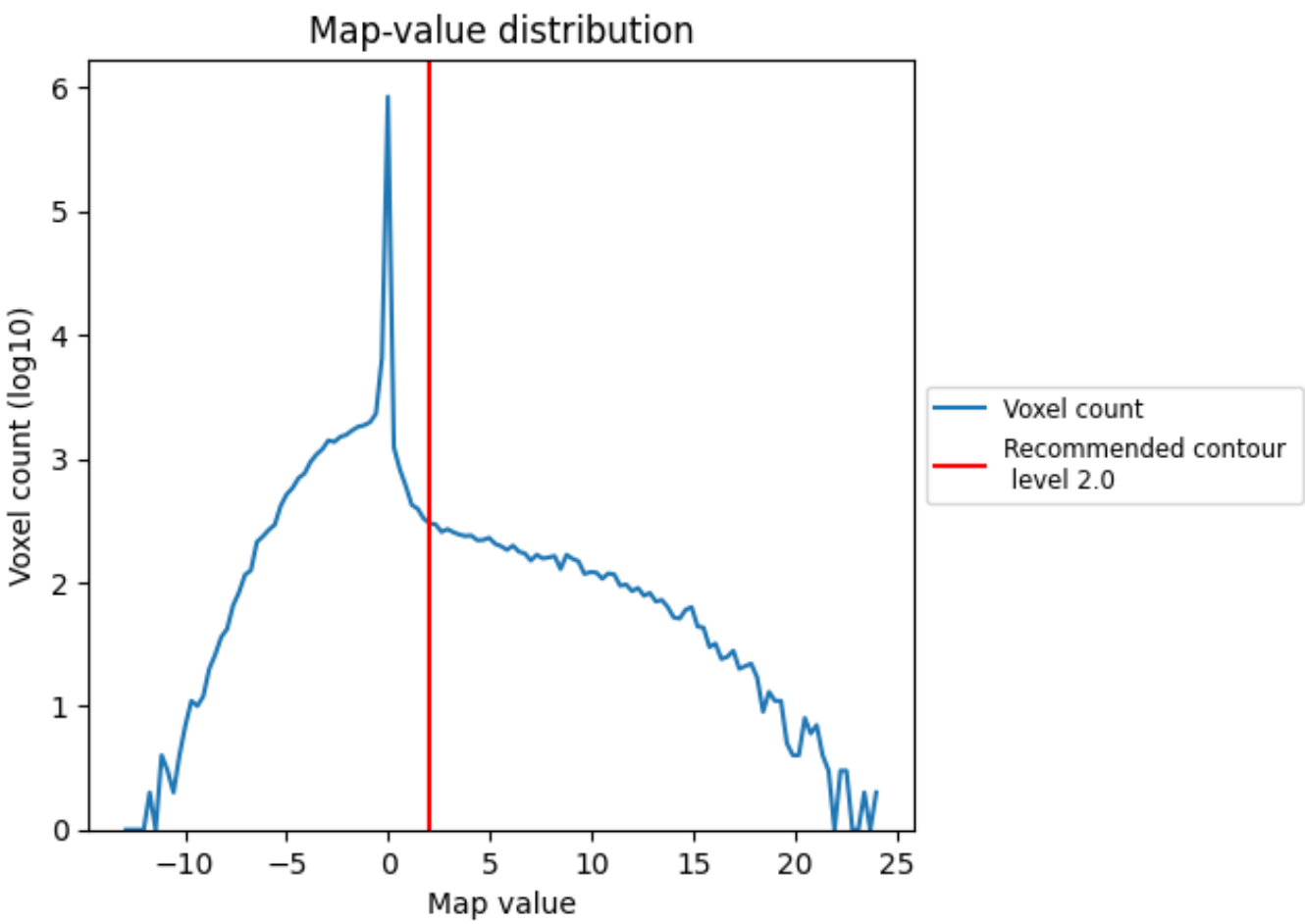
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

