# Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 05:34 PM EST

| | | |
|---|---|---|
| PDB ID | : | 1KP8 |
| Title | : | Structural Basis for GroEL-assisted Protein Folding from the Crystal Structure of (GroEL-KMgATP)14 at 2.0 A Resolution |
| Authors | : | Wang, J. |
| Deposited on | : | 2001-12-30 |
| Resolution | : | 2.00 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

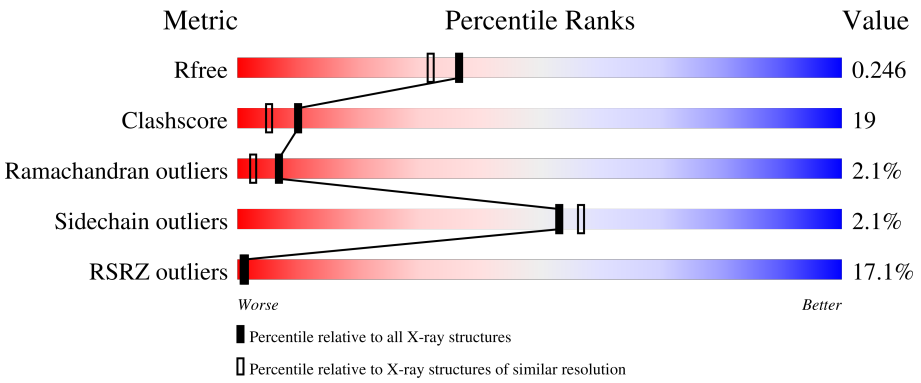
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 8085 (2.00-2.00) |
| Clashscore | 141614 | 9178 (2.00-2.00) |
| Ramachandran outliers | 138981 | 9054 (2.00-2.00) |
| Sidechain outliers | 138945 | 9053 (2.00-2.00) |
| RSRZ outliers | 127900 | 7900 (2.00-2.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 547 | 13% 63% 30% |
| 1 | B | 547 | 23% 64% 29% |
| 1 | C | 547 | 21% 64% 29% |
| 1 | D | 547 | 6% 67% 27% |
| 1 | E | 547 | 18% 64% 29% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 547 | 21% 66% 27% |
| 1 | G | 547 | 8% 65% 28% |
| 1 | H | 547 | 11% 65% 29% |
| 1 | I | 547 | 15% 65% 28% |
| 1 | J | 547 | 16% 65% 28% |
| 1 | K | 547 | 25% 64% 29% |
| 1 | L | 547 | 16% 64% 29% |
| 1 | M | 547 | 25% 64% 29% |
| 1 | N | 547 | 12% 67% 26% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 2 | SO4 | J | 4020 | - | - | - | X |
| 2 | SO4 | K | 4021 | - | - | - | X |

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 57085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called groEL protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | B | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | C | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | D | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | E | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | F | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | G | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | H | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | I | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | J | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | K | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | L | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | M | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |
| 1 | N | 525 | 3855 | 2399 | 664 | 772 | 20 | 0 | 0 | 0 |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |

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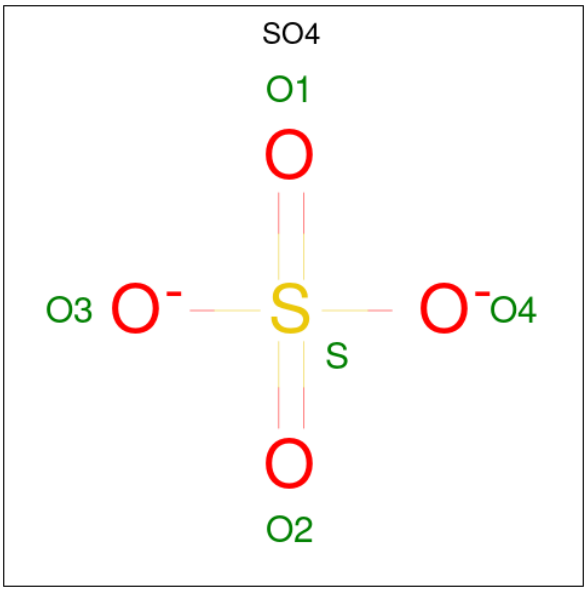
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| A | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| B | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| B | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| B | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| C | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| C | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| C | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| D | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| D | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| D | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| E | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| E | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| E | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| F | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| F | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| F | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| G | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| G | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| G | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| H | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| H | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| H | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| I | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| I | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| I | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| J | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| J | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| J | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| K | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| K | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| K | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| L | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| L | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| L | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| M | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| M | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| M | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |
| N | 13 | GLY | ARG | SEE REMARK 999 | UNP P0A6F5 |
| N | 126 | VAL | ALA | SEE REMARK 999 | UNP P0A6F5 |
| N | 434 | ALA | GLU | SEE REMARK 999 | UNP P0A6F5 |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: $O_4S$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | O | S | | | |
| 2 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | B | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | B | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | C | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | C | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | E | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | E | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | F | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | G | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | H | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | H | 1 | 5 | 4 | 1 | | 0 | 0 |
| | | | Total | O | S | | | |
| 2 | J | 1 | 5 | 4 | 1 | | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | J | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | K | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | K | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | L | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | M | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | M | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | N | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | N | 1 | Total O S<br>5 4 1 | 0 | 0 |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | B | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | C | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | D | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | E | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | F | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | G | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | H | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | I | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | J | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | K | 1 | Total Mg<br>1 1 | 0 | 0 |

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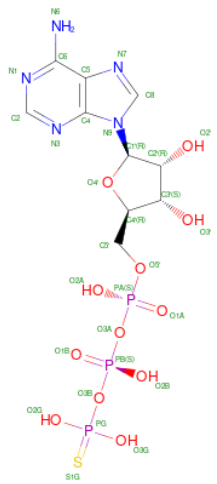
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | L | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | M | 1 | Total Mg<br>1 1 | 0 | 0 |
| 3 | N | 1 | Total Mg<br>1 1 | 0 | 0 |

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | A | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | B | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | C | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | D | 2 | Total K<br>2 2 | 0 | 0 |
| 4 | E | 2 | Total K<br>2 2 | 0 | 0 |
| 4 | F | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | G | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | H | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | I | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | J | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | K | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | L | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | M | 1 | Total K<br>1 1 | 0 | 0 |
| 4 | N | 1 | Total K<br>1 1 | 0 | 0 |

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

AGS



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | |
| 5 | A | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | B | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | C | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | D | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | E | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | F | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | G | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | H | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | I | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | J | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | K | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | L | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | M | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |
| 5 | N | 1 | 31 | 10 | 5 | 12 | 3 | 1 | 0 | 0 |

- Molecule 6 is water.

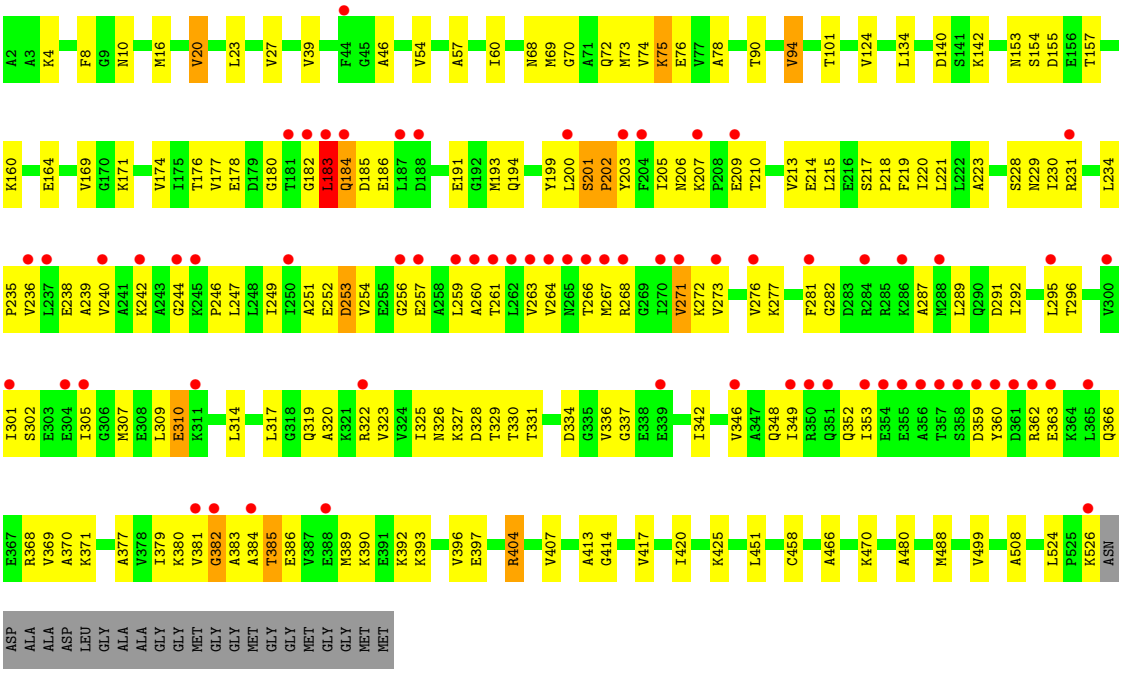
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 6 | A | 156 | Total O<br>156 156 | 0 | 0 |
| 6 | B | 214 | Total O<br>214 214 | 0 | 0 |
| 6 | C | 149 | Total O<br>149 149 | 0 | 0 |
| 6 | D | 261 | Total O<br>261 261 | 0 | 0 |
| 6 | E | 217 | Total O<br>217 217 | 0 | 0 |
| 6 | F | 200 | Total O<br>200 200 | 0 | 0 |
| 6 | G | 269 | Total O<br>269 269 | 0 | 0 |
| 6 | H | 204 | Total O<br>204 204 | 0 | 0 |
| 6 | I | 145 | Total O<br>145 145 | 0 | 0 |
| 6 | J | 139 | Total O<br>139 139 | 0 | 0 |
| 6 | K | 133 | Total O<br>133 133 | 0 | 0 |
| 6 | L | 163 | Total O<br>163 163 | 0 | 0 |
| 6 | M | 138 | Total O<br>138 138 | 0 | 0 |
| 6 | N | 153 | Total O<br>153 153 | 0 | 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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

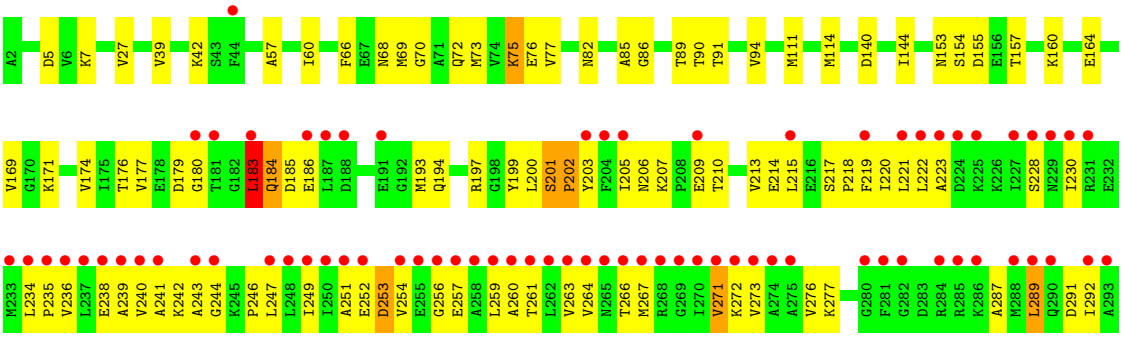
- Molecule 1: groEL protein

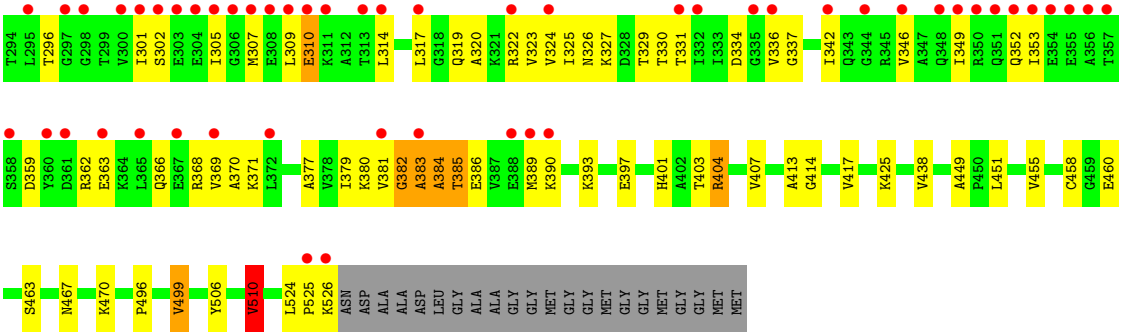
Chain A:




- Molecule 1: groEL protein

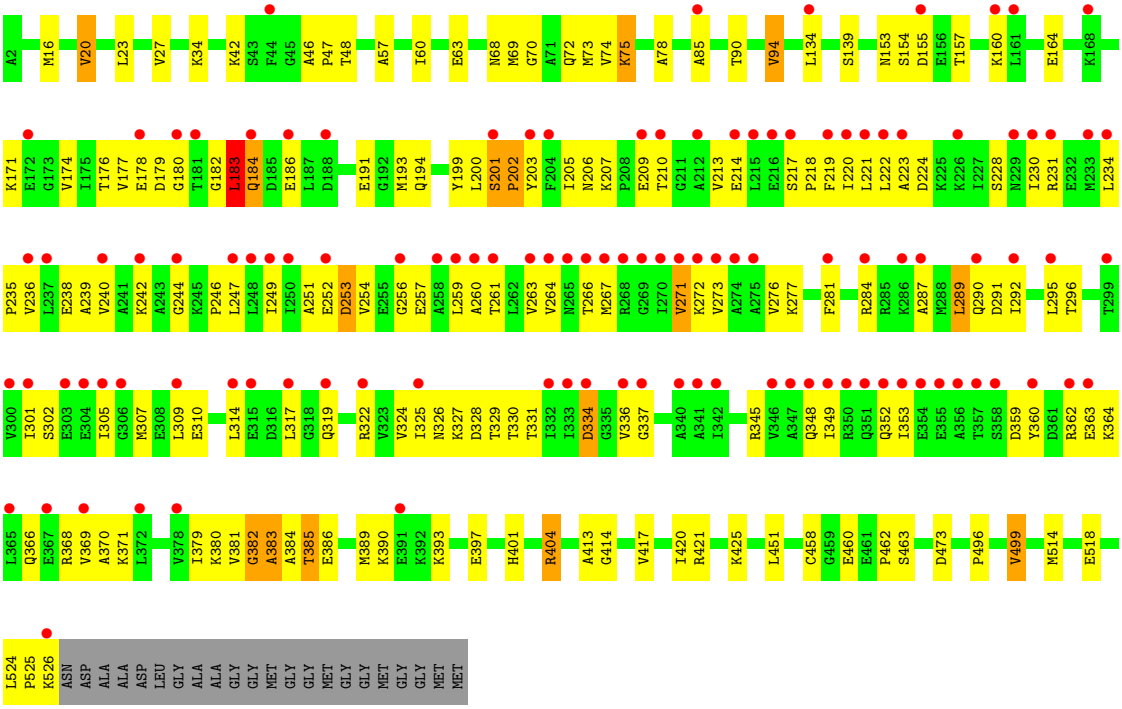
Chain B:





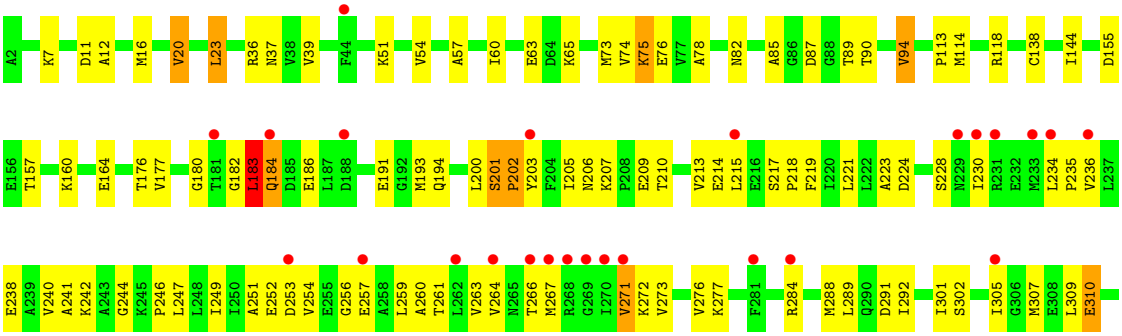

- Molecule 1: groEL protein

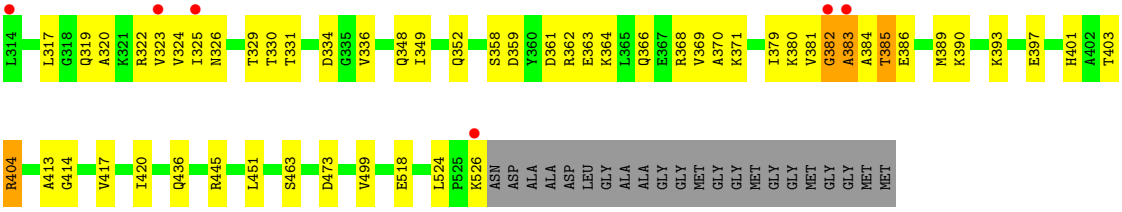
Chain C:




- Molecule 1: groEL protein

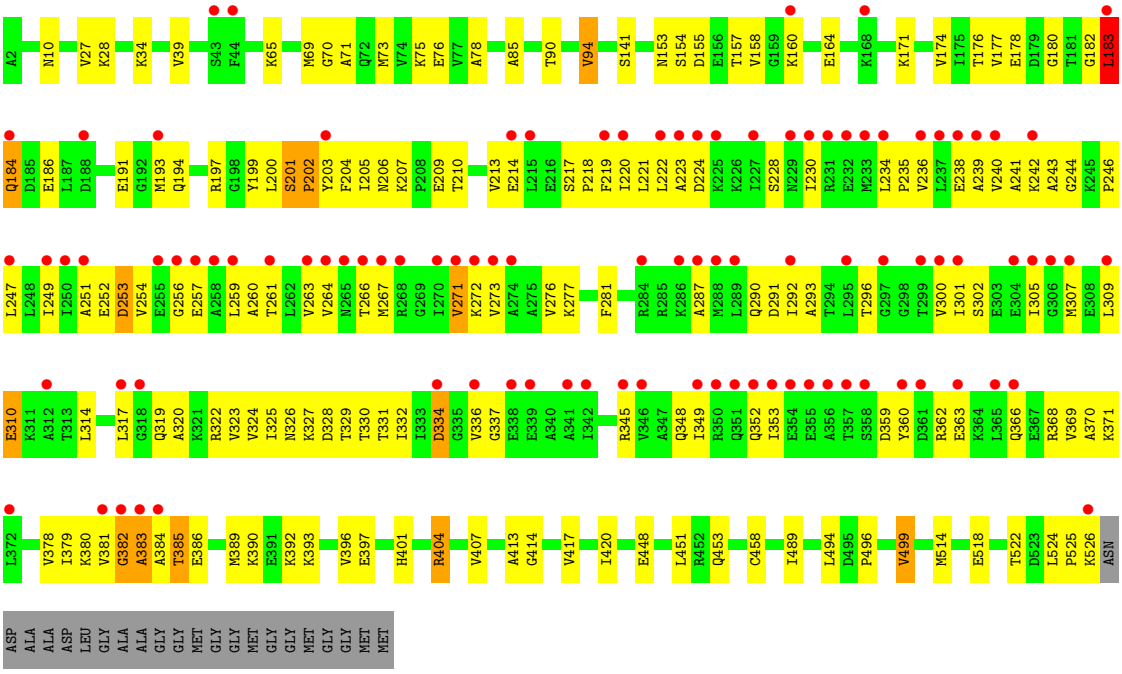
Chain D:





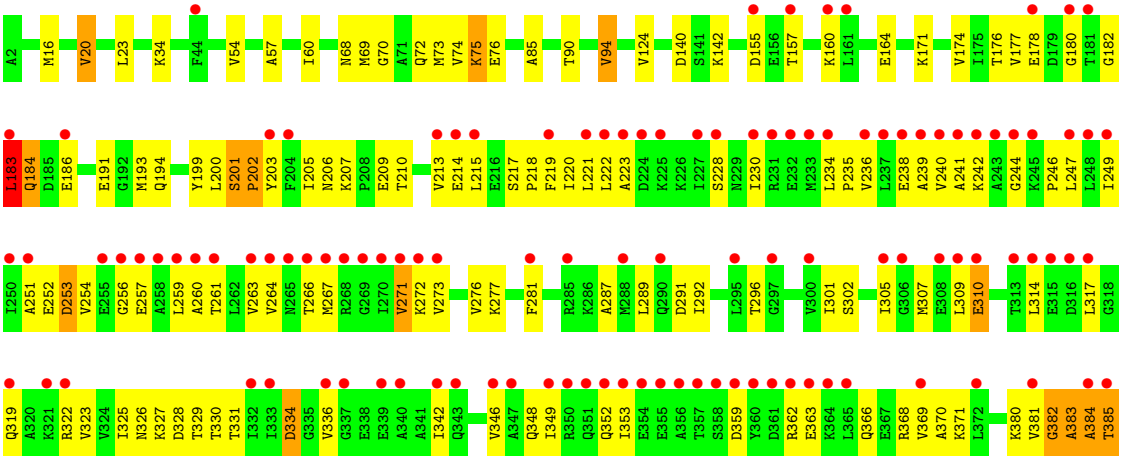

• Molecule 1: groEL protein

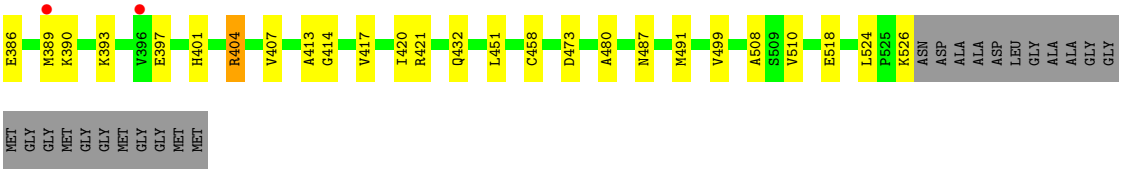
Chain E:




• Molecule 1: groEL protein

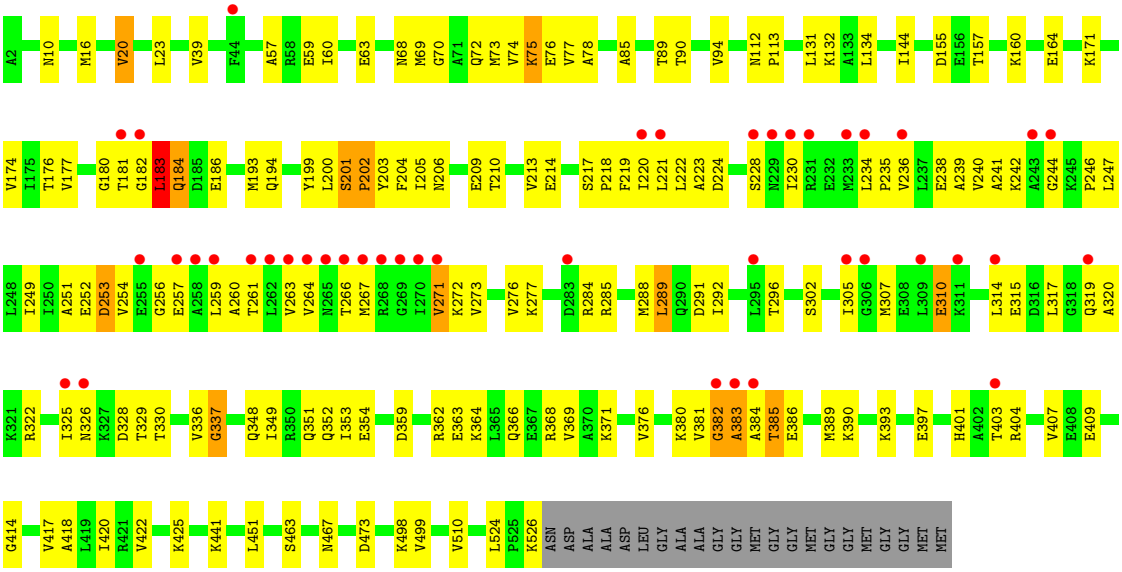
Chain F:





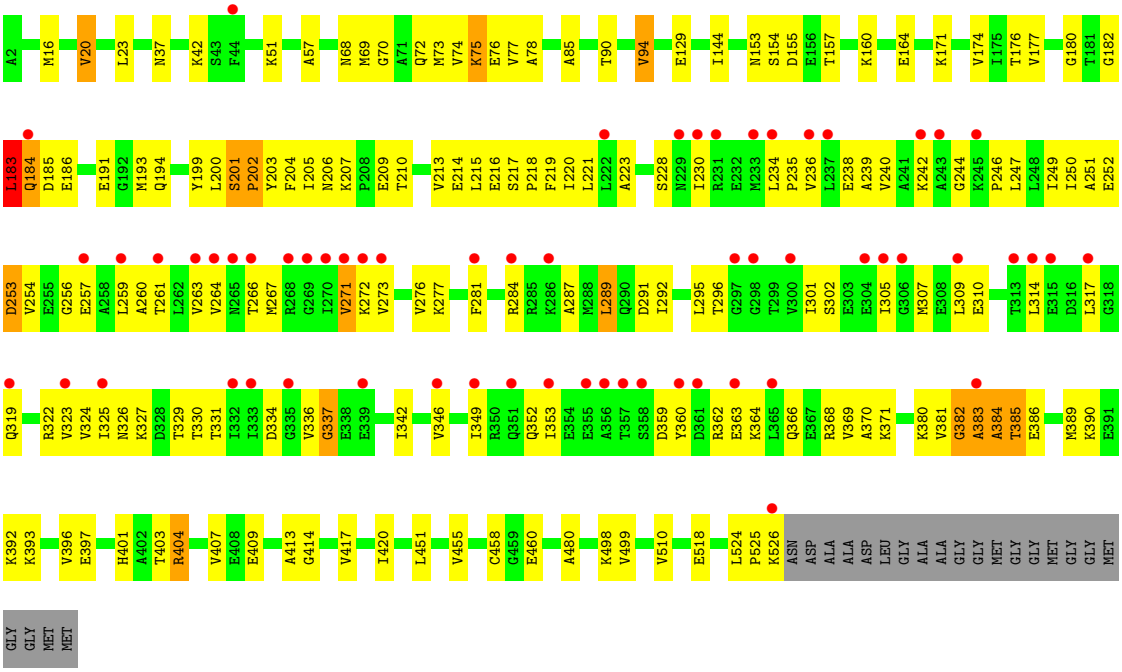

• Molecule 1: groEL protein

Chain G:



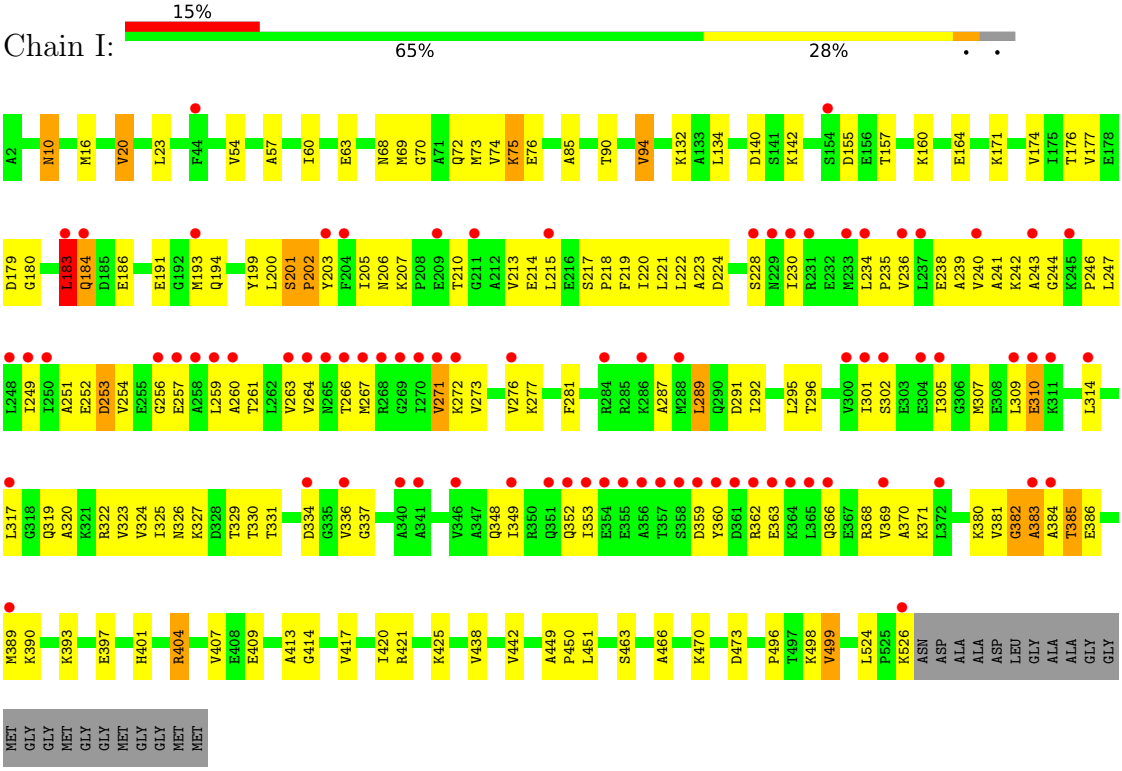

• Molecule 1: groEL protein

Chain H:



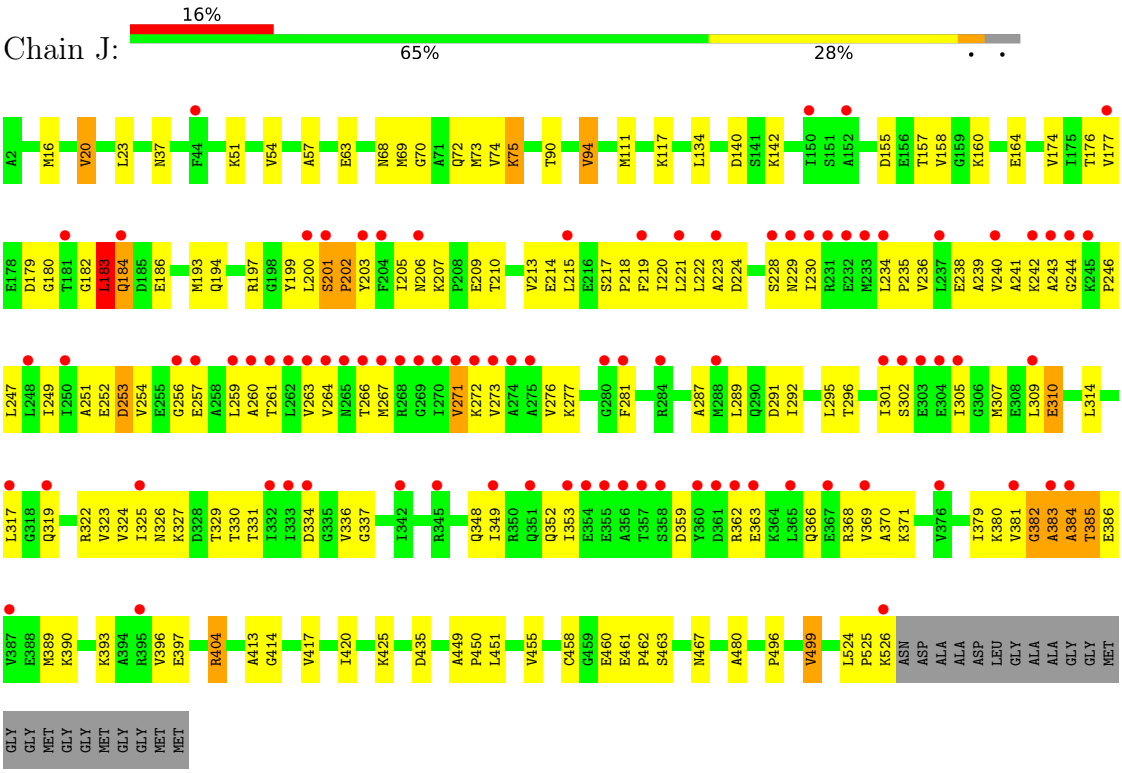
• Molecule 1: groEL protein

Chain I:



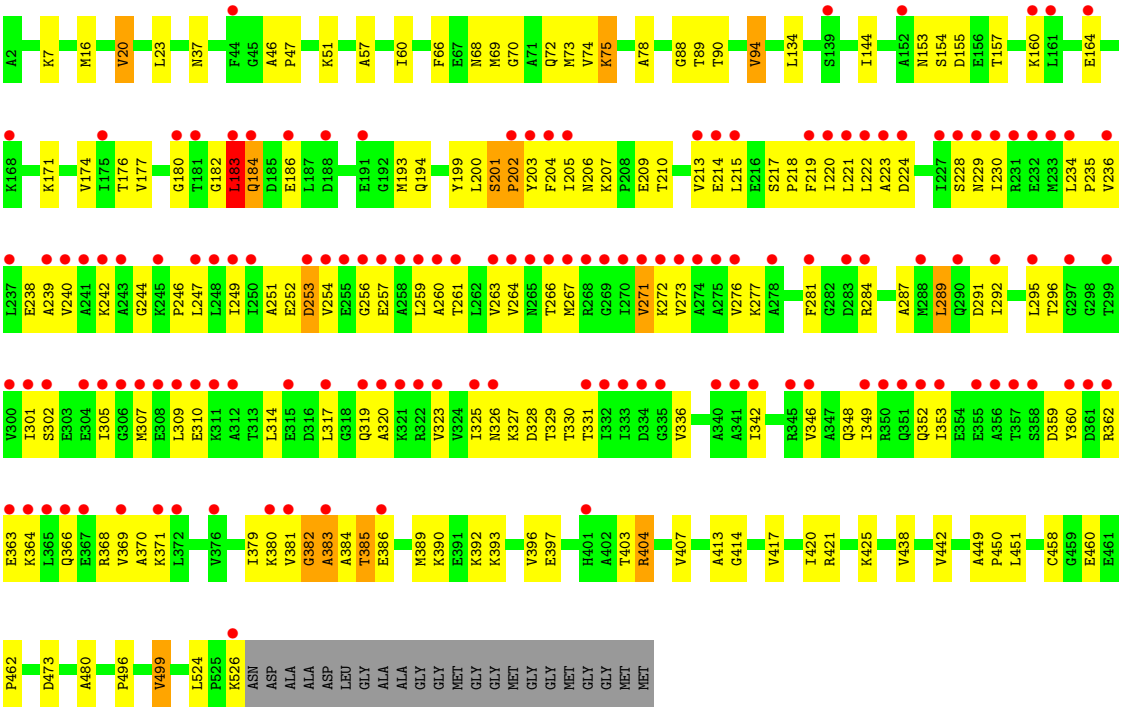

• Molecule 1: groEL protein

Chain J:



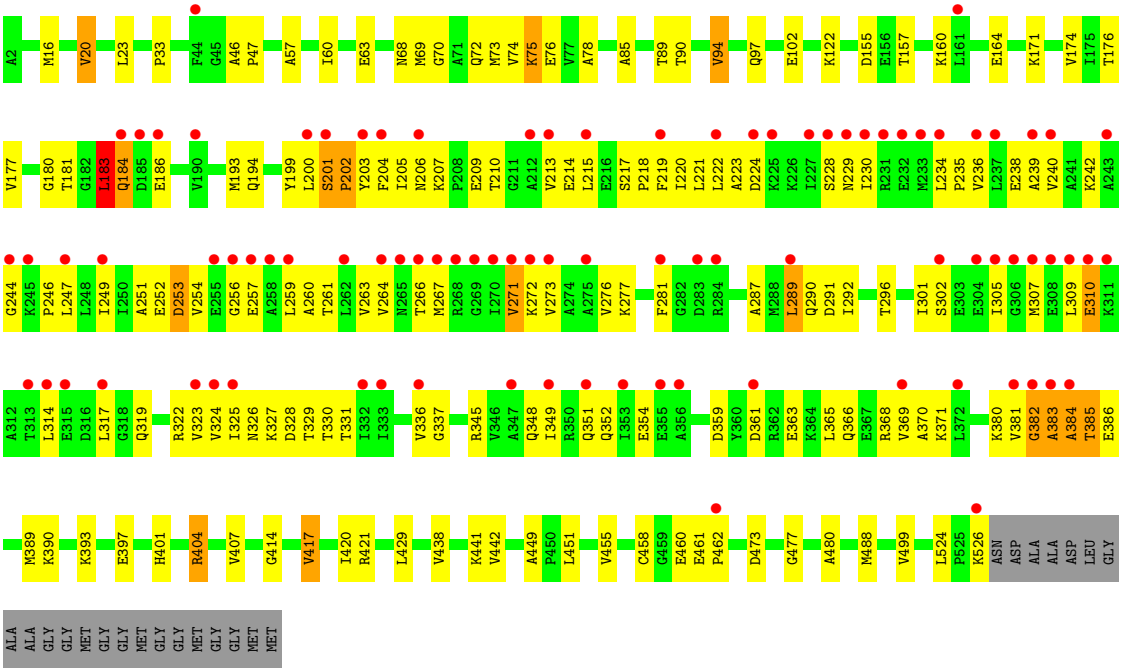

• Molecule 1: groEL protein

Chain K:



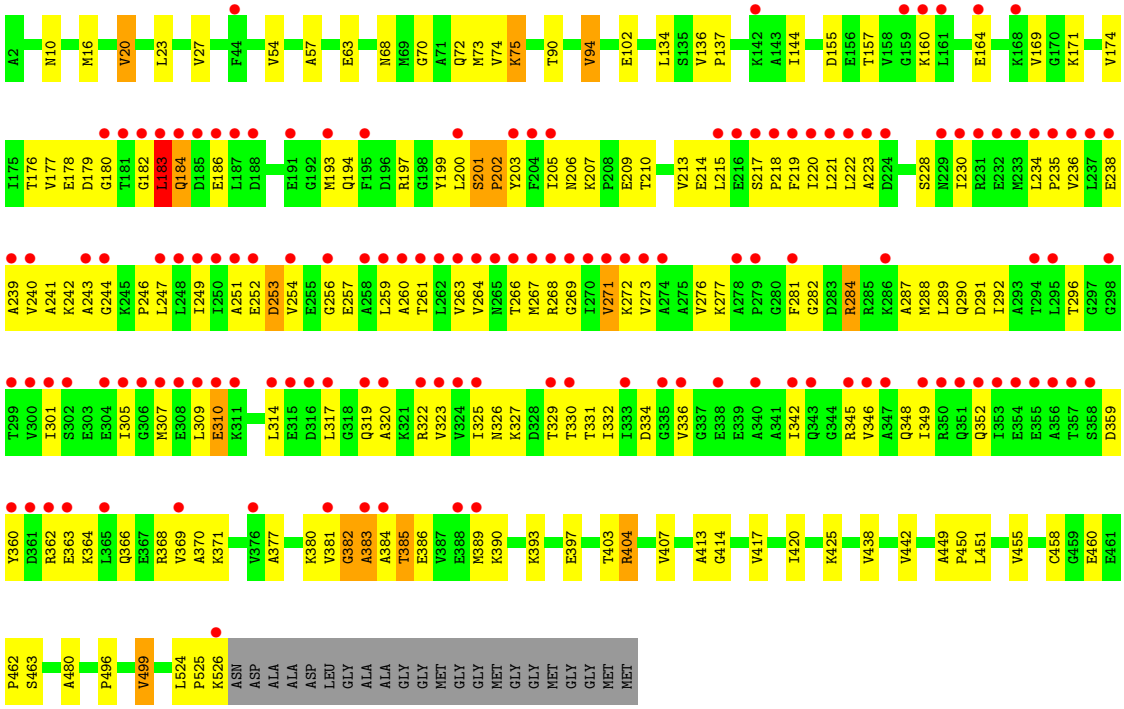

- Molecule 1: groEL protein

Chain L:



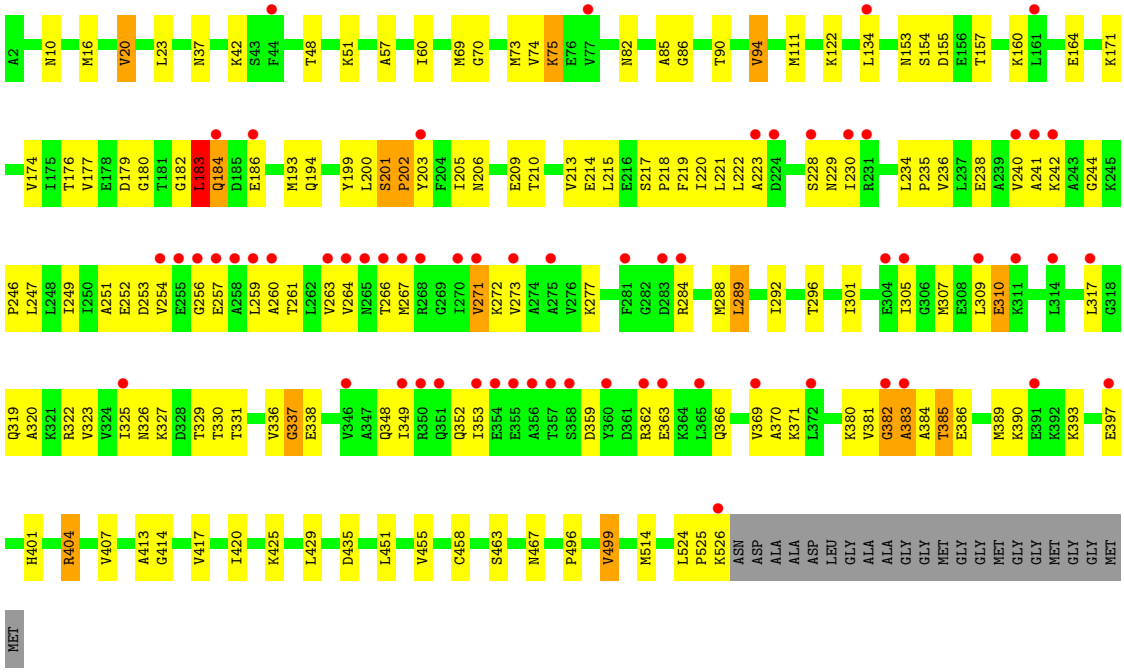

- Molecule 1: groEL protein

Chain M:



- Molecule 1: groEL protein

Chain N:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 135.57Å 260.11Å 150.20Å<br>90.00° 101.14° 90.00° | Depositor |
| Resolution (Å) | 39.89 – 2.00<br>39.89 – 2.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 78.9 (39.89-2.00)<br>79.1 (39.89-2.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.10 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.57 (at 2.00Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, $R_{free}$ | 0.243 , 0.258<br>0.229 , 0.246 | Depositor<br>DCC |
| $R_{free}$ test set | 12780 reflections (1.98%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 30.6 | Xtriage |
| Anisotropy | 0.362 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 60.3 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 57085 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 73.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, SO4, MG, K

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 | 0.32 | 0/3883 | 0.55 | 0/5243 |
| 1 | B | 0.35 | 0/3883 | 0.57 | 1/5243 (0.0%) |
| 1 | C | 0.32 | 0/3883 | 0.55 | 0/5243 |
| 1 | D | 0.36 | 0/3883 | 0.58 | 0/5243 |
| 1 | E | 0.34 | 0/3883 | 0.57 | 0/5243 |
| 1 | F | 0.32 | 0/3883 | 0.55 | 0/5243 |
| 1 | G | 0.36 | 0/3883 | 0.58 | 0/5243 |
| 1 | H | 0.33 | 0/3883 | 0.56 | 0/5243 |
| 1 | I | 0.30 | 0/3883 | 0.55 | 0/5243 |
| 1 | J | 0.30 | 0/3883 | 0.54 | 0/5243 |
| 1 | K | 0.30 | 0/3883 | 0.54 | 0/5243 |
| 1 | L | 0.32 | 0/3883 | 0.55 | 0/5243 |
| 1 | M | 0.30 | 0/3883 | 0.54 | 0/5243 |
| 1 | N | 0.31 | 0/3883 | 0.55 | 0/5243 |
| All | All | 0.32 | 0/54362 | 0.55 | 1/73402 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 510 | VAL | CB-CA-C | -5.51 | 100.94 | 111.40 |

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 | 3855 | 0 | 3982 | 161 | 0 |
| 1 | B | 3855 | 0 | 3982 | 170 | 0 |
| 1 | C | 3855 | 0 | 3982 | 153 | 0 |
| 1 | D | 3855 | 0 | 3982 | 146 | 0 |
| 1 | E | 3855 | 0 | 3982 | 154 | 0 |
| 1 | F | 3855 | 0 | 3982 | 136 | 0 |
| 1 | G | 3855 | 0 | 3982 | 153 | 1 |
| 1 | H | 3855 | 0 | 3982 | 149 | 0 |
| 1 | I | 3855 | 0 | 3982 | 150 | 0 |
| 1 | J | 3855 | 0 | 3982 | 149 | 0 |
| 1 | K | 3855 | 0 | 3982 | 154 | 0 |
| 1 | L | 3855 | 0 | 3982 | 149 | 0 |
| 1 | M | 3855 | 0 | 3982 | 151 | 0 |
| 1 | N | 3855 | 0 | 3982 | 145 | 1 |
| 2 | A | 15 | 0 | 0 | 0 | 0 |
| 2 | B | 10 | 0 | 0 | 0 | 0 |
| 2 | C | 10 | 0 | 0 | 0 | 0 |
| 2 | E | 10 | 0 | 0 | 1 | 0 |
| 2 | F | 5 | 0 | 0 | 0 | 0 |
| 2 | G | 5 | 0 | 0 | 0 | 0 |
| 2 | H | 10 | 0 | 0 | 0 | 0 |
| 2 | J | 10 | 0 | 0 | 0 | 0 |
| 2 | K | 10 | 0 | 0 | 0 | 0 |
| 2 | L | 5 | 0 | 0 | 0 | 0 |
| 2 | M | 10 | 0 | 0 | 0 | 0 |
| 2 | N | 10 | 0 | 0 | 0 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| 3 | I | 1 | 0 | 0 | 0 | 0 |
| 3 | J | 1 | 0 | 0 | 0 | 0 |
| 3 | K | 1 | 0 | 0 | 0 | 0 |
| 3 | L | 1 | 0 | 0 | 0 | 0 |
| 3 | M | 1 | 0 | 0 | 0 | 0 |
| 3 | N | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 2 | 0 | 0 | 0 | 0 |
| 4 | E | 2 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | I | 1 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| 4 | K | 1 | 0 | 0 | 0 | 0 |
| 4 | L | 1 | 0 | 0 | 0 | 0 |
| 4 | M | 1 | 0 | 0 | 0 | 0 |
| 4 | N | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 31 | 0 | 12 | 3 | 0 |
| 5 | B | 31 | 0 | 12 | 4 | 0 |
| 5 | C | 31 | 0 | 12 | 3 | 0 |
| 5 | D | 31 | 0 | 12 | 4 | 0 |
| 5 | E | 31 | 0 | 12 | 4 | 0 |
| 5 | F | 31 | 0 | 12 | 3 | 0 |
| 5 | G | 31 | 0 | 12 | 4 | 0 |
| 5 | H | 31 | 0 | 12 | 4 | 0 |
| 5 | I | 31 | 0 | 12 | 4 | 0 |
| 5 | J | 31 | 0 | 12 | 3 | 0 |
| 5 | K | 31 | 0 | 12 | 5 | 0 |
| 5 | L | 31 | 0 | 12 | 5 | 0 |
| 5 | M | 31 | 0 | 12 | 5 | 0 |
| 5 | N | 31 | 0 | 12 | 4 | 0 |
| 6 | A | 156 | 0 | 0 | 7 | 0 |
| 6 | B | 214 | 0 | 0 | 8 | 0 |
| 6 | C | 149 | 0 | 0 | 9 | 0 |
| 6 | D | 261 | 0 | 0 | 19 | 0 |
| 6 | E | 217 | 0 | 0 | 12 | 0 |
| 6 | F | 200 | 0 | 0 | 5 | 0 |
| 6 | G | 269 | 0 | 0 | 12 | 0 |
| 6 | H | 204 | 0 | 0 | 8 | 0 |
| 6 | I | 145 | 0 | 0 | 5 | 0 |
| 6 | J | 139 | 0 | 0 | 2 | 0 |
| 6 | K | 133 | 0 | 0 | 0 | 0 |
| 6 | L | 163 | 0 | 0 | 9 | 0 |
| 6 | M | 138 | 0 | 0 | 6 | 0 |
| 6 | N | 153 | 0 | 0 | 7 | 0 |
| All | All | 57085 | 0 | 55916 | 2099 | 1 |

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 19.

All (2099) 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) |
|---|---|---|---|
| 5:B:1:AGS:PG | 5:B:1:AGS:S1G | 1.50 | 1.50 |
| 5:A:1:AGS:PG | 5:A:1:AGS:S1G | 1.50 | 1.49 |
| 5:H:1:AGS:S1G | 5:H:1:AGS:PG | 1.49 | 1.49 |
| 5:M:1:AGS:PG | 5:M:1:AGS:S1G | 1.49 | 1.48 |
| 5:D:551:AGS:PG | 5:D:551:AGS:S1G | 1.48 | 1.48 |
| 5:K:1:AGS:S1G | 5:K:1:AGS:PG | 1.49 | 1.48 |
| 5:F:1:AGS:PG | 5:F:1:AGS:S1G | 1.49 | 1.48 |
| 5:J:1:AGS:PG | 5:J:1:AGS:S1G | 1.49 | 1.48 |
| 5:L:1:AGS:PG | 5:L:1:AGS:S1G | 1.49 | 1.47 |
| 5:N:1:AGS:PG | 5:N:1:AGS:S1G | 1.49 | 1.47 |
| 5:C:1:AGS:PG | 5:C:1:AGS:S1G | 1.49 | 1.47 |
| 5:E:1:AGS:PG | 5:E:1:AGS:S1G | 1.48 | 1.47 |
| 5:I:1:AGS:PG | 5:I:1:AGS:S1G | 1.49 | 1.47 |
| 5:G:1:AGS:PG | 5:G:1:AGS:S1G | 1.48 | 1.46 |
| 1:B:77:VAL:HG21 | 1:B:510:VAL:HG22 | 1.23 | 1.15 |
| 1:D:230:ILE:HD12 | 1:D:261:THR:HG21 | 1.31 | 1.10 |
| 1:I:183:LEU:H | 1:I:383:ALA:HB3 | 1.13 | 1.10 |
| 1:J:183:LEU:H | 1:J:383:ALA:HB3 | 1.12 | 1.10 |
| 1:B:230:ILE:HD12 | 1:B:261:THR:HG21 | 1.33 | 1.10 |
| 1:D:183:LEU:H | 1:D:383:ALA:HB3 | 1.15 | 1.10 |
| 1:D:7:LYS:HB3 | 6:D:2704:HOH:O | 1.47 | 1.10 |
| 1:C:230:ILE:HD12 | 1:C:261:THR:HG21 | 1.33 | 1.09 |
| 1:J:230:ILE:HD12 | 1:J:261:THR:HG21 | 1.33 | 1.09 |
| 1:G:230:ILE:HD12 | 1:G:261:THR:HG21 | 1.30 | 1.09 |
| 1:L:183:LEU:H | 1:L:383:ALA:HB3 | 1.08 | 1.09 |
| 1:B:183:LEU:H | 1:B:383:ALA:HB3 | 1.07 | 1.08 |
| 1:F:183:LEU:H | 1:F:383:ALA:HB3 | 1.19 | 1.08 |
| 1:M:230:ILE:HD12 | 1:M:261:THR:HG21 | 1.31 | 1.07 |
| 1:K:183:LEU:H | 1:K:383:ALA:HB3 | 1.19 | 1.07 |
| 1:L:230:ILE:HD12 | 1:L:261:THR:HG21 | 1.32 | 1.07 |
| 1:F:230:ILE:HD12 | 1:F:261:THR:HG21 | 1.31 | 1.06 |
| 1:H:183:LEU:H | 1:H:383:ALA:HB3 | 1.13 | 1.06 |
| 1:K:230:ILE:HD12 | 1:K:261:THR:HG21 | 1.36 | 1.06 |
| 1:N:183:LEU:H | 1:N:383:ALA:HB3 | 1.17 | 1.06 |
| 1:A:183:LEU:H | 1:A:383:ALA:HB3 | 1.20 | 1.06 |
| 1:N:230:ILE:HD12 | 1:N:261:THR:HG21 | 1.37 | 1.06 |
| 1:E:230:ILE:HD12 | 1:E:261:THR:HG21 | 1.32 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:230:ILE:HD12 | 1:A:261:THR:HG21 | 1.36 | 1.04 |
| 1:G:325:ILE:HB | 6:G:2628:HOH:O | 1.55 | 1.04 |
| 1:B:77:VAL:HG13 | 1:B:506:TYR:HB3 | 1.36 | 1.04 |
| 1:E:183:LEU:H | 1:E:383:ALA:HB3 | 1.19 | 1.03 |
| 1:C:183:LEU:H | 1:C:383:ALA:HB3 | 1.23 | 1.03 |
| 1:H:230:ILE:HD12 | 1:H:261:THR:HG21 | 1.33 | 1.03 |
| 1:I:230:ILE:HD12 | 1:I:261:THR:HG21 | 1.34 | 1.02 |
| 1:M:183:LEU:H | 1:M:383:ALA:HB3 | 1.27 | 0.99 |
| 1:G:183:LEU:H | 1:G:383:ALA:HB3 | 1.25 | 0.99 |
| 1:B:235:PRO:HG3 | 1:B:310:GLU:HA | 1.46 | 0.98 |
| 1:L:218:PRO:HB3 | 1:L:246:PRO:HG2 | 1.48 | 0.96 |
| 1:A:235:PRO:HG3 | 1:A:310:GLU:HA | 1.48 | 0.95 |
| 1:H:383:ALA:HB1 | 1:I:281:PHE:HZ | 1.31 | 0.95 |
| 1:I:218:PRO:HB3 | 1:I:246:PRO:HG2 | 1.48 | 0.95 |
| 1:K:218:PRO:HB3 | 1:K:246:PRO:HG2 | 1.49 | 0.95 |
| 1:H:218:PRO:HB3 | 1:H:246:PRO:HG2 | 1.50 | 0.94 |
| 1:F:235:PRO:HG3 | 1:F:310:GLU:HA | 1.49 | 0.94 |
| 1:J:383:ALA:HB1 | 1:K:281:PHE:HZ | 1.33 | 0.94 |
| 1:C:235:PRO:HG3 | 1:C:310:GLU:HA | 1.49 | 0.94 |
| 1:I:235:PRO:HG3 | 1:I:310:GLU:HA | 1.50 | 0.93 |
| 1:M:218:PRO:HB3 | 1:M:246:PRO:HG2 | 1.47 | 0.93 |
| 1:J:218:PRO:HB3 | 1:J:246:PRO:HG2 | 1.50 | 0.93 |
| 1:J:235:PRO:HG3 | 1:J:310:GLU:HA | 1.51 | 0.93 |
| 1:B:218:PRO:HB3 | 1:B:246:PRO:HG2 | 1.49 | 0.93 |
| 1:E:235:PRO:HG3 | 1:E:310:GLU:HA | 1.50 | 0.93 |
| 1:A:218:PRO:HB3 | 1:A:246:PRO:HG2 | 1.52 | 0.92 |
| 1:M:235:PRO:HG3 | 1:M:310:GLU:HA | 1.51 | 0.92 |
| 1:H:235:PRO:HG3 | 1:H:310:GLU:HA | 1.52 | 0.91 |
| 1:G:218:PRO:HB3 | 1:G:246:PRO:HG2 | 1.53 | 0.91 |
| 1:E:218:PRO:HB3 | 1:E:246:PRO:HG2 | 1.49 | 0.91 |
| 1:K:235:PRO:HG3 | 1:K:310:GLU:HA | 1.53 | 0.91 |
| 1:D:235:PRO:HG3 | 1:D:310:GLU:HA | 1.53 | 0.90 |
| 1:L:235:PRO:HG3 | 1:L:310:GLU:HA | 1.52 | 0.90 |
| 1:C:218:PRO:HB3 | 1:C:246:PRO:HG2 | 1.54 | 0.90 |
| 1:B:383:ALA:HB1 | 1:C:281:PHE:HZ | 1.36 | 0.90 |
| 1:F:218:PRO:HB3 | 1:F:246:PRO:HG2 | 1.51 | 0.89 |
| 1:N:218:PRO:HB3 | 1:N:246:PRO:HG2 | 1.55 | 0.89 |
| 1:A:281:PHE:HZ | 1:G:383:ALA:HB1 | 1.36 | 0.89 |
| 1:G:235:PRO:HG3 | 1:G:310:GLU:HA | 1.51 | 0.89 |
| 1:B:383:ALA:HB1 | 1:C:281:PHE:CZ | 2.07 | 0.89 |
| 1:N:235:PRO:HG3 | 1:N:310:GLU:HA | 1.54 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:94:VAL:HB | 6:B:2545:HOH:O | 1.70 | 0.88 |
| 1:L:383:ALA:HB1 | 1:M:281:PHE:HZ | 1.36 | 0.88 |
| 1:G:57:ALA:O | 1:G:75:LYS:HE2 | 1.73 | 0.88 |
| 1:C:171:LYS:HE2 | 6:C:2796:HOH:O | 1.74 | 0.88 |
| 1:D:218:PRO:HB3 | 1:D:246:PRO:HG2 | 1.55 | 0.88 |
| 1:D:359:ASP:O | 1:D:363:GLU:HG2 | 1.75 | 0.87 |
| 1:L:183:LEU:N | 1:L:383:ALA:HB3 | 1.89 | 0.86 |
| 1:B:183:LEU:N | 1:B:383:ALA:HB3 | 1.89 | 0.86 |
| 1:H:281:PHE:HZ | 1:N:383:ALA:HB1 | 1.38 | 0.86 |
| 1:L:383:ALA:HB1 | 1:M:281:PHE:CZ | 2.10 | 0.86 |
| 1:D:383:ALA:HB1 | 1:E:281:PHE:HZ | 1.42 | 0.85 |
| 1:H:404:ARG:HG2 | 1:H:404:ARG:HH11 | 1.40 | 0.85 |
| 1:G:359:ASP:O | 1:G:363:GLU:HG2 | 1.75 | 0.85 |
| 1:D:349:ILE:HA | 1:D:352:GLN:HG3 | 1.58 | 0.85 |
| 1:A:281:PHE:CZ | 1:G:383:ALA:HB1 | 2.12 | 0.84 |
| 1:D:57:ALA:O | 1:D:75:LYS:HE2 | 1.77 | 0.84 |
| 1:E:293:ALA:HB2 | 6:E:2717:HOH:O | 1.77 | 0.84 |
| 1:G:349:ILE:HA | 1:G:352:GLN:HG3 | 1.60 | 0.83 |
| 1:H:349:ILE:HA | 1:H:352:GLN:HG3 | 1.60 | 0.83 |
| 1:A:349:ILE:HA | 1:A:352:GLN:HG3 | 1.60 | 0.83 |
| 1:H:183:LEU:N | 1:H:383:ALA:HB3 | 1.93 | 0.82 |
| 1:E:222:LEU:HD13 | 6:E:2717:HOH:O | 1.79 | 0.82 |
| 1:H:289:LEU:HG | 6:H:2938:HOH:O | 1.77 | 0.82 |
| 1:M:420:ILE:HD12 | 1:M:451:LEU:HD13 | 1.60 | 0.82 |
| 1:J:57:ALA:O | 1:J:75:LYS:HE2 | 1.80 | 0.82 |
| 1:B:86:GLY:HA3 | 1:B:401:HIS:CE1 | 2.15 | 0.82 |
| 1:I:183:LEU:N | 1:I:383:ALA:HB3 | 1.93 | 0.82 |
| 1:D:183:LEU:N | 1:D:383:ALA:HB3 | 1.94 | 0.81 |
| 1:I:57:ALA:O | 1:I:75:LYS:HE2 | 1.80 | 0.81 |
| 1:C:200:LEU:HD21 | 1:C:277:LYS:HG3 | 1.62 | 0.81 |
| 1:B:77:VAL:CG2 | 1:B:510:VAL:HG22 | 2.07 | 0.81 |
| 1:J:183:LEU:N | 1:J:383:ALA:HB3 | 1.92 | 0.81 |
| 1:H:383:ALA:HB1 | 1:I:281:PHE:CZ | 2.16 | 0.80 |
| 1:K:420:ILE:HD12 | 1:K:451:LEU:HD13 | 1.63 | 0.80 |
| 1:N:420:ILE:HD12 | 1:N:451:LEU:HD13 | 1.62 | 0.80 |
| 1:J:383:ALA:HB1 | 1:K:281:PHE:CZ | 2.17 | 0.80 |
| 1:M:359:ASP:O | 1:M:363:GLU:HG2 | 1.82 | 0.80 |
| 1:B:200:LEU:HD21 | 1:B:277:LYS:HG3 | 1.64 | 0.80 |
| 1:J:200:LEU:HD21 | 1:J:277:LYS:HG3 | 1.64 | 0.80 |
| 1:N:57:ALA:O | 1:N:75:LYS:HE2 | 1.80 | 0.80 |
| 1:F:57:ALA:O | 1:F:75:LYS:HE2 | 1.81 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:200:LEU:HD21 | 1:M:277:LYS:HG3 | 1.64 | 0.79 |
| 1:K:200:LEU:HD21 | 1:K:277:LYS:HG3 | 1.64 | 0.79 |
| 1:J:359:ASP:O | 1:J:363:GLU:HG2 | 1.81 | 0.79 |
| 1:C:359:ASP:O | 1:C:363:GLU:HG2 | 1.83 | 0.79 |
| 1:C:463:SER:HB2 | 6:C:2549:HOH:O | 1.82 | 0.79 |
| 1:C:349:ILE:HA | 1:C:352:GLN:HG3 | 1.65 | 0.79 |
| 1:C:57:ALA:O | 1:C:75:LYS:HE2 | 1.83 | 0.78 |
| 1:E:349:ILE:HA | 1:E:352:GLN:HG3 | 1.64 | 0.78 |
| 1:N:200:LEU:HD21 | 1:N:277:LYS:HG3 | 1.65 | 0.78 |
| 1:N:349:ILE:HA | 1:N:352:GLN:HG3 | 1.66 | 0.78 |
| 1:J:349:ILE:HA | 1:J:352:GLN:HG3 | 1.65 | 0.78 |
| 1:K:183:LEU:N | 1:K:383:ALA:HB3 | 1.98 | 0.78 |
| 1:I:200:LEU:HD21 | 1:I:277:LYS:HG3 | 1.65 | 0.78 |
| 1:H:57:ALA:O | 1:H:75:LYS:HE2 | 1.83 | 0.78 |
| 1:M:349:ILE:HA | 1:M:352:GLN:HG3 | 1.66 | 0.78 |
| 1:N:183:LEU:N | 1:N:383:ALA:HB3 | 1.97 | 0.77 |
| 1:A:200:LEU:HD21 | 1:A:277:LYS:HG3 | 1.65 | 0.77 |
| 1:B:359:ASP:O | 1:B:363:GLU:HG2 | 1.85 | 0.77 |
| 1:M:57:ALA:O | 1:M:75:LYS:HE2 | 1.85 | 0.77 |
| 1:K:359:ASP:O | 1:K:363:GLU:HG2 | 1.85 | 0.77 |
| 1:I:349:ILE:HA | 1:I:352:GLN:HG3 | 1.66 | 0.77 |
| 1:F:349:ILE:HA | 1:F:352:GLN:HG3 | 1.66 | 0.77 |
| 1:F:359:ASP:O | 1:F:363:GLU:HG2 | 1.85 | 0.77 |
| 1:I:420:ILE:HD12 | 1:I:451:LEU:HD13 | 1.67 | 0.77 |
| 1:M:463:SER:HB2 | 6:M:3029:HOH:O | 1.85 | 0.77 |
| 1:N:359:ASP:O | 1:N:363:GLU:HG2 | 1.84 | 0.76 |
| 1:I:359:ASP:O | 1:I:363:GLU:HG2 | 1.86 | 0.76 |
| 1:L:349:ILE:HA | 1:L:352:GLN:HG3 | 1.68 | 0.76 |
| 1:F:414:GLY:O | 1:F:417:VAL:HG13 | 1.86 | 0.76 |
| 1:G:213:VAL:HB | 1:G:325:ILE:CG1 | 2.15 | 0.76 |
| 1:K:349:ILE:HA | 1:K:352:GLN:HG3 | 1.68 | 0.76 |
| 1:L:200:LEU:HD21 | 1:L:277:LYS:HG3 | 1.68 | 0.76 |
| 1:M:381:VAL:HG21 | 1:M:393:LYS:HA | 1.65 | 0.76 |
| 1:C:381:VAL:HG21 | 1:C:393:LYS:HA | 1.66 | 0.75 |
| 1:F:200:LEU:HD21 | 1:F:277:LYS:HG3 | 1.66 | 0.75 |
| 1:L:359:ASP:O | 1:L:363:GLU:HG2 | 1.85 | 0.75 |
| 1:N:381:VAL:HG21 | 1:N:393:LYS:HA | 1.68 | 0.75 |
| 1:E:194:GLN:O | 1:E:371:LYS:HE3 | 1.87 | 0.75 |
| 1:F:183:LEU:N | 1:F:383:ALA:HB3 | 1.97 | 0.75 |
| 1:J:381:VAL:HG21 | 1:J:393:LYS:HA | 1.68 | 0.75 |
| 1:B:349:ILE:HA | 1:B:352:GLN:HG3 | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:200:LEU:HD21 | 1:E:277:LYS:HG3 | 1.67 | 0.75 |
| 1:K:381:VAL:HG21 | 1:K:393:LYS:HA | 1.67 | 0.75 |
| 1:H:359:ASP:O | 1:H:363:GLU:HG2 | 1.86 | 0.75 |
| 1:E:359:ASP:O | 1:E:363:GLU:HG2 | 1.87 | 0.74 |
| 1:H:200:LEU:HD21 | 1:H:277:LYS:HG3 | 1.69 | 0.74 |
| 1:D:183:LEU:H | 1:D:383:ALA:CB | 1.99 | 0.74 |
| 1:E:183:LEU:N | 1:E:383:ALA:HB3 | 2.00 | 0.74 |
| 1:H:381:VAL:HG21 | 1:H:393:LYS:HA | 1.70 | 0.74 |
| 5:J:1:AGS:S1G | 5:J:1:AGS:O3B | 2.45 | 0.74 |
| 1:G:200:LEU:HD21 | 1:G:277:LYS:HG3 | 1.70 | 0.74 |
| 1:C:514:MET:HE3 | 6:C:2670:HOH:O | 1.88 | 0.73 |
| 1:I:194:GLN:O | 1:I:371:LYS:HE3 | 1.87 | 0.73 |
| 1:A:359:ASP:O | 1:A:363:GLU:HG2 | 1.88 | 0.73 |
| 1:C:183:LEU:N | 1:C:383:ALA:HB3 | 2.02 | 0.73 |
| 5:G:1:AGS:S1G | 5:G:1:AGS:O3B | 2.45 | 0.73 |
| 1:A:183:LEU:N | 1:A:383:ALA:HB3 | 1.99 | 0.73 |
| 1:N:186:GLU:HB2 | 1:N:380:LYS:HB2 | 1.69 | 0.73 |
| 1:G:473:ASP:HB2 | 6:G:2130:HOH:O | 1.89 | 0.73 |
| 1:L:414:GLY:O | 1:L:417:VAL:HG13 | 1.88 | 0.73 |
| 1:B:381:VAL:HG21 | 1:B:393:LYS:HA | 1.71 | 0.73 |
| 1:I:381:VAL:HG21 | 1:I:393:LYS:HA | 1.71 | 0.73 |
| 5:H:1:AGS:S1G | 5:H:1:AGS:O3B | 2.46 | 0.72 |
| 1:J:194:GLN:O | 1:J:371:LYS:HE3 | 1.88 | 0.72 |
| 1:A:57:ALA:O | 1:A:75:LYS:HE2 | 1.89 | 0.72 |
| 5:N:1:AGS:S1G | 5:N:1:AGS:O3G | 2.46 | 0.72 |
| 1:F:263:VAL:O | 1:F:267:MET:HB2 | 1.89 | 0.72 |
| 5:G:1:AGS:S1G | 5:G:1:AGS:O3G | 2.46 | 0.72 |
| 1:C:219:PHE:HB3 | 1:C:317:LEU:HD23 | 1.72 | 0.72 |
| 1:L:420:ILE:HD12 | 1:L:451:LEU:HD13 | 1.72 | 0.72 |
| 1:L:381:VAL:HG21 | 1:L:393:LYS:HA | 1.72 | 0.72 |
| 1:B:194:GLN:O | 1:B:371:LYS:HE3 | 1.89 | 0.72 |
| 5:D:551:AGS:S1G | 5:D:551:AGS:O3B | 2.46 | 0.72 |
| 1:G:221:LEU:HD23 | 1:G:249:ILE:HD12 | 1.71 | 0.72 |
| 1:K:57:ALA:O | 1:K:75:LYS:HE2 | 1.89 | 0.72 |
| 1:C:514:MET:HB3 | 6:C:2670:HOH:O | 1.89 | 0.72 |
| 1:I:383:ALA:HB1 | 1:J:281:PHE:HZ | 1.55 | 0.72 |
| 1:D:200:LEU:HD21 | 1:D:277:LYS:HG3 | 1.72 | 0.72 |
| 1:G:381:VAL:HG21 | 1:G:393:LYS:HA | 1.70 | 0.72 |
| 5:K:1:AGS:S1G | 5:K:1:AGS:O3G | 2.46 | 0.72 |
| 1:F:432:GLN:HG2 | 6:F:2120:HOH:O | 1.88 | 0.72 |
| 1:L:305:ILE:HD12 | 1:L:307:MET:HE2 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:1:AGS:S1G | 5:I:1:AGS:O3B | 2.47 | 0.71 |
| 1:A:414:GLY:O | 1:A:417:VAL:HG13 | 1.90 | 0.71 |
| 5:C:1:AGS:S1G | 5:C:1:AGS:O3B | 2.48 | 0.71 |
| 1:D:186:GLU:HB2 | 1:D:380:LYS:HB2 | 1.72 | 0.71 |
| 1:E:381:VAL:HG21 | 1:E:393:LYS:HA | 1.71 | 0.71 |
| 1:H:404:ARG:NH1 | 6:H:2827:HOH:O | 2.24 | 0.71 |
| 1:L:57:ALA:O | 1:L:75:LYS:HE2 | 1.89 | 0.71 |
| 1:G:177:VAL:HG21 | 1:G:397:GLU:CG | 2.21 | 0.71 |
| 1:M:183:LEU:N | 1:M:383:ALA:HB3 | 2.05 | 0.71 |
| 1:M:305:ILE:HD12 | 1:M:307:MET:HE2 | 1.73 | 0.71 |
| 1:B:305:ILE:HD12 | 1:B:307:MET:HE2 | 1.72 | 0.71 |
| 5:F:1:AGS:S1G | 5:F:1:AGS:O3B | 2.48 | 0.71 |
| 1:G:263:VAL:O | 1:G:267:MET:HB2 | 1.91 | 0.71 |
| 5:E:1:AGS:S1G | 5:E:1:AGS:O3B | 2.48 | 0.70 |
| 1:B:183:LEU:H | 1:B:383:ALA:CB | 1.95 | 0.70 |
| 1:D:263:VAL:O | 1:D:267:MET:HB2 | 1.91 | 0.70 |
| 1:D:305:ILE:HD12 | 1:D:307:MET:HE2 | 1.72 | 0.70 |
| 1:D:420:ILE:HD12 | 1:D:451:LEU:HD13 | 1.72 | 0.70 |
| 1:K:414:GLY:O | 1:K:417:VAL:HG13 | 1.91 | 0.70 |
| 1:I:183:LEU:H | 1:I:383:ALA:CB | 1.98 | 0.70 |
| 1:L:194:GLN:O | 1:L:371:LYS:HE3 | 1.91 | 0.70 |
| 1:M:194:GLN:O | 1:M:371:LYS:HE3 | 1.91 | 0.70 |
| 1:F:305:ILE:HD12 | 1:F:307:MET:HE2 | 1.72 | 0.70 |
| 1:A:183:LEU:H | 1:A:383:ALA:CB | 2.03 | 0.70 |
| 5:C:1:AGS:S1G | 5:C:1:AGS:O3G | 2.45 | 0.70 |
| 1:D:177:VAL:HG21 | 1:D:397:GLU:HG3 | 1.72 | 0.70 |
| 5:F:1:AGS:S1G | 5:F:1:AGS:O3G | 2.46 | 0.70 |
| 5:M:1:AGS:S1G | 5:M:1:AGS:O3B | 2.50 | 0.70 |
| 1:E:525:PRO:HD3 | 6:E:1182:HOH:O | 1.91 | 0.70 |
| 1:D:291:ASP:OD2 | 1:D:368:ARG:HD2 | 1.92 | 0.69 |
| 1:A:381:VAL:HG21 | 1:A:393:LYS:HA | 1.73 | 0.69 |
| 1:D:176:THR:HG21 | 1:D:322:ARG:HH12 | 1.58 | 0.69 |
| 1:K:263:VAL:O | 1:K:267:MET:HB2 | 1.92 | 0.69 |
| 1:L:183:LEU:H | 1:L:383:ALA:CB | 1.95 | 0.69 |
| 1:A:263:VAL:O | 1:A:267:MET:HB2 | 1.91 | 0.69 |
| 1:H:219:PHE:HB3 | 1:H:317:LEU:HD23 | 1.74 | 0.69 |
| 1:I:213:VAL:HB | 1:I:325:ILE:CG1 | 2.23 | 0.69 |
| 5:D:551:AGS:S1G | 5:D:551:AGS:O3G | 2.45 | 0.69 |
| 1:G:186:GLU:HB2 | 1:G:380:LYS:HB2 | 1.74 | 0.69 |
| 1:J:414:GLY:O | 1:J:417:VAL:HG13 | 1.92 | 0.69 |
| 5:J:1:AGS:S1G | 5:J:1:AGS:O3G | 2.47 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:194:GLN:O | 1:H:371:LYS:HE3 | 1.91 | 0.69 |
| 1:C:525:PRO:HD3 | 6:C:1993:HOH:O | 1.93 | 0.69 |
| 1:H:183:LEU:H | 1:H:383:ALA:CB | 1.98 | 0.69 |
| 5:I:1:AGS:S1G | 5:I:1:AGS:O3G | 2.45 | 0.69 |
| 1:M:414:GLY:O | 1:M:417:VAL:HG13 | 1.92 | 0.69 |
| 5:N:1:AGS:S1G | 5:N:1:AGS:O3B | 2.50 | 0.69 |
| 5:A:1:AGS:S1G | 5:A:1:AGS:O3B | 2.48 | 0.69 |
| 1:C:194:GLN:O | 1:C:371:LYS:HE3 | 1.91 | 0.69 |
| 1:D:213:VAL:HB | 1:D:325:ILE:CG1 | 2.23 | 0.69 |
| 1:H:525:PRO:HD3 | 6:H:2151:HOH:O | 1.93 | 0.69 |
| 1:K:305:ILE:HD12 | 1:K:307:MET:HE2 | 1.75 | 0.69 |
| 1:N:263:VAL:O | 1:N:267:MET:HB2 | 1.93 | 0.69 |
| 1:E:213:VAL:HB | 1:E:325:ILE:CG1 | 2.23 | 0.69 |
| 5:E:1:AGS:S1G | 5:E:1:AGS:O3G | 2.46 | 0.69 |
| 5:H:1:AGS:S1G | 5:H:1:AGS:O3G | 2.48 | 0.69 |
| 1:J:420:ILE:HD12 | 1:J:451:LEU:HD13 | 1.75 | 0.69 |
| 5:K:1:AGS:S1G | 5:K:1:AGS:O3B | 2.50 | 0.69 |
| 1:L:263:VAL:O | 1:L:267:MET:HB2 | 1.93 | 0.69 |
| 1:H:177:VAL:HG21 | 1:H:397:GLU:HG3 | 1.74 | 0.69 |
| 1:F:186:GLU:HB2 | 1:F:380:LYS:HB2 | 1.75 | 0.68 |
| 1:H:183:LEU:HD23 | 1:H:384:ALA:HB2 | 1.76 | 0.68 |
| 1:A:213:VAL:HB | 1:A:325:ILE:CG1 | 2.23 | 0.68 |
| 1:D:219:PHE:HB3 | 1:D:317:LEU:HD23 | 1.75 | 0.68 |
| 1:H:263:VAL:O | 1:H:267:MET:HB2 | 1.92 | 0.68 |
| 1:J:183:LEU:H | 1:J:383:ALA:CB | 1.98 | 0.68 |
| 1:L:449:ALA:HB1 | 6:L:2642:HOH:O | 1.93 | 0.68 |
| 1:B:263:VAL:O | 1:B:267:MET:HB2 | 1.93 | 0.68 |
| 1:C:186:GLU:HB2 | 1:C:380:LYS:HB2 | 1.75 | 0.68 |
| 1:C:263:VAL:O | 1:C:267:MET:HB2 | 1.93 | 0.68 |
| 1:H:305:ILE:HD12 | 1:H:307:MET:HE2 | 1.76 | 0.68 |
| 1:J:305:ILE:HD12 | 1:J:307:MET:HE2 | 1.76 | 0.68 |
| 1:B:414:GLY:O | 1:B:417:VAL:HG13 | 1.93 | 0.68 |
| 1:N:177:VAL:HG21 | 1:N:397:GLU:HG3 | 1.75 | 0.68 |
| 1:A:228:SER:O | 1:A:257:GLU:HB3 | 1.94 | 0.68 |
| 1:B:213:VAL:HB | 1:B:325:ILE:CG1 | 2.24 | 0.68 |
| 5:L:1:AGS:S1G | 5:L:1:AGS:O3B | 2.49 | 0.68 |
| 1:D:194:GLN:O | 1:D:371:LYS:HE3 | 1.94 | 0.67 |
| 1:J:263:VAL:O | 1:J:267:MET:HB2 | 1.93 | 0.67 |
| 1:F:381:VAL:HG21 | 1:F:393:LYS:HA | 1.74 | 0.67 |
| 1:M:263:VAL:O | 1:M:267:MET:HB2 | 1.93 | 0.67 |
| 1:K:383:ALA:HB1 | 1:L:281:PHE:HZ | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:263:VAL:O | 1:I:267:MET:HB2 | 1.93 | 0.67 |
| 5:B:1:AGS:S1G | 5:B:1:AGS:O3B | 2.50 | 0.67 |
| 1:G:183:LEU:N | 1:G:383:ALA:HB3 | 2.04 | 0.67 |
| 1:M:177:VAL:HG21 | 1:M:397:GLU:HG3 | 1.75 | 0.67 |
| 1:N:219:PHE:HB3 | 1:N:317:LEU:HD23 | 1.77 | 0.67 |
| 1:G:285:ARG:HD2 | 6:G:2626:HOH:O | 1.95 | 0.67 |
| 1:C:228:SER:O | 1:C:257:GLU:HB3 | 1.95 | 0.67 |
| 1:H:177:VAL:HG21 | 1:H:397:GLU:CG | 2.25 | 0.67 |
| 5:B:1:AGS:S1G | 5:B:1:AGS:O3G | 2.48 | 0.67 |
| 1:E:263:VAL:O | 1:E:267:MET:HB2 | 1.94 | 0.67 |
| 1:J:384:ALA:HA | 1:K:360:TYR:OH | 1.95 | 0.67 |
| 1:D:160:LYS:O | 1:D:164:GLU:HG3 | 1.95 | 0.66 |
| 1:D:381:VAL:HG21 | 1:D:393:LYS:HA | 1.76 | 0.66 |
| 1:N:305:ILE:HD12 | 1:N:307:MET:HE2 | 1.76 | 0.66 |
| 1:G:183:LEU:HD23 | 1:G:384:ALA:HB2 | 1.77 | 0.66 |
| 1:J:219:PHE:HB3 | 1:J:317:LEU:HD23 | 1.75 | 0.66 |
| 1:D:383:ALA:HB1 | 1:E:281:PHE:CZ | 2.29 | 0.66 |
| 1:D:23:LEU:HD22 | 1:D:74:VAL:HG13 | 1.78 | 0.66 |
| 1:D:414:GLY:O | 1:D:417:VAL:HG13 | 1.96 | 0.66 |
| 1:H:174:VAL:HG22 | 1:H:194:GLN:HE21 | 1.61 | 0.66 |
| 5:M:1:AGS:S1G | 5:M:1:AGS:O3G | 2.47 | 0.66 |
| 1:N:176:THR:HG21 | 1:N:322:ARG:HH12 | 1.60 | 0.66 |
| 1:E:414:GLY:O | 1:E:417:VAL:HG13 | 1.95 | 0.66 |
| 1:F:177:VAL:HG21 | 1:F:397:GLU:CG | 2.26 | 0.66 |
| 1:G:177:VAL:HG21 | 1:G:397:GLU:HG3 | 1.75 | 0.66 |
| 1:L:177:VAL:HG21 | 1:L:397:GLU:CG | 2.25 | 0.66 |
| 1:N:183:LEU:HD23 | 1:N:384:ALA:HB2 | 1.78 | 0.66 |
| 1:A:194:GLN:O | 1:A:371:LYS:HE3 | 1.94 | 0.66 |
| 1:B:183:LEU:HD23 | 1:B:384:ALA:HB2 | 1.77 | 0.66 |
| 5:A:1:AGS:S1G | 5:A:1:AGS:O3G | 2.47 | 0.66 |
| 1:C:414:GLY:O | 1:C:417:VAL:HG13 | 1.96 | 0.66 |
| 1:I:160:LYS:O | 1:I:164:GLU:HG3 | 1.96 | 0.66 |
| 1:L:183:LEU:HD23 | 1:L:384:ALA:HB2 | 1.78 | 0.66 |
| 1:E:392:LYS:HE3 | 6:E:2648:HOH:O | 1.96 | 0.66 |
| 1:I:183:LEU:HD23 | 1:I:384:ALA:HB2 | 1.78 | 0.66 |
| 1:K:247:LEU:HB3 | 1:K:273:VAL:HG22 | 1.76 | 0.66 |
| 1:F:228:SER:O | 1:F:257:GLU:HB3 | 1.95 | 0.66 |
| 1:K:219:PHE:HB3 | 1:K:317:LEU:HD23 | 1.77 | 0.66 |
| 1:L:186:GLU:HB2 | 1:L:380:LYS:HB2 | 1.78 | 0.65 |
| 1:D:404:ARG:HH11 | 1:D:404:ARG:HG2 | 1.60 | 0.65 |
| 1:F:247:LEU:HB3 | 1:F:273:VAL:HG22 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:228:SER:O | 1:H:257:GLU:HB3 | 1.97 | 0.65 |
| 1:I:414:GLY:O | 1:I:417:VAL:HG13 | 1.96 | 0.65 |
| 1:K:221:LEU:HD23 | 1:K:249:ILE:HD12 | 1.78 | 0.65 |
| 1:L:213:VAL:HB | 1:L:325:ILE:HG12 | 1.79 | 0.65 |
| 1:H:404:ARG:HH11 | 1:H:404:ARG:CG | 2.08 | 0.65 |
| 1:D:326:ASN:HD22 | 1:D:329:THR:HB | 1.61 | 0.65 |
| 1:F:178:GLU:OE2 | 1:F:322:ARG:HD3 | 1.96 | 0.65 |
| 1:I:305:ILE:HD12 | 1:I:307:MET:HE2 | 1.77 | 0.65 |
| 1:K:213:VAL:HB | 1:K:325:ILE:CG1 | 2.27 | 0.65 |
| 1:F:213:VAL:HB | 1:F:325:ILE:CG1 | 2.26 | 0.65 |
| 1:L:228:SER:O | 1:L:257:GLU:HB3 | 1.97 | 0.65 |
| 1:B:228:SER:O | 1:B:257:GLU:HB3 | 1.97 | 0.65 |
| 1:D:78:ALA:HB3 | 6:D:2581:HOH:O | 1.95 | 0.65 |
| 1:G:242:LYS:C | 1:G:244:GLY:H | 1.98 | 0.65 |
| 1:K:177:VAL:HG21 | 1:K:397:GLU:HG3 | 1.78 | 0.65 |
| 1:L:221:LEU:HD23 | 1:L:249:ILE:HD12 | 1.78 | 0.65 |
| 1:M:247:LEU:HB3 | 1:M:273:VAL:HG22 | 1.79 | 0.65 |
| 1:C:221:LEU:HD23 | 1:C:249:ILE:HD12 | 1.79 | 0.65 |
| 1:H:281:PHE:CZ | 1:N:383:ALA:HB1 | 2.28 | 0.65 |
| 1:B:91:THR:O | 1:B:94:VAL:HG22 | 1.96 | 0.65 |
| 1:C:420:ILE:HD12 | 1:C:451:LEU:HD13 | 1.79 | 0.65 |
| 1:H:42:LYS:HB2 | 6:H:2847:HOH:O | 1.96 | 0.65 |
| 1:I:186:GLU:HB2 | 1:I:380:LYS:HB2 | 1.77 | 0.65 |
| 1:K:228:SER:O | 1:K:257:GLU:HB3 | 1.97 | 0.65 |
| 1:B:60:ILE:O | 1:B:75:LYS:HE3 | 1.98 | 0.64 |
| 1:E:206:ASN:HD21 | 1:E:214:GLU:H | 1.45 | 0.64 |
| 1:C:305:ILE:HD12 | 1:C:307:MET:HE2 | 1.78 | 0.64 |
| 1:A:221:LEU:HD23 | 1:A:249:ILE:HD12 | 1.79 | 0.64 |
| 1:E:177:VAL:HG21 | 1:E:397:GLU:HG3 | 1.79 | 0.64 |
| 1:G:228:SER:O | 1:G:257:GLU:HB3 | 1.97 | 0.64 |
| 1:H:69:MET:O | 1:H:73:MET:HG3 | 1.96 | 0.64 |
| 1:F:194:GLN:O | 1:F:371:LYS:HE3 | 1.97 | 0.64 |
| 1:H:414:GLY:O | 1:H:417:VAL:HG13 | 1.98 | 0.64 |
| 1:L:219:PHE:HB3 | 1:L:317:LEU:HD23 | 1.79 | 0.64 |
| 1:A:349:ILE:HA | 1:A:352:GLN:CG | 2.27 | 0.64 |
| 1:B:160:LYS:O | 1:B:164:GLU:HG3 | 1.97 | 0.64 |
| 1:F:183:LEU:HD23 | 1:F:384:ALA:HB2 | 1.80 | 0.64 |
| 1:I:177:VAL:HG21 | 1:I:397:GLU:CG | 2.28 | 0.64 |
| 1:I:206:ASN:HD21 | 1:I:214:GLU:H | 1.43 | 0.64 |
| 1:I:383:ALA:HB1 | 1:J:281:PHE:CZ | 2.32 | 0.64 |
| 1:M:221:LEU:HD23 | 1:M:249:ILE:HD12 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:176:THR:HG21 | 1:B:322:ARG:HH12 | 1.63 | 0.64 |
| 1:D:183:LEU:O | 1:D:184:GLN:HB2 | 1.98 | 0.64 |
| 1:K:183:LEU:HD23 | 1:K:384:ALA:HB2 | 1.80 | 0.64 |
| 1:B:219:PHE:HB3 | 1:B:317:LEU:HD23 | 1.80 | 0.64 |
| 1:D:177:VAL:HG21 | 1:D:397:GLU:CG | 2.27 | 0.64 |
| 1:E:177:VAL:HG21 | 1:E:397:GLU:CG | 2.27 | 0.64 |
| 1:J:177:VAL:HG21 | 1:J:397:GLU:HG3 | 1.80 | 0.64 |
| 1:K:404:ARG:HG2 | 1:K:404:ARG:HH11 | 1.63 | 0.64 |
| 1:M:186:GLU:HB2 | 1:M:380:LYS:HB2 | 1.80 | 0.64 |
| 1:N:213:VAL:HB | 1:N:325:ILE:CG1 | 2.28 | 0.64 |
| 1:A:46:ALA:HB2 | 1:B:76:GLU:CG | 2.28 | 0.64 |
| 1:A:268:ARG:O | 1:B:257:GLU:HG3 | 1.97 | 0.64 |
| 1:D:213:VAL:HB | 1:D:325:ILE:HG12 | 1.79 | 0.64 |
| 1:L:213:VAL:HB | 1:L:325:ILE:CG1 | 2.28 | 0.64 |
| 1:A:177:VAL:HG21 | 1:A:397:GLU:HG3 | 1.80 | 0.63 |
| 1:H:213:VAL:HB | 1:H:325:ILE:CG1 | 2.28 | 0.63 |
| 1:K:183:LEU:H | 1:K:383:ALA:CB | 2.03 | 0.63 |
| 1:M:205:ILE:HA | 1:M:213:VAL:HG22 | 1.79 | 0.63 |
| 1:E:221:LEU:HD23 | 1:E:249:ILE:HD12 | 1.80 | 0.63 |
| 1:I:177:VAL:HG21 | 1:I:397:GLU:HG3 | 1.80 | 0.63 |
| 1:I:219:PHE:HB3 | 1:I:317:LEU:HD23 | 1.79 | 0.63 |
| 1:K:194:GLN:O | 1:K:371:LYS:HE3 | 1.98 | 0.63 |
| 1:L:177:VAL:HG21 | 1:L:397:GLU:HG3 | 1.80 | 0.63 |
| 1:M:326:ASN:HD22 | 1:M:329:THR:HB | 1.64 | 0.63 |
| 1:A:183:LEU:HD23 | 1:A:384:ALA:HB2 | 1.81 | 0.63 |
| 1:C:213:VAL:HB | 1:C:325:ILE:CG1 | 2.28 | 0.63 |
| 1:D:221:LEU:HD23 | 1:D:249:ILE:HD12 | 1.80 | 0.63 |
| 1:A:186:GLU:HB2 | 1:A:380:LYS:HB2 | 1.80 | 0.63 |
| 1:B:27:VAL:HG12 | 1:B:90:THR:HG23 | 1.81 | 0.63 |
| 1:C:90:THR:O | 1:C:94:VAL:HG13 | 1.98 | 0.63 |
| 1:A:247:LEU:HB3 | 1:A:273:VAL:HG22 | 1.79 | 0.63 |
| 1:D:193:MET:CE | 1:D:292:ILE:HG12 | 2.28 | 0.63 |
| 1:F:177:VAL:HG21 | 1:F:397:GLU:HG3 | 1.81 | 0.63 |
| 1:B:247:LEU:HB3 | 1:B:273:VAL:HG22 | 1.80 | 0.63 |
| 1:F:183:LEU:H | 1:F:383:ALA:CB | 2.03 | 0.63 |
| 1:N:177:VAL:HG21 | 1:N:397:GLU:CG | 2.29 | 0.63 |
| 1:E:305:ILE:HD12 | 1:E:307:MET:HE2 | 1.80 | 0.63 |
| 1:H:362:ARG:O | 1:H:366:GLN:HG3 | 1.99 | 0.63 |
| 1:D:193:MET:HE2 | 1:D:292:ILE:HG12 | 1.80 | 0.63 |
| 1:E:496:PRO:HB2 | 1:E:499:VAL:HG13 | 1.79 | 0.63 |
| 1:J:54:VAL:HG23 | 6:J:2067:HOH:O | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:183:LEU:HD23 | 1:J:384:ALA:HB2 | 1.81 | 0.63 |
| 1:J:213:VAL:HB | 1:J:325:ILE:CG1 | 2.29 | 0.63 |
| 1:G:194:GLN:O | 1:G:371:LYS:HE3 | 1.99 | 0.62 |
| 1:I:221:LEU:HD23 | 1:I:249:ILE:HD12 | 1.81 | 0.62 |
| 1:J:404:ARG:HG2 | 1:J:404:ARG:HH11 | 1.64 | 0.62 |
| 1:G:305:ILE:HD12 | 1:G:307:MET:HE2 | 1.81 | 0.62 |
| 1:H:213:VAL:HB | 1:H:325:ILE:HG12 | 1.81 | 0.62 |
| 1:M:228:SER:O | 1:M:257:GLU:HB3 | 1.99 | 0.62 |
| 1:N:228:SER:O | 1:N:257:GLU:HB3 | 1.99 | 0.62 |
| 1:B:186:GLU:HB2 | 1:B:380:LYS:HB2 | 1.80 | 0.62 |
| 1:C:139:SER:HB3 | 6:C:2796:HOH:O | 2.00 | 0.62 |
| 1:F:420:ILE:HD12 | 1:F:451:LEU:HD13 | 1.81 | 0.62 |
| 1:J:70:GLY:HA2 | 1:J:73:MET:HE3 | 1.80 | 0.62 |
| 1:K:200:LEU:O | 1:K:201:SER:HB3 | 1.99 | 0.62 |
| 5:L:1:AGS:S1G | 5:L:1:AGS:O3G | 2.49 | 0.62 |
| 1:E:186:GLU:HB2 | 1:E:380:LYS:HB2 | 1.82 | 0.62 |
| 1:E:228:SER:O | 1:E:257:GLU:HB3 | 1.99 | 0.62 |
| 1:F:160:LYS:O | 1:F:164:GLU:HG3 | 2.00 | 0.62 |
| 1:I:213:VAL:HB | 1:I:325:ILE:HG12 | 1.81 | 0.62 |
| 1:J:186:GLU:HB2 | 1:J:380:LYS:HB2 | 1.81 | 0.62 |
| 1:M:176:THR:HG21 | 1:M:322:ARG:HH12 | 1.63 | 0.62 |
| 1:M:213:VAL:HB | 1:M:325:ILE:CG1 | 2.27 | 0.62 |
| 1:A:213:VAL:HB | 1:A:325:ILE:HG12 | 1.81 | 0.62 |
| 1:A:360:TYR:OH | 1:G:384:ALA:HA | 2.00 | 0.62 |
| 1:C:404:ARG:HG2 | 1:C:404:ARG:HH11 | 1.63 | 0.62 |
| 1:D:82:ASN:HA | 6:D:2757:HOH:O | 1.98 | 0.62 |
| 1:B:68:ASN:O | 1:B:72:GLN:HG2 | 1.98 | 0.62 |
| 1:C:200:LEU:O | 1:C:201:SER:HB3 | 1.99 | 0.62 |
| 1:N:183:LEU:H | 1:N:383:ALA:CB | 2.02 | 0.62 |
| 1:D:200:LEU:O | 1:D:201:SER:HB3 | 2.00 | 0.62 |
| 1:F:221:LEU:HD23 | 1:F:249:ILE:HD12 | 1.81 | 0.62 |
| 1:F:413:ALA:HB3 | 1:F:417:VAL:HG22 | 1.82 | 0.62 |
| 1:H:420:ILE:HD12 | 1:H:451:LEU:HD13 | 1.80 | 0.62 |
| 1:M:178:GLU:OE2 | 1:M:322:ARG:HD3 | 2.00 | 0.62 |
| 1:N:272:LYS:N | 1:N:272:LYS:HD2 | 2.15 | 0.62 |
| 1:E:219:PHE:HB3 | 1:E:317:LEU:HD23 | 1.80 | 0.62 |
| 1:F:219:PHE:HB3 | 1:F:317:LEU:HD23 | 1.80 | 0.62 |
| 1:H:206:ASN:HD21 | 1:H:214:GLU:H | 1.46 | 0.62 |
| 1:H:384:ALA:HA | 1:I:360:TYR:OH | 2.00 | 0.62 |
| 1:L:218:PRO:CB | 1:L:246:PRO:HG2 | 2.27 | 0.62 |
| 1:J:221:LEU:HD23 | 1:J:249:ILE:HD12 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:205:ILE:HA | 1:K:213:VAL:HG22 | 1.82 | 0.61 |
| 1:B:77:VAL:CG1 | 1:B:506:TYR:HB3 | 2.22 | 0.61 |
| 1:H:349:ILE:HA | 1:H:352:GLN:CG | 2.28 | 0.61 |
| 1:L:78:ALA:HB3 | 6:L:2535:HOH:O | 1.99 | 0.61 |
| 1:N:404:ARG:HG2 | 1:N:404:ARG:HH11 | 1.65 | 0.61 |
| 1:E:205:ILE:HA | 1:E:213:VAL:HG22 | 1.81 | 0.61 |
| 1:F:16:MET:O | 1:F:20:VAL:HG13 | 2.00 | 0.61 |
| 1:M:525:PRO:HD3 | 6:M:2817:HOH:O | 1.99 | 0.61 |
| 1:N:414:GLY:O | 1:N:417:VAL:HG13 | 2.00 | 0.61 |
| 1:D:247:LEU:HB3 | 1:D:273:VAL:HG22 | 1.82 | 0.61 |
| 1:E:247:LEU:HB3 | 1:E:273:VAL:HG22 | 1.82 | 0.61 |
| 1:G:219:PHE:HB3 | 1:G:317:LEU:HD23 | 1.81 | 0.61 |
| 1:G:291:ASP:OD2 | 1:G:368:ARG:HD2 | 2.01 | 0.61 |
| 1:J:177:VAL:HG21 | 1:J:397:GLU:CG | 2.30 | 0.61 |
| 1:K:186:GLU:HB2 | 1:K:380:LYS:HB2 | 1.82 | 0.61 |
| 1:N:213:VAL:HB | 1:N:325:ILE:HG12 | 1.83 | 0.61 |
| 1:B:200:LEU:O | 1:B:201:SER:HB3 | 2.00 | 0.61 |
| 1:D:404:ARG:NH1 | 6:D:2552:HOH:O | 2.33 | 0.61 |
| 1:E:78:ALA:HB3 | 6:E:2338:HOH:O | 2.00 | 0.61 |
| 1:G:78:ALA:HB3 | 6:G:1724:HOH:O | 1.98 | 0.61 |
| 1:A:219:PHE:HB3 | 1:A:317:LEU:HD23 | 1.82 | 0.61 |
| 1:D:183:LEU:HD23 | 1:D:384:ALA:HB2 | 1.83 | 0.61 |
| 1:N:200:LEU:O | 1:N:201:SER:HB3 | 2.00 | 0.61 |
| 1:E:291:ASP:OD2 | 1:E:368:ARG:HD2 | 2.00 | 0.61 |
| 1:M:268:ARG:O | 1:N:257:GLU:HG3 | 1.99 | 0.61 |
| 1:B:205:ILE:HA | 1:B:213:VAL:HG22 | 1.83 | 0.61 |
| 1:G:213:VAL:HB | 1:G:325:ILE:HG12 | 1.83 | 0.61 |
| 1:J:160:LYS:O | 1:J:164:GLU:HG3 | 2.01 | 0.61 |
| 1:J:213:VAL:HB | 1:J:325:ILE:HG12 | 1.83 | 0.61 |
| 1:A:69:MET:O | 1:A:73:MET:HG3 | 2.00 | 0.61 |
| 1:G:183:LEU:O | 1:G:184:GLN:HB2 | 2.00 | 0.61 |
| 1:C:183:LEU:HD12 | 1:C:184:GLN:HG3 | 1.83 | 0.61 |
| 1:C:272:LYS:N | 1:C:272:LYS:HD2 | 2.16 | 0.61 |
| 1:M:177:VAL:HG21 | 1:M:397:GLU:CG | 2.30 | 0.61 |
| 1:M:319:GLN:O | 1:M:336:VAL:HG23 | 2.01 | 0.61 |
| 1:I:228:SER:O | 1:I:257:GLU:HB3 | 2.01 | 0.60 |
| 1:J:183:LEU:HD12 | 1:J:184:GLN:HG3 | 1.83 | 0.60 |
| 1:E:213:VAL:HB | 1:E:325:ILE:HG12 | 1.83 | 0.60 |
| 1:F:206:ASN:HD21 | 1:F:214:GLU:H | 1.49 | 0.60 |
| 1:M:70:GLY:HA2 | 1:M:73:MET:HE3 | 1.83 | 0.60 |
| 1:C:23:LEU:HD22 | 1:C:74:VAL:HG13 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:177:VAL:HG21 | 1:C:397:GLU:CG | 2.31 | 0.60 |
| 1:D:39:VAL:HG12 | 1:E:69:MET:HE2 | 1.83 | 0.60 |
| 1:J:291:ASP:OD2 | 1:J:368:ARG:HD2 | 2.01 | 0.60 |
| 1:B:90:THR:O | 1:B:94:VAL:HG13 | 2.02 | 0.60 |
| 1:I:218:PRO:CB | 1:I:246:PRO:HG2 | 2.28 | 0.60 |
| 1:M:213:VAL:HB | 1:M:325:ILE:HG12 | 1.82 | 0.60 |
| 1:M:219:PHE:HB3 | 1:M:317:LEU:HD23 | 1.81 | 0.60 |
| 1:M:362:ARG:O | 1:M:366:GLN:HG3 | 2.02 | 0.60 |
| 1:B:177:VAL:HG21 | 1:B:397:GLU:CG | 2.32 | 0.60 |
| 1:B:221:LEU:HD23 | 1:B:249:ILE:HD12 | 1.82 | 0.60 |
| 1:C:247:LEU:HB3 | 1:C:273:VAL:HG22 | 1.83 | 0.60 |
| 1:A:46:ALA:CB | 1:B:76:GLU:HG3 | 2.31 | 0.60 |
| 1:B:425:LYS:HB2 | 6:B:2916:HOH:O | 2.01 | 0.60 |
| 1:M:200:LEU:O | 1:M:201:SER:HB3 | 1.99 | 0.60 |
| 1:D:272:LYS:N | 1:D:272:LYS:HD2 | 2.17 | 0.60 |
| 1:G:414:GLY:O | 1:G:417:VAL:HG13 | 2.01 | 0.60 |
| 1:G:420:ILE:HD12 | 1:G:451:LEU:HD13 | 1.82 | 0.60 |
| 1:J:23:LEU:CD2 | 1:J:74:VAL:HG13 | 2.31 | 0.60 |
| 1:D:228:SER:O | 1:D:257:GLU:HB3 | 2.01 | 0.60 |
| 1:A:177:VAL:HG21 | 1:A:397:GLU:CG | 2.31 | 0.60 |
| 1:B:57:ALA:O | 1:B:75:LYS:HE2 | 2.01 | 0.60 |
| 1:F:213:VAL:HB | 1:F:325:ILE:HG12 | 1.83 | 0.60 |
| 1:J:228:SER:O | 1:J:257:GLU:HB3 | 2.02 | 0.60 |
| 1:N:194:GLN:O | 1:N:371:LYS:HE3 | 2.00 | 0.60 |
| 1:F:383:ALA:O | 1:F:384:ALA:HB3 | 2.01 | 0.59 |
| 1:J:272:LYS:HD2 | 1:J:272:LYS:N | 2.17 | 0.59 |
| 1:J:349:ILE:HA | 1:J:352:GLN:CG | 2.31 | 0.59 |
| 1:B:496:PRO:HB2 | 1:B:499:VAL:HG13 | 1.84 | 0.59 |
| 1:I:404:ARG:HG2 | 1:I:404:ARG:HH11 | 1.67 | 0.59 |
| 1:C:183:LEU:HD23 | 1:C:384:ALA:HB2 | 1.85 | 0.59 |
| 1:E:349:ILE:HA | 1:E:352:GLN:CG | 2.32 | 0.59 |
| 1:A:23:LEU:HD22 | 1:A:74:VAL:HG13 | 1.85 | 0.59 |
| 1:D:242:LYS:C | 1:D:244:GLY:H | 2.03 | 0.59 |
| 1:E:183:LEU:HD23 | 1:E:384:ALA:HB2 | 1.85 | 0.59 |
| 1:E:489:ILE:HD13 | 1:E:494:LEU:HD21 | 1.85 | 0.59 |
| 1:H:186:GLU:HB2 | 1:H:380:LYS:HB2 | 1.82 | 0.59 |
| 1:J:218:PRO:CB | 1:J:246:PRO:HG2 | 2.28 | 0.59 |
| 1:A:291:ASP:OD2 | 1:A:368:ARG:HD2 | 2.03 | 0.59 |
| 1:F:90:THR:O | 1:F:94:VAL:HG13 | 2.02 | 0.59 |
| 1:K:177:VAL:HG21 | 1:K:397:GLU:CG | 2.32 | 0.59 |
| 1:B:291:ASP:OD2 | 1:B:368:ARG:HD2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:213:VAL:HB | 1:C:325:ILE:HG12 | 1.85 | 0.59 |
| 1:M:206:ASN:HD21 | 1:M:214:GLU:H | 1.51 | 0.59 |
| 1:M:349:ILE:HA | 1:M:352:GLN:CG | 2.32 | 0.59 |
| 1:B:114:MET:HB3 | 6:B:2278:HOH:O | 2.02 | 0.59 |
| 1:B:449:ALA:HB1 | 6:B:2545:HOH:O | 2.02 | 0.59 |
| 1:I:272:LYS:N | 1:I:272:LYS:HD2 | 2.18 | 0.59 |
| 1:L:70:GLY:HA2 | 1:L:73:MET:HE3 | 1.83 | 0.59 |
| 1:M:160:LYS:O | 1:M:164:GLU:HG3 | 2.03 | 0.59 |
| 1:C:362:ARG:O | 1:C:366:GLN:HG3 | 2.03 | 0.59 |
| 1:F:205:ILE:HA | 1:F:213:VAL:HG22 | 1.84 | 0.59 |
| 1:H:247:LEU:HB3 | 1:H:273:VAL:HG22 | 1.84 | 0.59 |
| 1:E:272:LYS:HD2 | 1:E:272:LYS:N | 2.17 | 0.59 |
| 1:L:90:THR:O | 1:L:94:VAL:HG13 | 2.03 | 0.59 |
| 1:L:205:ILE:HA | 1:L:213:VAL:HG22 | 1.85 | 0.59 |
| 1:A:272:LYS:N | 1:A:272:LYS:HD2 | 2.18 | 0.58 |
| 1:A:362:ARG:O | 1:A:366:GLN:HG3 | 2.03 | 0.58 |
| 1:C:205:ILE:HA | 1:C:213:VAL:HG22 | 1.83 | 0.58 |
| 1:C:349:ILE:HA | 1:C:352:GLN:CG | 2.31 | 0.58 |
| 1:F:349:ILE:HA | 1:F:352:GLN:CG | 2.33 | 0.58 |
| 1:F:386:GLU:O | 1:F:390:LYS:HG2 | 2.03 | 0.58 |
| 1:C:155:ASP:OD1 | 1:C:157:THR:HB | 2.03 | 0.58 |
| 1:G:272:LYS:HD2 | 1:G:272:LYS:N | 2.17 | 0.58 |
| 1:J:174:VAL:HG22 | 1:J:194:GLN:HE21 | 1.68 | 0.58 |
| 1:D:362:ARG:O | 1:D:366:GLN:HG3 | 2.03 | 0.58 |
| 1:K:272:LYS:N | 1:K:272:LYS:HD2 | 2.18 | 0.58 |
| 1:A:404:ARG:HG2 | 1:A:404:ARG:HH11 | 1.69 | 0.58 |
| 1:B:213:VAL:HB | 1:B:325:ILE:HG12 | 1.84 | 0.58 |
| 1:F:362:ARG:O | 1:F:366:GLN:HG3 | 2.04 | 0.58 |
| 1:B:39:VAL:HG12 | 1:C:69:MET:HE2 | 1.85 | 0.58 |
| 1:D:11:ASP:HB2 | 6:D:2704:HOH:O | 2.02 | 0.58 |
| 1:I:200:LEU:O | 1:I:201:SER:HB3 | 2.03 | 0.58 |
| 1:A:404:ARG:NH1 | 6:A:2654:HOH:O | 2.36 | 0.58 |
| 1:G:183:LEU:H | 1:G:383:ALA:CB | 2.08 | 0.58 |
| 1:H:218:PRO:CB | 1:H:246:PRO:HG2 | 2.30 | 0.58 |
| 1:H:183:LEU:O | 1:H:184:GLN:HB2 | 2.03 | 0.58 |
| 1:I:183:LEU:HD12 | 1:I:184:GLN:HG3 | 1.85 | 0.58 |
| 1:K:218:PRO:CB | 1:K:246:PRO:HG2 | 2.30 | 0.58 |
| 1:N:160:LYS:O | 1:N:164:GLU:HG3 | 2.03 | 0.58 |
| 1:C:206:ASN:HD21 | 1:C:214:GLU:H | 1.50 | 0.58 |
| 1:H:272:LYS:HD2 | 1:H:272:LYS:N | 2.19 | 0.58 |
| 1:K:349:ILE:HA | 1:K:352:GLN:CG | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:417:VAL:HG11 | 1:L:488:MET:HG3 | 1.84 | 0.58 |
| 1:M:183:LEU:HD23 | 1:M:384:ALA:HB2 | 1.85 | 0.58 |
| 1:N:349:ILE:HA | 1:N:352:GLN:CG | 2.33 | 0.58 |
| 1:M:404:ARG:HG2 | 1:M:404:ARG:HH11 | 1.68 | 0.58 |
| 1:E:183:LEU:O | 1:E:184:GLN:HB2 | 2.04 | 0.57 |
| 1:F:200:LEU:O | 1:F:201:SER:HB3 | 2.02 | 0.57 |
| 1:H:174:VAL:HG22 | 1:H:194:GLN:NE2 | 2.18 | 0.57 |
| 1:K:213:VAL:HB | 1:K:325:ILE:HG12 | 1.86 | 0.57 |
| 1:A:305:ILE:HD12 | 1:A:307:MET:HE2 | 1.85 | 0.57 |
| 1:A:382:GLY:O | 1:A:389:MET:HG2 | 2.04 | 0.57 |
| 1:B:272:LYS:HD2 | 1:B:272:LYS:N | 2.19 | 0.57 |
| 1:D:463:SER:HB2 | 6:D:2645:HOH:O | 2.03 | 0.57 |
| 1:L:272:LYS:N | 1:L:272:LYS:HD2 | 2.19 | 0.57 |
| 1:L:349:ILE:HA | 1:L:352:GLN:CG | 2.34 | 0.57 |
| 1:L:383:ALA:O | 1:L:384:ALA:HB3 | 2.04 | 0.57 |
| 1:A:420:ILE:HD12 | 1:A:451:LEU:HD13 | 1.87 | 0.57 |
| 1:E:183:LEU:H | 1:E:383:ALA:CB | 2.05 | 0.57 |
| 1:G:213:VAL:HB | 1:G:325:ILE:HG13 | 1.86 | 0.57 |
| 1:G:382:GLY:O | 1:G:389:MET:HG2 | 2.04 | 0.57 |
| 1:M:218:PRO:CB | 1:M:246:PRO:HG2 | 2.27 | 0.57 |
| 1:J:206:ASN:HD21 | 1:J:214:GLU:H | 1.51 | 0.57 |
| 1:C:177:VAL:HG21 | 1:C:397:GLU:HG3 | 1.87 | 0.57 |
| 1:D:11:ASP:CB | 6:D:2704:HOH:O | 2.52 | 0.57 |
| 1:F:70:GLY:HA2 | 1:F:73:MET:HE3 | 1.87 | 0.57 |
| 1:F:85:ALA:O | 1:F:401:HIS:HE1 | 1.88 | 0.57 |
| 1:I:205:ILE:HA | 1:I:213:VAL:HG22 | 1.85 | 0.57 |
| 1:N:183:LEU:HD12 | 1:N:184:GLN:HG3 | 1.87 | 0.57 |
| 1:A:326:ASN:HD22 | 1:A:329:THR:HB | 1.70 | 0.57 |
| 1:D:90:THR:O | 1:D:94:VAL:HG13 | 2.05 | 0.57 |
| 1:H:360:TYR:OH | 1:N:384:ALA:HA | 2.04 | 0.57 |
| 1:I:349:ILE:HA | 1:I:352:GLN:CG | 2.33 | 0.57 |
| 1:K:183:LEU:HD12 | 1:K:184:GLN:HG3 | 1.87 | 0.57 |
| 1:L:386:GLU:O | 1:L:390:LYS:HG2 | 2.04 | 0.57 |
| 1:N:183:LEU:CD1 | 1:N:184:GLN:HG3 | 2.34 | 0.57 |
| 1:N:247:LEU:HB3 | 1:N:273:VAL:HG22 | 1.86 | 0.57 |
| 1:N:362:ARG:O | 1:N:366:GLN:HG3 | 2.05 | 0.57 |
| 1:A:218:PRO:CB | 1:A:246:PRO:HG2 | 2.32 | 0.57 |
| 1:A:235:PRO:CG | 1:A:310:GLU:HA | 2.29 | 0.57 |
| 1:C:326:ASN:HD22 | 1:C:329:THR:HB | 1.70 | 0.57 |
| 1:I:183:LEU:O | 1:I:184:GLN:HB2 | 2.05 | 0.57 |
| 1:N:206:ASN:HD21 | 1:N:214:GLU:H | 1.50 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:382:GLY:O | 1:B:389:MET:HG2 | 2.05 | 0.57 |
| 1:K:206:ASN:HD21 | 1:K:214:GLU:H | 1.51 | 0.57 |
| 1:N:205:ILE:HA | 1:N:213:VAL:HG22 | 1.85 | 0.57 |
| 1:A:16:MET:O | 1:A:20:VAL:HG13 | 2.04 | 0.57 |
| 1:A:205:ILE:HA | 1:A:213:VAL:HG22 | 1.85 | 0.57 |
| 1:E:200:LEU:O | 1:E:201:SER:HB3 | 2.03 | 0.57 |
| 1:I:326:ASN:HD22 | 1:I:329:THR:HB | 1.70 | 0.57 |
| 1:J:205:ILE:HA | 1:J:213:VAL:HG22 | 1.85 | 0.57 |
| 1:L:242:LYS:C | 1:L:244:GLY:H | 2.06 | 0.57 |
| 1:A:281:PHE:HZ | 1:G:383:ALA:CB | 2.15 | 0.57 |
| 1:D:160:LYS:HB2 | 1:D:160:LYS:NZ | 2.20 | 0.57 |
| 1:E:218:PRO:CB | 1:E:246:PRO:HG2 | 2.29 | 0.57 |
| 1:F:404:ARG:HG2 | 1:F:404:ARG:HH11 | 1.70 | 0.57 |
| 1:K:326:ASN:HD22 | 1:K:329:THR:HB | 1.70 | 0.57 |
| 1:L:193:MET:CE | 1:L:292:ILE:HG12 | 2.35 | 0.57 |
| 1:L:247:LEU:HB3 | 1:L:273:VAL:HG22 | 1.86 | 0.57 |
| 1:A:155:ASP:OD1 | 1:A:157:THR:HB | 2.04 | 0.56 |
| 1:A:200:LEU:O | 1:A:201:SER:HB3 | 2.04 | 0.56 |
| 1:A:46:ALA:HB2 | 1:B:76:GLU:HG3 | 1.87 | 0.56 |
| 6:B:1684:HOH:O | 1:C:518:GLU:HG2 | 2.04 | 0.56 |
| 1:N:183:LEU:O | 1:N:184:GLN:HB2 | 2.05 | 0.56 |
| 1:A:183:LEU:O | 1:A:184:GLN:HB2 | 2.06 | 0.56 |
| 1:D:138:CYS:HB2 | 6:D:2989:HOH:O | 2.05 | 0.56 |
| 1:D:386:GLU:O | 1:D:390:LYS:HG2 | 2.05 | 0.56 |
| 1:E:155:ASP:OD1 | 1:E:157:THR:HB | 2.03 | 0.56 |
| 1:J:247:LEU:HB3 | 1:J:273:VAL:HG22 | 1.85 | 0.56 |
| 1:J:383:ALA:O | 1:J:384:ALA:HB3 | 2.05 | 0.56 |
| 1:K:291:ASP:OD2 | 1:K:368:ARG:HD2 | 2.04 | 0.56 |
| 1:L:183:LEU:O | 1:L:184:GLN:HB2 | 2.06 | 0.56 |
| 1:L:384:ALA:HA | 1:M:360:TYR:OH | 2.05 | 0.56 |
| 1:H:70:GLY:HA2 | 1:H:73:MET:HE3 | 1.88 | 0.56 |
| 1:L:160:LYS:O | 1:L:164:GLU:HG3 | 2.05 | 0.56 |
| 1:M:220:ILE:HD12 | 1:M:296:THR:HG21 | 1.88 | 0.56 |
| 1:N:242:LYS:C | 1:N:244:GLY:H | 2.07 | 0.56 |
| 1:B:183:LEU:HD12 | 1:B:184:GLN:HG3 | 1.86 | 0.56 |
| 1:E:71:ALA:O | 1:E:75:LYS:HB2 | 2.05 | 0.56 |
| 1:G:77:VAL:HG23 | 1:G:510:VAL:HG21 | 1.88 | 0.56 |
| 1:A:282:GLY:HA3 | 1:G:181:THR:O | 2.05 | 0.56 |
| 1:E:34:LYS:HG3 | 1:E:458:CYS:SG | 2.46 | 0.56 |
| 1:H:68:ASN:O | 1:H:72:GLN:HG2 | 2.04 | 0.56 |
| 1:L:155:ASP:OD1 | 1:L:157:THR:HB | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:206:ASN:HD21 | 1:L:214:GLU:H | 1.52 | 0.56 |
| 1:M:272:LYS:HD2 | 1:M:272:LYS:N | 2.19 | 0.56 |
| 1:M:382:GLY:O | 1:M:389:MET:HG2 | 2.06 | 0.56 |
| 1:B:155:ASP:OD1 | 1:B:157:THR:HB | 2.05 | 0.56 |
| 1:J:242:LYS:C | 1:J:244:GLY:H | 2.09 | 0.56 |
| 1:B:349:ILE:HA | 1:B:352:GLN:CG | 2.34 | 0.56 |
| 1:E:300:VAL:HG22 | 6:E:2717:HOH:O | 2.04 | 0.56 |
| 1:I:23:LEU:CD2 | 1:I:74:VAL:HG13 | 2.35 | 0.56 |
| 1:D:284:ARG:HH12 | 1:D:364:LYS:NZ | 2.04 | 0.56 |
| 1:E:242:LYS:C | 1:E:244:GLY:H | 2.08 | 0.56 |
| 1:E:301:ILE:HG21 | 1:E:309:LEU:HD23 | 1.88 | 0.56 |
| 1:F:54:VAL:HG23 | 6:F:2017:HOH:O | 2.06 | 0.56 |
| 1:H:242:LYS:C | 1:H:244:GLY:H | 2.09 | 0.56 |
| 1:E:193:MET:CE | 1:E:292:ILE:HG12 | 2.37 | 0.56 |
| 1:G:252:GLU:O | 1:G:253:ASP:HB2 | 2.06 | 0.56 |
| 1:I:193:MET:HE1 | 1:I:292:ILE:HG12 | 1.88 | 0.56 |
| 1:I:362:ARG:O | 1:I:366:GLN:HG3 | 2.06 | 0.56 |
| 1:K:23:LEU:CD2 | 1:K:74:VAL:HG13 | 2.35 | 0.56 |
| 1:C:183:LEU:H | 1:C:383:ALA:CB | 2.08 | 0.55 |
| 1:D:114:MET:HG2 | 6:D:2375:HOH:O | 2.06 | 0.55 |
| 1:E:220:ILE:HD12 | 1:E:296:THR:HG21 | 1.88 | 0.55 |
| 1:F:326:ASN:HD22 | 1:F:329:THR:HB | 1.71 | 0.55 |
| 1:L:181:THR:O | 1:M:282:GLY:HA3 | 2.06 | 0.55 |
| 1:M:462:PRO:HD2 | 6:M:2751:HOH:O | 2.05 | 0.55 |
| 1:F:183:LEU:O | 1:F:184:GLN:HB2 | 2.07 | 0.55 |
| 1:G:176:THR:HG21 | 1:G:322:ARG:HH12 | 1.72 | 0.55 |
| 1:G:199:TYR:N | 6:G:2628:HOH:O | 2.39 | 0.55 |
| 1:H:205:ILE:HA | 1:H:213:VAL:HG22 | 1.86 | 0.55 |
| 1:J:23:LEU:HD22 | 1:J:74:VAL:HG13 | 1.88 | 0.55 |
| 1:M:242:LYS:C | 1:M:244:GLY:H | 2.10 | 0.55 |
| 1:H:23:LEU:CD2 | 1:H:74:VAL:HG13 | 2.37 | 0.55 |
| 1:H:386:GLU:O | 1:H:390:LYS:HG2 | 2.07 | 0.55 |
| 1:J:326:ASN:HD22 | 1:J:329:THR:HB | 1.71 | 0.55 |
| 1:K:242:LYS:C | 1:K:244:GLY:H | 2.08 | 0.55 |
| 1:K:383:ALA:HB1 | 1:L:281:PHE:CZ | 2.39 | 0.55 |
| 1:M:235:PRO:CG | 1:M:310:GLU:HA | 2.32 | 0.55 |
| 1:C:193:MET:CE | 1:C:292:ILE:HG12 | 2.37 | 0.55 |
| 1:I:266:THR:CG2 | 1:I:273:VAL:H | 2.19 | 0.55 |
| 1:J:180:GLY:HA3 | 1:J:381:VAL:O | 2.07 | 0.55 |
| 1:J:183:LEU:CD1 | 1:J:184:GLN:HG3 | 2.36 | 0.55 |
| 1:J:235:PRO:CG | 1:J:310:GLU:HA | 2.32 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:155:ASP:OD1 | 1:I:157:THR:HB | 2.06 | 0.55 |
| 1:I:383:ALA:O | 1:I:384:ALA:HB3 | 2.07 | 0.55 |
| 1:J:362:ARG:O | 1:J:366:GLN:HG3 | 2.06 | 0.55 |
| 1:K:155:ASP:OD1 | 1:K:157:THR:HB | 2.06 | 0.55 |
| 1:N:266:THR:CG2 | 1:N:273:VAL:H | 2.19 | 0.55 |
| 1:A:174:VAL:HG22 | 1:A:194:GLN:HE21 | 1.70 | 0.55 |
| 1:A:183:LEU:HD12 | 1:A:184:GLN:HG3 | 1.89 | 0.55 |
| 1:A:206:ASN:HD21 | 1:A:214:GLU:H | 1.54 | 0.55 |
| 1:D:60:ILE:O | 1:D:75:LYS:HE3 | 2.07 | 0.55 |
| 1:D:218:PRO:CB | 1:D:246:PRO:HG2 | 2.33 | 0.55 |
| 1:G:200:LEU:O | 1:G:201:SER:HB3 | 2.07 | 0.55 |
| 1:I:193:MET:CE | 1:I:292:ILE:HG12 | 2.36 | 0.55 |
| 1:K:272:LYS:NZ | 1:L:229:ASN:HD21 | 2.04 | 0.55 |
| 1:L:73:MET:O | 1:L:76:GLU:HB2 | 2.07 | 0.55 |
| 1:L:200:LEU:O | 1:L:201:SER:HB3 | 2.07 | 0.55 |
| 1:E:453:GLN:NE2 | 2:E:4005:SO4:O1 | 2.40 | 0.55 |
| 1:G:310:GLU:OE1 | 1:G:310:GLU:N | 2.40 | 0.55 |
| 1:K:386:GLU:O | 1:K:390:LYS:HG2 | 2.07 | 0.55 |
| 1:M:291:ASP:OD2 | 1:M:368:ARG:HD2 | 2.07 | 0.55 |
| 1:B:183:LEU:O | 1:B:184:GLN:HB2 | 2.06 | 0.55 |
| 1:E:160:LYS:O | 1:E:164:GLU:HG3 | 2.07 | 0.55 |
| 1:E:326:ASN:HD22 | 1:E:329:THR:HB | 1.72 | 0.55 |
| 1:M:180:GLY:HA3 | 1:M:381:VAL:O | 2.07 | 0.55 |
| 1:C:178:GLU:OE2 | 1:C:322:ARG:HD3 | 2.07 | 0.55 |
| 1:D:54:VAL:HG23 | 6:D:1693:HOH:O | 2.07 | 0.55 |
| 1:G:183:LEU:CD1 | 1:G:184:GLN:HG3 | 2.37 | 0.55 |
| 1:N:60:ILE:O | 1:N:75:LYS:HE3 | 2.07 | 0.55 |
| 1:A:331:THR:HG22 | 6:A:2839:HOH:O | 2.06 | 0.55 |
| 1:B:362:ARG:O | 1:B:366:GLN:HG3 | 2.07 | 0.55 |
| 1:C:218:PRO:CB | 1:C:246:PRO:HG2 | 2.35 | 0.55 |
| 1:G:23:LEU:HD22 | 1:G:74:VAL:HG13 | 1.89 | 0.55 |
| 1:G:386:GLU:O | 1:G:390:LYS:HG2 | 2.07 | 0.55 |
| 1:K:362:ARG:O | 1:K:366:GLN:HG3 | 2.07 | 0.55 |
| 1:B:384:ALA:O | 1:B:385:THR:HG23 | 2.08 | 0.54 |
| 1:F:183:LEU:HD12 | 1:F:184:GLN:HG3 | 1.89 | 0.54 |
| 1:I:291:ASP:OD2 | 1:I:368:ARG:HD2 | 2.06 | 0.54 |
| 1:J:200:LEU:O | 1:J:201:SER:HB3 | 2.05 | 0.54 |
| 1:A:160:LYS:O | 1:A:164:GLU:HG3 | 2.08 | 0.54 |
| 1:A:386:GLU:O | 1:A:390:LYS:HG2 | 2.08 | 0.54 |
| 1:D:114:MET:HB3 | 6:D:2178:HOH:O | 2.05 | 0.54 |
| 1:G:418:ALA:N | 6:G:2394:HOH:O | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:386:GLU:O | 1:B:390:LYS:HG2 | 2.07 | 0.54 |
| 1:C:260:ALA:O | 1:C:264:VAL:HG23 | 2.07 | 0.54 |
| 1:F:218:PRO:CB | 1:F:246:PRO:HG2 | 2.31 | 0.54 |
| 1:J:176:THR:HG21 | 1:J:322:ARG:HH12 | 1.71 | 0.54 |
| 1:N:382:GLY:O | 1:N:389:MET:HG2 | 2.07 | 0.54 |
| 1:B:218:PRO:CB | 1:B:246:PRO:HG2 | 2.29 | 0.54 |
| 1:C:183:LEU:CD1 | 1:C:184:GLN:HG3 | 2.38 | 0.54 |
| 1:H:160:LYS:O | 1:H:164:GLU:HG3 | 2.06 | 0.54 |
| 1:I:305:ILE:HB | 1:I:307:MET:HE2 | 1.89 | 0.54 |
| 1:B:235:PRO:CG | 1:B:310:GLU:HA | 2.30 | 0.54 |
| 1:G:362:ARG:O | 1:G:366:GLN:HG3 | 2.07 | 0.54 |
| 1:K:383:ALA:O | 1:K:384:ALA:HB3 | 2.08 | 0.54 |
| 1:C:291:ASP:OD2 | 1:C:368:ARG:HD2 | 2.07 | 0.54 |
| 1:E:489:ILE:HD13 | 1:E:494:LEU:CD2 | 2.38 | 0.54 |
| 1:G:236:VAL:O | 1:G:240:VAL:HG23 | 2.07 | 0.54 |
| 1:H:16:MET:O | 1:H:20:VAL:HG13 | 2.07 | 0.54 |
| 1:H:193:MET:CE | 1:H:292:ILE:HG12 | 2.38 | 0.54 |
| 1:H:200:LEU:O | 1:H:201:SER:HB3 | 2.07 | 0.54 |
| 1:J:183:LEU:O | 1:J:184:GLN:HB2 | 2.08 | 0.54 |
| 1:K:220:ILE:HD12 | 1:K:296:THR:HG21 | 1.90 | 0.54 |
| 1:N:218:PRO:CB | 1:N:246:PRO:HG2 | 2.34 | 0.54 |
| 1:H:305:ILE:HG22 | 1:H:305:ILE:O | 2.08 | 0.54 |
| 1:I:16:MET:O | 1:I:20:VAL:HG13 | 2.08 | 0.54 |
| 1:J:259:LEU:O | 1:J:263:VAL:HG23 | 2.08 | 0.54 |
| 1:B:206:ASN:HD21 | 1:B:214:GLU:H | 1.56 | 0.54 |
| 1:C:382:GLY:O | 1:C:389:MET:HG2 | 2.08 | 0.54 |
| 1:D:85:ALA:HB1 | 6:D:2188:HOH:O | 2.07 | 0.54 |
| 1:E:382:GLY:O | 1:E:389:MET:HG2 | 2.08 | 0.54 |
| 1:F:160:LYS:HB2 | 1:F:160:LYS:NZ | 2.23 | 0.54 |
| 1:F:242:LYS:C | 1:F:244:GLY:H | 2.10 | 0.54 |
| 1:J:305:ILE:O | 1:J:305:ILE:HG22 | 2.08 | 0.54 |
| 1:M:183:LEU:HD12 | 1:M:184:GLN:HG3 | 1.90 | 0.54 |
| 1:G:271:VAL:HG12 | 1:G:273:VAL:HG23 | 1.88 | 0.54 |
| 1:H:176:THR:HG22 | 1:H:177:VAL:N | 2.22 | 0.54 |
| 1:G:266:THR:CG2 | 1:G:273:VAL:H | 2.21 | 0.54 |
| 1:I:183:LEU:CD1 | 1:I:184:GLN:HG3 | 2.38 | 0.54 |
| 1:J:236:VAL:O | 1:J:240:VAL:HG23 | 2.08 | 0.54 |
| 1:M:183:LEU:O | 1:M:184:GLN:HB2 | 2.08 | 0.54 |
| 1:B:85:ALA:O | 1:B:401:HIS:HE1 | 1.90 | 0.53 |
| 1:B:242:LYS:C | 1:B:244:GLY:H | 2.11 | 0.53 |
| 1:B:383:ALA:O | 1:B:384:ALA:HB3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:305:ILE:O | 1:F:305:ILE:HG22 | 2.07 | 0.53 |
| 1:H:160:LYS:HB2 | 1:H:160:LYS:NZ | 2.23 | 0.53 |
| 1:H:382:GLY:O | 1:H:389:MET:HG2 | 2.08 | 0.53 |
| 1:L:16:MET:O | 1:L:20:VAL:HG13 | 2.08 | 0.53 |
| 1:N:221:LEU:HD23 | 1:N:249:ILE:HD12 | 1.90 | 0.53 |
| 1:A:281:PHE:CZ | 1:G:383:ALA:CB | 2.89 | 0.53 |
| 1:D:16:MET:O | 1:D:20:VAL:HG13 | 2.08 | 0.53 |
| 1:F:176:THR:HG22 | 1:F:177:VAL:N | 2.23 | 0.53 |
| 1:G:218:PRO:CB | 1:G:246:PRO:HG2 | 2.32 | 0.53 |
| 1:H:73:MET:O | 1:H:76:GLU:HB2 | 2.09 | 0.53 |
| 1:I:90:THR:O | 1:I:94:VAL:HG13 | 2.08 | 0.53 |
| 1:J:90:THR:O | 1:J:94:VAL:HG13 | 2.09 | 0.53 |
| 1:J:193:MET:CE | 1:J:292:ILE:HG12 | 2.38 | 0.53 |
| 1:A:305:ILE:O | 1:A:305:ILE:HG22 | 2.08 | 0.53 |
| 1:C:383:ALA:O | 1:C:384:ALA:HB3 | 2.08 | 0.53 |
| 1:H:183:LEU:HD12 | 1:H:184:GLN:HG3 | 1.91 | 0.53 |
| 1:H:319:GLN:O | 1:H:336:VAL:HG23 | 2.08 | 0.53 |
| 1:I:174:VAL:HG22 | 1:I:194:GLN:HE21 | 1.73 | 0.53 |
| 1:I:247:LEU:HB3 | 1:I:273:VAL:HG22 | 1.88 | 0.53 |
| 1:K:183:LEU:CD1 | 1:K:184:GLN:HG3 | 2.38 | 0.53 |
| 1:K:319:GLN:O | 1:K:336:VAL:HG23 | 2.08 | 0.53 |
| 1:M:176:THR:HG22 | 1:M:177:VAL:N | 2.24 | 0.53 |
| 1:M:183:LEU:CD1 | 1:M:184:GLN:HG3 | 2.38 | 0.53 |
| 1:N:319:GLN:HB3 | 1:N:336:VAL:HG21 | 1.88 | 0.53 |
| 1:A:229:ASN:ND2 | 1:G:244:GLY:CA | 2.71 | 0.53 |
| 1:A:301:ILE:HG21 | 1:A:309:LEU:HD23 | 1.90 | 0.53 |
| 1:G:206:ASN:HD21 | 1:G:214:GLU:H | 1.56 | 0.53 |
| 1:G:349:ILE:HA | 1:G:352:GLN:CG | 2.37 | 0.53 |
| 1:H:129:GLU:HG2 | 6:H:1634:HOH:O | 2.09 | 0.53 |
| 1:I:242:LYS:C | 1:I:244:GLY:H | 2.11 | 0.53 |
| 1:G:155:ASP:OD1 | 1:G:157:THR:HB | 2.08 | 0.53 |
| 1:J:310:GLU:OE1 | 1:J:310:GLU:N | 2.41 | 0.53 |
| 1:A:202:PRO:O | 1:A:203:TYR:HB2 | 2.08 | 0.53 |
| 1:B:177:VAL:HG21 | 1:B:397:GLU:HG3 | 1.90 | 0.53 |
| 1:B:219:PHE:O | 1:B:247:LEU:HD12 | 2.08 | 0.53 |
| 1:M:219:PHE:O | 1:M:247:LEU:HD12 | 2.09 | 0.53 |
| 1:M:301:ILE:HG21 | 1:M:309:LEU:HD23 | 1.90 | 0.53 |
| 1:A:252:GLU:O | 1:A:253:ASP:HB2 | 2.09 | 0.53 |
| 1:B:183:LEU:CD1 | 1:B:184:GLN:HG3 | 2.38 | 0.53 |
| 1:C:235:PRO:CG | 1:C:310:GLU:HA | 2.32 | 0.53 |
| 1:E:362:ARG:O | 1:E:366:GLN:HG3 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:90:THR:OG1 | 5:I:1:AGS:S1G | 2.65 | 0.53 |
| 1:L:176:THR:HG21 | 1:L:322:ARG:HH12 | 1.74 | 0.53 |
| 1:L:319:GLN:O | 1:L:336:VAL:HG23 | 2.09 | 0.53 |
| 1:M:155:ASP:OD1 | 1:M:157:THR:HB | 2.08 | 0.53 |
| 1:M:183:LEU:H | 1:M:383:ALA:CB | 2.10 | 0.53 |
| 1:N:23:LEU:CD2 | 1:N:74:VAL:HG13 | 2.38 | 0.53 |
| 1:N:326:ASN:HD22 | 1:N:329:THR:HB | 1.74 | 0.53 |
| 1:B:239:ALA:O | 1:B:314:LEU:HD11 | 2.09 | 0.53 |
| 1:B:301:ILE:HG21 | 1:B:309:LEU:HD23 | 1.91 | 0.53 |
| 1:B:319:GLN:O | 1:B:336:VAL:HG23 | 2.08 | 0.53 |
| 1:C:236:VAL:O | 1:C:240:VAL:HG23 | 2.09 | 0.53 |
| 1:D:247:LEU:HD21 | 1:D:249:ILE:HD11 | 1.90 | 0.53 |
| 1:E:386:GLU:O | 1:E:390:LYS:HG2 | 2.09 | 0.53 |
| 1:H:23:LEU:HD22 | 1:H:74:VAL:HG13 | 1.89 | 0.53 |
| 1:C:176:THR:HG22 | 1:C:177:VAL:N | 2.23 | 0.53 |
| 1:D:383:ALA:O | 1:D:384:ALA:HB3 | 2.09 | 0.53 |
| 1:G:183:LEU:HD12 | 1:G:184:GLN:HG3 | 1.90 | 0.53 |
| 1:G:325:ILE:HG22 | 1:G:330:THR:HA | 1.91 | 0.53 |
| 1:J:155:ASP:OD1 | 1:J:157:THR:HB | 2.09 | 0.53 |
| 1:K:16:MET:O | 1:K:20:VAL:HG13 | 2.09 | 0.53 |
| 1:K:239:ALA:O | 1:K:314:LEU:HD11 | 2.08 | 0.53 |
| 1:L:183:LEU:CD1 | 1:L:184:GLN:HG3 | 2.39 | 0.53 |
| 1:L:404:ARG:HG2 | 1:L:404:ARG:HH11 | 1.74 | 0.53 |
| 1:B:310:GLU:OE1 | 1:B:310:GLU:N | 2.42 | 0.53 |
| 1:C:386:GLU:O | 1:C:390:LYS:HG2 | 2.09 | 0.53 |
| 1:F:155:ASP:OD1 | 1:F:157:THR:HB | 2.08 | 0.53 |
| 1:F:183:LEU:CD1 | 1:F:184:GLN:HG3 | 2.39 | 0.53 |
| 1:G:16:MET:O | 1:G:20:VAL:HG13 | 2.09 | 0.53 |
| 1:G:193:MET:CE | 1:G:292:ILE:HG12 | 2.39 | 0.53 |
| 1:H:266:THR:CG2 | 1:H:273:VAL:H | 2.22 | 0.53 |
| 1:M:23:LEU:CD2 | 1:M:74:VAL:HG13 | 2.39 | 0.53 |
| 1:B:176:THR:HG22 | 1:B:177:VAL:N | 2.24 | 0.52 |
| 1:E:180:GLY:HA3 | 1:E:381:VAL:O | 2.09 | 0.52 |
| 1:E:383:ALA:O | 1:E:384:ALA:HB3 | 2.09 | 0.52 |
| 1:F:272:LYS:N | 1:F:272:LYS:HD2 | 2.24 | 0.52 |
| 1:G:160:LYS:O | 1:G:164:GLU:HG3 | 2.09 | 0.52 |
| 1:H:291:ASP:OD2 | 1:H:368:ARG:HD2 | 2.10 | 0.52 |
| 1:I:382:GLY:O | 1:I:389:MET:HG2 | 2.08 | 0.52 |
| 1:K:174:VAL:HG22 | 1:K:194:GLN:HE21 | 1.72 | 0.52 |
| 1:K:176:THR:HG22 | 1:K:177:VAL:N | 2.24 | 0.52 |
| 1:K:193:MET:CE | 1:K:292:ILE:HG12 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:319:GLN:HB3 | 1:M:336:VAL:HG21 | 1.92 | 0.52 |
| 1:M:383:ALA:O | 1:M:384:ALA:HB3 | 2.09 | 0.52 |
| 1:A:183:LEU:CD1 | 1:A:184:GLN:HG3 | 2.39 | 0.52 |
| 1:H:383:ALA:O | 1:H:384:ALA:HB3 | 2.09 | 0.52 |
| 1:K:524:LEU:O | 1:K:526:LYS:N | 2.41 | 0.52 |
| 1:N:219:PHE:O | 1:N:247:LEU:HD12 | 2.08 | 0.52 |
| 1:A:242:LYS:C | 1:A:244:GLY:H | 2.12 | 0.52 |
| 1:C:305:ILE:HG22 | 1:C:305:ILE:O | 2.09 | 0.52 |
| 1:G:235:PRO:CG | 1:G:310:GLU:HA | 2.32 | 0.52 |
| 1:K:90:THR:O | 1:K:94:VAL:HG13 | 2.09 | 0.52 |
| 1:C:242:LYS:C | 1:C:244:GLY:H | 2.11 | 0.52 |
| 1:G:160:LYS:NZ | 1:G:160:LYS:HB2 | 2.25 | 0.52 |
| 1:G:247:LEU:HB3 | 1:G:273:VAL:HG22 | 1.92 | 0.52 |
| 1:I:310:GLU:OE1 | 1:I:310:GLU:N | 2.42 | 0.52 |
| 1:M:23:LEU:HD22 | 1:M:74:VAL:HG13 | 1.90 | 0.52 |
| 1:A:178:GLU:OE2 | 1:A:322:ARG:HD3 | 2.10 | 0.52 |
| 1:B:90:THR:OG1 | 5:B:1:AGS:S1G | 2.67 | 0.52 |
| 1:C:239:ALA:O | 1:C:314:LEU:HD11 | 2.10 | 0.52 |
| 1:F:202:PRO:O | 1:F:203:TYR:HB2 | 2.10 | 0.52 |
| 1:H:183:LEU:CD1 | 1:H:184:GLN:HG3 | 2.40 | 0.52 |
| 1:L:193:MET:HE2 | 1:L:292:ILE:HG12 | 1.90 | 0.52 |
| 1:B:160:LYS:HB2 | 1:B:160:LYS:NZ | 2.24 | 0.52 |
| 1:B:470:LYS:HD3 | 6:B:2745:HOH:O | 2.10 | 0.52 |
| 1:K:254:VAL:HG12 | 1:K:259:LEU:HB2 | 1.92 | 0.52 |
| 1:H:90:THR:OG1 | 5:H:1:AGS:S1G | 2.63 | 0.52 |
| 1:J:252:GLU:O | 1:J:253:ASP:HB2 | 2.10 | 0.52 |
| 1:J:496:PRO:HB2 | 1:J:499:VAL:CG1 | 2.40 | 0.52 |
| 1:N:193:MET:CE | 1:N:292:ILE:HG12 | 2.39 | 0.52 |
| 1:E:310:GLU:OE1 | 1:E:310:GLU:N | 2.43 | 0.52 |
| 1:F:271:VAL:HG12 | 1:F:273:VAL:HG23 | 1.92 | 0.52 |
| 1:K:180:GLY:HA3 | 1:K:381:VAL:O | 2.10 | 0.52 |
| 1:K:382:GLY:O | 1:K:389:MET:HG2 | 2.10 | 0.52 |
| 1:M:90:THR:O | 1:M:94:VAL:HG13 | 2.10 | 0.52 |
| 1:M:134:LEU:HD21 | 1:M:425:LYS:NZ | 2.25 | 0.52 |
| 1:E:69:MET:O | 1:E:73:MET:HG3 | 2.09 | 0.52 |
| 1:I:235:PRO:CG | 1:I:310:GLU:HA | 2.33 | 0.52 |
| 1:J:386:GLU:O | 1:J:390:LYS:HG2 | 2.10 | 0.52 |
| 1:C:160:LYS:O | 1:C:164:GLU:HG3 | 2.10 | 0.52 |
| 1:C:180:GLY:HA3 | 1:C:381:VAL:O | 2.10 | 0.52 |
| 1:E:27:VAL:HG12 | 1:E:90:THR:HG23 | 1.92 | 0.52 |
| 1:E:193:MET:HE2 | 1:E:292:ILE:HG12 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:252:GLU:O | 1:E:253:ASP:HB2 | 2.10 | 0.52 |
| 1:E:319:GLN:O | 1:E:336:VAL:HG23 | 2.10 | 0.52 |
| 1:F:254:VAL:HG12 | 1:F:259:LEU:HB2 | 1.92 | 0.52 |
| 1:A:180:GLY:HA3 | 1:A:381:VAL:O | 2.10 | 0.51 |
| 1:F:291:ASP:OD2 | 1:F:368:ARG:HD2 | 2.10 | 0.51 |
| 1:G:305:ILE:O | 1:G:305:ILE:HG22 | 2.10 | 0.51 |
| 1:I:305:ILE:O | 1:I:305:ILE:HG22 | 2.10 | 0.51 |
| 1:K:235:PRO:CG | 1:K:310:GLU:HA | 2.35 | 0.51 |
| 1:M:284:ARG:NH1 | 1:M:364:LYS:NZ | 2.58 | 0.51 |
| 1:M:305:ILE:O | 1:M:305:ILE:HG22 | 2.09 | 0.51 |
| 1:A:383:ALA:O | 1:A:384:ALA:HB3 | 2.11 | 0.51 |
| 1:C:160:LYS:HB2 | 1:C:160:LYS:NZ | 2.24 | 0.51 |
| 1:D:215:LEU:HB2 | 1:D:323:VAL:HG22 | 1.92 | 0.51 |
| 1:E:524:LEU:O | 1:E:526:LYS:N | 2.43 | 0.51 |
| 1:F:68:ASN:O | 1:F:72:GLN:HG2 | 2.10 | 0.51 |
| 1:F:220:ILE:HD12 | 1:F:296:THR:HG21 | 1.92 | 0.51 |
| 1:I:68:ASN:O | 1:I:72:GLN:HG2 | 2.10 | 0.51 |
| 1:A:310:GLU:OE1 | 1:A:310:GLU:N | 2.44 | 0.51 |
| 1:B:193:MET:CE | 1:B:292:ILE:HG12 | 2.40 | 0.51 |
| 1:C:134:LEU:HD21 | 1:C:425:LYS:NZ | 2.25 | 0.51 |
| 1:C:266:THR:CG2 | 1:C:273:VAL:H | 2.24 | 0.51 |
| 1:E:174:VAL:HG22 | 1:E:194:GLN:HE21 | 1.74 | 0.51 |
| 1:F:382:GLY:O | 1:F:389:MET:HG2 | 2.10 | 0.51 |
| 1:I:239:ALA:O | 1:I:314:LEU:HD11 | 2.10 | 0.51 |
| 1:K:305:ILE:HG22 | 1:K:305:ILE:O | 2.10 | 0.51 |
| 1:N:70:GLY:HA2 | 1:N:73:MET:HE3 | 1.93 | 0.51 |
| 1:A:54:VAL:HG23 | 6:A:2015:HOH:O | 2.10 | 0.51 |
| 1:C:384:ALA:O | 1:C:385:THR:HG23 | 2.11 | 0.51 |
| 1:D:384:ALA:HA | 1:E:360:TYR:OH | 2.11 | 0.51 |
| 1:E:183:LEU:CD1 | 1:E:184:GLN:HG3 | 2.40 | 0.51 |
| 1:F:223:ALA:O | 1:F:251:ALA:HA | 2.10 | 0.51 |
| 1:I:219:PHE:O | 1:I:247:LEU:HD12 | 2.09 | 0.51 |
| 1:J:16:MET:O | 1:J:20:VAL:HG13 | 2.11 | 0.51 |
| 1:A:160:LYS:HB2 | 1:A:160:LYS:NZ | 2.26 | 0.51 |
| 1:E:305:ILE:HG22 | 1:E:305:ILE:O | 2.10 | 0.51 |
| 1:A:193:MET:CE | 1:A:292:ILE:HG12 | 2.41 | 0.51 |
| 1:B:305:ILE:O | 1:B:305:ILE:HG22 | 2.11 | 0.51 |
| 1:F:239:ALA:O | 1:F:314:LEU:HD11 | 2.10 | 0.51 |
| 1:I:176:THR:HG22 | 1:I:177:VAL:N | 2.25 | 0.51 |
| 1:L:266:THR:CG2 | 1:L:273:VAL:H | 2.24 | 0.51 |
| 1:L:305:ILE:O | 1:L:305:ILE:HG22 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:287:ALA:HB1 | 1:M:368:ARG:NH1 | 2.25 | 0.51 |
| 1:I:23:LEU:HD22 | 1:I:74:VAL:HG13 | 1.92 | 0.51 |
| 1:I:386:GLU:O | 1:I:390:LYS:HG2 | 2.11 | 0.51 |
| 1:J:193:MET:HE1 | 1:J:292:ILE:HG12 | 1.93 | 0.51 |
| 1:M:16:MET:O | 1:M:20:VAL:HG13 | 2.11 | 0.51 |
| 1:M:252:GLU:O | 1:M:253:ASP:HB2 | 2.10 | 0.51 |
| 1:A:200:LEU:HG | 1:A:276:VAL:HA | 1.93 | 0.51 |
| 1:A:458:CYS:SG | 1:A:480:ALA:HB1 | 2.51 | 0.51 |
| 1:B:254:VAL:HG12 | 1:B:259:LEU:HB2 | 1.92 | 0.51 |
| 1:E:183:LEU:HD12 | 1:E:184:GLN:HG3 | 1.93 | 0.51 |
| 1:E:271:VAL:HG12 | 1:E:273:VAL:HG23 | 1.93 | 0.51 |
| 1:A:176:THR:HG22 | 1:A:177:VAL:N | 2.25 | 0.51 |
| 1:D:155:ASP:OD1 | 1:D:157:THR:HB | 2.11 | 0.51 |
| 1:F:193:MET:CE | 1:F:292:ILE:HG12 | 2.41 | 0.51 |
| 1:G:319:GLN:O | 1:G:336:VAL:HG23 | 2.11 | 0.51 |
| 1:L:260:ALA:O | 1:L:264:VAL:HG23 | 2.11 | 0.51 |
| 1:N:266:THR:HG22 | 1:N:271:VAL:O | 2.11 | 0.51 |
| 1:N:383:ALA:O | 1:N:384:ALA:HB3 | 2.10 | 0.51 |
| 1:D:305:ILE:O | 1:D:305:ILE:HG22 | 2.10 | 0.51 |
| 1:F:310:GLU:OE1 | 1:F:310:GLU:N | 2.44 | 0.51 |
| 1:J:202:PRO:O | 1:J:203:TYR:HB2 | 2.11 | 0.51 |
| 1:K:183:LEU:O | 1:K:184:GLN:HB2 | 2.11 | 0.51 |
| 1:K:252:GLU:O | 1:K:253:ASP:HB2 | 2.11 | 0.51 |
| 1:A:70:GLY:HA2 | 1:A:73:MET:HE3 | 1.93 | 0.50 |
| 1:A:231:ARG:NH2 | 1:G:241:ALA:HB1 | 2.26 | 0.50 |
| 1:B:271:VAL:HG12 | 1:B:273:VAL:HG23 | 1.93 | 0.50 |
| 1:G:90:THR:O | 1:G:94:VAL:HG13 | 2.11 | 0.50 |
| 1:G:242:LYS:C | 1:G:244:GLY:N | 2.64 | 0.50 |
| 1:H:78:ALA:HB3 | 6:H:2660:HOH:O | 2.11 | 0.50 |
| 1:M:310:GLU:OE1 | 1:M:310:GLU:N | 2.44 | 0.50 |
| 1:N:496:PRO:HD2 | 6:N:2145:HOH:O | 2.10 | 0.50 |
| 1:C:85:ALA:O | 1:C:401:HIS:HE1 | 1.94 | 0.50 |
| 1:E:383:ALA:HB1 | 1:F:281:PHE:HZ | 1.75 | 0.50 |
| 1:I:54:VAL:HG23 | 6:I:2135:HOH:O | 2.11 | 0.50 |
| 1:I:319:GLN:HB3 | 1:I:336:VAL:HG21 | 1.92 | 0.50 |
| 1:N:23:LEU:HD22 | 1:N:74:VAL:HG13 | 1.93 | 0.50 |
| 1:N:215:LEU:HB2 | 1:N:323:VAL:HG22 | 1.93 | 0.50 |
| 1:N:305:ILE:HG22 | 1:N:305:ILE:O | 2.11 | 0.50 |
| 1:B:287:ALA:HB1 | 1:B:368:ARG:NH1 | 2.26 | 0.50 |
| 1:G:441:LYS:HE2 | 6:G:1481:HOH:O | 2.11 | 0.50 |
| 1:H:301:ILE:HG21 | 1:H:309:LEU:HD23 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:234:LEU:O | 1:I:238:GLU:HG3 | 2.12 | 0.50 |
| 1:L:310:GLU:OE1 | 1:L:310:GLU:N | 2.44 | 0.50 |
| 1:M:496:PRO:HB2 | 1:M:499:VAL:CG1 | 2.41 | 0.50 |
| 1:E:413:ALA:CB | 1:E:417:VAL:HG22 | 2.41 | 0.50 |
| 1:F:266:THR:CG2 | 1:F:273:VAL:H | 2.25 | 0.50 |
| 1:G:326:ASN:HD22 | 1:G:329:THR:HB | 1.75 | 0.50 |
| 1:J:271:VAL:HG12 | 1:J:273:VAL:HG23 | 1.92 | 0.50 |
| 1:K:193:MET:HE2 | 1:K:292:ILE:HG12 | 1.93 | 0.50 |
| 1:K:223:ALA:O | 1:K:251:ALA:HA | 2.12 | 0.50 |
| 1:N:202:PRO:O | 1:N:203:TYR:HB2 | 2.11 | 0.50 |
| 1:N:319:GLN:O | 1:N:336:VAL:HG23 | 2.12 | 0.50 |
| 1:C:325:ILE:HG22 | 1:C:330:THR:HA | 1.92 | 0.50 |
| 1:D:183:LEU:CD1 | 1:D:184:GLN:HG3 | 2.40 | 0.50 |
| 1:J:254:VAL:HG12 | 1:J:259:LEU:HB2 | 1.94 | 0.50 |
| 1:K:236:VAL:O | 1:K:240:VAL:HG23 | 2.11 | 0.50 |
| 1:K:266:THR:CG2 | 1:K:273:VAL:H | 2.24 | 0.50 |
| 1:L:183:LEU:HD12 | 1:L:184:GLN:HG3 | 1.93 | 0.50 |
| 1:N:514:MET:SD | 6:N:2800:HOH:O | 2.60 | 0.50 |
| 1:D:260:ALA:O | 1:D:264:VAL:HG23 | 2.11 | 0.50 |
| 1:H:90:THR:O | 1:H:94:VAL:HG13 | 2.10 | 0.50 |
| 1:I:176:THR:HG21 | 1:I:322:ARG:HH12 | 1.76 | 0.50 |
| 1:I:206:ASN:OD1 | 1:I:207:LYS:HG3 | 2.11 | 0.50 |
| 1:L:23:LEU:HD22 | 1:L:74:VAL:HG13 | 1.93 | 0.50 |
| 1:L:174:VAL:HG22 | 1:L:194:GLN:HE21 | 1.75 | 0.50 |
| 1:D:180:GLY:HA3 | 1:D:381:VAL:O | 2.12 | 0.50 |
| 1:D:381:VAL:O | 1:D:382:GLY:O | 2.30 | 0.50 |
| 1:F:301:ILE:HG21 | 1:F:309:LEU:HD23 | 1.93 | 0.50 |
| 1:H:252:GLU:O | 1:H:253:ASP:HB2 | 2.12 | 0.50 |
| 1:M:209:GLU:N | 1:M:209:GLU:OE1 | 2.44 | 0.50 |
| 1:D:271:VAL:HG12 | 1:D:273:VAL:HG23 | 1.92 | 0.50 |
| 1:I:202:PRO:O | 1:I:203:TYR:HB2 | 2.11 | 0.50 |
| 1:I:223:ALA:O | 1:I:251:ALA:HA | 2.12 | 0.50 |
| 1:K:271:VAL:HG12 | 1:K:273:VAL:HG23 | 1.93 | 0.50 |
| 1:K:310:GLU:N | 1:K:310:GLU:OE1 | 2.44 | 0.50 |
| 1:L:180:GLY:HA3 | 1:L:381:VAL:O | 2.11 | 0.50 |
| 1:M:266:THR:CG2 | 1:M:273:VAL:H | 2.25 | 0.50 |
| 1:N:310:GLU:OE1 | 1:N:310:GLU:N | 2.45 | 0.50 |
| 1:F:236:VAL:O | 1:F:240:VAL:HG23 | 2.12 | 0.50 |
| 1:G:383:ALA:O | 1:G:384:ALA:HB3 | 2.12 | 0.50 |
| 1:J:266:THR:CG2 | 1:J:273:VAL:H | 2.25 | 0.50 |
| 1:M:272:LYS:NZ | 1:N:228:SER:HB2 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:287:ALA:HB1 | 1:A:368:ARG:NH1 | 2.26 | 0.49 |
| 1:E:176:THR:HG21 | 1:E:322:ARG:HH12 | 1.75 | 0.49 |
| 1:E:239:ALA:O | 1:E:314:LEU:HD11 | 2.12 | 0.49 |
| 1:G:23:LEU:CD2 | 1:G:74:VAL:HG13 | 2.42 | 0.49 |
| 1:G:325:ILE:HG22 | 1:G:330:THR:HG23 | 1.94 | 0.49 |
| 1:L:301:ILE:HG21 | 1:L:309:LEU:HD23 | 1.94 | 0.49 |
| 1:M:413:ALA:HB3 | 1:M:417:VAL:HG22 | 1.94 | 0.49 |
| 1:A:319:GLN:O | 1:A:336:VAL:HG23 | 2.12 | 0.49 |
| 1:B:183:LEU:HD13 | 1:B:184:GLN:N | 2.26 | 0.49 |
| 1:C:219:PHE:O | 1:C:247:LEU:HD12 | 2.11 | 0.49 |
| 1:D:371:LYS:HG2 | 6:D:1228:HOH:O | 2.11 | 0.49 |
| 1:G:205:ILE:HA | 1:G:213:VAL:HG22 | 1.94 | 0.49 |
| 1:H:221:LEU:HD23 | 1:H:249:ILE:HD12 | 1.94 | 0.49 |
| 1:I:160:LYS:HB2 | 1:I:160:LYS:NZ | 2.27 | 0.49 |
| 1:M:236:VAL:O | 1:M:240:VAL:HG23 | 2.12 | 0.49 |
| 1:C:193:MET:HE1 | 1:C:292:ILE:HG12 | 1.93 | 0.49 |
| 1:D:78:ALA:HB1 | 1:D:89:THR:HB | 1.94 | 0.49 |
| 1:E:158:VAL:HG13 | 1:E:396:VAL:HG22 | 1.92 | 0.49 |
| 1:E:236:VAL:O | 1:E:240:VAL:HG23 | 2.12 | 0.49 |
| 1:F:174:VAL:HG22 | 1:F:194:GLN:HE21 | 1.77 | 0.49 |
| 1:G:202:PRO:O | 1:G:203:TYR:HB2 | 2.12 | 0.49 |
| 1:H:325:ILE:HG22 | 1:H:330:THR:HA | 1.95 | 0.49 |
| 1:L:252:GLU:O | 1:L:253:ASP:HB2 | 2.11 | 0.49 |
| 1:N:348:GLN:O | 1:N:352:GLN:HG2 | 2.13 | 0.49 |
| 1:C:254:VAL:HG12 | 1:C:259:LEU:HB2 | 1.94 | 0.49 |
| 1:E:266:THR:CG2 | 1:E:273:VAL:H | 2.25 | 0.49 |
| 1:F:23:LEU:HD22 | 1:F:74:VAL:HG13 | 1.94 | 0.49 |
| 1:H:176:THR:HG21 | 1:H:322:ARG:HH12 | 1.76 | 0.49 |
| 1:A:229:ASN:ND2 | 1:G:244:GLY:HA3 | 2.28 | 0.49 |
| 1:B:455:VAL:HG13 | 1:B:460:GLU:HB2 | 1.94 | 0.49 |
| 1:C:68:ASN:O | 1:C:72:GLN:HG2 | 2.12 | 0.49 |
| 1:C:202:PRO:O | 1:C:203:TYR:HB2 | 2.11 | 0.49 |
| 1:E:90:THR:OG1 | 5:E:1:AGS:S1G | 2.66 | 0.49 |
| 1:H:310:GLU:N | 1:H:310:GLU:OE1 | 2.45 | 0.49 |
| 1:H:413:ALA:HB3 | 1:H:417:VAL:HG22 | 1.93 | 0.49 |
| 1:L:287:ALA:HB1 | 1:L:368:ARG:NH1 | 2.27 | 0.49 |
| 1:M:386:GLU:O | 1:M:390:LYS:HG2 | 2.12 | 0.49 |
| 1:E:171:LYS:HB2 | 1:E:407:VAL:HG11 | 1.93 | 0.49 |
| 1:L:202:PRO:O | 1:L:203:TYR:HB2 | 2.12 | 0.49 |
| 1:A:266:THR:CG2 | 1:A:273:VAL:H | 2.26 | 0.49 |
| 1:B:202:PRO:O | 1:B:203:TYR:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:202:PRO:O | 1:D:203:TYR:HB2 | 2.12 | 0.49 |
| 1:K:69:MET:O | 1:K:73:MET:HG3 | 2.12 | 0.49 |
| 1:L:223:ALA:O | 1:L:251:ALA:HA | 2.12 | 0.49 |
| 1:B:326:ASN:HD22 | 1:B:329:THR:HB | 1.76 | 0.49 |
| 1:K:68:ASN:O | 1:K:72:GLN:HG2 | 2.13 | 0.49 |
| 1:L:102:GLU:HB2 | 1:L:442:VAL:HG13 | 1.95 | 0.49 |
| 1:L:524:LEU:O | 1:L:526:LYS:N | 2.45 | 0.49 |
| 1:B:5:ASP:HB2 | 1:B:524:LEU:HD12 | 1.95 | 0.49 |
| 1:B:223:ALA:O | 1:B:251:ALA:HA | 2.13 | 0.49 |
| 1:B:525:PRO:HD3 | 6:B:1427:HOH:O | 2.13 | 0.49 |
| 1:C:319:GLN:O | 1:C:336:VAL:HG23 | 2.13 | 0.49 |
| 6:C:2466:HOH:O | 1:D:518:GLU:HG2 | 2.12 | 0.49 |
| 1:F:413:ALA:CB | 1:F:417:VAL:HG22 | 2.42 | 0.49 |
| 1:H:287:ALA:HB1 | 1:H:368:ARG:NH1 | 2.27 | 0.49 |
| 1:I:252:GLU:O | 1:I:253:ASP:HB2 | 2.12 | 0.49 |
| 1:J:382:GLY:O | 1:J:389:MET:HG2 | 2.13 | 0.49 |
| 1:N:218:PRO:HD2 | 1:N:320:ALA:O | 2.13 | 0.49 |
| 1:A:60:ILE:O | 1:A:75:LYS:HE3 | 2.13 | 0.49 |
| 1:A:271:VAL:HG12 | 1:A:273:VAL:HG23 | 1.94 | 0.49 |
| 1:C:63:GLU:OE2 | 1:D:526:LYS:HE2 | 2.13 | 0.49 |
| 1:E:287:ALA:HB1 | 1:E:368:ARG:NH1 | 2.27 | 0.49 |
| 1:H:202:PRO:O | 1:H:203:TYR:HB2 | 2.11 | 0.49 |
| 1:J:63:GLU:OE2 | 1:K:526:LYS:HE2 | 2.12 | 0.49 |
| 1:M:271:VAL:HG12 | 1:M:273:VAL:HG23 | 1.95 | 0.49 |
| 1:N:234:LEU:O | 1:N:238:GLU:HG3 | 2.13 | 0.49 |
| 1:D:310:GLU:OE1 | 1:D:310:GLU:N | 2.46 | 0.48 |
| 1:E:206:ASN:OD1 | 1:E:207:LYS:HG3 | 2.13 | 0.48 |
| 1:F:235:PRO:CG | 1:F:310:GLU:HA | 2.31 | 0.48 |
| 1:I:266:THR:HG22 | 1:I:271:VAL:O | 2.13 | 0.48 |
| 1:I:319:GLN:O | 1:I:336:VAL:HG23 | 2.13 | 0.48 |
| 1:K:202:PRO:O | 1:K:203:TYR:HB2 | 2.12 | 0.48 |
| 1:M:223:ALA:O | 1:M:251:ALA:HA | 2.13 | 0.48 |
| 1:B:179:ASP:HB3 | 1:B:389:MET:CE | 2.44 | 0.48 |
| 1:B:404:ARG:HG2 | 1:B:404:ARG:HH11 | 1.78 | 0.48 |
| 1:D:259:LEU:O | 1:D:263:VAL:HG23 | 2.13 | 0.48 |
| 1:D:325:ILE:HG22 | 1:D:330:THR:HA | 1.94 | 0.48 |
| 1:E:202:PRO:O | 1:E:203:TYR:HB2 | 2.13 | 0.48 |
| 1:G:69:MET:O | 1:G:73:MET:HG3 | 2.13 | 0.48 |
| 1:G:259:LEU:O | 1:G:263:VAL:HG23 | 2.13 | 0.48 |
| 1:H:171:LYS:HB2 | 1:H:407:VAL:HG11 | 1.95 | 0.48 |
| 1:H:384:ALA:O | 1:H:385:THR:HG23 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:23:LEU:CD2 | 1:L:74:VAL:HG13 | 2.42 | 0.48 |
| 1:L:69:MET:O | 1:L:73:MET:HG3 | 2.13 | 0.48 |
| 1:L:326:ASN:HD22 | 1:L:329:THR:HB | 1.77 | 0.48 |
| 1:M:202:PRO:O | 1:M:203:TYR:HB2 | 2.13 | 0.48 |
| 1:N:413:ALA:HB3 | 1:N:417:VAL:HG22 | 1.94 | 0.48 |
| 1:C:183:LEU:O | 1:C:184:GLN:HB2 | 2.14 | 0.48 |
| 1:E:404:ARG:NH1 | 6:E:2208:HOH:O | 2.45 | 0.48 |
| 1:F:73:MET:O | 1:F:76:GLU:HB2 | 2.13 | 0.48 |
| 1:F:319:GLN:O | 1:F:336:VAL:HG23 | 2.12 | 0.48 |
| 1:H:234:LEU:O | 1:H:238:GLU:HG3 | 2.13 | 0.48 |
| 1:J:496:PRO:O | 1:J:499:VAL:HG13 | 2.12 | 0.48 |
| 1:A:234:LEU:O | 1:A:238:GLU:HG3 | 2.13 | 0.48 |
| 1:A:239:ALA:O | 1:A:314:LEU:HD11 | 2.13 | 0.48 |
| 1:B:70:GLY:HA2 | 1:B:73:MET:HE3 | 1.96 | 0.48 |
| 1:B:77:VAL:HG11 | 1:B:510:VAL:CG2 | 2.43 | 0.48 |
| 1:B:153:ASN:O | 1:B:154:SER:HB2 | 2.14 | 0.48 |
| 1:B:252:GLU:O | 1:B:253:ASP:HB2 | 2.13 | 0.48 |
| 1:C:220:ILE:HD12 | 1:C:296:THR:HG21 | 1.95 | 0.48 |
| 1:C:310:GLU:N | 1:C:310:GLU:OE1 | 2.46 | 0.48 |
| 1:C:524:LEU:O | 1:C:526:LYS:N | 2.45 | 0.48 |
| 1:E:404:ARG:HG2 | 1:E:404:ARG:HH11 | 1.78 | 0.48 |
| 6:E:1217:HOH:O | 1:F:518:GLU:HG2 | 2.12 | 0.48 |
| 1:G:425:LYS:NZ | 6:G:2070:HOH:O | 2.45 | 0.48 |
| 1:I:73:MET:O | 1:I:76:GLU:HB2 | 2.13 | 0.48 |
| 1:J:206:ASN:OD1 | 1:J:207:LYS:HG3 | 2.13 | 0.48 |
| 1:J:496:PRO:HB2 | 1:J:499:VAL:HG12 | 1.94 | 0.48 |
| 1:K:160:LYS:O | 1:K:164:GLU:HG3 | 2.12 | 0.48 |
| 1:L:176:THR:HG22 | 1:L:177:VAL:N | 2.28 | 0.48 |
| 1:L:384:ALA:O | 1:L:385:THR:HG23 | 2.14 | 0.48 |
| 1:M:193:MET:CE | 1:M:292:ILE:HG12 | 2.43 | 0.48 |
| 1:M:281:PHE:H | 1:M:284:ARG:HD2 | 1.76 | 0.48 |
| 1:A:266:THR:HG22 | 1:A:271:VAL:O | 2.13 | 0.48 |
| 1:B:236:VAL:O | 1:B:240:VAL:HG23 | 2.12 | 0.48 |
| 1:E:235:PRO:CG | 1:E:310:GLU:HA | 2.32 | 0.48 |
| 1:H:223:ALA:O | 1:H:251:ALA:HA | 2.12 | 0.48 |
| 1:M:200:LEU:HG | 1:M:276:VAL:HA | 1.95 | 0.48 |
| 1:M:266:THR:HG22 | 1:M:271:VAL:O | 2.14 | 0.48 |
| 1:N:499:VAL:HG11 | 6:N:2145:HOH:O | 2.13 | 0.48 |
| 1:A:260:ALA:O | 1:A:264:VAL:HG23 | 2.13 | 0.48 |
| 1:D:63:GLU:OE2 | 1:E:526:LYS:HE2 | 2.13 | 0.48 |
| 1:D:384:ALA:O | 1:D:385:THR:HG23 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:153:ASN:O | 1:E:154:SER:HB2 | 2.13 | 0.48 |
| 1:I:180:GLY:HA3 | 1:I:381:VAL:O | 2.13 | 0.48 |
| 1:I:524:LEU:O | 1:I:526:LYS:N | 2.46 | 0.48 |
| 1:J:413:ALA:HB3 | 1:J:417:VAL:HG22 | 1.95 | 0.48 |
| 1:L:174:VAL:HG22 | 1:L:194:GLN:NE2 | 2.28 | 0.48 |
| 1:L:254:VAL:HG12 | 1:L:259:LEU:HB2 | 1.95 | 0.48 |
| 1:N:222:LEU:HB3 | 1:N:289:LEU:CD2 | 2.43 | 0.48 |
| 1:A:46:ALA:HB2 | 1:B:76:GLU:HG2 | 1.93 | 0.48 |
| 1:A:176:THR:HG21 | 1:A:322:ARG:HH12 | 1.79 | 0.48 |
| 1:A:206:ASN:OD1 | 1:A:207:LYS:HG3 | 2.13 | 0.48 |
| 1:B:200:LEU:HG | 1:B:276:VAL:HA | 1.96 | 0.48 |
| 1:G:266:THR:HG22 | 1:G:271:VAL:O | 2.14 | 0.48 |
| 1:G:362:ARG:HD2 | 6:G:1728:HOH:O | 2.13 | 0.48 |
| 1:L:219:PHE:O | 1:L:247:LEU:HD12 | 2.13 | 0.48 |
| 1:L:291:ASP:OD2 | 1:L:368:ARG:HD2 | 2.14 | 0.48 |
| 1:L:441:LYS:HE2 | 6:L:2814:HOH:O | 2.13 | 0.48 |
| 1:N:16:MET:O | 1:N:20:VAL:HG13 | 2.13 | 0.48 |
| 1:B:144:ILE:HG23 | 1:B:403:THR:CG2 | 2.44 | 0.48 |
| 1:E:353:ILE:HD13 | 1:E:366:GLN:HG2 | 1.96 | 0.48 |
| 1:J:319:GLN:O | 1:J:336:VAL:HG23 | 2.14 | 0.48 |
| 1:K:384:ALA:O | 1:K:385:THR:HG23 | 2.14 | 0.48 |
| 1:L:209:GLU:OE1 | 1:L:209:GLU:N | 2.47 | 0.48 |
| 1:M:174:VAL:HG22 | 1:M:194:GLN:HE21 | 1.77 | 0.48 |
| 1:M:455:VAL:HG13 | 1:M:460:GLU:HB2 | 1.95 | 0.48 |
| 1:N:220:ILE:HD12 | 1:N:296:THR:HG21 | 1.95 | 0.48 |
| 1:N:325:ILE:HG22 | 1:N:330:THR:HA | 1.96 | 0.48 |
| 1:B:185:ASP:OD1 | 1:B:382:GLY:N | 2.47 | 0.48 |
| 1:C:266:THR:HG22 | 1:C:271:VAL:O | 2.14 | 0.48 |
| 1:D:113:PRO:HD2 | 6:D:2375:HOH:O | 2.14 | 0.48 |
| 1:D:524:LEU:O | 1:D:526:LYS:N | 2.46 | 0.48 |
| 1:E:259:LEU:O | 1:E:263:VAL:HG23 | 2.14 | 0.48 |
| 1:F:180:GLY:HA3 | 1:F:381:VAL:O | 2.13 | 0.48 |
| 1:F:252:GLU:O | 1:F:253:ASP:HB2 | 2.14 | 0.48 |
| 1:G:177:VAL:HG21 | 1:G:397:GLU:HG2 | 1.93 | 0.48 |
| 1:H:219:PHE:O | 1:H:247:LEU:HD12 | 2.13 | 0.48 |
| 1:I:199:TYR:CZ | 1:I:327:LYS:HA | 2.49 | 0.48 |
| 1:K:325:ILE:HG22 | 1:K:330:THR:HA | 1.96 | 0.48 |
| 1:N:223:ALA:O | 1:N:251:ALA:HA | 2.14 | 0.48 |
| 1:N:386:GLU:O | 1:N:390:LYS:HG2 | 2.14 | 0.48 |
| 1:D:144:ILE:HG23 | 1:D:403:THR:HG21 | 1.96 | 0.48 |
| 1:F:222:LEU:HB3 | 1:F:289:LEU:CD2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:73:MET:O | 1:G:76:GLU:HB2 | 2.13 | 0.48 |
| 1:G:254:VAL:HG12 | 1:G:259:LEU:HB2 | 1.96 | 0.48 |
| 1:H:266:THR:HG22 | 1:H:271:VAL:O | 2.14 | 0.48 |
| 1:I:413:ALA:HB3 | 1:I:417:VAL:HG22 | 1.94 | 0.48 |
| 1:A:223:ALA:O | 1:A:251:ALA:HA | 2.14 | 0.47 |
| 1:B:171:LYS:HB2 | 1:B:407:VAL:HG11 | 1.96 | 0.47 |
| 1:D:85:ALA:O | 1:D:401:HIS:HE1 | 1.95 | 0.47 |
| 1:G:239:ALA:O | 1:G:314:LEU:HD11 | 2.14 | 0.47 |
| 1:H:180:GLY:HA3 | 1:H:381:VAL:O | 2.14 | 0.47 |
| 1:J:220:ILE:HD12 | 1:J:296:THR:HG21 | 1.96 | 0.47 |
| 1:A:193:MET:HE2 | 1:A:292:ILE:HG12 | 1.96 | 0.47 |
| 1:A:254:VAL:HG12 | 1:A:259:LEU:HB2 | 1.95 | 0.47 |
| 1:A:413:ALA:HB3 | 1:A:417:VAL:HG22 | 1.95 | 0.47 |
| 1:B:260:ALA:O | 1:B:264:VAL:HG23 | 2.15 | 0.47 |
| 1:G:348:GLN:O | 1:G:352:GLN:HG2 | 2.14 | 0.47 |
| 1:H:206:ASN:ND2 | 1:H:214:GLU:H | 2.12 | 0.47 |
| 1:J:353:ILE:HD13 | 1:J:366:GLN:HG2 | 1.96 | 0.47 |
| 1:K:259:LEU:O | 1:K:263:VAL:HG23 | 2.14 | 0.47 |
| 1:L:177:VAL:HG21 | 1:L:397:GLU:HG2 | 1.94 | 0.47 |
| 1:B:220:ILE:HD12 | 1:B:296:THR:HG21 | 1.96 | 0.47 |
| 1:C:259:LEU:O | 1:C:263:VAL:HG23 | 2.14 | 0.47 |
| 1:D:23:LEU:CD2 | 1:D:74:VAL:HG13 | 2.44 | 0.47 |
| 1:I:236:VAL:O | 1:I:240:VAL:HG23 | 2.14 | 0.47 |
| 1:I:271:VAL:HG12 | 1:I:273:VAL:HG23 | 1.95 | 0.47 |
| 1:J:325:ILE:HG22 | 1:J:330:THR:HA | 1.97 | 0.47 |
| 1:K:37:ASN:HD21 | 1:K:51:LYS:HE3 | 1.80 | 0.47 |
| 1:K:206:ASN:OD1 | 1:K:207:LYS:HG3 | 2.13 | 0.47 |
| 1:K:287:ALA:HB1 | 1:K:368:ARG:NH1 | 2.28 | 0.47 |
| 1:M:366:GLN:O | 1:M:369:VAL:HG22 | 2.15 | 0.47 |
| 1:B:266:THR:CG2 | 1:B:273:VAL:H | 2.27 | 0.47 |
| 1:F:524:LEU:O | 1:F:526:LYS:N | 2.46 | 0.47 |
| 1:G:209:GLU:OE1 | 1:G:209:GLU:N | 2.44 | 0.47 |
| 1:G:234:LEU:N | 1:G:235:PRO:HD2 | 2.29 | 0.47 |
| 1:H:209:GLU:OE1 | 1:H:209:GLU:N | 2.46 | 0.47 |
| 1:I:10:ASN:ND2 | 6:I:2045:HOH:O | 2.47 | 0.47 |
| 1:I:287:ALA:HB1 | 1:I:368:ARG:NH1 | 2.29 | 0.47 |
| 1:I:449:ALA:HB3 | 1:I:450:PRO:HD3 | 1.97 | 0.47 |
| 1:J:287:ALA:HB1 | 1:J:368:ARG:NH1 | 2.29 | 0.47 |
| 1:K:219:PHE:O | 1:K:247:LEU:HD12 | 2.13 | 0.47 |
| 1:K:234:LEU:O | 1:K:238:GLU:HG3 | 2.13 | 0.47 |
| 1:L:206:ASN:OD1 | 1:L:207:LYS:HG3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:199:TYR:CZ | 1:N:327:LYS:HA | 2.50 | 0.47 |
| 1:A:209:GLU:OE1 | 1:A:209:GLU:N | 2.44 | 0.47 |
| 1:A:231:ARG:NH1 | 1:G:242:LYS:HG2 | 2.28 | 0.47 |
| 1:B:206:ASN:OD1 | 1:B:207:LYS:HG3 | 2.13 | 0.47 |
| 1:B:234:LEU:N | 1:B:235:PRO:HD2 | 2.29 | 0.47 |
| 1:D:217:SER:N | 1:D:218:PRO:CD | 2.78 | 0.47 |
| 1:H:239:ALA:O | 1:H:314:LEU:HD11 | 2.15 | 0.47 |
| 1:H:271:VAL:HG12 | 1:H:273:VAL:HG23 | 1.96 | 0.47 |
| 1:L:78:ALA:HB1 | 1:L:89:THR:HB | 1.97 | 0.47 |
| 1:M:524:LEU:O | 1:M:526:LYS:N | 2.46 | 0.47 |
| 1:N:160:LYS:HB2 | 1:N:160:LYS:NZ | 2.29 | 0.47 |
| 1:A:305:ILE:HB | 1:A:307:MET:HE2 | 1.95 | 0.47 |
| 1:B:383:ALA:HB1 | 1:C:281:PHE:CE2 | 2.49 | 0.47 |
| 1:C:301:ILE:HG21 | 1:C:309:LEU:HD23 | 1.95 | 0.47 |
| 1:D:89:THR:HG23 | 6:D:2757:HOH:O | 2.13 | 0.47 |
| 1:F:177:VAL:HG21 | 1:F:397:GLU:HG2 | 1.96 | 0.47 |
| 1:I:220:ILE:HD12 | 1:I:296:THR:HG21 | 1.95 | 0.47 |
| 1:L:234:LEU:O | 1:L:238:GLU:HG3 | 2.15 | 0.47 |
| 1:N:236:VAL:O | 1:N:240:VAL:HG23 | 2.14 | 0.47 |
| 1:A:183:LEU:CD2 | 1:A:384:ALA:HB2 | 2.44 | 0.47 |
| 1:B:215:LEU:HB2 | 1:B:323:VAL:HG22 | 1.96 | 0.47 |
| 1:D:12:ALA:N | 6:D:2704:HOH:O | 2.47 | 0.47 |
| 1:D:205:ILE:HA | 1:D:213:VAL:HG22 | 1.95 | 0.47 |
| 1:D:252:GLU:O | 1:D:253:ASP:HB2 | 2.15 | 0.47 |
| 1:G:302:SER:H | 1:G:307:MET:CE | 2.28 | 0.47 |
| 1:H:206:ASN:OD1 | 1:H:207:LYS:HG3 | 2.15 | 0.47 |
| 1:I:206:ASN:ND2 | 1:I:214:GLU:H | 2.12 | 0.47 |
| 1:I:234:LEU:N | 1:I:235:PRO:HD2 | 2.29 | 0.47 |
| 1:I:272:LYS:NZ | 1:J:229:ASN:OD1 | 2.47 | 0.47 |
| 1:J:176:THR:HG22 | 1:J:177:VAL:N | 2.29 | 0.47 |
| 1:J:266:THR:HG22 | 1:J:271:VAL:O | 2.15 | 0.47 |
| 1:J:369:VAL:HG23 | 1:J:370:ALA:N | 2.30 | 0.47 |
| 1:L:234:LEU:N | 1:L:235:PRO:HD2 | 2.30 | 0.47 |
| 1:L:366:GLN:HA | 1:L:369:VAL:HG22 | 1.95 | 0.47 |
| 1:M:199:TYR:CZ | 1:M:327:LYS:HA | 2.50 | 0.47 |
| 1:M:206:ASN:OD1 | 1:M:207:LYS:HG3 | 2.14 | 0.47 |
| 1:M:260:ALA:O | 1:M:264:VAL:HG23 | 2.15 | 0.47 |
| 1:N:183:LEU:HD13 | 1:N:184:GLN:N | 2.29 | 0.47 |
| 1:A:134:LEU:HD21 | 1:A:425:LYS:NZ | 2.30 | 0.47 |
| 1:B:7:LYS:HG3 | 1:B:66:PHE:CZ | 2.50 | 0.47 |
| 1:B:177:VAL:HG21 | 1:B:397:GLU:HG2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:382:GLY:O | 1:D:389:MET:HG2 | 2.15 | 0.47 |
| 1:E:70:GLY:HA2 | 1:E:73:MET:HE3 | 1.97 | 0.47 |
| 1:F:206:ASN:OD1 | 1:F:207:LYS:HG3 | 2.14 | 0.47 |
| 1:H:185:ASP:OD1 | 1:H:382:GLY:N | 2.46 | 0.47 |
| 1:H:193:MET:HE1 | 1:H:292:ILE:HG12 | 1.97 | 0.47 |
| 1:J:525:PRO:HD3 | 6:J:2970:HOH:O | 2.14 | 0.47 |
| 1:K:183:LEU:CD2 | 1:K:384:ALA:HB2 | 2.43 | 0.47 |
| 1:M:254:VAL:HG12 | 1:M:259:LEU:HB2 | 1.96 | 0.47 |
| 1:A:68:ASN:O | 1:A:72:GLN:HG2 | 2.15 | 0.47 |
| 1:C:183:LEU:HD13 | 1:C:184:GLN:N | 2.30 | 0.47 |
| 1:C:252:GLU:O | 1:C:253:ASP:HB2 | 2.14 | 0.47 |
| 1:E:90:THR:O | 1:E:94:VAL:HG13 | 2.14 | 0.47 |
| 1:E:260:ALA:O | 1:E:264:VAL:HG23 | 2.15 | 0.47 |
| 1:J:111:MET:HG2 | 1:J:435:ASP:OD1 | 2.15 | 0.47 |
| 1:K:160:LYS:HB2 | 1:K:160:LYS:NZ | 2.30 | 0.47 |
| 1:L:236:VAL:O | 1:L:240:VAL:HG23 | 2.15 | 0.47 |
| 1:L:325:ILE:HG22 | 1:L:330:THR:HA | 1.97 | 0.47 |
| 1:M:160:LYS:HB2 | 1:M:160:LYS:NZ | 2.29 | 0.47 |
| 1:A:236:VAL:O | 1:A:240:VAL:HG23 | 2.15 | 0.47 |
| 1:C:23:LEU:CD2 | 1:C:74:VAL:HG13 | 2.45 | 0.47 |
| 1:C:223:ALA:O | 1:C:251:ALA:HA | 2.15 | 0.47 |
| 1:D:206:ASN:HD21 | 1:D:214:GLU:H | 1.63 | 0.47 |
| 1:D:302:SER:H | 1:D:307:MET:HE1 | 1.80 | 0.47 |
| 1:J:234:LEU:O | 1:J:238:GLU:HG3 | 2.13 | 0.47 |
| 1:L:271:VAL:HG12 | 1:L:273:VAL:HG23 | 1.96 | 0.47 |
| 1:M:90:THR:OG1 | 5:M:1:AGS:S1G | 2.63 | 0.47 |
| 1:M:269:GLY:O | 1:N:229:ASN:OD1 | 2.33 | 0.47 |
| 1:A:73:MET:O | 1:A:76:GLU:HB2 | 2.15 | 0.46 |
| 1:D:238:GLU:O | 1:D:241:ALA:HB3 | 2.15 | 0.46 |
| 1:F:234:LEU:O | 1:F:238:GLU:HG3 | 2.14 | 0.46 |
| 1:F:384:ALA:O | 1:F:385:THR:HG23 | 2.14 | 0.46 |
| 1:G:240:VAL:HG11 | 1:G:247:LEU:HB2 | 1.96 | 0.46 |
| 1:H:199:TYR:CZ | 1:H:327:LYS:HA | 2.51 | 0.46 |
| 1:I:140:ASP:OD2 | 1:I:142:LYS:HB3 | 2.16 | 0.46 |
| 1:J:215:LEU:HB2 | 1:J:323:VAL:HG22 | 1.97 | 0.46 |
| 1:L:242:LYS:C | 1:L:244:GLY:N | 2.69 | 0.46 |
| 1:A:169:VAL:HG13 | 1:A:377:ALA:HB2 | 1.97 | 0.46 |
| 1:A:215:LEU:HB2 | 1:A:323:VAL:HG22 | 1.98 | 0.46 |
| 1:C:60:ILE:O | 1:C:75:LYS:HE3 | 2.15 | 0.46 |
| 1:C:176:THR:HG21 | 1:C:322:ARG:HH12 | 1.81 | 0.46 |
| 1:G:384:ALA:O | 1:G:385:THR:HG23 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:254:VAL:HG12 | 1:I:259:LEU:HB2 | 1.97 | 0.46 |
| 1:I:260:ALA:O | 1:I:264:VAL:HG23 | 2.14 | 0.46 |
| 1:I:325:ILE:HG22 | 1:I:330:THR:HA | 1.98 | 0.46 |
| 1:M:63:GLU:OE2 | 1:N:526:LYS:HE2 | 2.15 | 0.46 |
| 1:N:155:ASP:OD1 | 1:N:157:THR:HB | 2.14 | 0.46 |
| 1:C:234:LEU:N | 1:C:235:PRO:HD2 | 2.30 | 0.46 |
| 1:E:199:TYR:CZ | 1:E:327:LYS:HA | 2.50 | 0.46 |
| 1:E:451:LEU:HD23 | 1:E:451:LEU:C | 2.35 | 0.46 |
| 1:G:78:ALA:HB1 | 1:G:89:THR:HB | 1.96 | 0.46 |
| 1:G:144:ILE:HG23 | 1:G:403:THR:HG21 | 1.96 | 0.46 |
| 5:G:1:AGS:S1G | 5:G:1:AGS:O2G | 2.53 | 0.46 |
| 1:I:463:SER:HB2 | 6:I:2586:HOH:O | 2.14 | 0.46 |
| 1:M:239:ALA:O | 1:M:314:LEU:HD11 | 2.15 | 0.46 |
| 1:M:323:VAL:HG12 | 1:M:332:ILE:HA | 1.98 | 0.46 |
| 1:A:171:LYS:HB2 | 1:A:407:VAL:HG11 | 1.98 | 0.46 |
| 1:B:169:VAL:CG1 | 1:B:377:ALA:HB2 | 2.45 | 0.46 |
| 1:B:325:ILE:HG22 | 1:B:330:THR:HA | 1.96 | 0.46 |
| 1:D:209:GLU:OE1 | 1:D:209:GLU:N | 2.45 | 0.46 |
| 1:F:353:ILE:HD13 | 1:F:366:GLN:HG2 | 1.98 | 0.46 |
| 1:F:381:VAL:O | 1:F:382:GLY:O | 2.33 | 0.46 |
| 1:G:180:GLY:HA3 | 1:G:381:VAL:O | 2.16 | 0.46 |
| 1:G:218:PRO:HD2 | 1:G:320:ALA:O | 2.15 | 0.46 |
| 1:H:254:VAL:HG12 | 1:H:259:LEU:HB2 | 1.98 | 0.46 |
| 1:K:183:LEU:HD13 | 1:K:184:GLN:N | 2.30 | 0.46 |
| 1:N:122:LYS:HE2 | 1:N:429:LEU:HD11 | 1.97 | 0.46 |
| 1:A:90:THR:O | 1:A:94:VAL:HG13 | 2.14 | 0.46 |
| 1:H:234:LEU:N | 1:H:235:PRO:HD2 | 2.30 | 0.46 |
| 1:I:381:VAL:O | 1:I:382:GLY:O | 2.34 | 0.46 |
| 1:K:60:ILE:O | 1:K:75:LYS:HE3 | 2.16 | 0.46 |
| 1:K:144:ILE:HG23 | 1:K:403:THR:HG21 | 1.97 | 0.46 |
| 1:K:325:ILE:HA | 1:K:329:THR:O | 2.15 | 0.46 |
| 1:L:455:VAL:O | 1:L:458:CYS:HB2 | 2.14 | 0.46 |
| 1:M:234:LEU:N | 1:M:235:PRO:HD2 | 2.30 | 0.46 |
| 1:N:366:GLN:HA | 1:N:369:VAL:HG22 | 1.96 | 0.46 |
| 1:A:182:GLY:HA2 | 1:A:383:ALA:HB3 | 1.97 | 0.46 |
| 1:C:209:GLU:OE1 | 1:C:209:GLU:N | 2.45 | 0.46 |
| 1:D:235:PRO:CG | 1:D:310:GLU:HA | 2.34 | 0.46 |
| 1:E:10:ASN:HB2 | 6:E:1989:HOH:O | 2.14 | 0.46 |
| 1:E:223:ALA:O | 1:E:251:ALA:HA | 2.16 | 0.46 |
| 1:F:200:LEU:HG | 1:F:276:VAL:HA | 1.98 | 0.46 |
| 1:F:234:LEU:N | 1:F:235:PRO:HD2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:383:ALA:O | 1:F:384:ALA:CB | 2.63 | 0.46 |
| 1:H:250:ILE:HG22 | 6:H:2938:HOH:O | 2.15 | 0.46 |
| 1:H:404:ARG:NH1 | 1:H:404:ARG:CG | 2.71 | 0.46 |
| 1:J:234:LEU:N | 1:J:235:PRO:HD2 | 2.31 | 0.46 |
| 1:L:220:ILE:HD12 | 1:L:296:THR:HG21 | 1.96 | 0.46 |
| 1:M:234:LEU:O | 1:M:238:GLU:HG3 | 2.14 | 0.46 |
| 1:A:199:TYR:CZ | 1:A:327:LYS:HA | 2.51 | 0.46 |
| 1:A:366:GLN:O | 1:A:369:VAL:HG22 | 2.15 | 0.46 |
| 1:D:266:THR:CG2 | 1:D:273:VAL:H | 2.28 | 0.46 |
| 1:D:319:GLN:HB3 | 1:D:336:VAL:HG21 | 1.97 | 0.46 |
| 1:G:60:ILE:O | 1:G:75:LYS:HE3 | 2.16 | 0.46 |
| 1:J:174:VAL:HG22 | 1:J:194:GLN:NE2 | 2.31 | 0.46 |
| 1:M:10:ASN:HA | 6:M:2195:HOH:O | 2.15 | 0.46 |
| 1:A:78:ALA:HB3 | 6:A:2430:HOH:O | 2.15 | 0.46 |
| 1:C:234:LEU:O | 1:C:238:GLU:HG3 | 2.15 | 0.46 |
| 1:E:217:SER:N | 1:E:218:PRO:HD3 | 2.31 | 0.46 |
| 1:E:420:ILE:HG13 | 1:E:448:GLU:HG2 | 1.96 | 0.46 |
| 1:F:217:SER:N | 1:F:218:PRO:HD3 | 2.31 | 0.46 |
| 1:F:287:ALA:HB1 | 1:F:368:ARG:NH1 | 2.30 | 0.46 |
| 1:H:217:SER:N | 1:H:218:PRO:CD | 2.79 | 0.46 |
| 1:I:217:SER:N | 1:I:218:PRO:CD | 2.79 | 0.46 |
| 1:J:158:VAL:HG13 | 1:J:396:VAL:HG22 | 1.98 | 0.46 |
| 1:J:219:PHE:O | 1:J:247:LEU:HD12 | 2.15 | 0.46 |
| 1:J:223:ALA:O | 1:J:251:ALA:HA | 2.15 | 0.46 |
| 1:J:384:ALA:O | 1:J:385:THR:HG23 | 2.16 | 0.46 |
| 1:M:325:ILE:HA | 1:M:329:THR:O | 2.16 | 0.46 |
| 1:M:438:VAL:O | 1:M:442:VAL:HG23 | 2.16 | 0.46 |
| 1:N:234:LEU:N | 1:N:235:PRO:HD2 | 2.31 | 0.46 |
| 1:B:180:GLY:HA3 | 1:B:381:VAL:O | 2.15 | 0.46 |
| 1:C:290:GLN:HB3 | 1:C:345:ARG:NH2 | 2.31 | 0.46 |
| 1:E:234:LEU:N | 1:E:235:PRO:HD2 | 2.31 | 0.46 |
| 1:G:171:LYS:HB2 | 1:G:407:VAL:HG11 | 1.98 | 0.46 |
| 1:G:220:ILE:HD12 | 1:G:296:THR:HG21 | 1.97 | 0.46 |
| 1:H:183:LEU:CD2 | 1:H:384:ALA:HB2 | 2.45 | 0.46 |
| 1:H:353:ILE:HD13 | 1:H:366:GLN:HG2 | 1.98 | 0.46 |
| 1:I:301:ILE:HG21 | 1:I:309:LEU:HD23 | 1.97 | 0.46 |
| 1:J:319:GLN:HB3 | 1:J:336:VAL:HG21 | 1.97 | 0.46 |
| 1:K:78:ALA:HB1 | 1:K:89:THR:HB | 1.98 | 0.46 |
| 1:K:215:LEU:HB2 | 1:K:323:VAL:HG22 | 1.98 | 0.46 |
| 1:L:68:ASN:O | 1:L:72:GLN:HG2 | 2.16 | 0.46 |
| 1:A:325:ILE:HG22 | 1:A:330:THR:HA | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:524:LEU:O | 1:A:526:LYS:N | 2.48 | 0.46 |
| 1:I:69:MET:O | 1:I:73:MET:HG3 | 2.15 | 0.46 |
| 1:K:210:THR:O | 1:K:210:THR:HG22 | 2.16 | 0.46 |
| 1:K:234:LEU:N | 1:K:235:PRO:HD2 | 2.31 | 0.46 |
| 1:A:101:THR:HG23 | 6:A:2971:HOH:O | 2.16 | 0.45 |
| 1:A:353:ILE:HD13 | 1:A:366:GLN:HG2 | 1.97 | 0.45 |
| 1:B:404:ARG:NH1 | 6:B:2253:HOH:O | 2.48 | 0.45 |
| 1:F:458:CYS:SG | 1:F:480:ALA:HB1 | 2.57 | 0.45 |
| 1:G:193:MET:HG3 | 1:G:371:LYS:HB3 | 1.98 | 0.45 |
| 1:K:177:VAL:HA | 1:K:379:ILE:O | 2.16 | 0.45 |
| 1:K:302:SER:H | 1:K:307:MET:HE1 | 1.81 | 0.45 |
| 1:L:171:LYS:HB2 | 1:L:407:VAL:HG11 | 1.98 | 0.45 |
| 1:B:183:LEU:CD2 | 1:B:384:ALA:HB2 | 2.43 | 0.45 |
| 1:C:324:VAL:O | 1:C:331:THR:HG22 | 2.16 | 0.45 |
| 1:D:319:GLN:O | 1:D:336:VAL:HG23 | 2.17 | 0.45 |
| 1:G:234:LEU:O | 1:G:238:GLU:HG3 | 2.17 | 0.45 |
| 1:H:235:PRO:CG | 1:H:310:GLU:HA | 2.35 | 0.45 |
| 1:I:353:ILE:HD13 | 1:I:366:GLN:HG2 | 1.98 | 0.45 |
| 1:I:369:VAL:HG23 | 1:I:370:ALA:N | 2.31 | 0.45 |
| 1:J:183:LEU:HD13 | 1:J:184:GLN:N | 2.30 | 0.45 |
| 1:J:260:ALA:O | 1:J:264:VAL:HG23 | 2.16 | 0.45 |
| 1:K:369:VAL:HG23 | 1:K:370:ALA:N | 2.31 | 0.45 |
| 1:N:215:LEU:HB2 | 1:N:323:VAL:CG2 | 2.47 | 0.45 |
| 1:N:271:VAL:HG12 | 1:N:273:VAL:HG23 | 1.97 | 0.45 |
| 1:A:182:GLY:HA2 | 1:A:383:ALA:CB | 2.46 | 0.45 |
| 1:C:78:ALA:HB3 | 6:C:1582:HOH:O | 2.16 | 0.45 |
| 1:D:301:ILE:HG21 | 1:D:309:LEU:HD23 | 1.98 | 0.45 |
| 1:E:206:ASN:ND2 | 1:E:214:GLU:H | 2.11 | 0.45 |
| 1:E:219:PHE:O | 1:E:247:LEU:HD12 | 2.16 | 0.45 |
| 1:E:325:ILE:HG22 | 1:E:330:THR:HA | 1.97 | 0.45 |
| 1:F:160:LYS:HB2 | 1:F:160:LYS:HZ2 | 1.81 | 0.45 |
| 1:F:193:MET:HE2 | 1:F:292:ILE:HG12 | 1.99 | 0.45 |
| 1:F:217:SER:N | 1:F:218:PRO:CD | 2.79 | 0.45 |
| 1:I:60:ILE:O | 1:I:75:LYS:HE3 | 2.16 | 0.45 |
| 1:J:325:ILE:HA | 1:J:329:THR:O | 2.16 | 0.45 |
| 1:J:524:LEU:O | 1:J:526:LYS:N | 2.49 | 0.45 |
| 1:M:325:ILE:HG22 | 1:M:330:THR:HA | 1.97 | 0.45 |
| 1:N:266:THR:HG21 | 1:N:273:VAL:H | 1.80 | 0.45 |
| 1:A:384:ALA:O | 1:A:385:THR:HG23 | 2.16 | 0.45 |
| 1:B:319:GLN:HB3 | 1:B:336:VAL:HG21 | 1.99 | 0.45 |
| 1:C:413:ALA:HB3 | 1:C:417:VAL:HG22 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:290:GLN:HB3 | 1:E:345:ARG:NH2 | 2.31 | 0.45 |
| 1:G:68:ASN:O | 1:G:72:GLN:HG2 | 2.16 | 0.45 |
| 1:I:134:LEU:HD21 | 1:I:425:LYS:NZ | 2.31 | 0.45 |
| 1:I:217:SER:N | 1:I:218:PRO:HD3 | 2.31 | 0.45 |
| 1:K:37:ASN:ND2 | 1:K:51:LYS:HE3 | 2.32 | 0.45 |
| 1:K:217:SER:N | 1:K:218:PRO:CD | 2.80 | 0.45 |
| 1:L:224:ASP:HB3 | 1:L:302:SER:HB3 | 1.98 | 0.45 |
| 1:M:169:VAL:HG13 | 1:M:377:ALA:HB2 | 1.99 | 0.45 |
| 1:N:10:ASN:ND2 | 6:N:2158:HOH:O | 2.49 | 0.45 |
| 1:E:182:GLY:O | 1:E:183:LEU:O | 2.35 | 0.45 |
| 1:E:319:GLN:HB3 | 1:E:336:VAL:HG21 | 1.99 | 0.45 |
| 1:E:369:VAL:HG23 | 1:E:370:ALA:N | 2.30 | 0.45 |
| 1:F:171:LYS:HB2 | 1:F:407:VAL:HG11 | 1.98 | 0.45 |
| 1:F:219:PHE:O | 1:F:247:LEU:HD12 | 2.16 | 0.45 |
| 1:I:183:LEU:CD2 | 1:I:384:ALA:HB2 | 2.45 | 0.45 |
| 1:J:301:ILE:HG21 | 1:J:309:LEU:HD23 | 1.97 | 0.45 |
| 1:K:301:ILE:HG21 | 1:K:309:LEU:HD23 | 1.97 | 0.45 |
| 1:N:254:VAL:HG12 | 1:N:259:LEU:HB2 | 1.99 | 0.45 |
| 1:A:185:ASP:OD1 | 1:A:382:GLY:N | 2.48 | 0.45 |
| 1:D:90:THR:OG1 | 5:D:551:AGS:S1G | 2.68 | 0.45 |
| 1:E:217:SER:N | 1:E:218:PRO:CD | 2.79 | 0.45 |
| 1:H:524:LEU:O | 1:H:526:LYS:N | 2.49 | 0.45 |
| 1:I:183:LEU:HD13 | 1:I:184:GLN:N | 2.31 | 0.45 |
| 1:J:197:ARG:HD2 | 1:J:277:LYS:HB2 | 1.98 | 0.45 |
| 1:L:438:VAL:O | 1:L:442:VAL:HG23 | 2.17 | 0.45 |
| 1:M:217:SER:N | 1:M:218:PRO:HD3 | 2.32 | 0.45 |
| 1:A:39:VAL:HG12 | 1:B:69:MET:CE | 2.47 | 0.45 |
| 1:A:369:VAL:HG23 | 1:A:370:ALA:N | 2.32 | 0.45 |
| 1:C:42:LYS:HE3 | 1:C:48:THR:OG1 | 2.17 | 0.45 |
| 1:C:206:ASN:OD1 | 1:C:207:LYS:HG3 | 2.17 | 0.45 |
| 1:D:87:ASP:N | 6:D:2757:HOH:O | 2.49 | 0.45 |
| 1:E:158:VAL:HG22 | 6:E:2648:HOH:O | 2.16 | 0.45 |
| 1:G:238:GLU:O | 1:G:241:ALA:HB3 | 2.16 | 0.45 |
| 1:L:222:LEU:HB3 | 1:L:289:LEU:CD2 | 2.46 | 0.45 |
| 1:L:524:LEU:HD12 | 1:L:524:LEU:HA | 1.87 | 0.45 |
| 1:M:222:LEU:HB3 | 1:M:289:LEU:CD2 | 2.47 | 0.45 |
| 1:E:210:THR:HG22 | 1:E:210:THR:O | 2.17 | 0.45 |
| 1:F:124:VAL:HG21 | 1:F:508:ALA:CB | 2.47 | 0.45 |
| 1:F:325:ILE:HG22 | 1:F:330:THR:HA | 1.98 | 0.45 |
| 1:F:366:GLN:O | 1:F:369:VAL:HG22 | 2.16 | 0.45 |
| 1:G:463:SER:O | 1:G:467:ASN:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:242:LYS:C | 1:H:244:GLY:N | 2.70 | 0.45 |
| 1:M:218:PRO:HD2 | 1:M:320:ALA:O | 2.17 | 0.45 |
| 1:N:90:THR:O | 1:N:94:VAL:HG13 | 2.16 | 0.45 |
| 1:N:174:VAL:HG22 | 1:N:194:GLN:HE21 | 1.82 | 0.45 |
| 1:N:238:GLU:O | 1:N:241:ALA:HB3 | 2.17 | 0.45 |
| 1:N:252:GLU:O | 1:N:253:ASP:HB2 | 2.16 | 0.45 |
| 1:A:217:SER:N | 1:A:218:PRO:CD | 2.80 | 0.45 |
| 1:A:404:ARG:HH11 | 1:A:404:ARG:CG | 2.29 | 0.45 |
| 1:B:210:THR:HG22 | 1:B:210:THR:O | 2.16 | 0.45 |
| 1:B:217:SER:N | 1:B:218:PRO:HD3 | 2.32 | 0.45 |
| 1:C:239:ALA:C | 1:C:314:LEU:HD21 | 2.38 | 0.45 |
| 1:D:242:LYS:C | 1:D:244:GLY:N | 2.67 | 0.45 |
| 1:F:325:ILE:HA | 1:F:329:THR:O | 2.17 | 0.45 |
| 1:J:160:LYS:HB2 | 1:J:160:LYS:NZ | 2.32 | 0.45 |
| 1:J:239:ALA:O | 1:J:314:LEU:HD11 | 2.16 | 0.45 |
| 1:J:272:LYS:NZ | 1:K:229:ASN:OD1 | 2.50 | 0.45 |
| 1:K:88:GLY:HA2 | 5:K:1:AGS:PB | 2.57 | 0.45 |
| 1:K:174:VAL:HG22 | 1:K:194:GLN:NE2 | 2.32 | 0.45 |
| 1:K:217:SER:N | 1:K:218:PRO:HD3 | 2.31 | 0.45 |
| 1:K:260:ALA:O | 1:K:264:VAL:HG23 | 2.16 | 0.45 |
| 1:K:342:ILE:O | 1:K:346:VAL:HG23 | 2.16 | 0.45 |
| 1:L:325:ILE:HG22 | 1:L:330:THR:HG23 | 1.98 | 0.45 |
| 1:L:369:VAL:HG23 | 1:L:370:ALA:N | 2.32 | 0.45 |
| 1:N:242:LYS:C | 1:N:244:GLY:N | 2.69 | 0.45 |
| 1:A:217:SER:N | 1:A:218:PRO:HD3 | 2.32 | 0.45 |
| 1:A:392:LYS:O | 1:A:396:VAL:HG23 | 2.17 | 0.45 |
| 1:B:39:VAL:HG12 | 1:C:69:MET:CE | 2.47 | 0.45 |
| 1:B:342:ILE:O | 1:B:346:VAL:HG23 | 2.17 | 0.45 |
| 1:C:210:THR:O | 1:C:210:THR:HG22 | 2.17 | 0.45 |
| 1:E:141:SER:HB3 | 6:E:2603:HOH:O | 2.17 | 0.45 |
| 1:F:34:LYS:HG3 | 1:F:458:CYS:SG | 2.57 | 0.45 |
| 1:J:183:LEU:CD2 | 1:J:384:ALA:HB2 | 2.44 | 0.45 |
| 1:L:90:THR:OG1 | 5:L:1:AGS:S1G | 2.65 | 0.45 |
| 1:L:455:VAL:HG13 | 1:L:460:GLU:HB2 | 1.98 | 0.45 |
| 1:M:238:GLU:O | 1:M:241:ALA:HB3 | 2.17 | 0.45 |
| 1:C:182:GLY:HA2 | 1:C:383:ALA:HB3 | 1.97 | 0.44 |
| 1:C:305:ILE:HB | 1:C:307:MET:HE2 | 1.98 | 0.44 |
| 1:C:381:VAL:O | 1:C:382:GLY:O | 2.36 | 0.44 |
| 1:D:73:MET:O | 1:D:76:GLU:HB2 | 2.17 | 0.44 |
| 1:H:284:ARG:HH12 | 1:H:364:LYS:NZ | 2.14 | 0.44 |
| 1:J:37:ASN:HD21 | 1:J:51:LYS:HE3 | 1.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:209:GLU:OE1 | 1:K:209:GLU:N | 2.47 | 0.44 |
| 1:L:266:THR:HG22 | 1:L:271:VAL:O | 2.16 | 0.44 |
| 1:A:234:LEU:N | 1:A:235:PRO:HD2 | 2.32 | 0.44 |
| 1:B:209:GLU:OE1 | 1:B:209:GLU:N | 2.48 | 0.44 |
| 1:B:384:ALA:HA | 1:C:360:TYR:OH | 2.17 | 0.44 |
| 1:B:455:VAL:O | 1:B:458:CYS:HB2 | 2.17 | 0.44 |
| 1:D:247:LEU:CD2 | 1:D:249:ILE:HD11 | 2.47 | 0.44 |
| 1:D:358:SER:HB3 | 1:D:361:ASP:OD1 | 2.16 | 0.44 |
| 1:F:194:GLN:HG3 | 1:F:331:THR:HB | 1.99 | 0.44 |
| 1:I:70:GLY:HA2 | 1:I:73:MET:HE3 | 2.00 | 0.44 |
| 1:I:174:VAL:HG22 | 1:I:194:GLN:NE2 | 2.32 | 0.44 |
| 1:I:191:GLU:O | 1:I:334:ASP:HA | 2.16 | 0.44 |
| 1:N:301:ILE:HG21 | 1:N:309:LEU:HD23 | 1.99 | 0.44 |
| 1:N:353:ILE:HD13 | 1:N:366:GLN:HG2 | 1.99 | 0.44 |
| 1:C:319:GLN:HB3 | 1:C:336:VAL:HG21 | 2.00 | 0.44 |
| 1:E:325:ILE:HA | 1:E:329:THR:O | 2.18 | 0.44 |
| 1:E:381:VAL:O | 1:E:382:GLY:O | 2.36 | 0.44 |
| 1:G:302:SER:O | 1:G:307:MET:HE3 | 2.17 | 0.44 |
| 1:I:222:LEU:HB3 | 1:I:289:LEU:CD2 | 2.47 | 0.44 |
| 1:I:366:GLN:O | 1:I:369:VAL:HG22 | 2.16 | 0.44 |
| 1:K:182:GLY:HA2 | 1:K:383:ALA:HB3 | 1.99 | 0.44 |
| 1:N:496:PRO:HB2 | 1:N:499:VAL:CG1 | 2.47 | 0.44 |
| 1:C:287:ALA:HB1 | 1:C:368:ARG:NH1 | 2.32 | 0.44 |
| 1:D:183:LEU:HD12 | 1:D:184:GLN:HG3 | 1.99 | 0.44 |
| 1:E:413:ALA:HB3 | 1:E:417:VAL:HG22 | 1.99 | 0.44 |
| 1:G:305:ILE:HB | 1:G:307:MET:HE2 | 1.98 | 0.44 |
| 1:H:155:ASP:OD1 | 1:H:157:THR:HB | 2.18 | 0.44 |
| 1:H:336:VAL:O | 1:H:337:GLY:C | 2.56 | 0.44 |
| 1:I:215:LEU:HB2 | 1:I:323:VAL:HG22 | 1.99 | 0.44 |
| 1:I:325:ILE:HA | 1:I:329:THR:O | 2.17 | 0.44 |
| 1:J:463:SER:O | 1:J:467:ASN:HB2 | 2.18 | 0.44 |
| 1:K:222:LEU:HB3 | 1:K:289:LEU:CD2 | 2.48 | 0.44 |
| 1:K:266:THR:HG22 | 1:K:271:VAL:O | 2.17 | 0.44 |
| 1:L:302:SER:H | 1:L:307:MET:HE1 | 1.83 | 0.44 |
| 1:B:524:LEU:C | 1:B:526:LYS:H | 2.20 | 0.44 |
| 1:D:288:MET:HG2 | 1:D:368:ARG:HD3 | 1.99 | 0.44 |
| 1:E:254:VAL:HG12 | 1:E:259:LEU:HB2 | 1.99 | 0.44 |
| 1:H:236:VAL:O | 1:H:240:VAL:HG23 | 2.16 | 0.44 |
| 1:J:460:GLU:O | 1:J:462:PRO:HD3 | 2.18 | 0.44 |
| 1:N:325:ILE:HG22 | 1:N:330:THR:HG23 | 1.99 | 0.44 |
| 1:B:302:SER:O | 1:B:307:MET:HE3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:369:VAL:HG23 | 1:C:370:ALA:N | 2.32 | 0.44 |
| 1:D:218:PRO:HD2 | 1:D:320:ALA:O | 2.18 | 0.44 |
| 1:E:323:VAL:HG12 | 1:E:332:ILE:HA | 1.99 | 0.44 |
| 1:G:210:THR:O | 1:G:210:THR:HG22 | 2.17 | 0.44 |
| 1:I:348:GLN:O | 1:I:352:GLN:HG2 | 2.18 | 0.44 |
| 1:J:217:SER:N | 1:J:218:PRO:HD3 | 2.32 | 0.44 |
| 1:J:324:VAL:O | 1:J:331:THR:HG22 | 2.18 | 0.44 |
| 1:J:455:VAL:HG13 | 1:J:460:GLU:HB2 | 1.99 | 0.44 |
| 1:K:134:LEU:HD21 | 1:K:425:LYS:NZ | 2.32 | 0.44 |
| 1:K:413:ALA:HB3 | 1:K:417:VAL:HG22 | 1.98 | 0.44 |
| 5:K:1:AGS:S1G | 5:K:1:AGS:O2G | 2.55 | 0.44 |
| 1:L:319:GLN:HB3 | 1:L:336:VAL:HG21 | 1.99 | 0.44 |
| 1:M:73:MET:HB3 | 6:M:2221:HOH:O | 2.18 | 0.44 |
| 1:M:290:GLN:HB3 | 1:M:345:ARG:NH2 | 2.31 | 0.44 |
| 1:N:193:MET:HE2 | 1:N:292:ILE:HG12 | 1.99 | 0.44 |
| 1:N:384:ALA:O | 1:N:385:THR:HG23 | 2.17 | 0.44 |
| 1:A:69:MET:CE | 1:G:39:VAL:HG12 | 2.47 | 0.44 |
| 1:C:217:SER:N | 1:C:218:PRO:HD3 | 2.33 | 0.44 |
| 1:C:325:ILE:HA | 1:C:329:THR:O | 2.17 | 0.44 |
| 1:D:413:ALA:HB3 | 1:D:417:VAL:HG22 | 1.98 | 0.44 |
| 1:E:384:ALA:O | 1:E:385:THR:HG23 | 2.17 | 0.44 |
| 1:F:183:LEU:CD2 | 1:F:384:ALA:HB2 | 2.47 | 0.44 |
| 1:F:210:THR:O | 1:F:210:THR:HG22 | 2.17 | 0.44 |
| 1:F:369:VAL:HG23 | 1:F:370:ALA:N | 2.32 | 0.44 |
| 1:H:176:THR:HG22 | 1:H:177:VAL:H | 1.82 | 0.44 |
| 1:H:215:LEU:HB2 | 1:H:323:VAL:HG22 | 2.00 | 0.44 |
| 1:J:68:ASN:O | 1:J:72:GLN:HG2 | 2.17 | 0.44 |
| 1:J:217:SER:N | 1:J:218:PRO:CD | 2.81 | 0.44 |
| 1:K:23:LEU:HD22 | 1:K:74:VAL:HG13 | 1.99 | 0.44 |
| 1:L:253:ASP:OD1 | 1:L:277:LYS:HE2 | 2.18 | 0.44 |
| 1:M:182:GLY:HA2 | 1:M:383:ALA:HB3 | 2.00 | 0.44 |
| 1:A:218:PRO:HD2 | 1:A:320:ALA:O | 2.17 | 0.44 |
| 1:C:16:MET:O | 1:C:20:VAL:HG13 | 2.17 | 0.44 |
| 1:C:217:SER:N | 1:C:218:PRO:CD | 2.81 | 0.44 |
| 1:D:234:LEU:N | 1:D:235:PRO:HD2 | 2.33 | 0.44 |
| 1:H:392:LYS:O | 1:H:396:VAL:HG23 | 2.18 | 0.44 |
| 1:I:384:ALA:O | 1:I:385:THR:HG23 | 2.18 | 0.44 |
| 1:I:496:PRO:O | 1:I:499:VAL:HG13 | 2.17 | 0.44 |
| 1:J:224:ASP:HB3 | 1:J:302:SER:HB3 | 2.00 | 0.44 |
| 1:N:153:ASN:O | 1:N:154:SER:HB2 | 2.18 | 0.44 |
| 1:C:179:ASP:HB3 | 1:C:389:MET:CE | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:234:LEU:O | 1:E:238:GLU:HG3 | 2.17 | 0.44 |
| 1:E:242:LYS:C | 1:E:244:GLY:N | 2.71 | 0.44 |
| 1:F:389:MET:N | 6:F:2746:HOH:O | 2.50 | 0.44 |
| 1:G:336:VAL:O | 1:G:337:GLY:C | 2.55 | 0.44 |
| 1:K:242:LYS:C | 1:K:244:GLY:N | 2.71 | 0.44 |
| 1:M:369:VAL:HG23 | 1:M:370:ALA:N | 2.32 | 0.44 |
| 1:N:42:LYS:HE3 | 1:N:48:THR:OG1 | 2.18 | 0.44 |
| 1:N:217:SER:N | 1:N:218:PRO:CD | 2.81 | 0.44 |
| 1:B:217:SER:N | 1:B:218:PRO:CD | 2.80 | 0.43 |
| 1:B:259:LEU:O | 1:B:263:VAL:HG23 | 2.18 | 0.43 |
| 1:B:325:ILE:HA | 1:B:329:THR:O | 2.18 | 0.43 |
| 1:B:413:ALA:HB3 | 1:B:417:VAL:HG22 | 2.00 | 0.43 |
| 1:D:200:LEU:HD13 | 1:D:254:VAL:HB | 2.00 | 0.43 |
| 1:F:199:TYR:CZ | 1:F:327:LYS:HA | 2.53 | 0.43 |
| 1:F:260:ALA:O | 1:F:264:VAL:HG23 | 2.18 | 0.43 |
| 1:G:70:GLY:HA2 | 1:G:73:MET:HE3 | 2.01 | 0.43 |
| 1:G:381:VAL:O | 1:G:382:GLY:O | 2.36 | 0.43 |
| 1:H:217:SER:N | 1:H:218:PRO:HD3 | 2.33 | 0.43 |
| 1:H:302:SER:H | 1:H:307:MET:HE1 | 1.83 | 0.43 |
| 1:I:266:THR:HG22 | 1:I:273:VAL:H | 1.82 | 0.43 |
| 1:L:63:GLU:OE2 | 1:M:526:LYS:HE2 | 2.17 | 0.43 |
| 1:M:210:THR:HG22 | 1:M:210:THR:O | 2.18 | 0.43 |
| 1:B:451:LEU:HD23 | 1:B:451:LEU:C | 2.39 | 0.43 |
| 1:C:177:VAL:HG21 | 1:C:397:GLU:HG2 | 1.98 | 0.43 |
| 1:C:183:LEU:CD2 | 1:C:384:ALA:HB2 | 2.47 | 0.43 |
| 1:C:348:GLN:O | 1:C:352:GLN:HG2 | 2.18 | 0.43 |
| 1:D:236:VAL:O | 1:D:240:VAL:HG23 | 2.19 | 0.43 |
| 1:E:200:LEU:HG | 1:E:276:VAL:HA | 2.01 | 0.43 |
| 1:F:342:ILE:O | 1:F:346:VAL:HG23 | 2.18 | 0.43 |
| 1:G:260:ALA:O | 1:G:264:VAL:HG23 | 2.18 | 0.43 |
| 1:H:144:ILE:HG23 | 1:H:403:THR:HG21 | 1.99 | 0.43 |
| 1:H:518:GLU:HG2 | 6:N:1187:HOH:O | 2.18 | 0.43 |
| 1:J:242:LYS:C | 1:J:244:GLY:N | 2.71 | 0.43 |
| 1:L:199:TYR:CZ | 1:L:327:LYS:HA | 2.53 | 0.43 |
| 1:L:417:VAL:CG1 | 6:L:2905:HOH:O | 2.66 | 0.43 |
| 1:L:417:VAL:HB | 6:L:2905:HOH:O | 2.18 | 0.43 |
| 1:L:421:ARG:CZ | 1:L:473:ASP:HA | 2.48 | 0.43 |
| 1:A:348:GLN:O | 1:A:352:GLN:HG2 | 2.17 | 0.43 |
| 1:B:242:LYS:O | 1:B:243:ALA:HB3 | 2.19 | 0.43 |
| 1:E:73:MET:O | 1:E:76:GLU:HB2 | 2.18 | 0.43 |
| 1:G:351:GLN:HA | 1:G:354:GLU:HG2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:260:ALA:O | 1:H:264:VAL:HG23 | 2.18 | 0.43 |
| 1:K:348:GLN:O | 1:K:352:GLN:HG2 | 2.19 | 0.43 |
| 1:L:325:ILE:HA | 1:L:329:THR:O | 2.18 | 0.43 |
| 1:N:210:THR:O | 1:N:210:THR:HG22 | 2.18 | 0.43 |
| 1:N:217:SER:N | 1:N:218:PRO:HD3 | 2.33 | 0.43 |
| 1:N:525:PRO:HD3 | 6:N:2033:HOH:O | 2.18 | 0.43 |
| 1:A:210:THR:O | 1:A:210:THR:HG22 | 2.18 | 0.43 |
| 1:A:526:LYS:HE2 | 1:G:63:GLU:OE2 | 2.19 | 0.43 |
| 1:I:409:GLU:OE2 | 1:I:498:LYS:HG3 | 2.19 | 0.43 |
| 1:N:171:LYS:HB2 | 1:N:407:VAL:HG11 | 2.01 | 0.43 |
| 1:A:191:GLU:O | 1:A:334:ASP:HA | 2.18 | 0.43 |
| 1:B:218:PRO:HD2 | 1:B:320:ALA:O | 2.18 | 0.43 |
| 1:B:266:THR:HG22 | 1:B:271:VAL:O | 2.19 | 0.43 |
| 1:D:193:MET:HG3 | 1:D:371:LYS:HB3 | 2.01 | 0.43 |
| 1:G:224:ASP:HB3 | 1:G:302:SER:HB3 | 2.00 | 0.43 |
| 1:H:384:ALA:C | 1:H:385:THR:HG23 | 2.39 | 0.43 |
| 1:J:69:MET:O | 1:J:73:MET:HG3 | 2.19 | 0.43 |
| 1:J:199:TYR:CZ | 1:J:327:LYS:HA | 2.54 | 0.43 |
| 1:M:217:SER:N | 1:M:218:PRO:CD | 2.82 | 0.43 |
| 1:N:180:GLY:HA3 | 1:N:381:VAL:O | 2.18 | 0.43 |
| 1:N:284:ARG:O | 1:N:288:MET:HG3 | 2.19 | 0.43 |
| 1:N:366:GLN:O | 1:N:369:VAL:HG22 | 2.18 | 0.43 |
| 1:N:381:VAL:O | 1:N:382:GLY:O | 2.37 | 0.43 |
| 1:B:369:VAL:HG23 | 1:B:370:ALA:N | 2.33 | 0.43 |
| 1:C:242:LYS:C | 1:C:244:GLY:N | 2.72 | 0.43 |
| 1:D:325:ILE:HG22 | 1:D:330:THR:HG23 | 1.99 | 0.43 |
| 1:F:178:GLU:OE2 | 1:F:322:ARG:NH1 | 2.51 | 0.43 |
| 1:F:240:VAL:HG11 | 1:F:247:LEU:HB2 | 2.00 | 0.43 |
| 1:H:183:LEU:HD13 | 1:H:184:GLN:N | 2.33 | 0.43 |
| 1:H:409:GLU:OE2 | 1:H:498:LYS:HG3 | 2.19 | 0.43 |
| 1:I:210:THR:O | 1:I:210:THR:HG22 | 2.19 | 0.43 |
| 1:J:210:THR:HG22 | 1:J:210:THR:O | 2.18 | 0.43 |
| 1:J:240:VAL:HG11 | 1:J:247:LEU:HB2 | 1.99 | 0.43 |
| 1:J:449:ALA:HB3 | 1:J:450:PRO:HD3 | 2.01 | 0.43 |
| 1:K:205:ILE:CA | 1:K:213:VAL:HG22 | 2.49 | 0.43 |
| 1:M:259:LEU:O | 1:M:263:VAL:HG23 | 2.19 | 0.43 |
| 1:N:37:ASN:HD21 | 1:N:51:LYS:HE3 | 1.84 | 0.43 |
| 1:N:82:ASN:O | 1:N:86:GLY:N | 2.49 | 0.43 |
| 1:A:194:GLN:OE1 | 1:A:329:THR:HG21 | 2.18 | 0.43 |
| 1:A:384:ALA:O | 1:A:385:THR:OG1 | 2.33 | 0.43 |
| 1:B:199:TYR:CZ | 1:B:327:LYS:HA | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:234:LEU:O | 1:B:238:GLU:HG3 | 2.18 | 0.43 |
| 1:E:176:THR:HG22 | 1:E:177:VAL:N | 2.33 | 0.43 |
| 1:E:218:PRO:HD2 | 1:E:320:ALA:O | 2.19 | 0.43 |
| 1:F:383:ALA:HA | 6:F:2746:HOH:O | 2.19 | 0.43 |
| 1:G:132:LYS:HG3 | 6:G:1971:HOH:O | 2.19 | 0.43 |
| 1:H:369:VAL:HG23 | 1:H:370:ALA:N | 2.34 | 0.43 |
| 1:J:209:GLU:OE1 | 1:J:209:GLU:N | 2.47 | 0.43 |
| 1:L:85:ALA:O | 1:L:401:HIS:HE1 | 2.01 | 0.43 |
| 1:A:69:MET:HE2 | 1:G:39:VAL:HG12 | 2.01 | 0.43 |
| 1:B:215:LEU:HB2 | 1:B:323:VAL:CG2 | 2.48 | 0.43 |
| 1:B:463:SER:O | 1:B:467:ASN:HB2 | 2.19 | 0.43 |
| 1:C:272:LYS:NZ | 1:D:228:SER:HB2 | 2.34 | 0.43 |
| 1:D:349:ILE:CG2 | 1:D:369:VAL:HG13 | 2.48 | 0.43 |
| 1:E:324:VAL:O | 1:E:331:THR:HG22 | 2.17 | 0.43 |
| 1:G:223:ALA:O | 1:G:251:ALA:HA | 2.19 | 0.43 |
| 1:H:37:ASN:ND2 | 1:H:51:LYS:HE3 | 2.34 | 0.43 |
| 1:I:259:LEU:O | 1:I:263:VAL:HG23 | 2.18 | 0.43 |
| 1:K:144:ILE:HG23 | 1:K:403:THR:CG2 | 2.49 | 0.43 |
| 1:K:449:ALA:HB3 | 1:K:450:PRO:HD3 | 2.00 | 0.43 |
| 1:L:239:ALA:O | 1:L:314:LEU:HD11 | 2.18 | 0.43 |
| 1:C:70:GLY:HA2 | 1:C:73:MET:HE3 | 2.01 | 0.43 |
| 1:E:65:LYS:HE3 | 1:E:522:THR:OG1 | 2.19 | 0.43 |
| 1:F:209:GLU:OE1 | 1:F:209:GLU:N | 2.49 | 0.43 |
| 1:F:348:GLN:O | 1:F:352:GLN:HG2 | 2.18 | 0.43 |
| 1:F:420:ILE:CD1 | 1:F:451:LEU:HD13 | 2.49 | 0.43 |
| 1:G:217:SER:N | 1:G:218:PRO:CD | 2.82 | 0.43 |
| 1:L:217:SER:N | 1:L:218:PRO:CD | 2.82 | 0.43 |
| 1:L:381:VAL:O | 1:L:382:GLY:O | 2.37 | 0.43 |
| 1:M:68:ASN:O | 1:M:72:GLN:HG2 | 2.18 | 0.43 |
| 1:N:222:LEU:HB3 | 1:N:289:LEU:HD21 | 2.01 | 0.43 |
| 1:A:124:VAL:HG21 | 1:A:508:ALA:CB | 2.49 | 0.43 |
| 1:A:417:VAL:HG11 | 1:A:488:MET:HG3 | 2.00 | 0.43 |
| 1:B:241:ALA:HB1 | 1:C:231:ARG:NH1 | 2.33 | 0.43 |
| 1:B:384:ALA:C | 1:B:385:THR:HG23 | 2.38 | 0.43 |
| 1:D:65:LYS:HG2 | 6:D:1200:HOH:O | 2.19 | 0.43 |
| 1:D:234:LEU:O | 1:D:238:GLU:HG3 | 2.18 | 0.43 |
| 1:E:177:VAL:HG21 | 1:E:397:GLU:HG2 | 1.99 | 0.43 |
| 1:I:496:PRO:HB2 | 1:I:499:VAL:CG1 | 2.49 | 0.43 |
| 1:K:220:ILE:CD1 | 1:K:296:THR:HG21 | 2.49 | 0.43 |
| 1:L:217:SER:N | 1:L:218:PRO:HD3 | 2.33 | 0.43 |
| 1:N:524:LEU:O | 1:N:526:LYS:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:329:THR:HG22 | 6:A:2839:HOH:O | 2.18 | 0.42 |
| 1:B:353:ILE:HD13 | 1:B:366:GLN:HG2 | 2.01 | 0.42 |
| 1:C:421:ARG:CZ | 1:C:473:ASP:HA | 2.49 | 0.42 |
| 1:E:177:VAL:HA | 1:E:379:ILE:O | 2.19 | 0.42 |
| 1:F:191:GLU:O | 1:F:334:ASP:HA | 2.18 | 0.42 |
| 1:F:266:THR:HG22 | 1:F:271:VAL:O | 2.18 | 0.42 |
| 1:J:179:ASP:HB3 | 1:J:389:MET:CE | 2.48 | 0.42 |
| 1:K:70:GLY:HA2 | 1:K:73:MET:HE3 | 2.01 | 0.42 |
| 1:K:182:GLY:HA2 | 1:K:383:ALA:CB | 2.49 | 0.42 |
| 1:L:60:ILE:O | 1:L:75:LYS:HE3 | 2.19 | 0.42 |
| 1:L:383:ALA:O | 1:L:384:ALA:CB | 2.66 | 0.42 |
| 1:M:27:VAL:HG12 | 1:M:90:THR:HG23 | 2.00 | 0.42 |
| 1:M:284:ARG:HH11 | 1:M:364:LYS:CE | 2.32 | 0.42 |
| 5:N:1:AGS:S1G | 5:N:1:AGS:O2G | 2.54 | 0.42 |
| 1:A:366:GLN:HA | 1:A:369:VAL:HG22 | 2.00 | 0.42 |
| 1:E:240:VAL:HG11 | 1:E:247:LEU:HB2 | 2.00 | 0.42 |
| 1:G:302:SER:H | 1:G:307:MET:HE1 | 1.83 | 0.42 |
| 1:I:466:ALA:O | 1:I:470:LYS:HG3 | 2.19 | 0.42 |
| 1:J:222:LEU:HB3 | 1:J:289:LEU:CD2 | 2.50 | 0.42 |
| 1:K:319:GLN:HB3 | 1:K:336:VAL:HG21 | 2.00 | 0.42 |
| 1:K:384:ALA:C | 1:K:385:THR:HG23 | 2.39 | 0.42 |
| 1:M:496:PRO:O | 1:M:499:VAL:HG13 | 2.19 | 0.42 |
| 1:A:253:ASP:OD1 | 1:A:277:LYS:HE2 | 2.19 | 0.42 |
| 1:B:193:MET:HE3 | 1:B:292:ILE:HG12 | 2.02 | 0.42 |
| 1:C:496:PRO:O | 1:C:499:VAL:HG13 | 2.19 | 0.42 |
| 1:D:37:ASN:HD21 | 1:D:51:LYS:HE3 | 1.84 | 0.42 |
| 1:D:284:ARG:O | 1:D:288:MET:HG3 | 2.19 | 0.42 |
| 1:E:220:ILE:CD1 | 1:E:296:THR:HG21 | 2.48 | 0.42 |
| 1:I:238:GLU:O | 1:I:241:ALA:HB3 | 2.19 | 0.42 |
| 1:I:496:PRO:HD2 | 1:I:499:VAL:CG1 | 2.49 | 0.42 |
| 1:J:200:LEU:HG | 1:J:276:VAL:HA | 2.01 | 0.42 |
| 1:K:421:ARG:CZ | 1:K:473:ASP:HA | 2.49 | 0.42 |
| 1:K:438:VAL:O | 1:K:442:VAL:HG23 | 2.18 | 0.42 |
| 1:L:324:VAL:O | 1:L:331:THR:HG22 | 2.19 | 0.42 |
| 1:N:272:LYS:N | 1:N:272:LYS:CD | 2.83 | 0.42 |
| 1:N:336:VAL:O | 1:N:337:GLY:C | 2.58 | 0.42 |
| 1:A:8:PHE:HB3 | 6:A:1960:HOH:O | 2.20 | 0.42 |
| 1:A:177:VAL:HA | 1:A:379:ILE:O | 2.19 | 0.42 |
| 1:B:169:VAL:HG13 | 1:B:377:ALA:HB2 | 2.00 | 0.42 |
| 1:C:271:VAL:HG12 | 1:C:273:VAL:HG23 | 2.00 | 0.42 |
| 1:D:36:ARG:HG3 | 1:E:518:GLU:HG2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:206:ASN:OD1 | 1:D:207:LYS:HG3 | 2.19 | 0.42 |
| 1:E:348:GLN:O | 1:E:352:GLN:HG2 | 2.19 | 0.42 |
| 1:F:253:ASP:OD1 | 1:F:277:LYS:HE2 | 2.19 | 0.42 |
| 1:F:384:ALA:C | 1:F:385:THR:HG23 | 2.40 | 0.42 |
| 1:G:85:ALA:O | 1:G:401:HIS:HE1 | 2.02 | 0.42 |
| 1:G:524:LEU:O | 1:G:526:LYS:N | 2.52 | 0.42 |
| 1:I:200:LEU:HG | 1:I:276:VAL:HA | 2.00 | 0.42 |
| 1:I:224:ASP:HB3 | 1:I:302:SER:HB3 | 2.02 | 0.42 |
| 1:L:94:VAL:HB | 6:L:2642:HOH:O | 2.20 | 0.42 |
| 1:M:288:MET:HA | 1:M:291:ASP:OD2 | 2.19 | 0.42 |
| 1:M:325:ILE:HG22 | 1:M:330:THR:HG23 | 2.01 | 0.42 |
| 1:N:193:MET:HE1 | 1:N:292:ILE:HG12 | 2.01 | 0.42 |
| 1:N:206:ASN:ND2 | 1:N:214:GLU:H | 2.16 | 0.42 |
| 1:A:183:LEU:HD13 | 1:A:184:GLN:N | 2.34 | 0.42 |
| 1:A:240:VAL:HG11 | 1:A:247:LEU:HB2 | 2.00 | 0.42 |
| 1:C:23:LEU:HD13 | 1:C:75:LYS:HD2 | 2.01 | 0.42 |
| 1:C:27:VAL:HG12 | 1:C:90:THR:HG23 | 2.01 | 0.42 |
| 1:D:445:ARG:HD3 | 6:D:2123:HOH:O | 2.19 | 0.42 |
| 1:F:60:ILE:O | 1:F:75:LYS:HE3 | 2.19 | 0.42 |
| 1:F:183:LEU:HD13 | 1:F:184:GLN:N | 2.34 | 0.42 |
| 1:G:134:LEU:HD22 | 6:G:2213:HOH:O | 2.19 | 0.42 |
| 1:H:342:ILE:O | 1:H:346:VAL:HG23 | 2.19 | 0.42 |
| 6:I:2009:HOH:O | 1:J:117:LYS:HE3 | 2.18 | 0.42 |
| 1:J:215:LEU:HB2 | 1:J:323:VAL:CG2 | 2.50 | 0.42 |
| 1:J:238:GLU:O | 1:J:241:ALA:HB3 | 2.20 | 0.42 |
| 1:L:183:LEU:HD13 | 1:L:184:GLN:N | 2.34 | 0.42 |
| 1:L:202:PRO:O | 1:L:204:PHE:N | 2.46 | 0.42 |
| 1:M:284:ARG:HH11 | 1:M:364:LYS:NZ | 2.18 | 0.42 |
| 6:C:2549:HOH:O | 1:J:463:SER:HB2 | 2.19 | 0.42 |
| 1:D:404:ARG:HH11 | 1:D:404:ARG:CG | 2.27 | 0.42 |
| 1:E:209:GLU:OE1 | 1:E:209:GLU:N | 2.49 | 0.42 |
| 1:E:266:THR:HG22 | 1:E:271:VAL:O | 2.19 | 0.42 |
| 1:F:319:GLN:HB3 | 1:F:336:VAL:HG21 | 2.02 | 0.42 |
| 1:G:112:ASN:HA | 1:G:113:PRO:HD3 | 1.91 | 0.42 |
| 1:G:131:LEU:HD13 | 1:G:422:VAL:HG21 | 2.02 | 0.42 |
| 1:G:242:LYS:O | 1:G:244:GLY:N | 2.52 | 0.42 |
| 1:G:266:THR:HG21 | 1:G:273:VAL:H | 1.84 | 0.42 |
| 1:H:160:LYS:HB2 | 1:H:160:LYS:HZ3 | 1.84 | 0.42 |
| 1:J:182:GLY:HA2 | 1:J:383:ALA:HB3 | 2.02 | 0.42 |
| 1:J:348:GLN:O | 1:J:352:GLN:HG2 | 2.19 | 0.42 |
| 1:K:458:CYS:SG | 1:K:480:ALA:HB1 | 2.60 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:460:GLU:O | 1:K:462:PRO:HD3 | 2.18 | 0.42 |
| 1:L:259:LEU:O | 1:L:263:VAL:HG23 | 2.19 | 0.42 |
| 1:M:220:ILE:CD1 | 1:M:296:THR:HG21 | 2.48 | 0.42 |
| 1:N:194:GLN:HG3 | 1:N:331:THR:HB | 2.00 | 0.42 |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:HB2 | 2.02 | 0.42 |
| 1:N:259:LEU:O | 1:N:263:VAL:HG23 | 2.20 | 0.42 |
| 1:B:144:ILE:HG23 | 1:B:403:THR:HG21 | 2.02 | 0.42 |
| 1:C:191:GLU:O | 1:C:334:ASP:HA | 2.20 | 0.42 |
| 1:D:182:GLY:HA2 | 1:D:383:ALA:CB | 2.50 | 0.42 |
| 1:H:182:GLY:HA2 | 1:H:383:ALA:HB3 | 2.02 | 0.42 |
| 1:I:179:ASP:HB3 | 1:I:389:MET:CE | 2.49 | 0.42 |
| 1:I:336:VAL:O | 1:I:337:GLY:C | 2.58 | 0.42 |
| 1:J:206:ASN:ND2 | 1:J:214:GLU:H | 2.17 | 0.42 |
| 1:K:496:PRO:O | 1:K:499:VAL:HG13 | 2.19 | 0.42 |
| 1:M:242:LYS:O | 1:M:243:ALA:HB3 | 2.20 | 0.42 |
| 1:N:111:MET:HG2 | 1:N:435:ASP:OD1 | 2.19 | 0.42 |
| 1:A:302:SER:O | 1:A:307:MET:HE3 | 2.20 | 0.42 |
| 1:B:140:ASP:O | 1:B:144:ILE:HG13 | 2.20 | 0.42 |
| 1:B:197:ARG:HD2 | 1:B:277:LYS:HB2 | 2.01 | 0.42 |
| 1:F:206:ASN:ND2 | 1:F:214:GLU:H | 2.16 | 0.42 |
| 1:G:193:MET:HE2 | 1:G:292:ILE:HG12 | 2.00 | 0.42 |
| 1:H:210:THR:HG22 | 1:H:210:THR:O | 2.20 | 0.42 |
| 1:H:319:GLN:HB3 | 1:H:336:VAL:HG21 | 2.01 | 0.42 |
| 1:H:325:ILE:HA | 1:H:329:THR:O | 2.19 | 0.42 |
| 1:H:381:VAL:O | 1:H:382:GLY:O | 2.38 | 0.42 |
| 1:I:266:THR:HG21 | 1:I:273:VAL:H | 1.84 | 0.42 |
| 1:J:305:ILE:HB | 1:J:307:MET:HE2 | 2.01 | 0.42 |
| 1:J:331:THR:HG23 | 1:J:331:THR:O | 2.20 | 0.42 |
| 1:M:144:ILE:HG23 | 1:M:403:THR:HG21 | 2.01 | 0.42 |
| 1:M:179:ASP:HB3 | 1:M:389:MET:CE | 2.50 | 0.42 |
| 1:M:524:LEU:HD12 | 1:M:524:LEU:HA | 1.87 | 0.42 |
| 1:A:4:LYS:HG3 | 1:G:59:GLU:O | 2.19 | 0.42 |
| 1:B:77:VAL:HG11 | 1:B:506:TYR:O | 2.18 | 0.42 |
| 1:B:324:VAL:O | 1:B:331:THR:HG22 | 2.20 | 0.42 |
| 1:I:366:GLN:HA | 1:I:369:VAL:HG22 | 2.01 | 0.42 |
| 1:L:206:ASN:ND2 | 1:L:214:GLU:H | 2.18 | 0.42 |
| 1:L:382:GLY:O | 1:L:389:MET:HG2 | 2.20 | 0.42 |
| 1:M:348:GLN:O | 1:M:352:GLN:HG2 | 2.20 | 0.42 |
| 1:N:305:ILE:HB | 1:N:307:MET:HE2 | 2.01 | 0.42 |
| 1:N:369:VAL:HG23 | 1:N:370:ALA:N | 2.35 | 0.42 |
| 1:C:384:ALA:C | 1:C:385:THR:HG23 | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:223:ALA:O | 1:D:251:ALA:HA | 2.20 | 0.42 |
| 1:E:76:GLU:HG3 | 6:E:2322:HOH:O | 2.20 | 0.42 |
| 1:F:259:LEU:O | 1:F:263:VAL:HG23 | 2.19 | 0.42 |
| 1:G:219:PHE:O | 1:G:247:LEU:HD12 | 2.19 | 0.42 |
| 1:H:240:VAL:HG11 | 1:H:247:LEU:HB2 | 2.01 | 0.42 |
| 1:J:461:GLU:HA | 1:J:462:PRO:HD3 | 1.91 | 0.42 |
| 1:L:33:PRO:CG | 1:L:480:ALA:HB3 | 2.50 | 0.42 |
| 1:N:37:ASN:ND2 | 1:N:51:LYS:HE3 | 2.35 | 0.42 |
| 1:A:336:VAL:O | 1:A:337:GLY:C | 2.59 | 0.41 |
| 1:B:305:ILE:HB | 1:B:307:MET:HE2 | 2.02 | 0.41 |
| 1:C:222:LEU:HB3 | 1:C:289:LEU:CD2 | 2.50 | 0.41 |
| 1:D:191:GLU:O | 1:D:334:ASP:HA | 2.20 | 0.41 |
| 1:F:242:LYS:C | 1:F:244:GLY:N | 2.73 | 0.41 |
| 1:F:510:VAL:CG2 | 6:F:2556:HOH:O | 2.67 | 0.41 |
| 1:G:417:VAL:HG13 | 6:G:2394:HOH:O | 2.20 | 0.41 |
| 1:H:220:ILE:HD12 | 1:H:296:THR:HG21 | 2.02 | 0.41 |
| 1:I:177:VAL:HG21 | 1:I:397:GLU:HG2 | 1.99 | 0.41 |
| 1:J:37:ASN:ND2 | 1:J:51:LYS:HE3 | 2.34 | 0.41 |
| 1:N:183:LEU:CD2 | 1:N:384:ALA:HB2 | 2.49 | 0.41 |
| 1:N:325:ILE:HA | 1:N:329:THR:O | 2.18 | 0.41 |
| 1:A:176:THR:HG22 | 1:A:177:VAL:H | 1.84 | 0.41 |
| 1:B:366:GLN:HA | 1:B:369:VAL:HG22 | 2.02 | 0.41 |
| 1:C:200:LEU:HG | 1:C:276:VAL:HA | 2.02 | 0.41 |
| 1:D:160:LYS:HB2 | 1:D:160:LYS:HZ2 | 1.84 | 0.41 |
| 1:D:177:VAL:HA | 1:D:379:ILE:O | 2.20 | 0.41 |
| 1:F:487:ASN:O | 1:F:491:MET:HG3 | 2.20 | 0.41 |
| 1:G:353:ILE:HD13 | 1:G:366:GLN:HG2 | 2.02 | 0.41 |
| 1:G:409:GLU:OE2 | 1:G:498:LYS:HG3 | 2.20 | 0.41 |
| 1:L:97:GLN:HG2 | 6:L:2018:HOH:O | 2.19 | 0.41 |
| 5:L:1:AGS:S1G | 5:L:1:AGS:O2G | 2.55 | 0.41 |
| 1:M:171:LYS:HB2 | 1:M:407:VAL:HG11 | 2.02 | 0.41 |
| 1:M:242:LYS:C | 1:M:244:GLY:N | 2.72 | 0.41 |
| 1:M:496:PRO:HB2 | 1:M:499:VAL:HG12 | 2.02 | 0.41 |
| 1:A:140:ASP:OD2 | 1:A:142:LYS:HB3 | 2.21 | 0.41 |
| 1:A:153:ASN:O | 1:A:154:SER:HB2 | 2.19 | 0.41 |
| 1:A:220:ILE:HD12 | 1:A:296:THR:HG21 | 2.02 | 0.41 |
| 1:B:194:GLN:OE1 | 1:B:329:THR:HG21 | 2.20 | 0.41 |
| 1:B:222:LEU:HB3 | 1:B:289:LEU:CD2 | 2.49 | 0.41 |
| 1:C:224:ASP:HB3 | 1:C:302:SER:HB3 | 2.02 | 0.41 |
| 1:C:353:ILE:HD13 | 1:C:366:GLN:HG2 | 2.01 | 0.41 |
| 1:D:217:SER:N | 1:D:218:PRO:HD3 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:183:LEU:CD2 | 1:E:384:ALA:HB2 | 2.50 | 0.41 |
| 1:E:191:GLU:O | 1:E:334:ASP:HA | 2.20 | 0.41 |
| 1:E:238:GLU:O | 1:E:241:ALA:HB3 | 2.19 | 0.41 |
| 1:F:182:GLY:HA2 | 1:F:383:ALA:HB3 | 2.01 | 0.41 |
| 1:G:222:LEU:HB3 | 1:G:289:LEU:CD2 | 2.50 | 0.41 |
| 1:G:384:ALA:C | 1:G:385:THR:HG23 | 2.40 | 0.41 |
| 1:J:336:VAL:O | 1:J:337:GLY:C | 2.58 | 0.41 |
| 1:K:239:ALA:C | 1:K:314:LEU:HD21 | 2.41 | 0.41 |
| 1:L:122:LYS:HE2 | 1:L:429:LEU:HD11 | 2.02 | 0.41 |
| 1:L:210:THR:O | 1:L:210:THR:HG22 | 2.20 | 0.41 |
| 1:M:193:MET:HE2 | 1:M:292:ILE:HG12 | 2.02 | 0.41 |
| 1:N:69:MET:O | 1:N:73:MET:HG3 | 2.19 | 0.41 |
| 1:N:209:GLU:OE1 | 1:N:209:GLU:N | 2.48 | 0.41 |
| 1:N:524:LEU:HD12 | 1:N:524:LEU:HA | 1.91 | 0.41 |
| 1:B:240:VAL:HG11 | 1:B:247:LEU:HB2 | 2.01 | 0.41 |
| 1:B:242:LYS:C | 1:B:244:GLY:N | 2.73 | 0.41 |
| 1:G:351:GLN:HA | 1:G:354:GLU:CG | 2.49 | 0.41 |
| 1:H:16:MET:HE3 | 6:H:2854:HOH:O | 2.21 | 0.41 |
| 1:I:217:SER:HA | 1:I:320:ALA:O | 2.20 | 0.41 |
| 1:J:177:VAL:HA | 1:J:379:ILE:O | 2.20 | 0.41 |
| 1:J:295:LEU:O | 1:J:295:LEU:HD13 | 2.20 | 0.41 |
| 1:K:171:LYS:HB2 | 1:K:407:VAL:HG11 | 2.02 | 0.41 |
| 1:K:366:GLN:HA | 1:K:369:VAL:HG22 | 2.01 | 0.41 |
| 1:N:176:THR:HG22 | 1:N:177:VAL:N | 2.35 | 0.41 |
| 1:A:182:GLY:O | 1:A:183:LEU:O | 2.39 | 0.41 |
| 1:A:219:PHE:O | 1:A:247:LEU:HD12 | 2.20 | 0.41 |
| 1:B:325:ILE:HG22 | 1:B:330:THR:HG23 | 2.03 | 0.41 |
| 1:B:524:LEU:HD12 | 1:B:524:LEU:HA | 1.87 | 0.41 |
| 1:C:177:VAL:HA | 1:C:379:ILE:O | 2.20 | 0.41 |
| 1:C:460:GLU:O | 1:C:462:PRO:HD3 | 2.21 | 0.41 |
| 1:D:182:GLY:HA2 | 1:D:383:ALA:HB3 | 2.03 | 0.41 |
| 1:D:284:ARG:NH1 | 1:D:364:LYS:NZ | 2.67 | 0.41 |
| 1:E:28:LYS:HD2 | 1:E:453:GLN:NE2 | 2.36 | 0.41 |
| 1:E:178:GLU:OE1 | 1:E:378:VAL:HG11 | 2.20 | 0.41 |
| 1:E:182:GLY:HA2 | 1:E:383:ALA:HB3 | 2.02 | 0.41 |
| 1:E:325:ILE:HG22 | 1:E:330:THR:HG23 | 2.02 | 0.41 |
| 1:G:144:ILE:HG23 | 1:G:403:THR:CG2 | 2.50 | 0.41 |
| 1:H:153:ASN:O | 1:H:154:SER:HB2 | 2.20 | 0.41 |
| 1:H:295:LEU:HD13 | 1:H:295:LEU:C | 2.41 | 0.41 |
| 1:J:134:LEU:HD21 | 1:J:425:LYS:NZ | 2.35 | 0.41 |
| 1:J:458:CYS:SG | 1:J:480:ALA:HB1 | 2.60 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:461:GLU:HA | 1:L:462:PRO:HD3 | 1.91 | 0.41 |
| 1:M:54:VAL:HG23 | 6:M:2164:HOH:O | 2.20 | 0.41 |
| 1:M:63:GLU:HB2 | 1:N:524:LEU:CD2 | 2.50 | 0.41 |
| 1:N:463:SER:O | 1:N:467:ASN:HB2 | 2.19 | 0.41 |
| 1:B:193:MET:HE1 | 1:B:292:ILE:HG12 | 2.02 | 0.41 |
| 1:B:336:VAL:O | 1:B:337:GLY:C | 2.59 | 0.41 |
| 1:C:182:GLY:HA2 | 1:C:383:ALA:CB | 2.50 | 0.41 |
| 1:C:272:LYS:HZ3 | 1:D:228:SER:HB2 | 1.85 | 0.41 |
| 1:D:200:LEU:HG | 1:D:276:VAL:HA | 2.01 | 0.41 |
| 1:D:210:THR:O | 1:D:210:THR:HG22 | 2.19 | 0.41 |
| 1:F:140:ASP:OD2 | 1:F:142:LYS:HB3 | 2.20 | 0.41 |
| 1:H:85:ALA:O | 1:H:401:HIS:HE1 | 2.03 | 0.41 |
| 1:I:324:VAL:O | 1:I:331:THR:HG22 | 2.21 | 0.41 |
| 1:K:199:TYR:CZ | 1:K:327:LYS:HA | 2.56 | 0.41 |
| 1:K:204:PHE:C | 1:K:213:VAL:HG22 | 2.41 | 0.41 |
| 1:K:295:LEU:HD13 | 1:K:295:LEU:O | 2.20 | 0.41 |
| 1:K:366:GLN:O | 1:K:369:VAL:HG22 | 2.20 | 0.41 |
| 1:L:477:GLY:CA | 6:L:2905:HOH:O | 2.68 | 0.41 |
| 1:M:136:VAL:HA | 1:M:137:PRO:HD3 | 1.87 | 0.41 |
| 1:M:215:LEU:HB2 | 1:M:323:VAL:HG22 | 2.03 | 0.41 |
| 1:A:231:ARG:NH1 | 1:G:242:LYS:HA | 2.35 | 0.41 |
| 1:A:242:LYS:C | 1:A:244:GLY:N | 2.73 | 0.41 |
| 1:A:266:THR:HG21 | 1:A:273:VAL:H | 1.86 | 0.41 |
| 1:B:69:MET:O | 1:B:73:MET:HG3 | 2.20 | 0.41 |
| 1:E:305:ILE:HB | 1:E:307:MET:HE2 | 2.02 | 0.41 |
| 1:N:455:VAL:O | 1:N:458:CYS:HB2 | 2.21 | 0.41 |
| 1:B:302:SER:H | 1:B:307:MET:HE1 | 1.85 | 0.41 |
| 1:D:201:SER:O | 1:D:202:PRO:O | 2.39 | 0.41 |
| 1:D:324:VAL:HB | 1:D:331:THR:CG2 | 2.51 | 0.41 |
| 1:D:348:GLN:O | 1:D:352:GLN:HG2 | 2.21 | 0.41 |
| 1:E:39:VAL:HG12 | 1:F:69:MET:CE | 2.51 | 0.41 |
| 1:E:85:ALA:O | 1:E:401:HIS:HE1 | 2.03 | 0.41 |
| 1:E:336:VAL:O | 1:E:337:GLY:C | 2.58 | 0.41 |
| 1:F:238:GLU:O | 1:F:241:ALA:HB3 | 2.20 | 0.41 |
| 1:G:183:LEU:CD2 | 1:G:384:ALA:HB2 | 2.48 | 0.41 |
| 1:G:202:PRO:C | 1:G:204:PHE:H | 2.23 | 0.41 |
| 1:G:266:THR:HG22 | 1:G:273:VAL:H | 1.86 | 0.41 |
| 1:I:242:LYS:O | 1:I:243:ALA:HB3 | 2.20 | 0.41 |
| 1:J:140:ASP:OD2 | 1:J:142:LYS:HB3 | 2.21 | 0.41 |
| 1:K:153:ASN:O | 1:K:154:SER:HB2 | 2.20 | 0.41 |
| 1:K:381:VAL:O | 1:K:382:GLY:O | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:194:GLN:HG3 | 1:L:331:THR:HB | 2.03 | 0.41 |
| 1:M:458:CYS:SG | 1:M:480:ALA:HB1 | 2.61 | 0.41 |
| 1:N:260:ALA:O | 1:N:264:VAL:HG23 | 2.21 | 0.41 |
| 1:A:194:GLN:HG3 | 1:A:331:THR:HB | 2.02 | 0.41 |
| 1:B:77:VAL:CB | 1:B:510:VAL:HG22 | 2.51 | 0.41 |
| 1:B:174:VAL:HG22 | 1:B:194:GLN:NE2 | 2.36 | 0.41 |
| 1:B:177:VAL:HA | 1:B:379:ILE:O | 2.21 | 0.41 |
| 1:B:194:GLN:HG3 | 1:B:331:THR:HB | 2.03 | 0.41 |
| 1:B:205:ILE:CA | 1:B:213:VAL:HG22 | 2.50 | 0.41 |
| 1:C:496:PRO:HB2 | 1:C:499:VAL:CG1 | 2.50 | 0.41 |
| 1:D:39:VAL:HG12 | 1:E:69:MET:CE | 2.50 | 0.41 |
| 1:E:160:LYS:HB2 | 1:E:160:LYS:NZ | 2.36 | 0.41 |
| 1:E:366:GLN:HA | 1:E:369:VAL:HG22 | 2.03 | 0.41 |
| 1:F:421:ARG:CZ | 1:F:473:ASP:HA | 2.51 | 0.41 |
| 1:G:77:VAL:CG2 | 1:G:510:VAL:HG21 | 2.51 | 0.41 |
| 1:G:200:LEU:HG | 1:G:276:VAL:HA | 2.02 | 0.41 |
| 1:G:284:ARG:HH12 | 1:G:364:LYS:NZ | 2.19 | 0.41 |
| 1:G:284:ARG:O | 1:G:288:MET:HG3 | 2.21 | 0.41 |
| 1:G:366:GLN:HA | 1:G:369:VAL:HG22 | 2.03 | 0.41 |
| 1:H:177:VAL:HG21 | 1:H:397:GLU:HG2 | 2.00 | 0.41 |
| 1:H:191:GLU:O | 1:H:334:ASP:HA | 2.19 | 0.41 |
| 1:H:324:VAL:O | 1:H:331:THR:HG22 | 2.21 | 0.41 |
| 1:H:458:CYS:SG | 1:H:480:ALA:HB1 | 2.60 | 0.41 |
| 1:I:63:GLU:HB2 | 1:J:524:LEU:CD2 | 2.50 | 0.41 |
| 1:I:171:LYS:HB2 | 1:I:407:VAL:HG11 | 2.02 | 0.41 |
| 1:I:421:ARG:CZ | 1:I:473:ASP:HA | 2.51 | 0.41 |
| 1:J:182:GLY:HA2 | 1:J:383:ALA:CB | 2.50 | 0.41 |
| 1:J:242:LYS:O | 1:J:243:ALA:HB3 | 2.20 | 0.41 |
| 1:J:381:VAL:O | 1:J:382:GLY:O | 2.39 | 0.41 |
| 1:K:353:ILE:HD13 | 1:K:366:GLN:HG2 | 2.01 | 0.41 |
| 1:K:404:ARG:HG2 | 1:K:404:ARG:NH1 | 2.34 | 0.41 |
| 1:K:524:LEU:HD12 | 1:K:524:LEU:HA | 1.87 | 0.41 |
| 1:L:46:ALA:HA | 1:L:47:PRO:HD3 | 1.93 | 0.41 |
| 1:L:183:LEU:CD2 | 1:L:384:ALA:HB2 | 2.49 | 0.41 |
| 1:L:200:LEU:HG | 1:L:276:VAL:HA | 2.02 | 0.41 |
| 1:L:215:LEU:HB2 | 1:L:323:VAL:HG22 | 2.03 | 0.41 |
| 1:L:235:PRO:CG | 1:L:310:GLU:HA | 2.34 | 0.41 |
| 1:L:290:GLN:HB3 | 1:L:345:ARG:NH2 | 2.35 | 0.41 |
| 1:L:351:GLN:HA | 1:L:354:GLU:HG2 | 2.02 | 0.41 |
| 1:L:384:ALA:C | 1:L:385:THR:HG23 | 2.40 | 0.41 |
| 1:L:477:GLY:HA2 | 6:L:2905:HOH:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:253:ASP:OD1 | 1:M:277:LYS:HE2 | 2.20 | 0.41 |
| 1:M:449:ALA:HB3 | 1:M:450:PRO:HD3 | 2.03 | 0.41 |
| 1:N:85:ALA:O | 1:N:401:HIS:HE1 | 2.03 | 0.41 |
| 1:N:134:LEU:HD21 | 1:N:425:LYS:NZ | 2.35 | 0.41 |
| 1:N:194:GLN:OE1 | 1:N:329:THR:HG21 | 2.21 | 0.41 |
| 1:A:325:ILE:HA | 1:A:329:THR:O | 2.20 | 0.41 |
| 1:C:153:ASN:O | 1:C:154:SER:HB2 | 2.21 | 0.41 |
| 1:E:197:ARG:HD2 | 1:E:277:LYS:HB2 | 2.03 | 0.41 |
| 1:E:202:PRO:C | 1:E:204:PHE:H | 2.23 | 0.41 |
| 1:E:224:ASP:HB3 | 1:E:302:SER:HB3 | 2.01 | 0.41 |
| 1:F:23:LEU:CD2 | 1:F:74:VAL:HG13 | 2.51 | 0.41 |
| 1:M:102:GLU:HB2 | 1:M:442:VAL:HG13 | 2.03 | 0.41 |
| 1:N:193:MET:HG3 | 1:N:371:LYS:HB3 | 2.03 | 0.41 |
| 1:A:466:ALA:O | 1:A:470:LYS:HG3 | 2.21 | 0.40 |
| 1:B:82:ASN:HB2 | 1:B:89:THR:CG2 | 2.51 | 0.40 |
| 1:H:77:VAL:HG23 | 1:H:510:VAL:HG21 | 2.03 | 0.40 |
| 1:K:46:ALA:HA | 1:K:47:PRO:HD3 | 1.88 | 0.40 |
| 1:L:160:LYS:HB2 | 1:L:160:LYS:NZ | 2.36 | 0.40 |
| 1:M:205:ILE:CA | 1:M:213:VAL:HG22 | 2.48 | 0.40 |
| 1:M:384:ALA:C | 1:M:385:THR:HG23 | 2.42 | 0.40 |
| 1:A:27:VAL:HG12 | 1:A:90:THR:HG23 | 2.03 | 0.40 |
| 1:C:284:ARG:HH12 | 1:C:364:LYS:NZ | 2.19 | 0.40 |
| 1:D:224:ASP:HB3 | 1:D:302:SER:HB3 | 2.04 | 0.40 |
| 1:E:242:LYS:O | 1:E:243:ALA:HB3 | 2.21 | 0.40 |
| 1:F:302:SER:O | 1:F:307:MET:HE3 | 2.21 | 0.40 |
| 1:G:182:GLY:HA2 | 1:G:383:ALA:HB3 | 2.04 | 0.40 |
| 1:H:200:LEU:HG | 1:H:276:VAL:HA | 2.02 | 0.40 |
| 1:I:325:ILE:HG22 | 1:I:330:THR:HG23 | 2.02 | 0.40 |
| 1:I:496:PRO:HD2 | 1:I:499:VAL:HG11 | 2.03 | 0.40 |
| 1:J:366:GLN:O | 1:J:369:VAL:HG22 | 2.20 | 0.40 |
| 1:K:7:LYS:HE2 | 1:K:66:PHE:CE2 | 2.56 | 0.40 |
| 1:K:194:GLN:OE1 | 1:K:329:THR:HG21 | 2.21 | 0.40 |
| 1:K:215:LEU:HB2 | 1:K:323:VAL:CG2 | 2.51 | 0.40 |
| 1:K:224:ASP:HB3 | 1:K:302:SER:HB3 | 2.03 | 0.40 |
| 1:K:404:ARG:HH11 | 1:K:404:ARG:CG | 2.31 | 0.40 |
| 1:K:451:LEU:HD23 | 1:K:451:LEU:C | 2.41 | 0.40 |
| 1:M:197:ARG:HD2 | 1:M:277:LYS:HB2 | 2.04 | 0.40 |
| 1:N:384:ALA:C | 1:N:385:THR:HG23 | 2.41 | 0.40 |
| 1:A:342:ILE:O | 1:A:346:VAL:HG23 | 2.21 | 0.40 |
| 1:C:174:VAL:HG22 | 1:C:194:GLN:HE21 | 1.87 | 0.40 |
| 1:C:199:TYR:CZ | 1:C:327:LYS:HA | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:295:LEU:HD13 | 1:C:295:LEU:O | 2.21 | 0.40 |
| 1:C:336:VAL:O | 1:C:337:GLY:C | 2.60 | 0.40 |
| 1:H:144:ILE:HG23 | 1:H:403:THR:CG2 | 2.51 | 0.40 |
| 1:H:455:VAL:HG13 | 1:H:460:GLU:HB2 | 2.02 | 0.40 |
| 1:I:240:VAL:HG11 | 1:I:247:LEU:HB2 | 2.02 | 0.40 |
| 1:I:242:LYS:C | 1:I:244:GLY:N | 2.73 | 0.40 |
| 1:I:295:LEU:C | 1:I:295:LEU:HD13 | 2.42 | 0.40 |
| 1:K:284:ARG:HH12 | 1:K:364:LYS:NZ | 2.20 | 0.40 |
| 1:M:183:LEU:HD13 | 1:M:184:GLN:N | 2.35 | 0.40 |
| 1:M:342:ILE:O | 1:M:346:VAL:HG23 | 2.22 | 0.40 |
| 1:A:295:LEU:HD13 | 1:A:295:LEU:C | 2.42 | 0.40 |
| 1:B:111:MET:SD | 1:B:438:VAL:HG21 | 2.62 | 0.40 |
| 1:B:253:ASP:OD1 | 1:B:277:LYS:HE2 | 2.21 | 0.40 |
| 1:C:34:LYS:HG3 | 1:C:458:CYS:SG | 2.62 | 0.40 |
| 1:C:46:ALA:HA | 1:C:47:PRO:HD3 | 1.94 | 0.40 |
| 1:C:160:LYS:HB2 | 1:C:160:LYS:HZ2 | 1.87 | 0.40 |
| 1:C:201:SER:O | 1:C:202:PRO:O | 2.40 | 0.40 |
| 1:C:266:THR:HG21 | 1:C:273:VAL:H | 1.86 | 0.40 |
| 1:C:524:LEU:HD12 | 1:C:524:LEU:HA | 1.92 | 0.40 |
| 1:D:118:ARG:HD2 | 1:D:436:GLN:NE2 | 2.36 | 0.40 |
| 1:D:369:VAL:HG23 | 1:D:370:ALA:N | 2.36 | 0.40 |
| 1:E:384:ALA:C | 1:E:385:THR:HG23 | 2.42 | 0.40 |
| 1:F:215:LEU:HB2 | 1:F:323:VAL:HG22 | 2.03 | 0.40 |
| 1:H:202:PRO:C | 1:H:204:PHE:H | 2.24 | 0.40 |
| 1:I:194:GLN:HG3 | 1:I:331:THR:HB | 2.02 | 0.40 |
| 1:I:384:ALA:C | 1:I:385:THR:HG23 | 2.41 | 0.40 |
| 1:I:438:VAL:O | 1:I:442:VAL:HG23 | 2.21 | 0.40 |
| 1:I:524:LEU:HD12 | 1:I:524:LEU:HA | 1.93 | 0.40 |
| 1:K:200:LEU:HG | 1:K:276:VAL:HA | 2.03 | 0.40 |
| 1:K:240:VAL:HG11 | 1:K:247:LEU:HB2 | 2.02 | 0.40 |
| 1:K:392:LYS:O | 1:K:396:VAL:HG23 | 2.22 | 0.40 |
| 1:L:361:ASP:O | 1:L:365:LEU:HG | 2.20 | 0.40 |
| 1:N:10:ASN:HA | 6:N:2143:HOH:O | 2.21 | 0.40 |
| 1:N:179:ASP:HB3 | 1:N:389:MET:CE | 2.51 | 0.40 |
| 1:N:182:GLY:O | 1:N:183:LEU:O | 2.40 | 0.40 |
| 1:B:42:LYS:HB3 | 1:B:42:LYS:HE2 | 1.95 | 0.40 |
| 1:C:206:ASN:ND2 | 1:C:214:GLU:H | 2.18 | 0.40 |
| 1:C:331:THR:HG23 | 1:C:331:THR:O | 2.22 | 0.40 |
| 1:D:404:ARG:HG2 | 1:D:404:ARG:NH1 | 2.33 | 0.40 |
| 1:G:174:VAL:HG12 | 1:G:376:VAL:HG13 | 2.04 | 0.40 |
| 1:H:182:GLY:HA2 | 1:H:383:ALA:CB | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:216:GLU:C | 1:H:218:PRO:HD3 | 2.41 | 0.40 |
| 1:H:266:THR:HG21 | 1:H:273:VAL:H | 1.85 | 0.40 |
| 1:H:326:ASN:HD22 | 1:H:329:THR:HB | 1.86 | 0.40 |
| 1:I:85:ALA:O | 1:I:401:HIS:HE1 | 2.04 | 0.40 |
| 1:I:132:LYS:HE2 | 6:I:1912:HOH:O | 2.21 | 0.40 |
| 1:J:253:ASP:OD1 | 1:J:277:LYS:HE2 | 2.22 | 0.40 |
| 1:K:194:GLN:HG3 | 1:K:331:THR:HB | 2.03 | 0.40 |
| 1:K:217:SER:HA | 1:K:320:ALA:O | 2.21 | 0.40 |
| 1:K:302:SER:O | 1:K:307:MET:HE3 | 2.22 | 0.40 |
| 1:L:348:GLN:O | 1:L:352:GLN:HG2 | 2.21 | 0.40 |
| 1:M:194:GLN:HG3 | 1:M:331:THR:HB | 2.03 | 0.40 |
| 5:M:1:AGS:S1G | 5:M:1:AGS:O2G | 2.54 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:315:GLU:OE2 | 1:N:338:GLU:OE1[1_554] | 2.17 | 0.03 |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 523/547 (96%) | 487 (93%) | 27 (5%) | 9 (2%) | 9 4 |
| 1 | B | 523/547 (96%) | 487 (93%) | 24 (5%) | 12 (2%) | 6 2 |
| 1 | C | 523/547 (96%) | 488 (93%) | 24 (5%) | 11 (2%) | 7 2 |
| 1 | D | 523/547 (96%) | 492 (94%) | 22 (4%) | 9 (2%) | 9 4 |
| 1 | E | 523/547 (96%) | 485 (93%) | 27 (5%) | 11 (2%) | 7 2 |
| 1 | F | 523/547 (96%) | 487 (93%) | 24 (5%) | 12 (2%) | 6 2 |
| 1 | G | 523/547 (96%) | 489 (94%) | 23 (4%) | 11 (2%) | 7 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | H | 523/547 (96%) | 487 (93%) | 24 (5%) | 12 (2%) | 6 | 2 |
| 1 | I | 523/547 (96%) | 486 (93%) | 27 (5%) | 10 (2%) | 8 | 3 |
| 1 | J | 523/547 (96%) | 486 (93%) | 25 (5%) | 12 (2%) | 6 | 2 |
| 1 | K | 523/547 (96%) | 484 (92%) | 29 (6%) | 10 (2%) | 8 | 3 |
| 1 | L | 523/547 (96%) | 488 (93%) | 23 (4%) | 12 (2%) | 6 | 2 |
| 1 | M | 523/547 (96%) | 487 (93%) | 25 (5%) | 11 (2%) | 7 | 2 |
| 1 | N | 523/547 (96%) | 487 (93%) | 26 (5%) | 10 (2%) | 8 | 3 |
| All | All | 7322/7658 (96%) | 6820 (93%) | 350 (5%) | 152 (2%) | 7 | 2 |