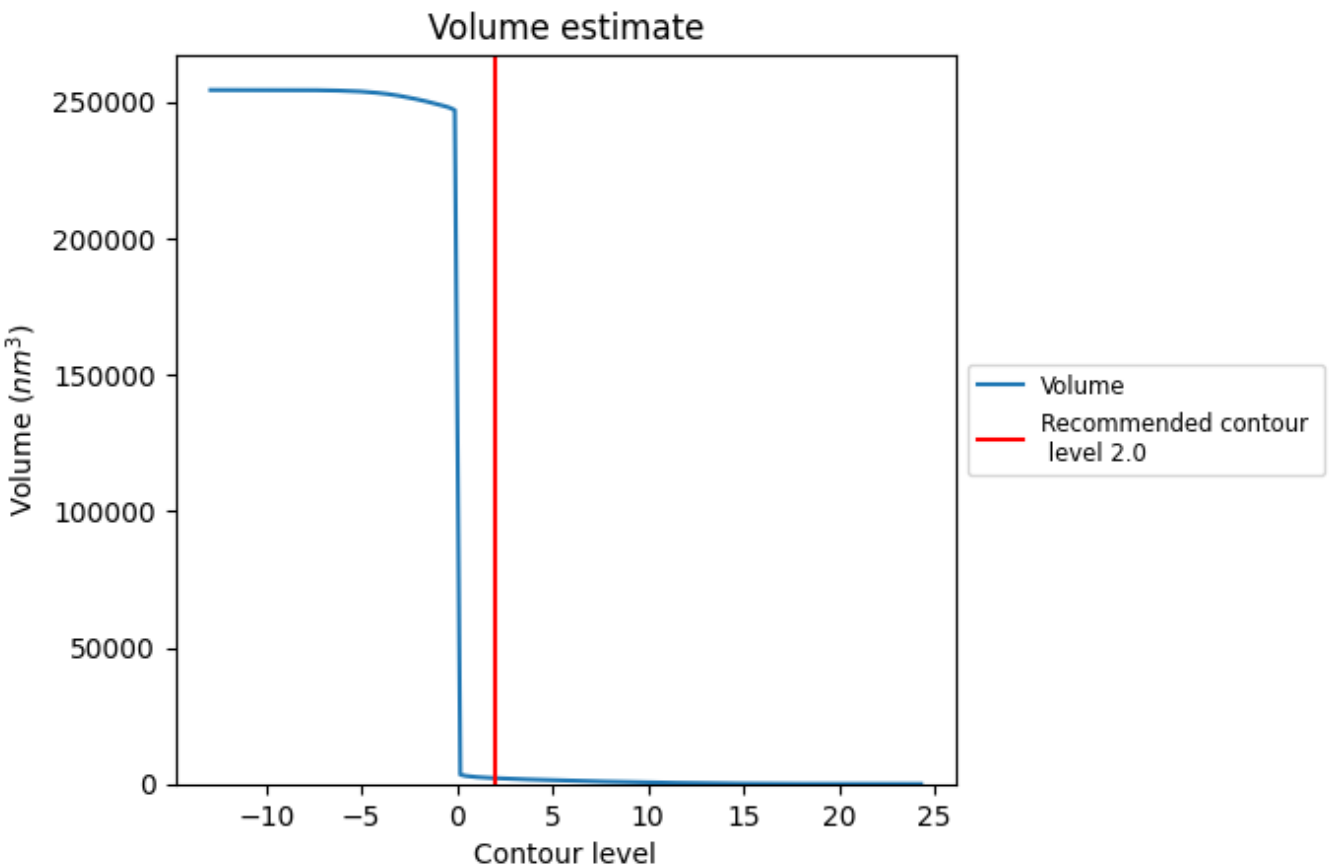
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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.