All (152) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 183 | LEU |
| 1 | E | 183 | LEU |
| 1 | A | 183 | LEU |
| 1 | A | 256 | GLY |
| 1 | A | 271 | VAL |
| 1 | B | 256 | GLY |
| 1 | B | 385 | THR |
| 1 | C | 183 | LEU |
| 1 | C | 256 | GLY |
| 1 | D | 183 | LEU |
| 1 | D | 256 | GLY |
| 1 | D | 382 | GLY |
| 1 | E | 256 | GLY |
| 1 | F | 183 | LEU |
| 1 | F | 256 | GLY |
| 1 | F | 271 | VAL |
| 1 | F | 382 | GLY |
| 1 | G | 183 | LEU |
| 1 | G | 256 | GLY |
| 1 | G | 382 | GLY |
| 1 | H | 183 | LEU |
| 1 | H | 256 | GLY |
| 1 | H | 382 | GLY |
| 1 | I | 183 | LEU |
| 1 | I | 256 | GLY |
| 1 | I | 382 | GLY |
| 1 | J | 183 | LEU |
| 1 | J | 256 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 183 | LEU |
| 1 | K | 256 | GLY |
| 1 | L | 183 | LEU |
| 1 | L | 256 | GLY |
| 1 | L | 382 | GLY |
| 1 | M | 183 | LEU |
| 1 | M | 256 | GLY |
| 1 | M | 271 | VAL |
| 1 | N | 183 | LEU |
| 1 | N | 256 | GLY |
| 1 | N | 382 | GLY |
| 1 | A | 202 | PRO |
| 1 | A | 385 | THR |
| 1 | B | 202 | PRO |
| 1 | B | 271 | VAL |
| 1 | C | 202 | PRO |
| 1 | C | 271 | VAL |
| 1 | C | 382 | GLY |
| 1 | C | 385 | THR |
| 1 | D | 202 | PRO |
| 1 | D | 271 | VAL |
| 1 | D | 385 | THR |
| 1 | E | 202 | PRO |
| 1 | E | 271 | VAL |
| 1 | E | 382 | GLY |
| 1 | E | 385 | THR |
| 1 | F | 202 | PRO |
| 1 | F | 384 | ALA |
| 1 | F | 385 | THR |
| 1 | G | 202 | PRO |
| 1 | G | 271 | VAL |
| 1 | G | 385 | THR |
| 1 | H | 202 | PRO |
| 1 | H | 271 | VAL |
| 1 | H | 385 | THR |
| 1 | I | 202 | PRO |
| 1 | I | 271 | VAL |
| 1 | I | 385 | THR |
| 1 | J | 202 | PRO |
| 1 | J | 271 | VAL |
| 1 | J | 382 | GLY |
| 1 | J | 385 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 202 | PRO |
| 1 | K | 271 | VAL |
| 1 | K | 385 | THR |
| 1 | L | 202 | PRO |
| 1 | L | 271 | VAL |
| 1 | L | 384 | ALA |
| 1 | L | 385 | THR |
| 1 | M | 202 | PRO |
| 1 | M | 385 | THR |
| 1 | N | 202 | PRO |
| 1 | N | 271 | VAL |
| 1 | N | 385 | THR |
| 1 | A | 253 | ASP |
| 1 | B | 382 | GLY |
| 1 | B | 384 | ALA |
| 1 | C | 184 | GLN |
| 1 | C | 201 | SER |
| 1 | C | 383 | ALA |
| 1 | D | 201 | SER |
| 1 | D | 383 | ALA |
| 1 | E | 253 | ASP |
| 1 | F | 334 | ASP |
| 1 | F | 383 | ALA |
| 1 | G | 253 | ASP |
| 1 | G | 337 | GLY |
| 1 | I | 253 | ASP |
| 1 | I | 383 | ALA |
| 1 | J | 253 | ASP |
| 1 | J | 383 | ALA |
| 1 | J | 384 | ALA |
| 1 | K | 184 | GLN |
| 1 | K | 201 | SER |
| 1 | K | 253 | ASP |
| 1 | K | 382 | GLY |
| 1 | L | 253 | ASP |
| 1 | L | 383 | ALA |
| 1 | M | 201 | SER |
| 1 | M | 253 | ASP |
| 1 | M | 382 | GLY |
| 1 | B | 184 | GLN |
| 1 | B | 201 | SER |
| 1 | B | 253 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 383 | ALA |
| 1 | C | 253 | ASP |
| 1 | C | 334 | ASP |
| 1 | E | 184 | GLN |
| 1 | E | 334 | ASP |
| 1 | E | 383 | ALA |
| 1 | F | 184 | GLN |
| 1 | F | 201 | SER |
| 1 | F | 253 | ASP |
| 1 | G | 184 | GLN |
| 1 | H | 337 | GLY |
| 1 | H | 383 | ALA |
| 1 | I | 184 | GLN |
| 1 | J | 184 | GLN |
| 1 | J | 334 | ASP |
| 1 | K | 383 | ALA |
| 1 | L | 184 | GLN |
| 1 | M | 334 | ASP |
| 1 | M | 383 | ALA |
| 1 | N | 184 | GLN |
| 1 | N | 201 | SER |
| 1 | N | 383 | ALA |
| 1 | A | 184 | GLN |
| 1 | A | 201 | SER |
| 1 | B | 334 | ASP |
| 1 | D | 184 | GLN |
| 1 | E | 201 | SER |
| 1 | G | 201 | SER |
| 1 | G | 383 | ALA |
| 1 | H | 184 | GLN |
| 1 | H | 253 | ASP |
| 1 | H | 384 | ALA |
| 1 | I | 201 | SER |
| 1 | J | 201 | SER |
| 1 | M | 184 | GLN |
| 1 | A | 382 | GLY |
| 1 | N | 337 | GLY |
| 1 | H | 201 | SER |
| 1 | L | 201 | SER |
| 1 | L | 337 | GLY |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 404/413 (98%) | 394 (98%) | 10 (2%) | 47 | 49 |
| 1 | B | 404/413 (98%) | 397 (98%) | 7 (2%) | 60 | 65 |
| 1 | C | 404/413 (98%) | 396 (98%) | 8 (2%) | 55 | 58 |
| 1 | D | 404/413 (98%) | 394 (98%) | 10 (2%) | 47 | 49 |
| 1 | E | 404/413 (98%) | 397 (98%) | 7 (2%) | 60 | 65 |
| 1 | F | 404/413 (98%) | 396 (98%) | 8 (2%) | 55 | 58 |
| 1 | G | 404/413 (98%) | 395 (98%) | 9 (2%) | 52 | 55 |
| 1 | H | 404/413 (98%) | 397 (98%) | 7 (2%) | 60 | 65 |
| 1 | I | 404/413 (98%) | 395 (98%) | 9 (2%) | 52 | 55 |
| 1 | J | 404/413 (98%) | 397 (98%) | 7 (2%) | 60 | 65 |
| 1 | K | 404/413 (98%) | 396 (98%) | 8 (2%) | 55 | 58 |
| 1 | L | 404/413 (98%) | 394 (98%) | 10 (2%) | 47 | 49 |
| 1 | M | 404/413 (98%) | 396 (98%) | 8 (2%) | 55 | 58 |
| 1 | N | 404/413 (98%) | 396 (98%) | 8 (2%) | 55 | 58 |
| All | All | 5656/5782 (98%) | 5540 (98%) | 116 (2%) | 53 | 57 |