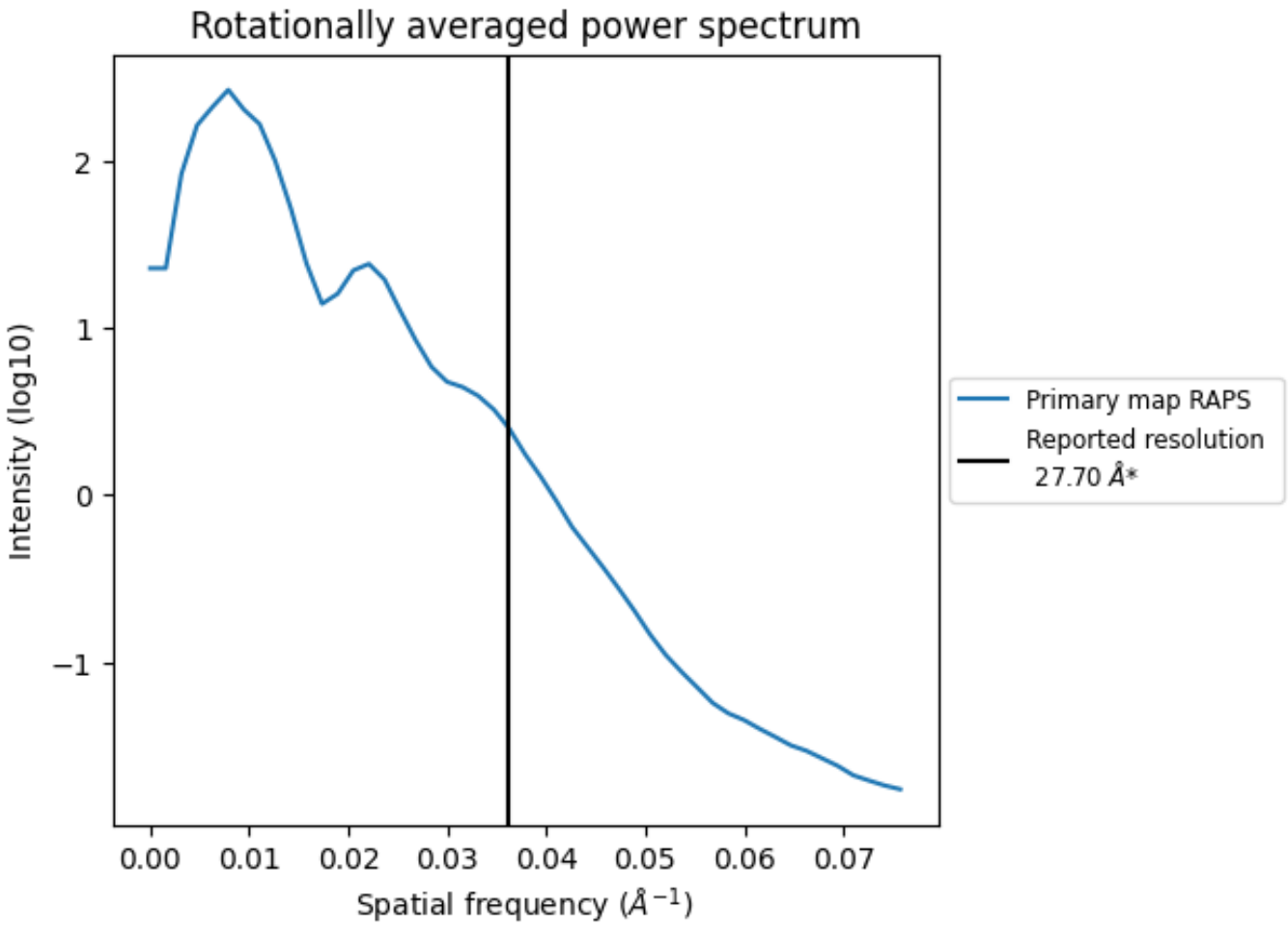
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 2126 $nm^3$; this corresponds to an approximate mass of 1920 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 0.036 Å$^{-1}$

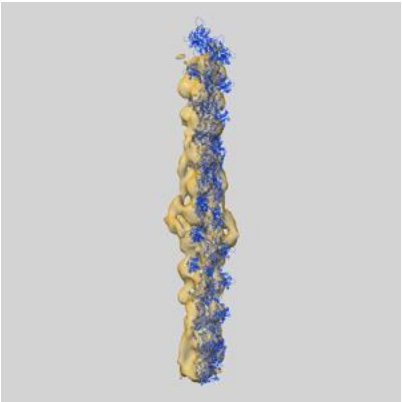
# 8 Fourier-Shell correlation (i)

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

# 9 Map-model fit (i)

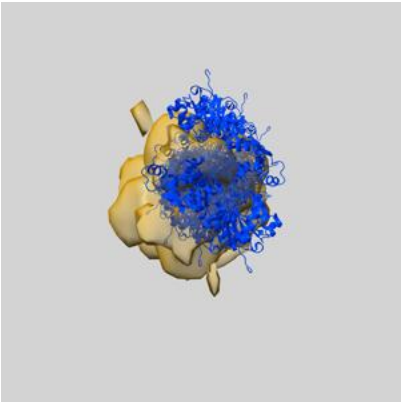
This section contains information regarding the fit between EMDB map EMD-3576 and PDB model 5MVA. Per-residue inclusion information can be found in section 3 on page 7.