All (116) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 10 | ASN |
| 1 | A | 20 | VAL |
| 1 | A | 75 | LYS |
| 1 | A | 94 | VAL |
| 1 | A | 183 | LEU |
| 1 | A | 289 | LEU |
| 1 | A | 310 | GLU |
| 1 | A | 328 | ASP |
| 1 | A | 404 | ARG |
| 1 | A | 499 | VAL |
| 1 | B | 75 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 183 | LEU |
| 1 | B | 289 | LEU |
| 1 | B | 310 | GLU |
| 1 | B | 404 | ARG |
| 1 | B | 499 | VAL |
| 1 | B | 510 | VAL |
| 1 | C | 20 | VAL |
| 1 | C | 75 | LYS |
| 1 | C | 94 | VAL |
| 1 | C | 183 | LEU |
| 1 | C | 289 | LEU |
| 1 | C | 328 | ASP |
| 1 | C | 404 | ARG |
| 1 | C | 499 | VAL |
| 1 | D | 20 | VAL |
| 1 | D | 23 | LEU |
| 1 | D | 75 | LYS |
| 1 | D | 94 | VAL |
| 1 | D | 183 | LEU |
| 1 | D | 289 | LEU |
| 1 | D | 310 | GLU |
| 1 | D | 404 | ARG |
| 1 | D | 473 | ASP |
| 1 | D | 499 | VAL |
| 1 | E | 94 | VAL |
| 1 | E | 183 | LEU |
| 1 | E | 310 | GLU |
| 1 | E | 328 | ASP |
| 1 | E | 404 | ARG |
| 1 | E | 499 | VAL |
| 1 | E | 514 | MET |
| 1 | F | 20 | VAL |
| 1 | F | 75 | LYS |
| 1 | F | 94 | VAL |
| 1 | F | 183 | LEU |
| 1 | F | 310 | GLU |
| 1 | F | 328 | ASP |
| 1 | F | 404 | ARG |
| 1 | F | 499 | VAL |
| 1 | G | 10 | ASN |
| 1 | G | 20 | VAL |
| 1 | G | 75 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 183 | LEU |
| 1 | G | 289 | LEU |
| 1 | G | 310 | GLU |
| 1 | G | 328 | ASP |
| 1 | G | 404 | ARG |
| 1 | G | 499 | VAL |
| 1 | H | 20 | VAL |
| 1 | H | 75 | LYS |
| 1 | H | 94 | VAL |
| 1 | H | 183 | LEU |
| 1 | H | 289 | LEU |
| 1 | H | 404 | ARG |
| 1 | H | 499 | VAL |
| 1 | I | 10 | ASN |
| 1 | I | 20 | VAL |
| 1 | I | 75 | LYS |
| 1 | I | 94 | VAL |
| 1 | I | 183 | LEU |
| 1 | I | 289 | LEU |
| 1 | I | 310 | GLU |
| 1 | I | 404 | ARG |
| 1 | I | 499 | VAL |
| 1 | J | 20 | VAL |
| 1 | J | 75 | LYS |
| 1 | J | 94 | VAL |
| 1 | J | 183 | LEU |
| 1 | J | 310 | GLU |
| 1 | J | 404 | ARG |
| 1 | J | 499 | VAL |
| 1 | K | 20 | VAL |
| 1 | K | 75 | LYS |
| 1 | K | 94 | VAL |
| 1 | K | 183 | LEU |
| 1 | K | 289 | LEU |
| 1 | K | 328 | ASP |
| 1 | K | 404 | ARG |
| 1 | K | 499 | VAL |
| 1 | L | 20 | VAL |
| 1 | L | 75 | LYS |
| 1 | L | 94 | VAL |
| 1 | L | 183 | LEU |
| 1 | L | 289 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L | 310 | GLU |
| 1 | L | 328 | ASP |
| 1 | L | 404 | ARG |
| 1 | L | 417 | VAL |
| 1 | L | 499 | VAL |
| 1 | M | 20 | VAL |
| 1 | M | 75 | LYS |
| 1 | M | 94 | VAL |
| 1 | M | 183 | LEU |
| 1 | M | 284 | ARG |
| 1 | M | 310 | GLU |
| 1 | M | 404 | ARG |
| 1 | M | 499 | VAL |
| 1 | N | 20 | VAL |
| 1 | N | 75 | LYS |
| 1 | N | 94 | VAL |
| 1 | N | 183 | LEU |
| 1 | N | 289 | LEU |
| 1 | N | 310 | GLU |
| 1 | N | 404 | ARG |
| 1 | N | 499 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 37 | ASN |
| 1 | A | 146 | GLN |
| 1 | A | 229 | ASN |
| 1 | A | 265 | ASN |
| 1 | A | 319 | GLN |
| 1 | A | 326 | ASN |
| 1 | A | 348 | GLN |
| 1 | A | 351 | GLN |
| 1 | B | 146 | GLN |
| 1 | B | 265 | ASN |
| 1 | B | 319 | GLN |
| 1 | B | 326 | ASN |
| 1 | B | 348 | GLN |
| 1 | B | 351 | GLN |
| 1 | B | 366 | GLN |
| 1 | B | 401 | HIS |
| 1 | B | 475 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 37 | ASN |
| 1 | C | 146 | GLN |
| 1 | C | 265 | ASN |
| 1 | C | 319 | GLN |
| 1 | C | 326 | ASN |
| 1 | C | 348 | GLN |
| 1 | C | 351 | GLN |
| 1 | C | 366 | GLN |
| 1 | C | 401 | HIS |
| 1 | D | 37 | ASN |
| 1 | D | 146 | GLN |
| 1 | D | 229 | ASN |
| 1 | D | 265 | ASN |
| 1 | D | 319 | GLN |
| 1 | D | 326 | ASN |
| 1 | D | 348 | GLN |
| 1 | D | 351 | GLN |
| 1 | D | 366 | GLN |
| 1 | D | 401 | HIS |
| 1 | D | 453 | GLN |
| 1 | D | 475 | ASN |
| 1 | E | 37 | ASN |
| 1 | E | 146 | GLN |
| 1 | E | 265 | ASN |
| 1 | E | 319 | GLN |
| 1 | E | 326 | ASN |
| 1 | E | 348 | GLN |
| 1 | E | 351 | GLN |
| 1 | E | 401 | HIS |
| 1 | E | 453 | GLN |
| 1 | E | 475 | ASN |
| 1 | F | 146 | GLN |
| 1 | F | 265 | ASN |
| 1 | F | 319 | GLN |
| 1 | F | 326 | ASN |
| 1 | F | 348 | GLN |
| 1 | F | 351 | GLN |
| 1 | F | 401 | HIS |
| 1 | G | 37 | ASN |
| 1 | G | 146 | GLN |
| 1 | G | 265 | ASN |
| 1 | G | 319 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 326 | ASN |
| 1 | G | 348 | GLN |
| 1 | G | 351 | GLN |
| 1 | G | 401 | HIS |
| 1 | G | 453 | GLN |
| 1 | G | 475 | ASN |
| 1 | H | 37 | ASN |
| 1 | H | 146 | GLN |
| 1 | H | 265 | ASN |
| 1 | H | 319 | GLN |
| 1 | H | 326 | ASN |
| 1 | H | 348 | GLN |
| 1 | H | 351 | GLN |
| 1 | H | 401 | HIS |
| 1 | I | 37 | ASN |
| 1 | I | 146 | GLN |
| 1 | I | 265 | ASN |
| 1 | I | 319 | GLN |
| 1 | I | 326 | ASN |
| 1 | I | 348 | GLN |
| 1 | I | 351 | GLN |
| 1 | I | 401 | HIS |
| 1 | J | 37 | ASN |
| 1 | J | 146 | GLN |
| 1 | J | 265 | ASN |
| 1 | J | 319 | GLN |
| 1 | J | 326 | ASN |
| 1 | J | 348 | GLN |
| 1 | J | 351 | GLN |
| 1 | J | 453 | GLN |
| 1 | K | 37 | ASN |
| 1 | K | 146 | GLN |
| 1 | K | 265 | ASN |
| 1 | K | 319 | GLN |
| 1 | K | 326 | ASN |
| 1 | K | 348 | GLN |
| 1 | K | 351 | GLN |
| 1 | K | 401 | HIS |
| 1 | L | 37 | ASN |
| 1 | L | 146 | GLN |
| 1 | L | 229 | ASN |
| 1 | L | 265 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L | 319 | GLN |
| 1 | L | 326 | ASN |
| 1 | L | 348 | GLN |
| 1 | L | 351 | GLN |
| 1 | L | 401 | HIS |
| 1 | L | 453 | GLN |
| 1 | M | 37 | ASN |
| 1 | M | 146 | GLN |
| 1 | M | 229 | ASN |
| 1 | M | 265 | ASN |
| 1 | M | 319 | GLN |
| 1 | M | 326 | ASN |
| 1 | M | 348 | GLN |
| 1 | M | 351 | GLN |
| 1 | M | 401 | HIS |
| 1 | M | 453 | GLN |
| 1 | N | 37 | ASN |
| 1 | N | 146 | GLN |
| 1 | N | 265 | ASN |
| 1 | N | 319 | GLN |
| 1 | N | 326 | ASN |
| 1 | N | 348 | GLN |
| 1 | N | 351 | GLN |
| 1 | N | 401 | HIS |
| 1 | N | 453 | 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)

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 30 are monoatomic - leaving 36 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | AGS | E | 1 | 4,3 | 26,33,33 | 3.96 | 3 (11%) | 26,52,52 | 1.13 | 2 (7%) |
| 2 | SO4 | M | 4013 | - | 4,4,4 | 1.58 | 1 (25%) | 6,6,6 | 1.15 | 0 |
| 2 | SO4 | J | 4019 | - | 4,4,4 | 1.52 | 1 (25%) | 6,6,6 | 1.12 | 0 |
| 5 | AGS | C | 1 | 4,3 | 26,33,33 | 3.87 | 2 (7%) | 26,52,52 | 1.12 | 2 (7%) |
| 5 | AGS | N | 1 | 4,3 | 26,33,33 | 3.90 | 3 (11%) | 26,52,52 | 1.11 | 2 (7%) |
| 2 | SO4 | M | 4014 | - | 4,4,4 | 1.55 | 1 (25%) | 6,6,6 | 1.13 | 0 |
| 5 | AGS | H | 1 | 4,3 | 26,33,33 | 3.85 | 1 (3%) | 26,52,52 | 1.18 | 2 (7%) |
| 2 | SO4 | E | 4006 | - | 4,4,4 | 1.53 | 1 (25%) | 6,6,6 | 1.12 | 0 |
| 2 | SO4 | A | 4008 | - | 4,4,4 | 1.52 | 1 (25%) | 6,6,6 | 1.13 | 0 |
| 2 | SO4 | C | 4011 | - | 4,4,4 | 1.53 | 1 (25%) | 6,6,6 | 1.13 | 0 |
| 2 | SO4 | J | 4020 | - | 4,4,4 | 1.54 | 1 (25%) | 6,6,6 | 1.13 | 0 |
| 2 | SO4 | B | 4009 | - | 4,4,4 | 1.52 | 1 (25%) | 6,6,6 | 1.11 | 0 |
| 5 | AGS | A | 1 | 4,3 | 26,33,33 | 3.76 | 1 (3%) | 26,52,52 | 1.20 | 2 (7%) |
| 2 | SO4 | A | 4007 | - | 4,4,4 | 1.50 | 1 (25%) | 6,6,6 | 1.16 | 0 |
| 2 | SO4 | G | 4002 | - | 4,4,4 | 1.53 | 1 (25%) | 6,6,6 | 1.17 | 0 |
| 5 | AGS | J | 1 | 4,3 | 26,33,33 | 3.88 | 4 (15%) | 26,52,52 | 1.11 | 2 (7%) |
| 2 | SO4 | K | 4022 | - | 4,4,4 | 1.51 | 1 (25%) | 6,6,6 | 1.14 | 0 |
| 5 | AGS | D | 551 | 4,3 | 26,33,33 | 3.96 | 5 (19%) | 26,52,52 | 1.07 | 1 (3%) |
| 5 | AGS | F | 1 | 4,3 | 26,33,33 | 3.86 | 3 (11%) | 26,52,52 | 1.04 | 1 (3%) |
| 2 | SO4 | K | 4021 | - | 4,4,4 | 1.56 | 1 (25%) | 6,6,6 | 1.14 | 0 |
| 2 | SO4 | N | 4016 | - | 4,4,4 | 1.53 | 1 (25%) | 6,6,6 | 1.14 | 0 |
| 2 | SO4 | A | 4001 | - | 4,4,4 | 1.52 | 1 (25%) | 6,6,6 | 1.16 | 0 |
| 2 | SO4 | H | 4018 | - | 4,4,4 | 1.53 | 1 (25%) | 6,6,6 | 1.11 | 0 |
| 5 | AGS | B | 1 | 4,3 | 26,33,33 | 3.81 | 2 (7%) | 26,52,52 | 1.12 | 2 (7%) |
| 5 | AGS | G | 1 | 4,3 | 26,33,33 | 3.99 | 2 (7%) | 26,52,52 | 1.18 | 2 (7%) |
| 5 | AGS | L | 1 | 4,3 | 26,33,33 | 3.85 | 2 (7%) | 26,52,52 | 1.11 | 2 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | AGS | M | 1 | 4,3 | 26,33,33 | 3.86 | 1 (3%) | 26,52,52 | 1.11 | 2 (7%) |
| 2 | SO4 | C | 4012 | - | 4,4,4 | 1.56 | 1 (25%) | 6,6,6 | 1.16 | 0 |
| 2 | SO4 | E | 4005 | - | 4,4,4 | 1.43 | 1 (25%) | 6,6,6 | 1.16 | 0 |
| 5 | AGS | K | 1 | 4,3 | 26,33,33 | 3.88 | 4 (15%) | 26,52,52 | 1.08 | 2 (7%) |
| 2 | SO4 | L | 4003 | - | 4,4,4 | 1.52 | 1 (25%) | 6,6,6 | 1.16 | 0 |
| 2 | SO4 | N | 4015 | - | 4,4,4 | 1.54 | 1 (25%) | 6,6,6 | 1.16 | 0 |
| 2 | SO4 | B | 4010 | - | 4,4,4 | 1.54 | 1 (25%) | 6,6,6 | 1.13 | 0 |
| 2 | SO4 | H | 4017 | - | 4,4,4 | 1.53 | 1 (25%) | 6,6,6 | 1.14 | 0 |
| 2 | SO4 | F | 4004 | - | 4,4,4 | 1.45 | 1 (25%) | 6,6,6 | 1.18 | 0 |
| 5 | AGS | I | 1 | 4,3 | 26,33,33 | 3.89 | 2 (7%) | 26,52,52 | 1.09 | 2 (7%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 5 | AGS | B | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | E | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | A | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | G | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | J | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | L | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | M | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | K | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | C | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | D | 551 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | F | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | N | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | H | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |
| 5 | AGS | I | 1 | 4,3 | - | 3/17/38/38 | 0/3/3/3 |