## 9.1 Map-model overlay (i)



X

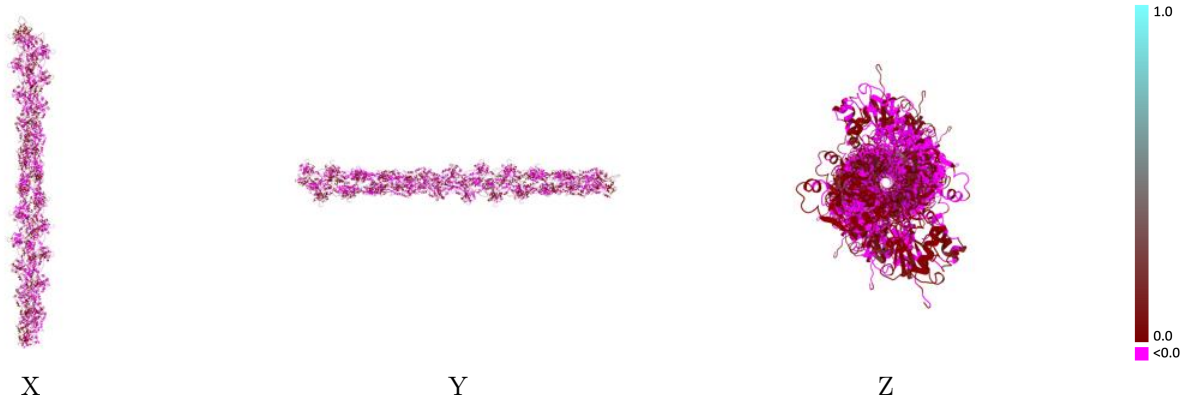
Y



Z

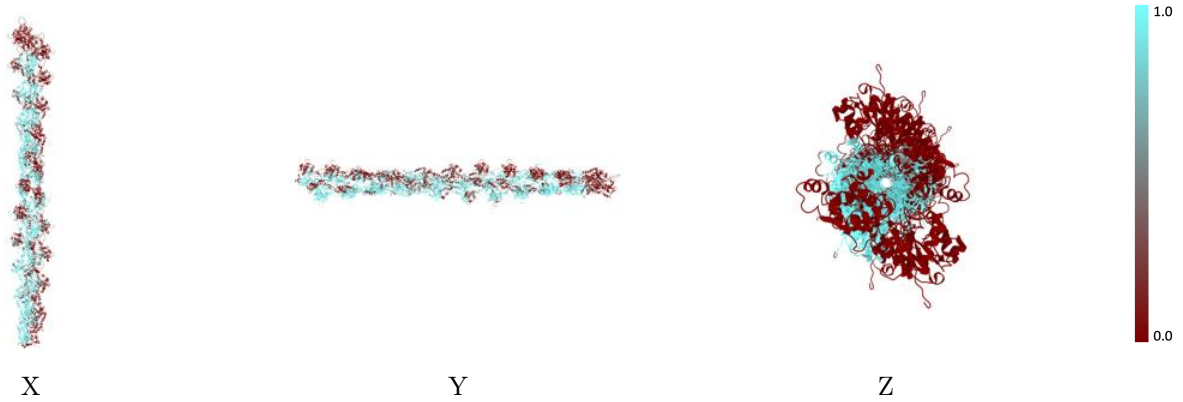
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