All (57) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | G | 1 | AGS | PG-S1G | -19.57 | 1.48 | 1.90 |
| 5 | E | 1 | AGS | PG-S1G | -19.49 | 1.48 | 1.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | D | 551 | AGS | PG-S1G | -19.39 | 1.48 | 1.90 |
| 5 | N | 1 | AGS | PG-S1G | -19.10 | 1.49 | 1.90 |
| 5 | I | 1 | AGS | PG-S1G | -19.09 | 1.49 | 1.90 |
| 5 | H | 1 | AGS | PG-S1G | -18.99 | 1.49 | 1.90 |
| 5 | C | 1 | AGS | PG-S1G | -18.98 | 1.49 | 1.90 |
| 5 | J | 1 | AGS | PG-S1G | -18.97 | 1.49 | 1.90 |
| 5 | K | 1 | AGS | PG-S1G | -18.95 | 1.49 | 1.90 |
| 5 | M | 1 | AGS | PG-S1G | -18.92 | 1.49 | 1.90 |
| 5 | F | 1 | AGS | PG-S1G | -18.83 | 1.49 | 1.90 |
| 5 | L | 1 | AGS | PG-S1G | -18.82 | 1.49 | 1.90 |
| 5 | B | 1 | AGS | PG-S1G | -18.66 | 1.50 | 1.90 |
| 5 | A | 1 | AGS | PG-S1G | -18.55 | 1.50 | 1.90 |
| 5 | K | 1 | AGS | O4'-C1' | 3.14 | 1.45 | 1.41 |
| 2 | M | 4013 | SO4 | O1-S | 3.08 | 1.62 | 1.46 |
| 2 | K | 4021 | SO4 | O1-S | 3.02 | 1.62 | 1.46 |
| 2 | C | 4012 | SO4 | O1-S | 3.01 | 1.62 | 1.46 |
| 2 | B | 4010 | SO4 | O1-S | 3.00 | 1.62 | 1.46 |
| 2 | M | 4014 | SO4 | O1-S | 2.99 | 1.62 | 1.46 |
| 2 | N | 4015 | SO4 | O1-S | 2.98 | 1.62 | 1.46 |
| 2 | C | 4011 | SO4 | O1-S | 2.98 | 1.62 | 1.46 |
| 2 | H | 4018 | SO4 | O1-S | 2.98 | 1.62 | 1.46 |
| 2 | J | 4019 | SO4 | O1-S | 2.97 | 1.62 | 1.46 |
| 2 | J | 4020 | SO4 | O1-S | 2.97 | 1.62 | 1.46 |
| 2 | E | 4006 | SO4 | O1-S | 2.97 | 1.62 | 1.46 |
| 2 | H | 4017 | SO4 | O1-S | 2.97 | 1.62 | 1.46 |
| 2 | B | 4009 | SO4 | O1-S | 2.96 | 1.62 | 1.46 |
| 2 | N | 4016 | SO4 | O1-S | 2.96 | 1.62 | 1.46 |
| 2 | A | 4008 | SO4 | O1-S | 2.96 | 1.62 | 1.46 |
| 2 | A | 4001 | SO4 | O1-S | 2.95 | 1.62 | 1.46 |
| 2 | G | 4002 | SO4 | O1-S | 2.95 | 1.62 | 1.46 |
| 2 | L | 4003 | SO4 | O1-S | 2.93 | 1.61 | 1.46 |
| 2 | K | 4022 | SO4 | O1-S | 2.93 | 1.61 | 1.46 |
| 2 | A | 4007 | SO4 | O1-S | 2.89 | 1.61 | 1.46 |
| 2 | F | 4004 | SO4 | O1-S | 2.81 | 1.61 | 1.46 |
| 2 | E | 4005 | SO4 | O1-S | 2.77 | 1.61 | 1.46 |
| 5 | F | 1 | AGS | C2-N3 | 2.29 | 1.35 | 1.32 |
| 5 | D | 551 | AGS | C2'-C1' | -2.29 | 1.50 | 1.53 |
| 5 | D | 551 | AGS | C2-N3 | 2.22 | 1.35 | 1.32 |
| 5 | F | 1 | AGS | PG-O3G | -2.22 | 1.47 | 1.54 |
| 5 | J | 1 | AGS | C2-N3 | 2.17 | 1.35 | 1.32 |
| 5 | J | 1 | AGS | O4'-C1' | 2.16 | 1.44 | 1.41 |
| 5 | L | 1 | AGS | C2'-C1' | -2.13 | 1.50 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | G | 1 | AGS | C2-N3 | 2.12 | 1.35 | 1.32 |
| 5 | N | 1 | AGS | C2-N3 | 2.12 | 1.35 | 1.32 |
| 5 | D | 551 | AGS | PG-O3G | -2.10 | 1.48 | 1.54 |
| 5 | E | 1 | AGS | PG-O3G | -2.08 | 1.48 | 1.54 |
| 5 | K | 1 | AGS | C2-N3 | 2.07 | 1.35 | 1.32 |
| 5 | I | 1 | AGS | C2'-C1' | -2.07 | 1.50 | 1.53 |
| 5 | J | 1 | AGS | PG-O3G | -2.05 | 1.48 | 1.54 |
| 5 | C | 1 | AGS | PG-O3G | -2.04 | 1.48 | 1.54 |
| 5 | B | 1 | AGS | PG-O3G | -2.04 | 1.48 | 1.54 |
| 5 | N | 1 | AGS | PG-O3G | -2.04 | 1.48 | 1.54 |
| 5 | K | 1 | AGS | PG-O3G | -2.03 | 1.48 | 1.54 |
| 5 | D | 551 | AGS | C4-N3 | 2.02 | 1.38 | 1.35 |
| 5 | E | 1 | AGS | C2-N3 | 2.01 | 1.35 | 1.32 |

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | H | 1 | AGS | C5-C6-N6 | 3.11 | 125.08 | 120.35 |
| 5 | M | 1 | AGS | C5-C6-N6 | 3.10 | 125.06 | 120.35 |
| 5 | G | 1 | AGS | C5-C6-N6 | 3.06 | 125.00 | 120.35 |
| 5 | A | 1 | AGS | C5-C6-N6 | 2.95 | 124.83 | 120.35 |
| 5 | L | 1 | AGS | C5-C6-N6 | 2.85 | 124.69 | 120.35 |
| 5 | C | 1 | AGS | C5-C6-N6 | 2.85 | 124.68 | 120.35 |
| 5 | K | 1 | AGS | C5-C6-N6 | 2.81 | 124.63 | 120.35 |
| 5 | K | 1 | AGS | O4'-C1'-C2' | -2.79 | 102.84 | 106.93 |
| 5 | B | 1 | AGS | C5-C6-N6 | 2.79 | 124.59 | 120.35 |
| 5 | E | 1 | AGS | C5-C6-N6 | 2.77 | 124.57 | 120.35 |
| 5 | N | 1 | AGS | C5-C6-N6 | 2.70 | 124.46 | 120.35 |
| 5 | J | 1 | AGS | C5-C6-N6 | 2.69 | 124.44 | 120.35 |
| 5 | J | 1 | AGS | O4'-C1'-C2' | -2.66 | 103.04 | 106.93 |
| 5 | F | 1 | AGS | C5-C6-N6 | 2.64 | 124.36 | 120.35 |
| 5 | G | 1 | AGS | O4'-C1'-C2' | -2.60 | 103.13 | 106.93 |
| 5 | I | 1 | AGS | C5-C6-N6 | 2.56 | 124.24 | 120.35 |
| 5 | A | 1 | AGS | O4'-C1'-C2' | -2.53 | 103.23 | 106.93 |
| 5 | D | 551 | AGS | C5-C6-N6 | 2.36 | 123.94 | 120.35 |
| 5 | N | 1 | AGS | O4'-C1'-C2' | -2.36 | 103.48 | 106.93 |
| 5 | B | 1 | AGS | O4'-C1'-C2' | -2.20 | 103.71 | 106.93 |
| 5 | M | 1 | AGS | O4'-C1'-C2' | -2.18 | 103.73 | 106.93 |
| 5 | C | 1 | AGS | O4'-C1'-C2' | -2.16 | 103.77 | 106.93 |
| 5 | E | 1 | AGS | O4'-C1'-C2' | -2.12 | 103.82 | 106.93 |
| 5 | L | 1 | AGS | O4'-C1'-C2' | -2.10 | 103.86 | 106.93 |
| 5 | H | 1 | AGS | O4'-C1'-C2' | -2.06 | 103.91 | 106.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | I | 1 | AGS | O4'-C1'-C2' | -2.03 | 103.95 | 106.93 |

There are no chirality outliers.

All (42) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | A | 1 | AGS | PB-O3B-PG-O2G |
| 5 | A | 1 | AGS | PB-O3B-PG-O3G |
| 5 | B | 1 | AGS | PB-O3B-PG-O2G |
| 5 | B | 1 | AGS | PB-O3B-PG-O3G |
| 5 | C | 1 | AGS | PB-O3B-PG-O2G |
| 5 | C | 1 | AGS | PB-O3B-PG-O3G |
| 5 | D | 551 | AGS | PB-O3B-PG-O2G |
| 5 | D | 551 | AGS | PB-O3B-PG-O3G |
| 5 | E | 1 | AGS | PB-O3B-PG-O2G |
| 5 | E | 1 | AGS | PB-O3B-PG-O3G |
| 5 | F | 1 | AGS | PB-O3B-PG-O2G |
| 5 | F | 1 | AGS | PB-O3B-PG-O3G |
| 5 | G | 1 | AGS | PB-O3B-PG-O2G |
| 5 | G | 1 | AGS | PB-O3B-PG-O3G |
| 5 | H | 1 | AGS | PB-O3B-PG-O2G |
| 5 | H | 1 | AGS | PB-O3B-PG-O3G |
| 5 | I | 1 | AGS | PB-O3B-PG-O2G |
| 5 | I | 1 | AGS | PB-O3B-PG-O3G |
| 5 | J | 1 | AGS | PB-O3B-PG-O2G |
| 5 | J | 1 | AGS | PB-O3B-PG-O3G |
| 5 | K | 1 | AGS | PB-O3B-PG-O2G |
| 5 | K | 1 | AGS | PB-O3B-PG-O3G |
| 5 | L | 1 | AGS | PB-O3B-PG-O2G |
| 5 | L | 1 | AGS | PB-O3B-PG-O3G |
| 5 | M | 1 | AGS | PB-O3B-PG-O2G |
| 5 | M | 1 | AGS | PB-O3B-PG-O3G |
| 5 | N | 1 | AGS | PB-O3B-PG-O2G |
| 5 | N | 1 | AGS | PB-O3B-PG-O3G |
| 5 | A | 1 | AGS | PA-O3A-PB-O1B |
| 5 | B | 1 | AGS | PA-O3A-PB-O1B |
| 5 | C | 1 | AGS | PA-O3A-PB-O1B |
| 5 | D | 551 | AGS | PA-O3A-PB-O1B |
| 5 | E | 1 | AGS | PA-O3A-PB-O1B |
| 5 | F | 1 | AGS | PA-O3A-PB-O1B |
| 5 | G | 1 | AGS | PA-O3A-PB-O1B |
| 5 | H | 1 | AGS | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | I | 1 | AGS | PA-O3A-PB-O1B |
| 5 | J | 1 | AGS | PA-O3A-PB-O1B |
| 5 | K | 1 | AGS | PA-O3A-PB-O1B |
| 5 | L | 1 | AGS | PA-O3A-PB-O1B |
| 5 | M | 1 | AGS | PA-O3A-PB-O1B |
| 5 | N | 1 | AGS | PA-O3A-PB-O1B |

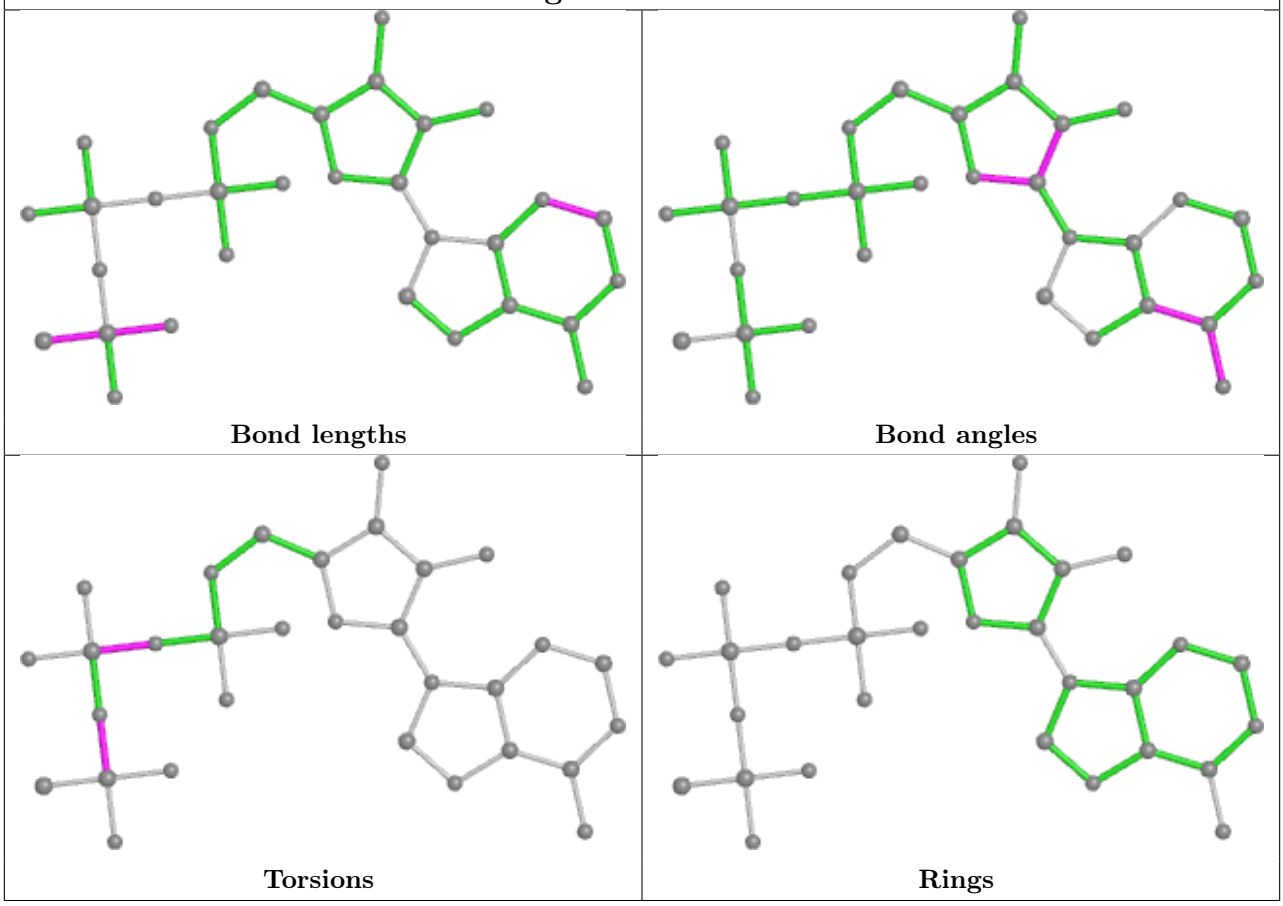
There are no ring outliers.

15 monomers are involved in 56 short contacts:

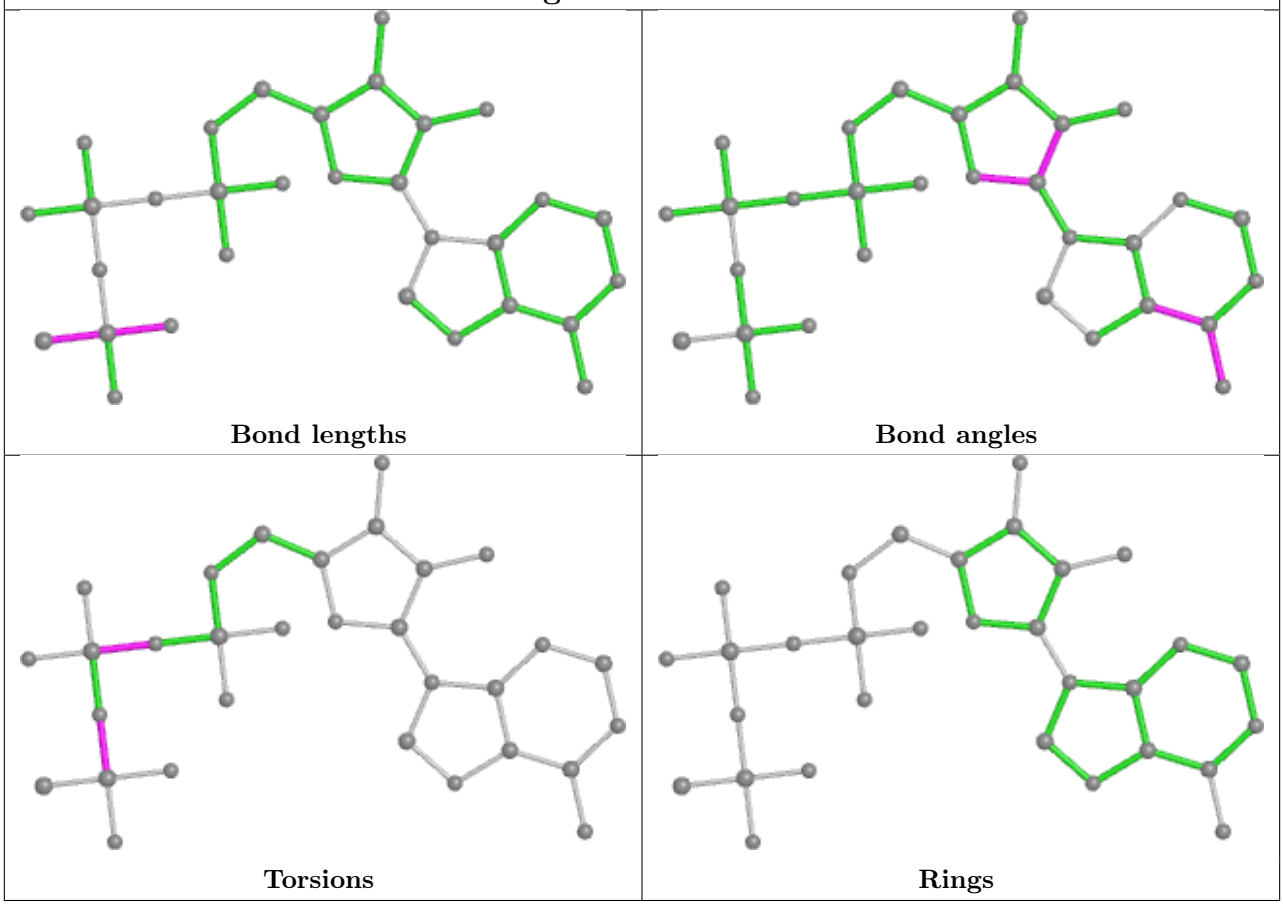
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | E | 1 | AGS | 4 | 0 |
| 5 | C | 1 | AGS | 3 | 0 |
| 5 | N | 1 | AGS | 4 | 0 |
| 5 | H | 1 | AGS | 4 | 0 |
| 5 | A | 1 | AGS | 3 | 0 |
| 5 | J | 1 | AGS | 3 | 0 |
| 5 | D | 551 | AGS | 4 | 0 |
| 5 | F | 1 | AGS | 3 | 0 |
| 5 | B | 1 | AGS | 4 | 0 |
| 5 | G | 1 | AGS | 4 | 0 |
| 5 | L | 1 | AGS | 5 | 0 |
| 5 | M | 1 | AGS | 5 | 0 |
| 2 | E | 4005 | SO4 | 1 | 0 |
| 5 | K | 1 | AGS | 5 | 0 |
| 5 | I | 1 | AGS | 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.

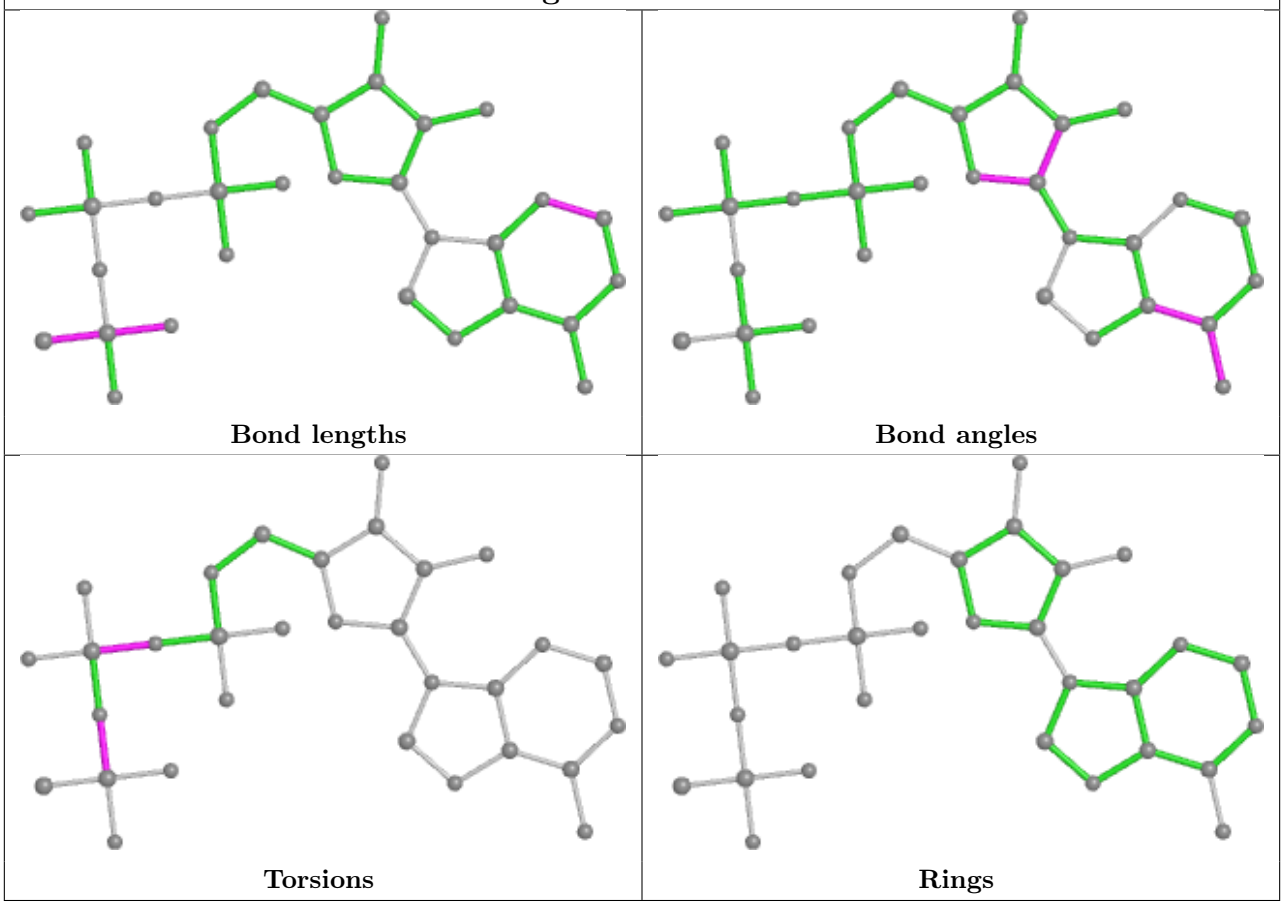
**Ligand AGS E 1**



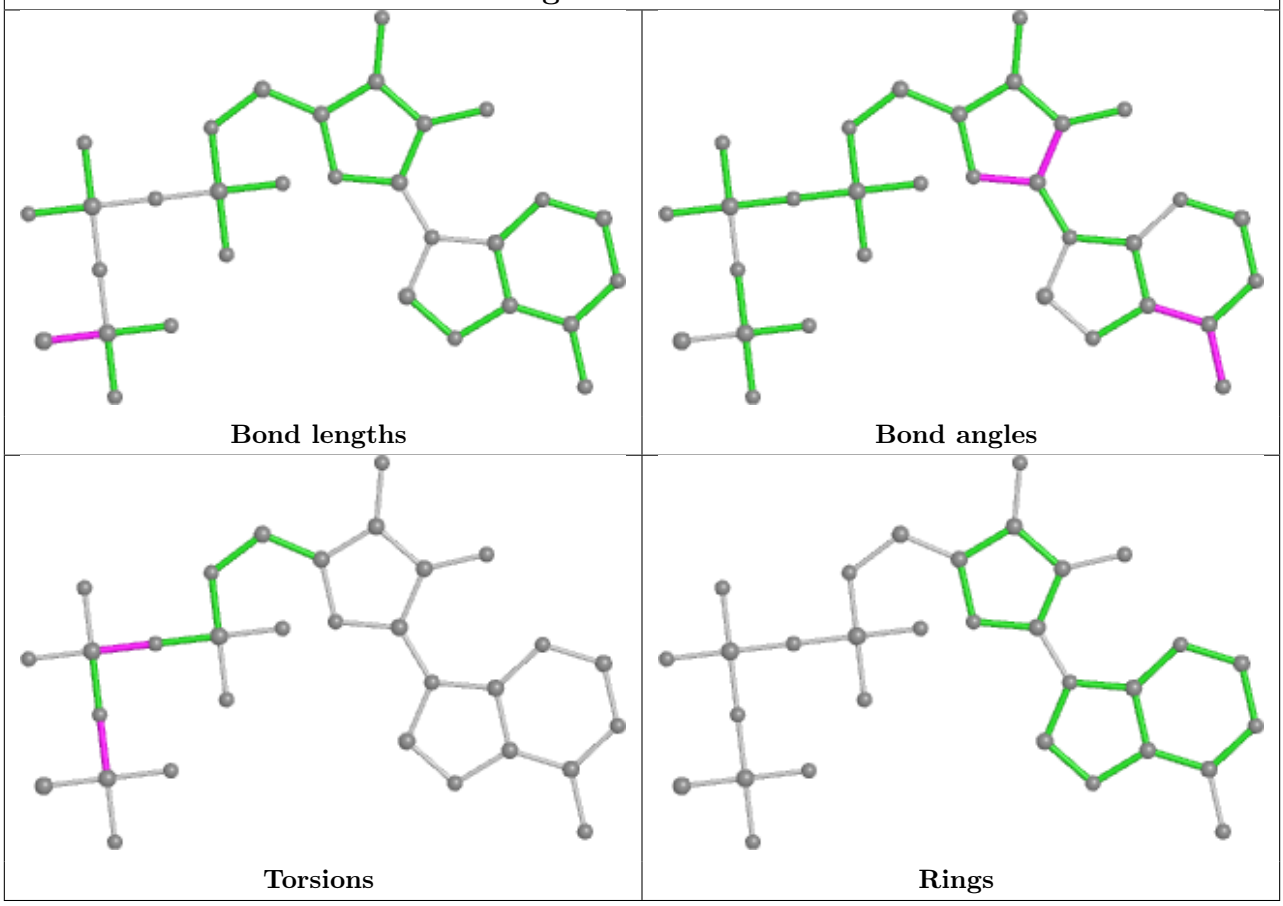
**Ligand AGS C 1**



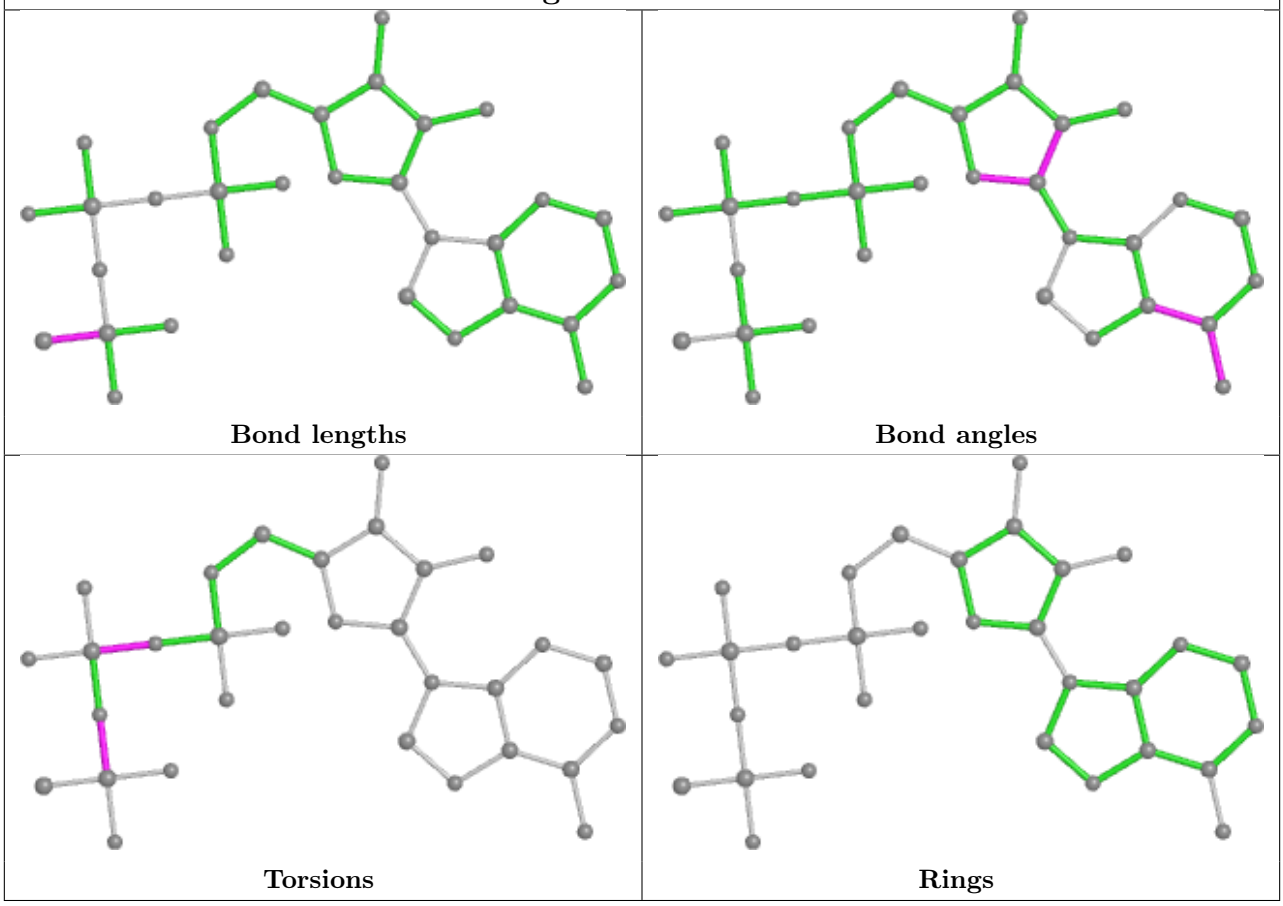
**Ligand AGS N 1**



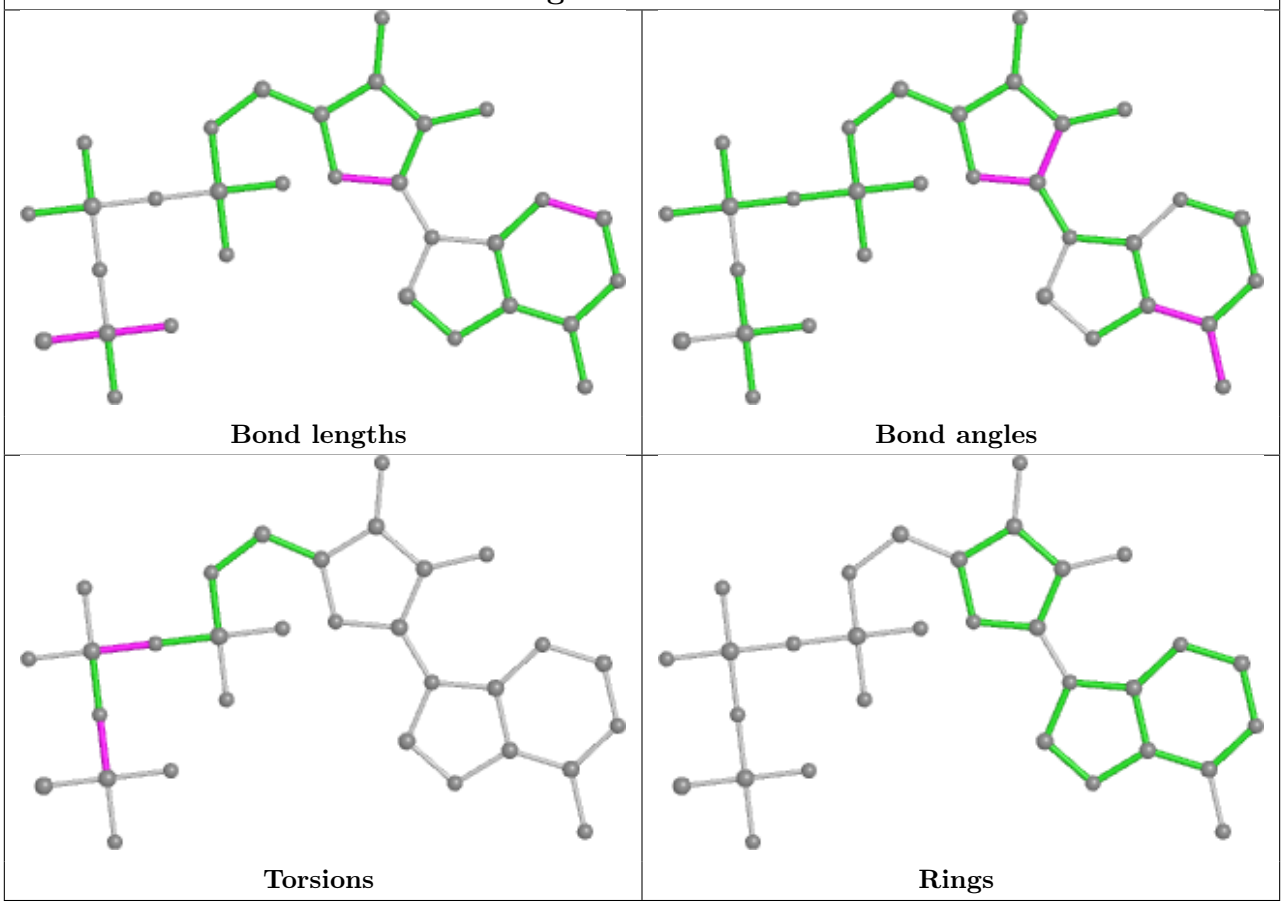
**Ligand AGS H 1**



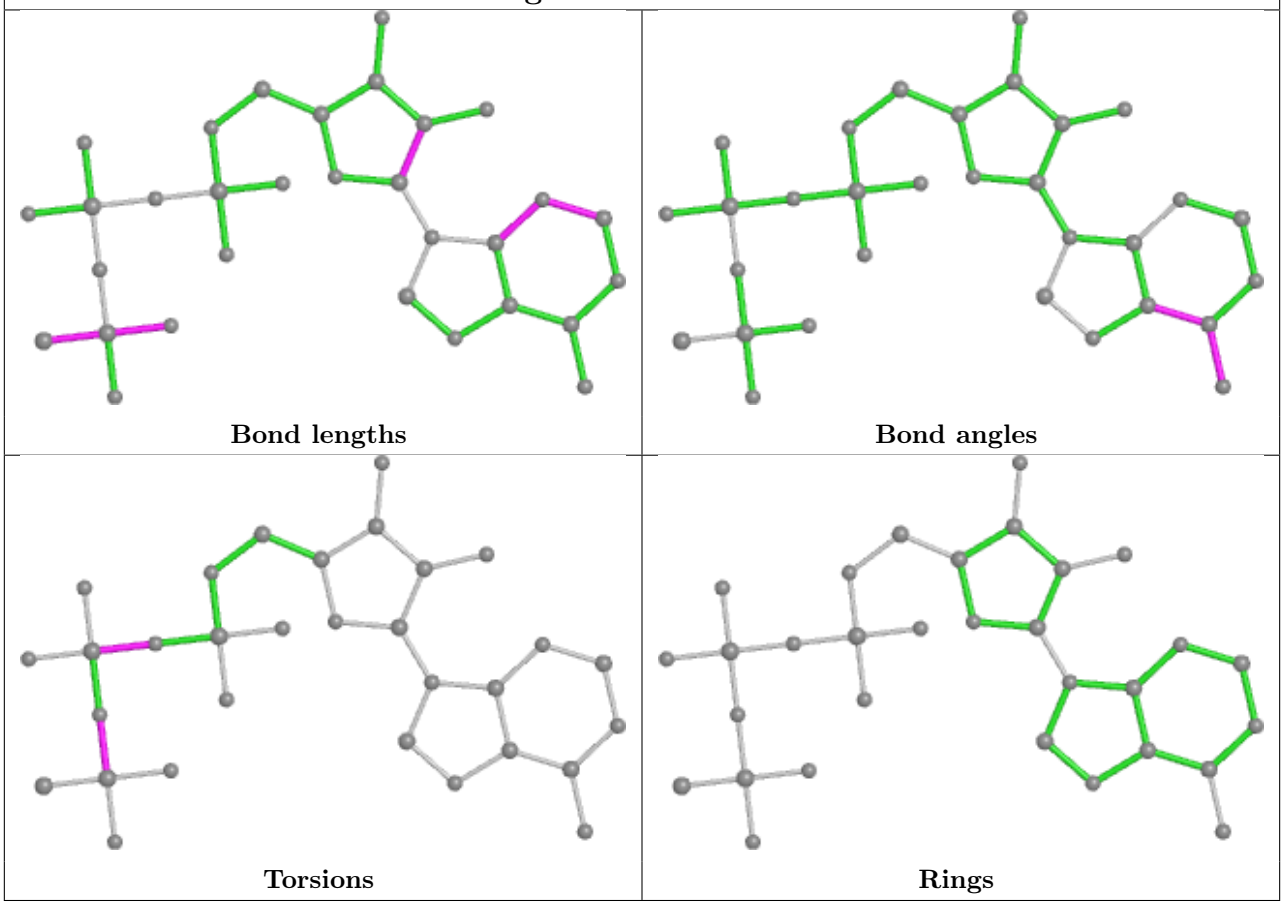
**Ligand AGS A 1**



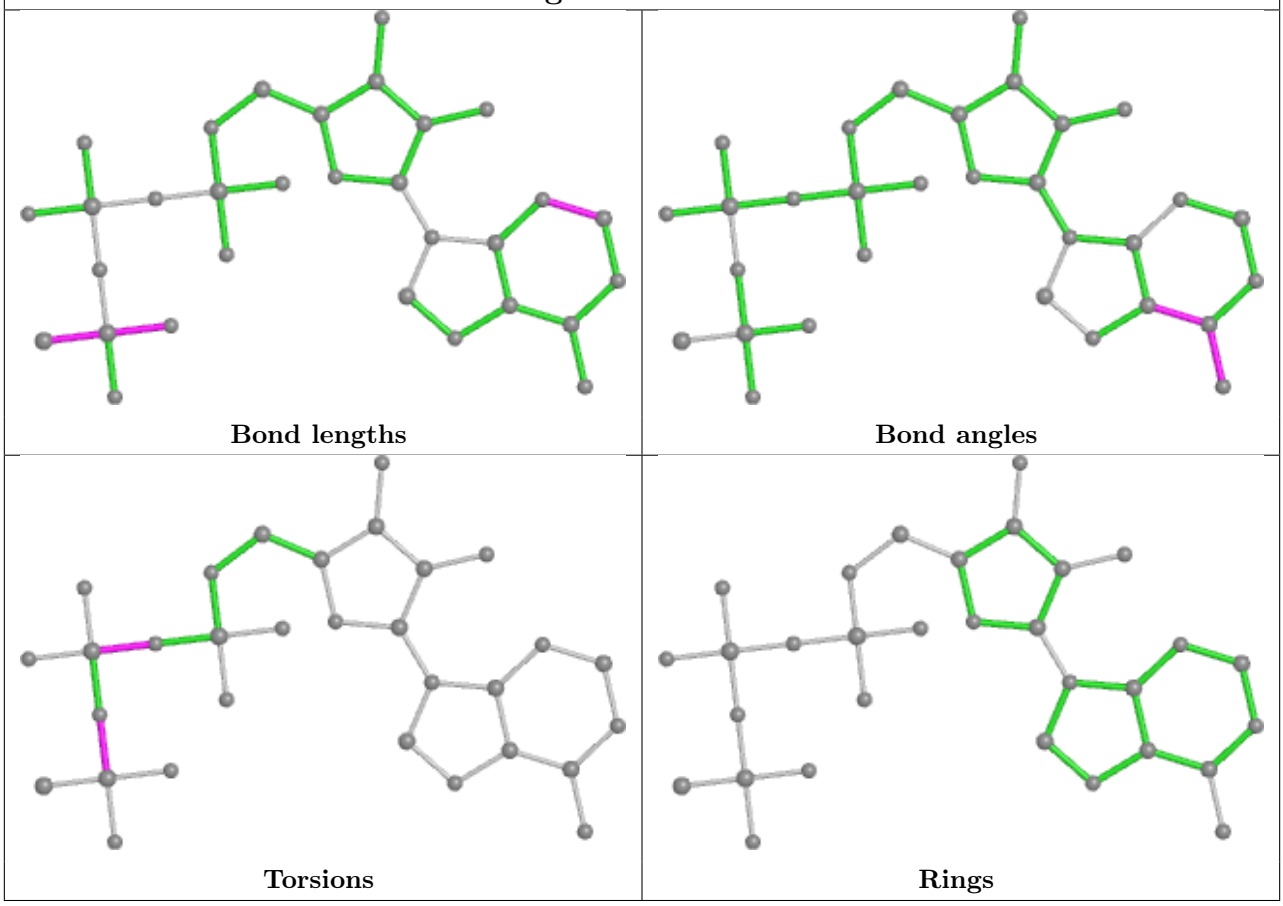
**Ligand AGS J 1**



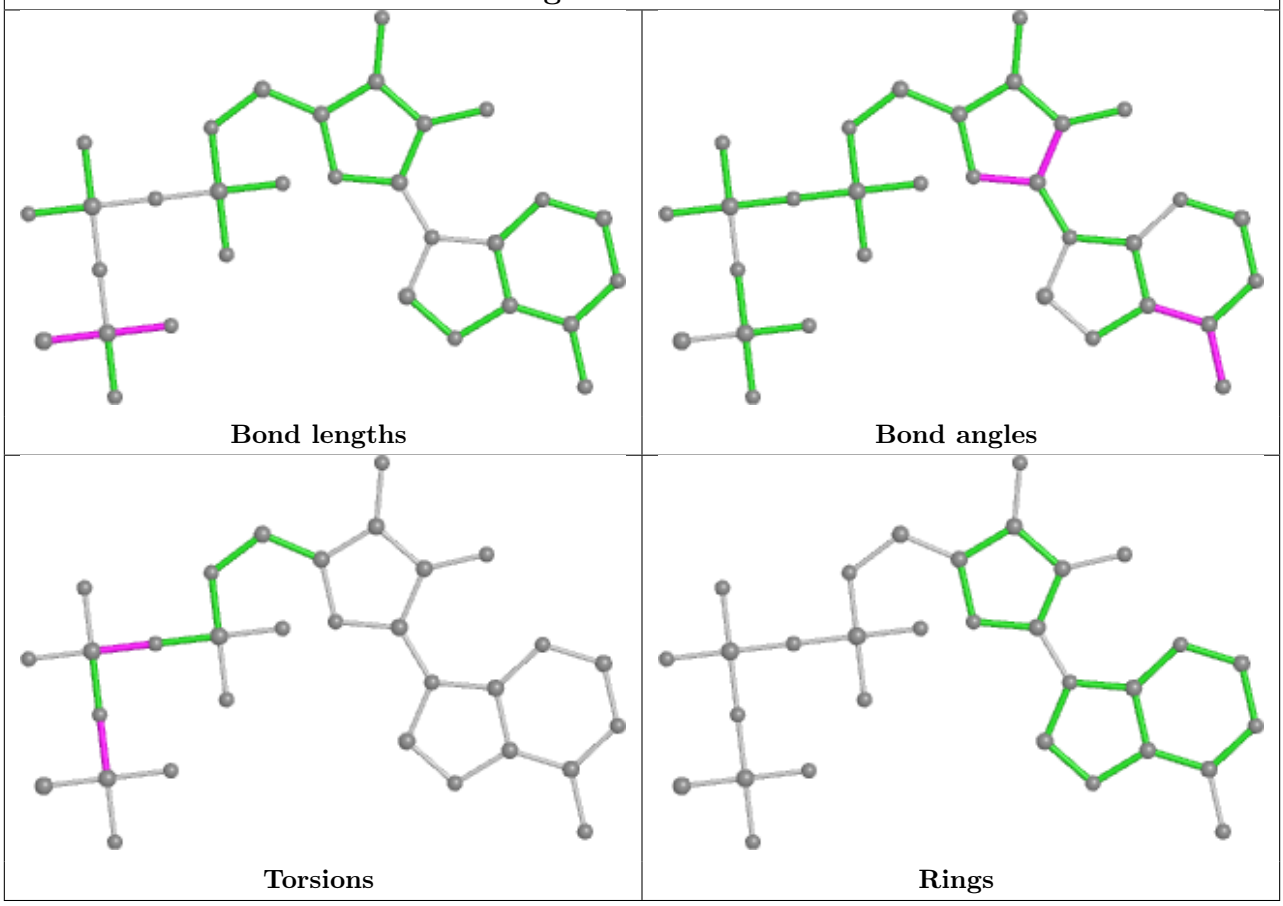
**Ligand AGS D 551**



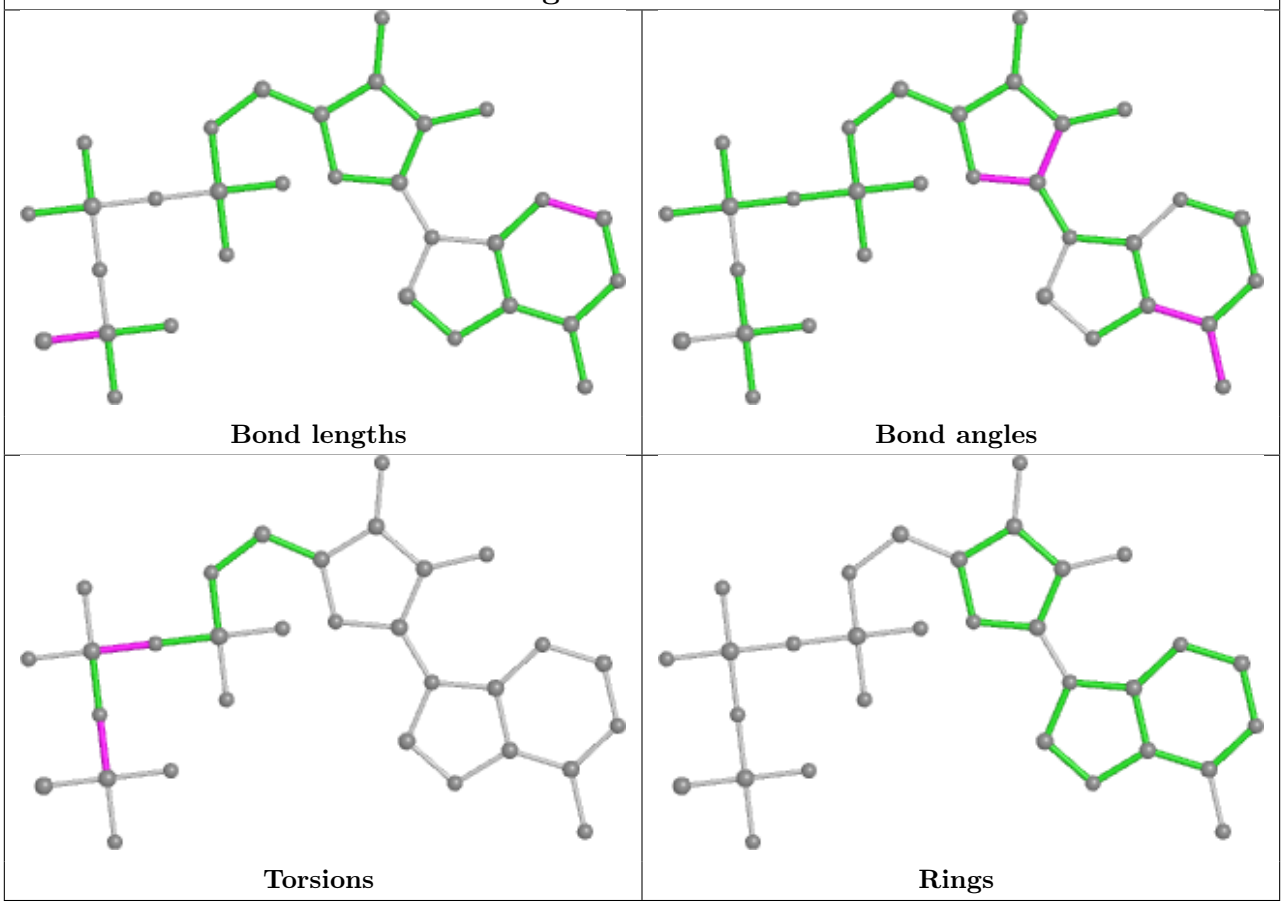
**Ligand AGS F 1**



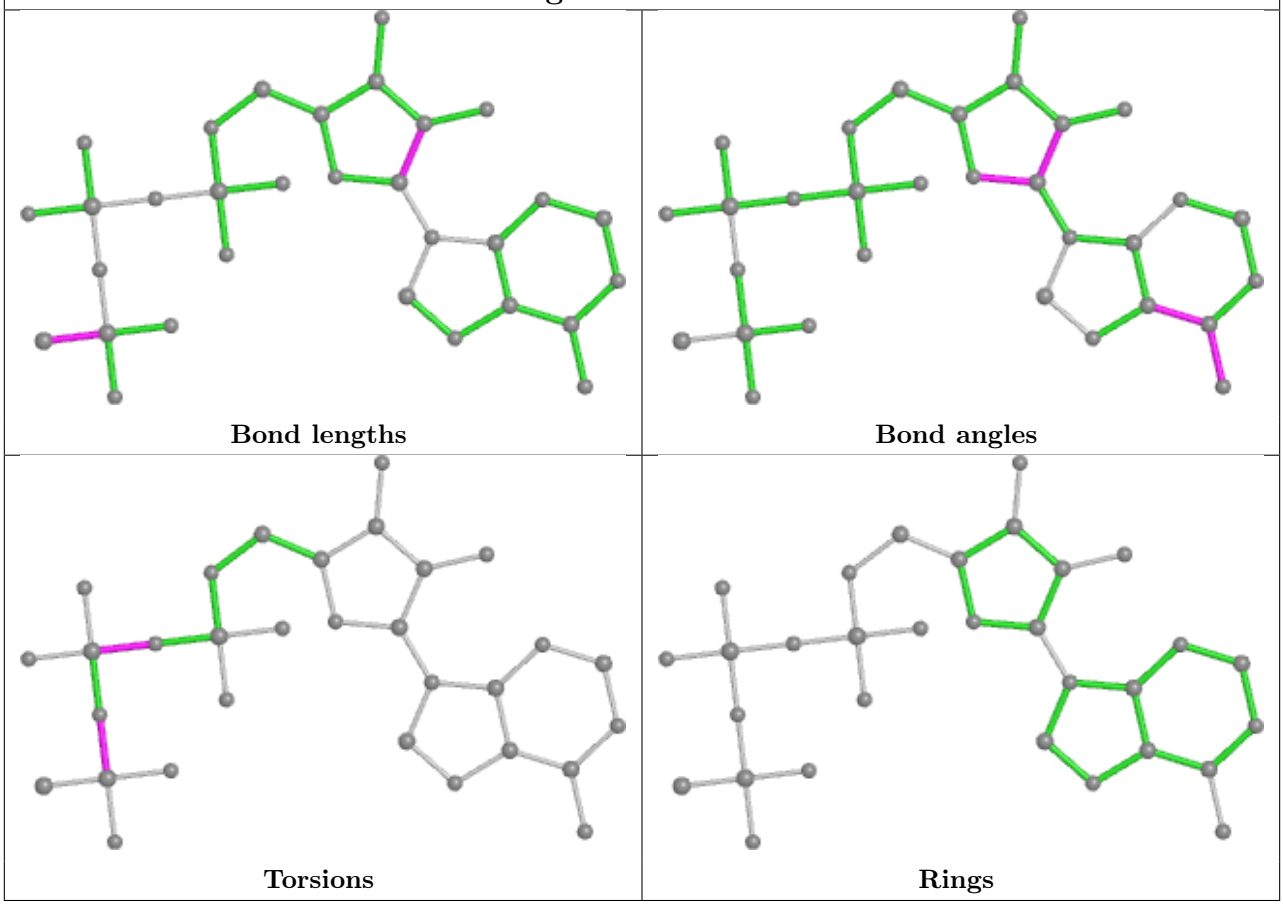
**Ligand AGS B 1**



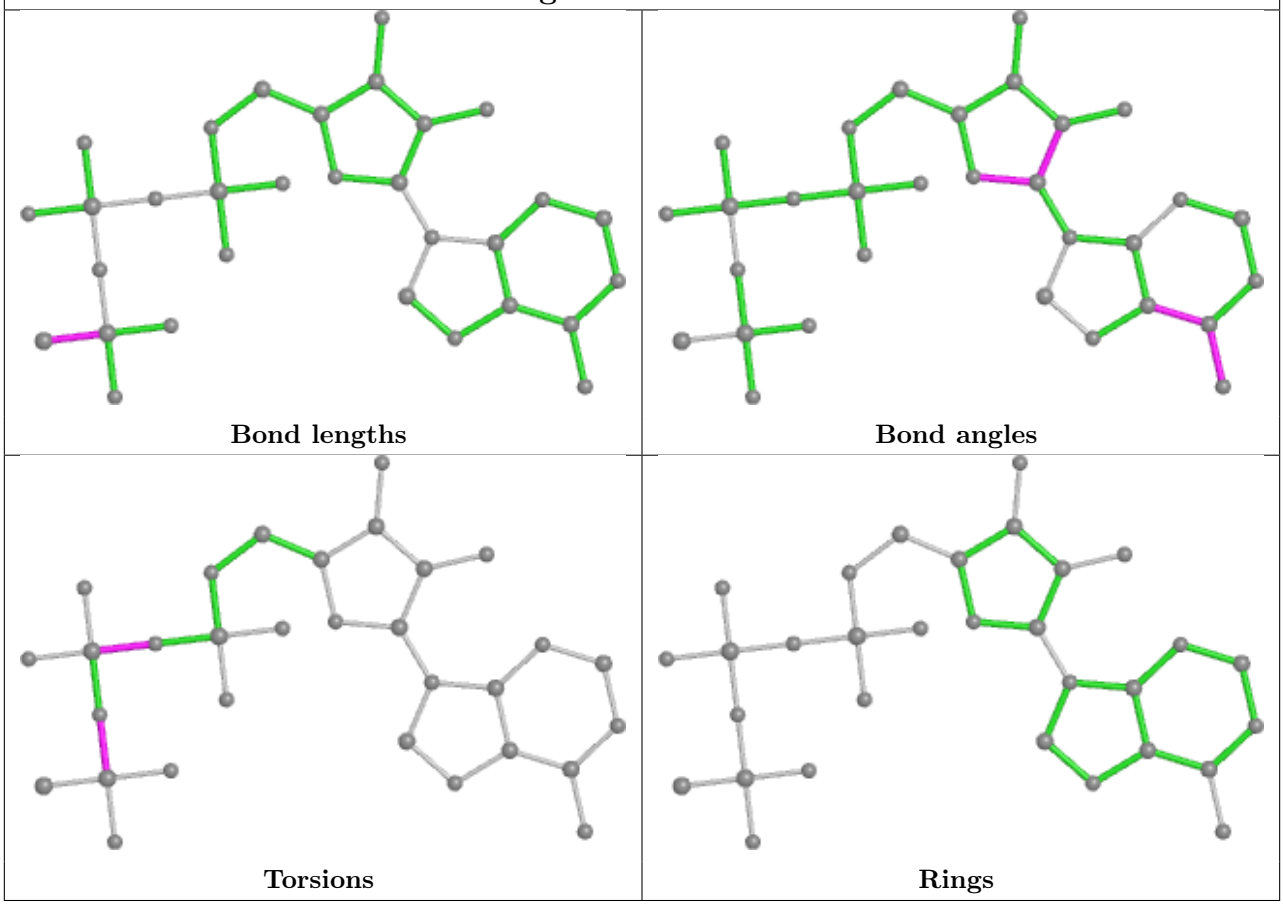
**Ligand AGS G 1**



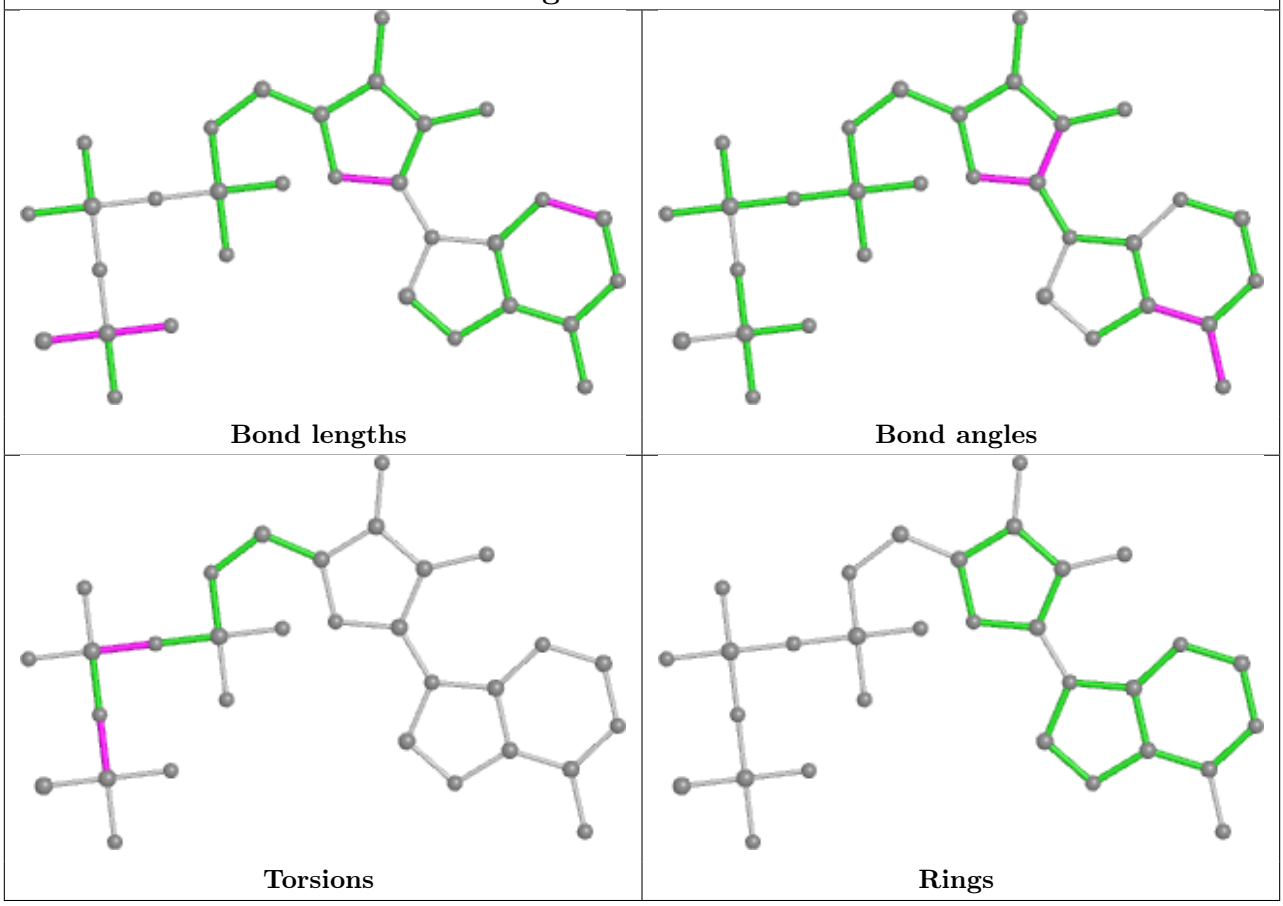
**Ligand AGS L 1**



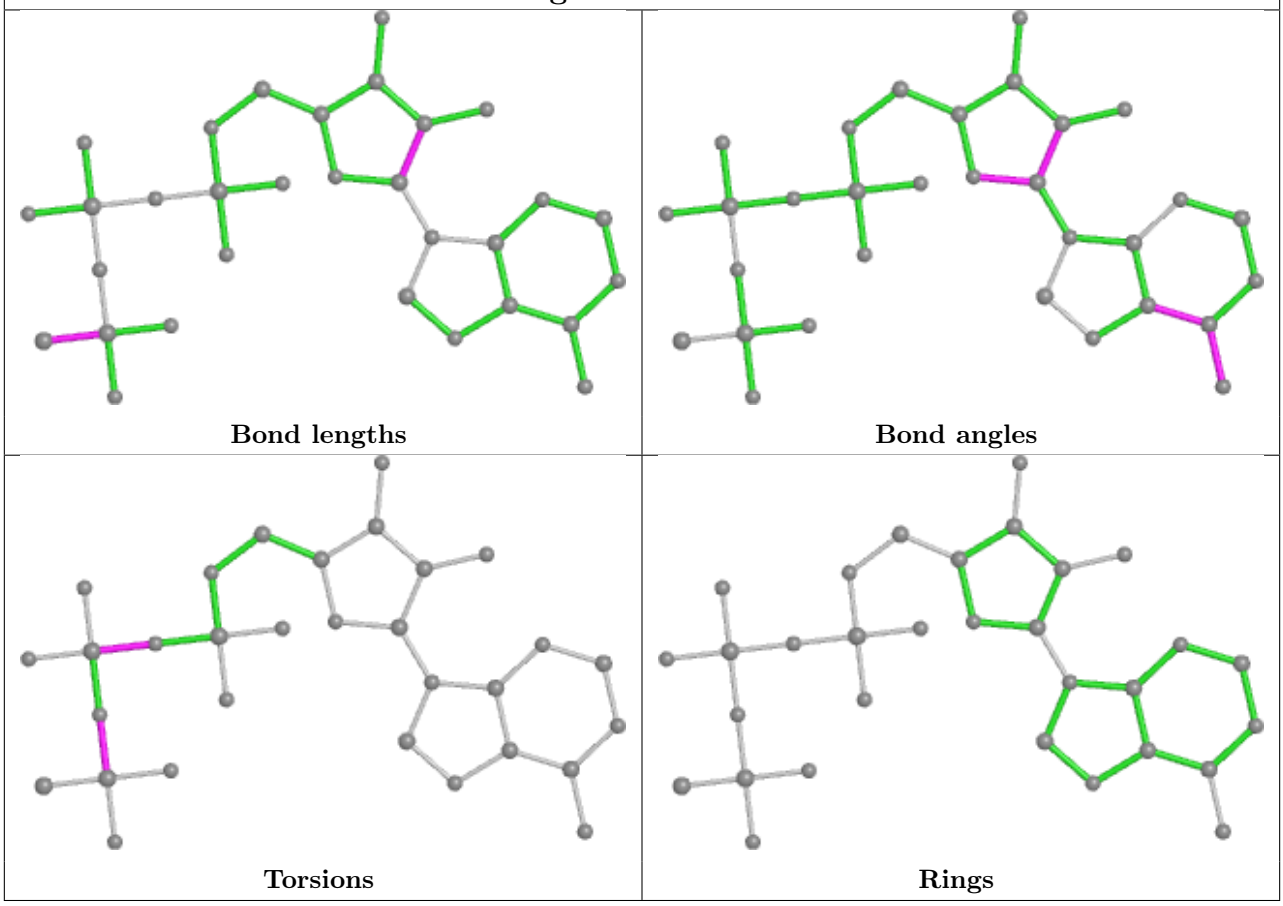
**Ligand AGS M 1**



**Ligand AGS K 1**



**Ligand AGS I 1**




## 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 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 525/547 (95%) | 0.72 | 69 (13%) | 3 | 3 | 28, 64, 121, 132 | 0 |
| 1 | B | 525/547 (95%) | 1.34 | 126 (24%) | 0 | 0 | 24, 59, 149, 159 | 0 |
| 1 | C | 525/547 (95%) | 1.15 | 115 (21%) | 0 | 0 | 29, 71, 141, 152 | 0 |
| 1 | D | 525/547 (95%) | 0.47 | 31 (5%) | 22 | 21 | 25, 48, 99, 115 | 0 |
| 1 | E | 525/547 (95%) | 0.99 | 99 (18%) | 1 | 1 | 23, 55, 134, 145 | 0 |
| 1 | F | 525/547 (95%) | 1.27 | 115 (21%) | 0 | 0 | 27, 66, 150, 159 | 0 |
| 1 | G | 525/547 (95%) | 0.58 | 43 (8%) | 11 | 11 | 26, 50, 113, 126 | 0 |
| 1 | H | 525/547 (95%) | 0.64 | 61 (11%) | 4 | 4 | 26, 56, 118, 130 | 0 |
| 1 | I | 525/547 (95%) | 0.96 | 81 (15%) | 2 | 1 | 31, 69, 132, 143 | 0 |
| 1 | J | 525/547 (95%) | 1.02 | 89 (16%) | 1 | 1 | 31, 73, 138, 146 | 0 |
| 1 | K | 525/547 (95%) | 1.43 | 139 (26%) | 0 | 0 | 31, 78, 151, 159 | 0 |
| 1 | L | 525/547 (95%) | 0.90 | 90 (17%) | 1 | 1 | 29, 66, 136, 149 | 0 |
| 1 | M | 525/547 (95%) | 1.35 | 136 (25%) | 0 | 0 | 30, 77, 152, 160 | 0 |
| 1 | N | 525/547 (95%) | 0.71 | 63 (12%) | 4 | 3 | 28, 65, 118, 129 | 0 |
| All | All | 7350/7658 (95%) | 0.97 | 1257 (17%) | 1 | 1 | 23, 60, 140, 160 | 0 |