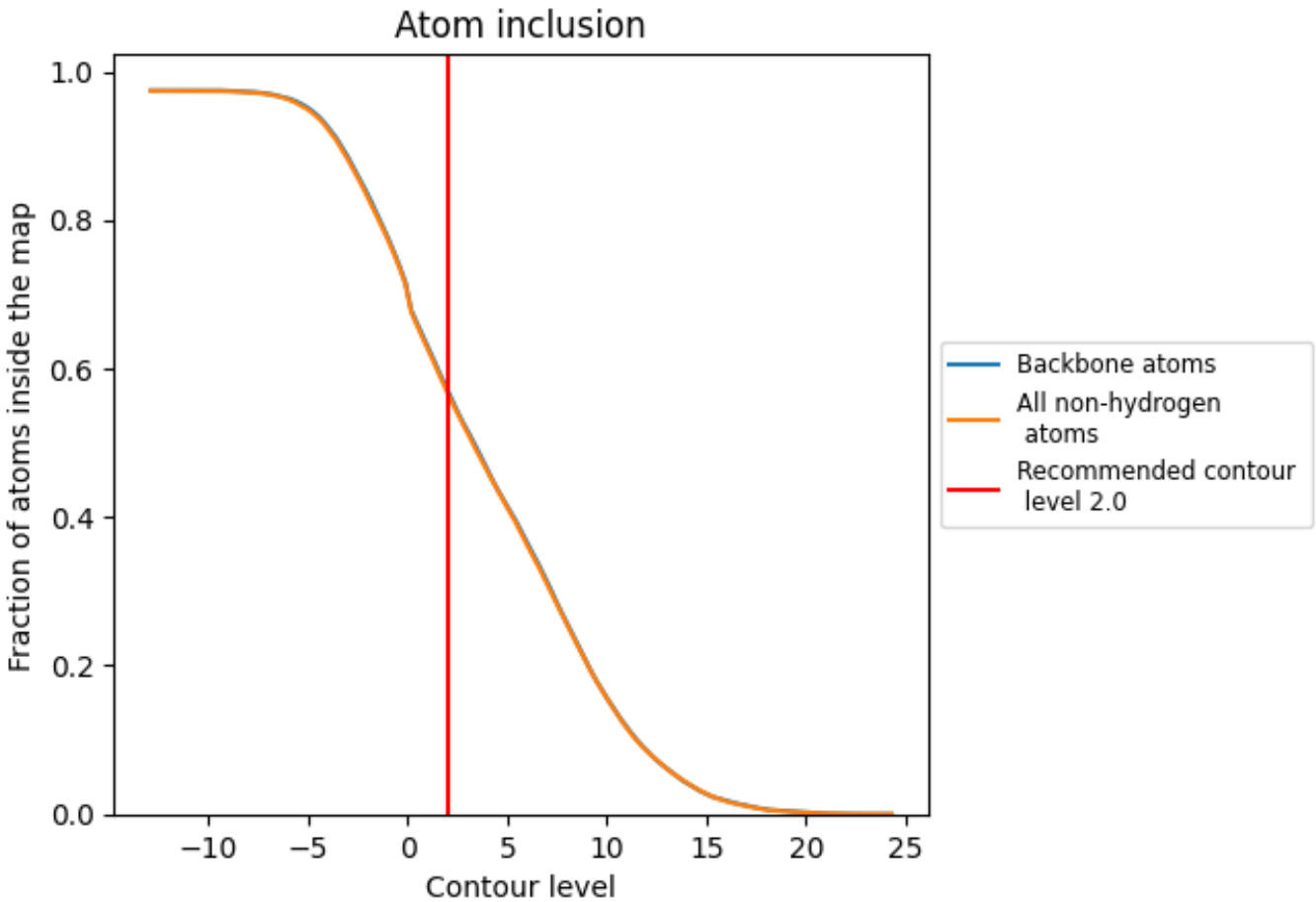

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)




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 (2.0).

## 9.4 Atom inclusion (i)




At the recommended contour level, 57% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5674 | -0.0000 |
| A | 0.0324 | 0.0020 |
| B | 0.1477 | -0.0120 |
| C | 0.7012 | 0.0080 |
| D | 0.3115 | -0.0080 |
| E | 0.8871 | 0.0150 |
| F | 0.4379 | -0.0160 |
| G | 0.8127 | 0.0080 |
| H | 0.5508 | 0.0170 |
| I | 0.6313 | 0.0010 |
| J | 0.6282 | 0.0150 |
| K | 0.5504 | -0.0070 |
| L | 0.5752 | -0.0170 |
| M | 0.5308 | -0.0010 |
| N | 0.5793 | -0.0220 |
| O | 0.5157 | -0.0050 |
| P | 0.7480 | -0.0160 |
| Q | 0.4100 | -0.0110 |
| R | 0.9129 | 0.0110 |
| S | 0.4571 | -0.0240 |
| T | 0.7886 | 0.0120 |
| U | 0.5487 | 0.0180 |
| V | 0.7126 | 0.0090 |
| W | 0.5793 | 0.0220 |