All (1257) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 349 | ILE | 13.6 |
| 1 | F | 309 | LEU | 12.7 |
| 1 | K | 270 | ILE | 12.2 |
| 1 | K | 271 | VAL | 12.0 |
| 1 | K | 305 | ILE | 11.7 |
| 1 | B | 349 | ILE | 11.6 |
| 1 | M | 270 | ILE | 11.5 |
| 1 | K | 349 | ILE | 11.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 240 | VAL | 10.9 |
| 1 | F | 233 | MET | 10.7 |
| 1 | J | 356 | ALA | 10.6 |
| 1 | B | 233 | MET | 10.5 |
| 1 | E | 353 | ILE | 10.5 |
| 1 | E | 356 | ALA | 10.4 |
| 1 | F | 353 | ILE | 10.2 |
| 1 | M | 353 | ILE | 10.2 |
| 1 | J | 271 | VAL | 10.2 |
| 1 | B | 356 | ALA | 10.2 |
| 1 | I | 270 | ILE | 10.1 |
| 1 | J | 270 | ILE | 10.0 |
| 1 | C | 356 | ALA | 10.0 |
| 1 | L | 266 | THR | 10.0 |
| 1 | M | 259 | LEU | 9.9 |
| 1 | K | 309 | LEU | 9.8 |
| 1 | F | 314 | LEU | 9.7 |
| 1 | B | 230 | ILE | 9.5 |
| 1 | M | 233 | MET | 9.5 |
| 1 | N | 349 | ILE | 9.4 |
| 1 | K | 259 | LEU | 9.3 |
| 1 | B | 353 | ILE | 9.3 |
| 1 | K | 260 | ALA | 9.3 |
| 1 | E | 309 | LEU | 9.2 |
| 1 | E | 271 | VAL | 9.2 |
| 1 | M | 237 | LEU | 9.2 |
| 1 | J | 269 | GLY | 9.2 |
| 1 | F | 259 | LEU | 9.1 |
| 1 | C | 270 | ILE | 9.1 |
| 1 | K | 236 | VAL | 9.1 |
| 1 | M | 221 | LEU | 9.0 |
| 1 | K | 237 | LEU | 8.9 |
| 1 | C | 353 | ILE | 8.8 |
| 1 | K | 233 | MET | 8.8 |
| 1 | M | 271 | VAL | 8.8 |
| 1 | F | 349 | ILE | 8.7 |
| 1 | M | 223 | ALA | 8.6 |
| 1 | J | 349 | ILE | 8.6 |
| 1 | B | 264 | VAL | 8.5 |
| 1 | D | 271 | VAL | 8.3 |
| 1 | M | 314 | LEU | 8.3 |
| 1 | M | 240 | VAL | 8.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 270 | ILE | 8.2 |
| 1 | K | 231 | ARG | 8.2 |
| 1 | K | 360 | TYR | 8.1 |
| 1 | B | 301 | ILE | 8.1 |
| 1 | I | 305 | ILE | 8.0 |
| 1 | K | 267 | MET | 8.0 |
| 1 | J | 357 | THR | 8.0 |
| 1 | J | 268 | ARG | 8.0 |
| 1 | B | 227 | ILE | 7.9 |
| 1 | M | 267 | MET | 7.9 |
| 1 | I | 271 | VAL | 7.8 |
| 1 | J | 233 | MET | 7.8 |
| 1 | B | 365 | LEU | 7.8 |
| 1 | B | 258 | ALA | 7.7 |
| 1 | M | 309 | LEU | 7.7 |
| 1 | K | 356 | ALA | 7.7 |
| 1 | A | 270 | ILE | 7.7 |
| 1 | B | 281 | PHE | 7.7 |
| 1 | F | 360 | TYR | 7.7 |
| 1 | M | 272 | LYS | 7.7 |
| 1 | K | 264 | VAL | 7.7 |
| 1 | M | 357 | THR | 7.6 |
| 1 | M | 268 | ARG | 7.6 |
| 1 | M | 349 | ILE | 7.5 |
| 1 | B | 268 | ARG | 7.5 |
| 1 | K | 265 | ASN | 7.4 |
| 1 | L | 271 | VAL | 7.4 |
| 1 | K | 203 | TYR | 7.4 |
| 1 | M | 266 | THR | 7.3 |
| 1 | H | 309 | LEU | 7.3 |
| 1 | M | 356 | ALA | 7.3 |
| 1 | J | 309 | LEU | 7.3 |
| 1 | K | 268 | ARG | 7.2 |
| 1 | A | 356 | ALA | 7.2 |
| 1 | I | 264 | VAL | 7.2 |
| 1 | L | 270 | ILE | 7.1 |
| 1 | K | 353 | ILE | 7.0 |
| 1 | C | 271 | VAL | 7.0 |
| 1 | M | 239 | ALA | 6.9 |
| 1 | A | 353 | ILE | 6.9 |
| 1 | I | 265 | ASN | 6.9 |
| 1 | I | 356 | ALA | 6.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | K | 340 | ALA | 6.9 |
| 1 | E | 234 | LEU | 6.8 |
| 1 | E | 230 | ILE | 6.8 |
| 1 | I | 268 | ARG | 6.7 |
| 1 | E | 233 | MET | 6.7 |
| 1 | F | 227 | ILE | 6.7 |
| 1 | N | 263 | VAL | 6.7 |
| 1 | B | 259 | LEU | 6.7 |
| 1 | E | 349 | ILE | 6.7 |
| 1 | M | 244 | GLY | 6.7 |
| 1 | L | 231 | ARG | 6.7 |
| 1 | M | 264 | VAL | 6.7 |
| 1 | J | 353 | ILE | 6.7 |
| 1 | C | 268 | ARG | 6.7 |
| 1 | M | 358 | SER | 6.6 |
| 1 | F | 219 | PHE | 6.6 |
| 1 | J | 44 | PHE | 6.6 |
| 1 | F | 203 | TYR | 6.6 |
| 1 | L | 264 | VAL | 6.6 |
| 1 | M | 273 | VAL | 6.6 |
| 1 | M | 251 | ALA | 6.6 |
| 1 | F | 268 | ARG | 6.6 |
| 1 | J | 317 | LEU | 6.6 |
| 1 | F | 230 | ILE | 6.6 |
| 1 | F | 272 | LYS | 6.5 |
| 1 | F | 357 | THR | 6.5 |
| 1 | F | 267 | MET | 6.5 |
| 1 | B | 271 | VAL | 6.5 |
| 1 | K | 227 | ILE | 6.5 |
| 1 | E | 223 | ALA | 6.4 |
| 1 | J | 526 | LYS | 6.4 |
| 1 | B | 229 | ASN | 6.4 |
| 1 | B | 257 | GLU | 6.4 |
| 1 | F | 255 | GLU | 6.4 |
| 1 | B | 265 | ASN | 6.4 |
| 1 | I | 349 | ILE | 6.4 |
| 1 | B | 355 | GLU | 6.3 |
| 1 | K | 240 | VAL | 6.3 |
| 1 | E | 268 | ARG | 6.3 |
| 1 | N | 270 | ILE | 6.3 |
| 1 | B | 309 | LEU | 6.3 |
| 1 | M | 204 | PHE | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 237 | LEU | 6.3 |
| 1 | J | 264 | VAL | 6.3 |
| 1 | E | 266 | THR | 6.3 |
| 1 | B | 307 | MET | 6.3 |
| 1 | G | 230 | ILE | 6.2 |
| 1 | I | 230 | ILE | 6.2 |
| 1 | J | 266 | THR | 6.2 |
| 1 | M | 263 | VAL | 6.2 |
| 1 | K | 204 | PHE | 6.2 |
| 1 | L | 383 | ALA | 6.2 |
| 1 | F | 222 | LEU | 6.2 |
| 1 | E | 270 | ILE | 6.1 |
| 1 | K | 232 | GLU | 6.1 |
| 1 | C | 342 | ILE | 6.1 |
| 1 | E | 305 | ILE | 6.1 |
| 1 | L | 305 | ILE | 6.1 |
| 1 | H | 233 | MET | 6.1 |
| 1 | I | 353 | ILE | 6.1 |
| 1 | B | 357 | THR | 6.1 |
| 1 | K | 230 | ILE | 6.0 |
| 1 | F | 342 | ILE | 6.0 |
| 1 | M | 305 | ILE | 6.0 |
| 1 | F | 305 | ILE | 5.9 |
| 1 | N | 230 | ILE | 5.9 |
| 1 | C | 263 | VAL | 5.9 |
| 1 | B | 286 | LYS | 5.9 |
| 1 | B | 270 | ILE | 5.9 |
| 1 | F | 237 | LEU | 5.9 |
| 1 | N | 264 | VAL | 5.9 |
| 1 | F | 317 | LEU | 5.8 |
| 1 | E | 300 | VAL | 5.8 |
| 1 | F | 271 | VAL | 5.8 |
| 1 | C | 266 | THR | 5.8 |
| 1 | F | 231 | ARG | 5.8 |
| 1 | L | 269 | GLY | 5.8 |
| 1 | C | 249 | ILE | 5.8 |
| 1 | J | 305 | ILE | 5.8 |
| 1 | K | 256 | GLY | 5.8 |
| 1 | E | 357 | THR | 5.8 |
| 1 | F | 234 | LEU | 5.7 |
| 1 | L | 230 | ILE | 5.7 |
| 1 | K | 223 | ALA | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | M | 336 | VAL | 5.7 |
| 1 | I | 266 | THR | 5.7 |
| 1 | G | 383 | ALA | 5.7 |
| 1 | B | 240 | VAL | 5.7 |
| 1 | I | 352 | GLN | 5.6 |
| 1 | M | 265 | ASN | 5.6 |
| 1 | B | 203 | TYR | 5.6 |
| 1 | K | 219 | PHE | 5.6 |
| 1 | L | 309 | LEU | 5.6 |
| 1 | L | 268 | ARG | 5.6 |
| 1 | I | 526 | LYS | 5.6 |
| 1 | B | 269 | GLY | 5.6 |
| 1 | K | 306 | GLY | 5.6 |
| 1 | C | 369 | VAL | 5.5 |
| 1 | L | 234 | LEU | 5.5 |
| 1 | B | 342 | ILE | 5.5 |
| 1 | F | 389 | MET | 5.5 |
| 1 | G | 44 | PHE | 5.5 |
| 1 | H | 270 | ILE | 5.5 |
| 1 | C | 203 | TYR | 5.5 |
| 1 | C | 237 | LEU | 5.5 |
| 1 | C | 259 | LEU | 5.5 |
| 1 | K | 228 | SER | 5.5 |
| 1 | E | 312 | ALA | 5.4 |
| 1 | J | 351 | GLN | 5.4 |
| 1 | K | 269 | GLY | 5.4 |
| 1 | F | 245 | LYS | 5.4 |
| 1 | I | 360 | TYR | 5.4 |
| 1 | J | 263 | VAL | 5.4 |
| 1 | J | 358 | SER | 5.4 |
| 1 | B | 236 | VAL | 5.4 |
| 1 | M | 249 | ILE | 5.4 |
| 1 | E | 272 | LYS | 5.4 |
| 1 | B | 305 | ILE | 5.4 |
| 1 | K | 188 | ASP | 5.4 |
| 1 | M | 203 | TYR | 5.4 |
| 1 | I | 203 | TYR | 5.3 |
| 1 | B | 251 | ALA | 5.3 |
| 1 | B | 231 | ARG | 5.3 |
| 1 | J | 229 | ASN | 5.3 |
| 1 | M | 365 | LEU | 5.3 |
| 1 | M | 342 | ILE | 5.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | K | 241 | ALA | 5.3 |
| 1 | M | 335 | GLY | 5.3 |
| 1 | I | 272 | LYS | 5.3 |
| 1 | E | 351 | GLN | 5.3 |
| 1 | F | 44 | PHE | 5.2 |
| 1 | C | 365 | LEU | 5.2 |
| 1 | E | 203 | TYR | 5.2 |
| 1 | C | 261 | THR | 5.2 |
| 1 | C | 357 | THR | 5.2 |
| 1 | K | 234 | LEU | 5.2 |
| 1 | G | 271 | VAL | 5.2 |
| 1 | H | 234 | LEU | 5.2 |
| 1 | I | 234 | LEU | 5.2 |
| 1 | F | 273 | VAL | 5.2 |
| 1 | K | 383 | ALA | 5.2 |
| 1 | B | 351 | GLN | 5.2 |
| 1 | F | 355 | GLU | 5.2 |
| 1 | B | 237 | LEU | 5.2 |
| 1 | K | 272 | LYS | 5.2 |
| 1 | C | 256 | GLY | 5.1 |
| 1 | I | 355 | GLU | 5.1 |
| 1 | C | 295 | LEU | 5.1 |
| 1 | L | 259 | LEU | 5.1 |
| 1 | K | 273 | VAL | 5.1 |
| 1 | J | 219 | PHE | 5.1 |
| 1 | I | 267 | MET | 5.1 |
| 1 | C | 230 | ILE | 5.1 |
| 1 | H | 526 | LYS | 5.1 |
| 1 | C | 44 | PHE | 5.1 |
| 1 | I | 231 | ARG | 5.1 |
| 1 | M | 317 | LEU | 5.1 |
| 1 | B | 273 | VAL | 5.1 |
| 1 | K | 44 | PHE | 5.1 |
| 1 | B | 306 | GLY | 5.1 |
| 1 | C | 244 | GLY | 5.1 |
| 1 | H | 243 | ALA | 5.1 |
| 1 | F | 263 | VAL | 5.0 |
| 1 | F | 264 | VAL | 5.0 |
| 1 | C | 304 | GLU | 5.0 |
| 1 | K | 281 | PHE | 5.0 |
| 1 | M | 219 | PHE | 5.0 |
| 1 | B | 234 | LEU | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 231 | ARG | 5.0 |
| 1 | M | 260 | ALA | 5.0 |
| 1 | M | 186 | GLU | 5.0 |
| 1 | F | 241 | ALA | 5.0 |
| 1 | A | 44 | PHE | 5.0 |
| 1 | A | 263 | VAL | 5.0 |
| 1 | E | 301 | ILE | 5.0 |
| 1 | G | 270 | ILE | 5.0 |
| 1 | C | 372 | LEU | 4.9 |
| 1 | C | 264 | VAL | 4.9 |
| 1 | L | 258 | ALA | 4.9 |
| 1 | H | 229 | ASN | 4.9 |
| 1 | L | 227 | ILE | 4.9 |
| 1 | B | 262 | LEU | 4.9 |
| 1 | A | 349 | ILE | 4.9 |
| 1 | B | 44 | PHE | 4.9 |
| 1 | C | 333 | ILE | 4.9 |
| 1 | B | 526 | LYS | 4.9 |
| 1 | M | 195 | PHE | 4.9 |
| 1 | J | 265 | ASN | 4.9 |
| 1 | D | 270 | ILE | 4.9 |
| 1 | H | 353 | ILE | 4.9 |
| 1 | H | 356 | ALA | 4.8 |
| 1 | K | 275 | ALA | 4.8 |
| 1 | M | 340 | ALA | 4.8 |
| 1 | C | 360 | TYR | 4.8 |
| 1 | D | 44 | PHE | 4.8 |
| 1 | F | 365 | LEU | 4.8 |
| 1 | J | 281 | PHE | 4.8 |
| 1 | H | 268 | ARG | 4.8 |
| 1 | G | 267 | MET | 4.8 |
| 1 | I | 363 | GLU | 4.8 |
| 1 | I | 309 | LEU | 4.8 |
| 1 | L | 317 | LEU | 4.8 |
| 1 | K | 335 | GLY | 4.8 |
| 1 | L | 233 | MET | 4.8 |
| 1 | B | 266 | THR | 4.8 |
| 1 | C | 362 | ARG | 4.8 |
| 1 | D | 230 | ILE | 4.8 |
| 1 | M | 250 | ILE | 4.8 |
| 1 | J | 256 | GLY | 4.8 |
| 1 | K | 263 | VAL | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 355 | GLU | 4.7 |
| 1 | I | 243 | ALA | 4.7 |
| 1 | C | 233 | MET | 4.7 |
| 1 | I | 233 | MET | 4.7 |
| 1 | J | 204 | PHE | 4.7 |
| 1 | F | 243 | ALA | 4.7 |
| 1 | G | 265 | ASN | 4.7 |
| 1 | K | 358 | SER | 4.7 |
| 1 | M | 355 | GLU | 4.7 |
| 1 | B | 250 | ILE | 4.6 |
| 1 | F | 306 | GLY | 4.6 |
| 1 | H | 357 | THR | 4.6 |
| 1 | B | 317 | LEU | 4.6 |
| 1 | G | 259 | LEU | 4.6 |
| 1 | F | 315 | GLU | 4.6 |
| 1 | B | 372 | LEU | 4.6 |
| 1 | L | 356 | ALA | 4.6 |
| 1 | K | 160 | LYS | 4.6 |
| 1 | A | 182 | GLY | 4.6 |
| 1 | K | 247 | LEU | 4.6 |
| 1 | M | 351 | GLN | 4.6 |
| 1 | K | 302 | SER | 4.6 |
| 1 | L | 203 | TYR | 4.6 |
| 1 | C | 274 | ALA | 4.6 |
| 1 | E | 247 | LEU | 4.6 |
| 1 | E | 358 | SER | 4.6 |
| 1 | A | 268 | ARG | 4.6 |
| 1 | K | 357 | THR | 4.6 |
| 1 | B | 243 | ALA | 4.6 |
| 1 | F | 269 | GLY | 4.5 |
| 1 | F | 336 | VAL | 4.5 |
| 1 | E | 44 | PHE | 4.5 |
| 1 | M | 218 | PRO | 4.5 |
| 1 | A | 358 | SER | 4.5 |
| 1 | A | 361 | ASP | 4.5 |
| 1 | E | 231 | ARG | 4.5 |
| 1 | B | 295 | LEU | 4.5 |
| 1 | M | 222 | LEU | 4.5 |
| 1 | H | 44 | PHE | 4.5 |
| 1 | I | 357 | THR | 4.5 |
| 1 | F | 356 | ALA | 4.5 |
| 1 | G | 258 | ALA | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 273 | VAL | 4.5 |
| 1 | B | 223 | ALA | 4.5 |
| 1 | F | 258 | ALA | 4.5 |
| 1 | A | 357 | THR | 4.5 |
| 1 | I | 351 | GLN | 4.4 |
| 1 | J | 262 | LEU | 4.4 |
| 1 | C | 346 | VAL | 4.4 |
| 1 | E | 264 | VAL | 4.4 |
| 1 | D | 526 | LYS | 4.4 |
| 1 | E | 384 | ALA | 4.4 |
| 1 | F | 242 | LYS | 4.4 |
| 1 | L | 255 | GLU | 4.4 |
| 1 | M | 238 | GLU | 4.4 |
| 1 | K | 362 | ARG | 4.4 |
| 1 | A | 271 | VAL | 4.4 |
| 1 | B | 383 | ALA | 4.4 |
| 1 | G | 306 | GLY | 4.4 |
| 1 | K | 283 | ASP | 4.4 |
| 1 | E | 263 | VAL | 4.4 |
| 1 | C | 265 | ASN | 4.4 |
| 1 | E | 265 | ASN | 4.4 |
| 1 | B | 358 | SER | 4.4 |
| 1 | B | 363 | GLU | 4.4 |
| 1 | L | 267 | MET | 4.4 |
| 1 | N | 281 | PHE | 4.4 |
| 1 | B | 221 | LEU | 4.4 |
| 1 | B | 300 | VAL | 4.4 |
| 1 | H | 383 | ALA | 4.3 |
| 1 | F | 244 | GLY | 4.3 |
| 1 | D | 305 | ILE | 4.3 |
| 1 | C | 350 | ARG | 4.3 |
| 1 | K | 334 | ASP | 4.3 |
| 1 | L | 244 | GLY | 4.3 |
| 1 | C | 284 | ARG | 4.3 |
| 1 | M | 230 | ILE | 4.3 |
| 1 | F | 236 | VAL | 4.3 |
| 1 | M | 231 | ARG | 4.3 |
| 1 | A | 257 | GLU | 4.3 |
| 1 | B | 209 | GLU | 4.3 |
| 1 | C | 355 | GLU | 4.3 |
| 1 | J | 260 | ALA | 4.3 |
| 1 | K | 365 | LEU | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 260 | ALA | 4.3 |
| 1 | C | 267 | MET | 4.3 |
| 1 | M | 526 | LYS | 4.3 |
| 1 | B | 261 | THR | 4.2 |
| 1 | C | 292 | ILE | 4.2 |
| 1 | K | 351 | GLN | 4.2 |
| 1 | G | 264 | VAL | 4.2 |
| 1 | B | 180 | GLY | 4.2 |
| 1 | L | 526 | LYS | 4.2 |
| 1 | F | 266 | THR | 4.2 |
| 1 | E | 237 | LEU | 4.2 |
| 1 | F | 249 | ILE | 4.2 |
| 1 | F | 260 | ALA | 4.2 |
| 1 | H | 305 | ILE | 4.2 |
| 1 | B | 304 | GLU | 4.2 |
| 1 | J | 257 | GLU | 4.2 |
| 1 | J | 383 | ALA | 4.2 |
| 1 | F | 224 | ASP | 4.2 |
| 1 | E | 383 | ALA | 4.2 |
| 1 | B | 302 | SER | 4.2 |
| 1 | F | 351 | GLN | 4.2 |
| 1 | J | 362 | ARG | 4.1 |
| 1 | B | 225 | LYS | 4.1 |
| 1 | F | 346 | VAL | 4.1 |
| 1 | K | 346 | VAL | 4.1 |
| 1 | F | 228 | SER | 4.1 |
| 1 | C | 340 | ALA | 4.1 |
| 1 | L | 314 | LEU | 4.1 |
| 1 | M | 295 | LEU | 4.1 |
| 1 | E | 346 | VAL | 4.1 |
| 1 | B | 354 | GLU | 4.1 |
| 1 | C | 351 | GLN | 4.1 |
| 1 | M | 262 | LEU | 4.1 |
| 1 | D | 268 | ARG | 4.1 |
| 1 | C | 273 | VAL | 4.1 |
| 1 | E | 354 | GLU | 4.1 |
| 1 | J | 360 | TYR | 4.1 |
| 1 | M | 258 | ALA | 4.1 |
| 1 | K | 299 | THR | 4.1 |
| 1 | F | 225 | LYS | 4.1 |
| 1 | F | 358 | SER | 4.1 |
| 1 | F | 261 | THR | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 311 | LYS | 4.0 |
| 1 | M | 44 | PHE | 4.0 |
| 1 | H | 265 | ASN | 4.0 |
| 1 | E | 240 | VAL | 4.0 |
| 1 | I | 184 | GLN | 4.0 |
| 1 | K | 355 | GLU | 4.0 |
| 1 | E | 360 | TYR | 4.0 |
| 1 | L | 229 | ASN | 4.0 |
| 1 | D | 264 | VAL | 4.0 |
| 1 | F | 369 | VAL | 4.0 |
| 1 | I | 384 | ALA | 4.0 |
| 1 | K | 331 | THR | 4.0 |
| 1 | A | 187 | LEU | 4.0 |
| 1 | C | 231 | ARG | 4.0 |
| 1 | G | 268 | ARG | 4.0 |
| 1 | J | 203 | TYR | 4.0 |
| 1 | H | 349 | ILE | 4.0 |
| 1 | K | 332 | ILE | 4.0 |
| 1 | I | 44 | PHE | 4.0 |
| 1 | J | 333 | ILE | 4.0 |
| 1 | K | 350 | ARG | 4.0 |
| 1 | H | 355 | GLU | 4.0 |
| 1 | D | 266 | THR | 3.9 |
| 1 | B | 289 | LEU | 3.9 |
| 1 | F | 221 | LEU | 3.9 |
| 1 | M | 161 | LEU | 3.9 |
| 1 | I | 358 | SER | 3.9 |
| 1 | B | 244 | GLY | 3.9 |
| 1 | F | 256 | GLY | 3.9 |
| 1 | C | 161 | LEU | 3.9 |
| 1 | C | 526 | LYS | 3.9 |
| 1 | N | 356 | ALA | 3.9 |
| 1 | J | 367 | GLU | 3.9 |
| 1 | L | 311 | LYS | 3.9 |
| 1 | K | 307 | MET | 3.9 |
| 1 | E | 295 | LEU | 3.9 |
| 1 | B | 224 | ASP | 3.9 |
| 1 | M | 307 | MET | 3.9 |
| 1 | I | 269 | GLY | 3.9 |
| 1 | J | 355 | GLU | 3.9 |
| 1 | M | 180 | GLY | 3.9 |
| 1 | B | 293 | ALA | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | J | 361 | ASP | 3.8 |
| 1 | G | 229 | ASN | 3.8 |
| 1 | F | 265 | ASN | 3.8 |
| 1 | K | 258 | ALA | 3.8 |
| 1 | J | 267 | MET | 3.8 |
| 1 | B | 219 | PHE | 3.8 |
| 1 | C | 286 | LYS | 3.8 |
| 1 | L | 44 | PHE | 3.8 |
| 1 | E | 255 | GLU | 3.8 |
| 1 | K | 301 | ILE | 3.8 |
| 1 | M | 160 | LYS | 3.8 |
| 1 | C | 309 | LEU | 3.8 |
| 1 | M | 347 | ALA | 3.8 |
| 1 | C | 181 | THR | 3.8 |
| 1 | E | 257 | GLU | 3.8 |
| 1 | J | 365 | LEU | 3.8 |
| 1 | M | 350 | ARG | 3.8 |
| 1 | B | 282 | GLY | 3.8 |
| 1 | C | 219 | PHE | 3.8 |
| 1 | E | 242 | LYS | 3.8 |
| 1 | I | 211 | GLY | 3.8 |
| 1 | M | 269 | GLY | 3.8 |
| 1 | G | 233 | MET | 3.8 |
| 1 | L | 224 | ASP | 3.8 |
| 1 | K | 181 | THR | 3.7 |
| 1 | G | 182 | GLY | 3.7 |
| 1 | F | 381 | VAL | 3.7 |
| 1 | K | 274 | ALA | 3.7 |
| 1 | G | 325 | ILE | 3.7 |
| 1 | J | 342 | ILE | 3.7 |
| 1 | K | 372 | LEU | 3.7 |
| 1 | H | 264 | VAL | 3.7 |
| 1 | K | 369 | VAL | 3.7 |
| 1 | M | 301 | ILE | 3.7 |
| 1 | H | 346 | VAL | 3.7 |
| 1 | J | 381 | VAL | 3.7 |
| 1 | F | 214 | GLU | 3.7 |
| 1 | A | 261 | THR | 3.7 |
| 1 | F | 181 | THR | 3.7 |
| 1 | G | 266 | THR | 3.7 |
| 1 | K | 266 | THR | 3.7 |
| 1 | K | 250 | ILE | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | M | 333 | ILE | 3.6 |
| 1 | E | 345 | ARG | 3.6 |
| 1 | C | 347 | ALA | 3.6 |
| 1 | K | 304 | GLU | 3.6 |
| 1 | L | 239 | ALA | 3.6 |
| 1 | N | 256 | GLY | 3.6 |
| 1 | B | 314 | LEU | 3.6 |
| 1 | M | 261 | THR | 3.6 |
| 1 | B | 191 | GLU | 3.6 |
| 1 | C | 229 | ASN | 3.6 |
| 1 | J | 319 | GLN | 3.6 |
| 1 | K | 276 | VAL | 3.6 |
| 1 | I | 204 | PHE | 3.6 |
| 1 | B | 241 | ALA | 3.6 |
| 1 | F | 248 | LEU | 3.6 |
| 1 | I | 237 | LEU | 3.6 |
| 1 | J | 272 | LYS | 3.6 |
| 1 | K | 311 | LYS | 3.6 |
| 1 | F | 396 | VAL | 3.6 |
| 1 | A | 183 | LEU | 3.6 |
| 1 | G | 262 | LEU | 3.6 |
| 1 | A | 265 | ASN | 3.6 |
| 1 | J | 280 | GLY | 3.6 |
| 1 | L | 219 | PHE | 3.5 |
| 1 | L | 186 | GLU | 3.5 |
| 1 | K | 222 | LEU | 3.5 |
| 1 | F | 178 | GLU | 3.5 |
| 1 | F | 232 | GLU | 3.5 |
| 1 | J | 243 | ALA | 3.5 |
| 1 | L | 353 | ILE | 3.5 |
| 1 | H | 266 | THR | 3.5 |
| 1 | B | 238 | GLU | 3.5 |
| 1 | M | 236 | VAL | 3.5 |
| 1 | N | 258 | ALA | 3.5 |
| 1 | E | 220 | ILE | 3.5 |
| 1 | J | 273 | VAL | 3.5 |
| 1 | L | 185 | ASP | 3.5 |
| 1 | M | 254 | VAL | 3.5 |
| 1 | A | 231 | ARG | 3.5 |
| 1 | A | 237 | LEU | 3.5 |
| 1 | F | 340 | ALA | 3.5 |
| 1 | H | 242 | LYS | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 204 | PHE | 3.5 |
| 1 | C | 281 | PHE | 3.5 |
| 1 | H | 259 | LEU | 3.5 |
| 1 | B | 275 | ALA | 3.5 |
| 1 | I | 369 | VAL | 3.5 |
| 1 | A | 203 | TYR | 3.5 |
| 1 | L | 228 | SER | 3.5 |
| 1 | M | 188 | ASP | 3.4 |
| 1 | M | 286 | LYS | 3.4 |
| 1 | F | 251 | ALA | 3.4 |
| 1 | K | 215 | LEU | 3.4 |
| 1 | M | 383 | ALA | 3.4 |
| 1 | B | 298 | GLY | 3.4 |
| 1 | K | 345 | ARG | 3.4 |
| 1 | K | 213 | VAL | 3.4 |
| 1 | K | 352 | GLN | 3.4 |
| 1 | N | 266 | THR | 3.4 |
| 1 | L | 349 | ILE | 3.4 |
| 1 | M | 384 | ALA | 3.4 |
| 1 | N | 526 | LYS | 3.4 |
| 1 | F | 372 | LEU | 3.4 |
| 1 | L | 247 | LEU | 3.4 |
| 1 | K | 310 | GLU | 3.4 |
| 1 | B | 360 | TYR | 3.4 |
| 1 | F | 337 | GLY | 3.4 |
| 1 | M | 168 | LYS | 3.4 |
| 1 | F | 215 | LEU | 3.4 |
| 1 | J | 261 | THR | 3.4 |
| 1 | K | 191 | GLU | 3.4 |
| 1 | E | 284 | ARG | 3.4 |
| 1 | I | 258 | ALA | 3.4 |
| 1 | K | 152 | ALA | 3.4 |
| 1 | M | 235 | PRO | 3.4 |
| 1 | E | 215 | LEU | 3.4 |
| 1 | L | 222 | LEU | 3.4 |
| 1 | C | 300 | VAL | 3.4 |
| 1 | F | 300 | VAL | 3.4 |
| 1 | I | 240 | VAL | 3.4 |
| 1 | I | 263 | VAL | 3.4 |
| 1 | M | 346 | VAL | 3.4 |
| 1 | N | 363 | GLU | 3.4 |
| 1 | M | 389 | MET | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 223 | ALA | 3.3 |
| 1 | M | 354 | GLU | 3.3 |
| 1 | C | 332 | ILE | 3.3 |
| 1 | N | 365 | LEU | 3.3 |
| 1 | F | 180 | GLY | 3.3 |
| 1 | A | 284 | ARG | 3.3 |
| 1 | B | 263 | VAL | 3.3 |
| 1 | N | 44 | PHE | 3.3 |
| 1 | D | 325 | ILE | 3.3 |
| 1 | B | 222 | LEU | 3.3 |
| 1 | M | 217 | SER | 3.3 |
| 1 | A | 276 | VAL | 3.3 |
| 1 | A | 381 | VAL | 3.3 |
| 1 | C | 186 | GLU | 3.3 |
| 1 | L | 307 | MET | 3.3 |
| 1 | C | 212 | ALA | 3.3 |
| 1 | K | 243 | ALA | 3.3 |
| 1 | L | 275 | ALA | 3.3 |
| 1 | A | 266 | THR | 3.3 |
| 1 | G | 181 | THR | 3.3 |
| 1 | B | 249 | ILE | 3.3 |
| 1 | K | 221 | LEU | 3.3 |
| 1 | E | 267 | MET | 3.3 |
| 1 | N | 231 | ARG | 3.3 |
| 1 | H | 360 | TYR | 3.3 |
| 1 | K | 224 | ASP | 3.3 |
| 1 | D | 281 | PHE | 3.3 |
| 1 | C | 322 | ARG | 3.3 |
| 1 | L | 310 | GLU | 3.3 |
| 1 | M | 229 | ASN | 3.3 |
| 1 | H | 361 | ASP | 3.3 |
| 1 | C | 319 | GLN | 3.3 |
| 1 | C | 358 | SER | 3.3 |
| 1 | H | 358 | SER | 3.3 |
| 1 | K | 245 | LYS | 3.3 |
| 1 | A | 204 | PHE | 3.3 |
| 1 | E | 219 | PHE | 3.3 |
| 1 | K | 342 | ILE | 3.3 |
| 1 | B | 525 | PRO | 3.3 |
| 1 | E | 229 | ASN | 3.3 |
| 1 | K | 202 | PRO | 3.3 |
| 1 | C | 240 | VAL | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 263 | VAL | 3.3 |
| 1 | M | 320 | ALA | 3.3 |
| 1 | A | 188 | ASP | 3.2 |
| 1 | C | 306 | GLY | 3.2 |
| 1 | I | 245 | LYS | 3.2 |
| 1 | M | 343 | GLN | 3.2 |
| 1 | J | 363 | GLU | 3.2 |
| 1 | M | 322 | ARG | 3.2 |
| 1 | A | 365 | LEU | 3.2 |
| 1 | J | 354 | GLU | 3.2 |
| 1 | K | 376 | VAL | 3.2 |
| 1 | C | 242 | LYS | 3.2 |
| 1 | J | 248 | LEU | 3.2 |
| 1 | I | 340 | ALA | 3.2 |
| 1 | M | 300 | VAL | 3.2 |
| 1 | J | 242 | LYS | 3.2 |
| 1 | K | 297 | GLY | 3.2 |
| 1 | M | 360 | TYR | 3.2 |
| 1 | I | 259 | LEU | 3.2 |
| 1 | E | 304 | GLU | 3.2 |
| 1 | F | 361 | ASP | 3.2 |
| 1 | A | 355 | GLU | 3.2 |
| 1 | F | 186 | GLU | 3.2 |
| 1 | K | 214 | GLU | 3.2 |
| 1 | K | 255 | GLU | 3.2 |
| 1 | I | 215 | LEU | 3.2 |
| 1 | B | 346 | VAL | 3.2 |
| 1 | D | 231 | ARG | 3.2 |
| 1 | F | 322 | ARG | 3.2 |
| 1 | K | 242 | LYS | 3.2 |
| 1 | L | 272 | LYS | 3.2 |
| 1 | C | 272 | LYS | 3.1 |
| 1 | A | 304 | GLU | 3.1 |
| 1 | A | 363 | GLU | 3.1 |
| 1 | E | 342 | ILE | 3.1 |
| 1 | H | 230 | ILE | 3.1 |
| 1 | L | 324 | VAL | 3.1 |
| 1 | H | 351 | GLN | 3.1 |
| 1 | L | 206 | ASN | 3.1 |
| 1 | F | 354 | GLU | 3.1 |
| 1 | A | 260 | ALA | 3.1 |
| 1 | N | 203 | TYR | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 361 | ASP | 3.1 |
| 1 | D | 236 | VAL | 3.1 |
| 1 | K | 288 | MET | 3.1 |
| 1 | K | 300 | VAL | 3.1 |
| 1 | N | 362 | ARG | 3.1 |
| 1 | D | 383 | ALA | 3.1 |
| 1 | I | 383 | ALA | 3.1 |
| 1 | B | 256 | GLY | 3.1 |
| 1 | M | 224 | ASP | 3.1 |
| 1 | M | 181 | THR | 3.1 |
| 1 | B | 187 | LEU | 3.1 |
| 1 | G | 305 | ILE | 3.1 |
| 1 | K | 139 | SER | 3.1 |
| 1 | A | 264 | VAL | 3.1 |
| 1 | J | 240 | VAL | 3.1 |
| 1 | L | 381 | VAL | 3.1 |
| 1 | C | 260 | ALA | 3.1 |
| 1 | B | 284 | ARG | 3.1 |
| 1 | C | 363 | GLU | 3.1 |
| 1 | G | 257 | GLU | 3.1 |
| 1 | L | 382 | GLY | 3.1 |
| 1 | B | 215 | LEU | 3.1 |
| 1 | F | 161 | LEU | 3.1 |
| 1 | D | 323 | VAL | 3.1 |
| 1 | G | 311 | LYS | 3.1 |
| 1 | F | 384 | ALA | 3.1 |
| 1 | N | 357 | THR | 3.1 |
| 1 | B | 352 | GLN | 3.1 |
| 1 | E | 184 | GLN | 3.1 |
| 1 | A | 384 | ALA | 3.0 |
| 1 | E | 382 | GLY | 3.0 |
| 1 | F | 352 | GLN | 3.0 |
| 1 | K | 257 | GLU | 3.0 |
| 1 | K | 308 | GLU | 3.0 |
| 1 | M | 247 | LEU | 3.0 |
| 1 | E | 292 | ILE | 3.0 |
| 1 | F | 332 | ILE | 3.0 |
| 1 | N | 325 | ILE | 3.0 |
| 1 | M | 304 | GLU | 3.0 |
| 1 | L | 302 | SER | 3.0 |
| 1 | B | 267 | MET | 3.0 |
| 1 | E | 526 | LYS | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 180 | GLY | 3.0 |
| 1 | C | 247 | LEU | 3.0 |
| 1 | C | 317 | LEU | 3.0 |
| 1 | I | 336 | VAL | 3.0 |
| 1 | K | 320 | ALA | 3.0 |
| 1 | M | 323 | VAL | 3.0 |
| 1 | G | 231 | ARG | 3.0 |
| 1 | A | 181 | THR | 3.0 |
| 1 | A | 388 | GLU | 3.0 |
| 1 | C | 315 | GLU | 3.0 |
| 1 | J | 234 | LEU | 3.0 |
| 1 | K | 361 | ASP | 3.0 |
| 1 | A | 382 | GLY | 3.0 |
| 1 | D | 269 | GLY | 3.0 |
| 1 | N | 351 | GLN | 3.0 |
| 1 | C | 341 | ALA | 3.0 |
| 1 | N | 257 | GLU | 3.0 |
| 1 | A | 273 | VAL | 3.0 |
| 1 | A | 281 | PHE | 3.0 |
| 1 | E | 236 | VAL | 3.0 |
| 1 | L | 249 | ILE | 3.0 |
| 1 | L | 265 | ASN | 3.0 |
| 1 | F | 155 | ASP | 3.0 |
| 1 | K | 380 | LYS | 3.0 |
| 1 | H | 304 | GLU | 3.0 |
| 1 | B | 248 | LEU | 3.0 |
| 1 | F | 295 | LEU | 3.0 |
| 1 | F | 347 | ALA | 3.0 |
| 1 | K | 312 | ALA | 3.0 |
| 1 | K | 381 | VAL | 2.9 |
| 1 | M | 369 | VAL | 2.9 |
| 1 | F | 204 | PHE | 2.9 |
| 1 | F | 362 | ARG | 2.9 |
| 1 | D | 267 | MET | 2.9 |
| 1 | N | 354 | GLU | 2.9 |
| 1 | F | 319 | GLN | 2.9 |
| 1 | E | 258 | ALA | 2.9 |
| 1 | K | 341 | ALA | 2.9 |
| 1 | A | 245 | LYS | 2.9 |
| 1 | I | 310 | GLU | 2.9 |
| 1 | M | 216 | GLU | 2.9 |
| 1 | B | 313 | THR | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 325 | ILE | 2.9 |
| 1 | I | 302 | SER | 2.9 |
| 1 | H | 286 | LYS | 2.9 |
| 1 | H | 363 | GLU | 2.9 |
| 1 | C | 222 | LEU | 2.9 |
| 1 | B | 254 | VAL | 2.9 |
| 1 | D | 229 | ASN | 2.9 |
| 1 | B | 188 | ASP | 2.9 |
| 1 | L | 161 | LEU | 2.9 |
| 1 | M | 299 | THR | 2.9 |
| 1 | B | 390 | LYS | 2.9 |
| 1 | F | 238 | GLU | 2.9 |
| 1 | H | 300 | VAL | 2.9 |
| 1 | N | 284 | ARG | 2.9 |
| 1 | E | 224 | ASP | 2.9 |
| 1 | E | 274 | ALA | 2.9 |
| 1 | M | 243 | ALA | 2.9 |
| 1 | B | 255 | GLU | 2.9 |
| 1 | I | 257 | GLU | 2.9 |
| 1 | C | 220 | ILE | 2.9 |
| 1 | M | 363 | GLU | 2.9 |
| 1 | H | 269 | GLY | 2.9 |
| 1 | G | 243 | ALA | 2.9 |
| 1 | G | 234 | LEU | 2.9 |
| 1 | C | 172 | GLU | 2.9 |
| 1 | L | 308 | GLU | 2.9 |
| 1 | C | 301 | ILE | 2.8 |
| 1 | C | 305 | ILE | 2.8 |
| 1 | J | 184 | GLN | 2.8 |
| 1 | M | 308 | GLU | 2.8 |
| 1 | H | 314 | LEU | 2.8 |
| 1 | I | 314 | LEU | 2.8 |
| 1 | K | 323 | VAL | 2.8 |
| 1 | L | 240 | VAL | 2.8 |
| 1 | M | 182 | GLY | 2.8 |
| 1 | B | 332 | ILE | 2.8 |
| 1 | J | 250 | ILE | 2.8 |
| 1 | F | 223 | ALA | 2.8 |
| 1 | C | 221 | LEU | 2.8 |
| 1 | G | 269 | GLY | 2.8 |
| 1 | C | 226 | LYS | 2.8 |
| 1 | N | 346 | VAL | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | N | 369 | VAL | 2.8 |
| 1 | L | 325 | ILE | 2.8 |
| 1 | F | 385 | THR | 2.8 |
| 1 | B | 252 | GLU | 2.8 |
| 1 | I | 365 | LEU | 2.8 |
| 1 | K | 317 | LEU | 2.8 |
| 1 | C | 352 | GLN | 2.8 |
| 1 | A | 362 | ARG | 2.8 |
| 1 | G | 384 | ALA | 2.8 |
| 1 | M | 362 | ARG | 2.8 |
| 1 | K | 526 | LYS | 2.8 |
| 1 | E | 307 | MET | 2.8 |
| 1 | E | 188 | ASP | 2.8 |
| 1 | I | 229 | ASN | 2.8 |
| 1 | I | 361 | ASP | 2.8 |
| 1 | N | 265 | ASN | 2.8 |
| 1 | N | 360 | TYR | 2.8 |
| 1 | H | 271 | VAL | 2.8 |
| 1 | K | 164 | GLU | 2.8 |
| 1 | N | 304 | GLU | 2.8 |
| 1 | C | 250 | ILE | 2.8 |
| 1 | K | 205 | ILE | 2.8 |
| 1 | D | 203 | TYR | 2.8 |
| 1 | H | 365 | LEU | 2.8 |
| 1 | L | 336 | VAL | 2.7 |
| 1 | L | 304 | GLU | 2.7 |
| 1 | B | 228 | SER | 2.7 |
| 1 | B | 183 | LEU | 2.7 |
| 1 | C | 334 | ASP | 2.7 |
| 1 | N | 309 | LEU | 2.7 |
| 1 | B | 274 | ALA | 2.7 |
| 1 | E | 251 | ALA | 2.7 |
| 1 | B | 348 | GLN | 2.7 |
| 1 | C | 336 | VAL | 2.7 |
| 1 | B | 280 | GLY | 2.7 |
| 1 | I | 284 | ARG | 2.7 |
| 1 | M | 193 | MET | 2.7 |
| 1 | A | 301 | ILE | 2.7 |
| 1 | E | 250 | ILE | 2.7 |
| 1 | M | 220 | ILE | 2.7 |
| 1 | N | 283 | ASP | 2.7 |
| 1 | A | 209 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 184 | GLN | 2.7 |
| 1 | B | 336 | VAL | 2.7 |
| 1 | C | 299 | THR | 2.7 |
| 1 | K | 220 | ILE | 2.7 |
| 1 | L | 184 | GLN | 2.7 |
| 1 | M | 319 | GLN | 2.7 |
| 1 | B | 350 | ARG | 2.7 |
| 1 | I | 260 | ALA | 2.7 |
| 1 | A | 295 | LEU | 2.7 |
| 1 | A | 346 | VAL | 2.7 |
| 1 | H | 315 | GLU | 2.7 |
| 1 | B | 272 | LYS | 2.7 |
| 1 | K | 325 | ILE | 2.7 |
| 1 | L | 333 | ILE | 2.7 |
| 1 | C | 269 | GLY | 2.7 |
| 1 | C | 367 | GLU | 2.7 |
| 1 | I | 209 | GLU | 2.7 |
| 1 | D | 262 | LEU | 2.7 |
| 1 | H | 237 | LEU | 2.7 |
| 1 | M | 248 | LEU | 2.7 |
| 1 | M | 205 | ILE | 2.7 |
| 1 | J | 303 | GLU | 2.7 |
| 1 | M | 279 | PRO | 2.7 |
| 1 | N | 241 | ALA | 2.7 |
| 1 | L | 284 | ARG | 2.7 |
| 1 | I | 389 | MET | 2.7 |
| 1 | K | 295 | LEU | 2.7 |
| 1 | E | 232 | GLU | 2.6 |
| 1 | N | 311 | LYS | 2.6 |
| 1 | B | 205 | ILE | 2.6 |
| 1 | I | 250 | ILE | 2.6 |
| 1 | J | 301 | ILE | 2.6 |
| 1 | N | 353 | ILE | 2.6 |
| 1 | I | 304 | GLU | 2.6 |
| 1 | L | 315 | GLU | 2.6 |
| 1 | G | 314 | LEU | 2.6 |
| 1 | M | 234 | LEU | 2.6 |
| 1 | N | 382 | GLY | 2.6 |
| 1 | A | 250 | ILE | 2.6 |
| 1 | E | 249 | ILE | 2.6 |
| 1 | F | 250 | ILE | 2.6 |
| 1 | B | 186 | GLU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | L | 313 | THR | 2.6 |
| 1 | F | 343 | GLN | 2.6 |
| 1 | K | 253 | ASP | 2.6 |
| 1 | E | 339 | GLU | 2.6 |
| 1 | J | 177 | VAL | 2.6 |
| 1 | L | 273 | VAL | 2.6 |
| 1 | L | 462 | PRO | 2.6 |
| 1 | M | 315 | GLU | 2.6 |
| 1 | I | 286 | LYS | 2.6 |
| 1 | A | 305 | ILE | 2.6 |
| 1 | F | 350 | ARG | 2.6 |
| 1 | H | 297 | GLY | 2.6 |
| 1 | H | 335 | GLY | 2.6 |
| 1 | I | 256 | GLY | 2.6 |
| 1 | C | 248 | LEU | 2.6 |
| 1 | G | 309 | LEU | 2.6 |
| 1 | H | 317 | LEU | 2.6 |
| 1 | L | 232 | GLU | 2.6 |
| 1 | A | 256 | GLY | 2.6 |
| 1 | E | 381 | VAL | 2.6 |
| 1 | B | 322 | ARG | 2.6 |
| 1 | D | 257 | GLU | 2.6 |
| 1 | I | 301 | ILE | 2.6 |
| 1 | N | 267 | MET | 2.6 |
| 1 | E | 318 | GLY | 2.6 |
| 1 | C | 354 | GLU | 2.6 |
| 1 | J | 232 | GLU | 2.6 |
| 1 | A | 259 | LEU | 2.6 |
| 1 | A | 242 | LYS | 2.5 |
| 1 | E | 361 | ASP | 2.5 |
| 1 | M | 215 | LEU | 2.6 |
| 1 | A | 300 | VAL | 2.5 |
| 1 | M | 376 | VAL | 2.5 |
| 1 | I | 154 | SER | 2.5 |
| 1 | C | 209 | GLU | 2.5 |
| 1 | F | 281 | PHE | 2.5 |
| 1 | C | 215 | LEU | 2.5 |
| 1 | L | 200 | LEU | 2.5 |
| 1 | L | 262 | LEU | 2.5 |
| 1 | M | 183 | LEU | 2.5 |
| 1 | B | 381 | VAL | 2.5 |
| 1 | C | 85 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | N | 254 | VAL | 2.5 |
| 1 | M | 256 | GLY | 2.5 |
| 1 | E | 352 | GLN | 2.5 |
| 1 | M | 184 | GLN | 2.5 |
| 1 | D | 234 | LEU | 2.5 |
| 1 | E | 317 | LEU | 2.5 |
| 1 | M | 200 | LEU | 2.5 |
| 1 | D | 382 | GLY | 2.5 |
| 1 | H | 261 | THR | 2.5 |
| 1 | C | 391 | GLU | 2.5 |
| 1 | E | 214 | GLU | 2.5 |
| 1 | J | 304 | GLU | 2.5 |
| 1 | C | 160 | LYS | 2.5 |
| 1 | K | 180 | GLY | 2.5 |
| 1 | E | 261 | THR | 2.5 |
| 1 | G | 261 | THR | 2.5 |
| 1 | J | 288 | MET | 2.5 |
| 1 | J | 387 | VAL | 2.5 |
| 1 | B | 303 | GLU | 2.5 |
| 1 | B | 335 | GLY | 2.5 |
| 1 | F | 359 | ASP | 2.5 |
| 1 | B | 239 | ALA | 2.5 |
| 1 | F | 239 | ALA | 2.5 |
| 1 | F | 339 | GLU | 2.5 |
| 1 | J | 275 | ALA | 2.5 |
| 1 | H | 245 | LYS | 2.5 |
| 1 | H | 284 | ARG | 2.5 |
| 1 | N | 268 | ARG | 2.5 |
| 1 | C | 217 | SER | 2.5 |
| 1 | C | 337 | GLY | 2.5 |
| 1 | F | 363 | GLU | 2.5 |
| 1 | M | 298 | GLY | 2.5 |
| 1 | N | 305 | ILE | 2.5 |
| 1 | K | 321 | LYS | 2.5 |
| 1 | J | 384 | ALA | 2.5 |
| 1 | L | 281 | PHE | 2.5 |
| 1 | I | 183 | LEU | 2.4 |
| 1 | K | 248 | LEU | 2.4 |
| 1 | M | 330 | THR | 2.4 |
| 1 | B | 367 | GLU | 2.4 |
| 1 | J | 334 | ASP | 2.4 |
| 1 | L | 283 | ASP | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | M | 361 | ASP | 2.4 |
| 1 | J | 152 | ALA | 2.4 |
| 1 | N | 260 | ALA | 2.4 |
| 1 | J | 181 | THR | 2.4 |
| 1 | K | 284 | ARG | 2.4 |
| 1 | I | 372 | LEU | 2.4 |
| 1 | M | 232 | GLU | 2.4 |
| 1 | G | 283 | ASP | 2.4 |
| 1 | G | 236 | VAL | 2.4 |
| 1 | F | 285 | ARG | 2.4 |
| 1 | J | 332 | ILE | 2.4 |
| 1 | K | 333 | ILE | 2.4 |
| 1 | L | 351 | GLN | 2.4 |
| 1 | E | 299 | THR | 2.4 |
| 1 | H | 313 | THR | 2.4 |
| 1 | K | 261 | THR | 2.4 |
| 1 | M | 311 | LYS | 2.4 |
| 1 | E | 365 | LEU | 2.4 |
| 1 | G | 221 | LEU | 2.4 |
| 1 | H | 306 | GLY | 2.4 |
| 1 | L | 306 | GLY | 2.4 |
| 1 | M | 159 | GLY | 2.4 |
| 1 | H | 236 | VAL | 2.4 |
| 1 | I | 276 | VAL | 2.4 |
| 1 | B | 308 | GLU | 2.4 |
| 1 | C | 214 | GLU | 2.4 |
| 1 | A | 286 | LYS | 2.4 |
| 1 | M | 316 | ASP | 2.4 |
| 1 | K | 175 | ILE | 2.4 |
| 1 | J | 228 | SER | 2.4 |
| 1 | A | 354 | GLU | 2.4 |
| 1 | B | 344 | GLY | 2.4 |
| 1 | E | 338 | GLU | 2.4 |
| 1 | L | 215 | LEU | 2.4 |
| 1 | K | 364 | LYS | 2.4 |
| 1 | C | 155 | ASP | 2.4 |
| 1 | M | 185 | ASP | 2.4 |
| 1 | F | 333 | ILE | 2.4 |
| 1 | J | 302 | SER | 2.4 |
| 1 | M | 302 | SER | 2.4 |
| 1 | M | 310 | GLU | 2.4 |
| 1 | M | 329 | THR | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 184 | GLN | 2.4 |
| 1 | D | 284 | ARG | 2.4 |
| 1 | G | 382 | GLY | 2.4 |
| 1 | I | 362 | ARG | 2.4 |
| 1 | L | 204 | PHE | 2.4 |
| 1 | N | 259 | LEU | 2.4 |
| 1 | N | 317 | LEU | 2.4 |
| 1 | M | 324 | VAL | 2.4 |
| 1 | M | 164 | GLU | 2.4 |
| 1 | I | 288 | MET | 2.4 |
| 1 | L | 384 | ALA | 2.4 |
| 1 | B | 285 | ARG | 2.4 |
| 1 | C | 184 | GLN | 2.4 |
| 1 | F | 157 | THR | 2.4 |
| 1 | H | 272 | LYS | 2.4 |
| 1 | L | 361 | ASP | 2.4 |
| 1 | E | 289 | LEU | 2.3 |
| 1 | J | 215 | LEU | 2.3 |
| 1 | K | 161 | LEU | 2.3 |
| 1 | K | 326 | ASN | 2.3 |
| 1 | C | 168 | LYS | 2.3 |
| 1 | E | 225 | LYS | 2.3 |
| 1 | L | 256 | GLY | 2.3 |
| 1 | I | 334 | ASP | 2.3 |
| 1 | I | 354 | GLU | 2.3 |
| 1 | L | 332 | ILE | 2.3 |
| 1 | J | 245 | LYS | 2.3 |
| 1 | K | 290 | GLN | 2.3 |
| 1 | N | 350 | ARG | 2.3 |
| 1 | C | 236 | VAL | 2.3 |
| 1 | M | 381 | VAL | 2.3 |
| 1 | B | 310 | GLU | 2.3 |
| 1 | K | 249 | ILE | 2.3 |
| 1 | A | 360 | TYR | 2.3 |
| 1 | B | 204 | PHE | 2.3 |
| 1 | B | 247 | LEU | 2.3 |
| 1 | J | 200 | LEU | 2.3 |
| 1 | M | 187 | LEU | 2.3 |
| 1 | N | 161 | LEU | 2.3 |
| 1 | N | 314 | LEU | 2.3 |
| 1 | I | 346 | VAL | 2.3 |
| 1 | N | 77 | VAL | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 287 | ALA | 2.3 |
| 1 | E | 286 | LYS | 2.3 |
| 1 | E | 287 | ALA | 2.3 |
| 1 | C | 325 | ILE | 2.3 |
| 1 | H | 333 | ILE | 2.3 |
| 1 | J | 150 | ILE | 2.3 |
| 1 | L | 257 | GLU | 2.3 |
| 1 | M | 325 | ILE | 2.3 |
| 1 | E | 168 | LYS | 2.3 |
| 1 | I | 364 | LYS | 2.3 |
| 1 | L | 237 | LEU | 2.3 |
| 1 | N | 358 | SER | 2.3 |
| 1 | E | 341 | ALA | 2.3 |
| 1 | H | 273 | VAL | 2.3 |
| 1 | J | 274 | ALA | 2.3 |
| 1 | N | 240 | VAL | 2.3 |
| 1 | M | 191 | GLU | 2.3 |
| 1 | A | 322 | ARG | 2.3 |
| 1 | B | 389 | MET | 2.3 |
| 1 | F | 288 | MET | 2.3 |
| 1 | K | 239 | ALA | 2.3 |
| 1 | L | 347 | ALA | 2.3 |
| 1 | I | 300 | VAL | 2.3 |
| 1 | G | 244 | GLY | 2.3 |
| 1 | B | 292 | ILE | 2.3 |
| 1 | H | 339 | GLU | 2.3 |
| 1 | A | 288 | MET | 2.2 |
| 1 | A | 311 | LYS | 2.2 |
| 1 | E | 222 | LEU | 2.2 |
| 1 | F | 321 | LYS | 2.2 |
| 1 | G | 295 | LEU | 2.2 |
| 1 | K | 371 | LYS | 2.2 |
| 1 | N | 275 | ALA | 2.2 |
| 1 | N | 224 | ASP | 2.2 |
| 1 | A | 351 | GLN | 2.2 |
| 1 | K | 184 | GLN | 2.2 |
| 1 | K | 322 | ARG | 2.2 |
| 1 | M | 388 | GLU | 2.2 |
| 1 | N | 255 | GLU | 2.2 |
| 1 | E | 256 | GLY | 2.2 |
| 1 | A | 359 | ASP | 2.2 |
| 1 | I | 359 | ASP | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 200 | LEU | 2.2 |
| 1 | C | 275 | ALA | 2.2 |
| 1 | M | 274 | ALA | 2.2 |
| 1 | N | 383 | ALA | 2.2 |
| 1 | F | 257 | GLU | 2.2 |
| 1 | K | 367 | GLU | 2.2 |
| 1 | K | 386 | GLU | 2.2 |
| 1 | N | 186 | GLU | 2.2 |
| 1 | B | 369 | VAL | 2.2 |
| 1 | C | 290 | GLN | 2.2 |
| 1 | C | 378 | VAL | 2.2 |
| 1 | E | 350 | ARG | 2.2 |
| 1 | J | 345 | ARG | 2.2 |
| 1 | N | 273 | VAL | 2.2 |
| 1 | K | 229 | ASN | 2.2 |
| 1 | D | 233 | MET | 2.2 |
| 1 | E | 193 | MET | 2.2 |
| 1 | H | 231 | ARG | 2.2 |
| 1 | K | 278 | ALA | 2.2 |
| 1 | K | 319 | GLN | 2.2 |
| 1 | K | 366 | GLN | 2.2 |
| 1 | A | 262 | LEU | 2.2 |
| 1 | C | 234 | LEU | 2.2 |
| 1 | K | 183 | LEU | 2.2 |
| 1 | C | 201 | SER | 2.2 |
| 1 | F | 213 | VAL | 2.2 |
| 1 | E | 334 | ASP | 2.2 |
| 1 | E | 238 | GLU | 2.2 |
| 1 | E | 363 | GLU | 2.2 |
| 1 | B | 288 | MET | 2.2 |
| 1 | E | 288 | MET | 2.2 |
| 1 | I | 193 | MET | 2.2 |
| 1 | L | 225 | LYS | 2.2 |
| 1 | D | 181 | THR | 2.2 |
| 1 | J | 325 | ILE | 2.2 |
| 1 | A | 244 | GLY | 2.2 |
| 1 | D | 314 | LEU | 2.2 |
| 1 | F | 183 | LEU | 2.2 |
| 1 | I | 317 | LEU | 2.2 |
| 1 | G | 228 | SER | 2.2 |
| 1 | L | 201 | SER | 2.2 |
| 1 | F | 310 | GLU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | N | 184 | GLN | 2.2 |
| 1 | G | 326 | ASN | 2.2 |
| 1 | C | 258 | ALA | 2.2 |
| 1 | E | 227 | ILE | 2.2 |
| 1 | F | 297 | GLY | 2.2 |
| 1 | K | 363 | GLU | 2.2 |
| 1 | L | 355 | GLU | 2.2 |
| 1 | H | 332 | ILE | 2.2 |
| 1 | A | 526 | LYS | 2.2 |
| 1 | F | 160 | LYS | 2.2 |
| 1 | I | 311 | LYS | 2.2 |
| 1 | J | 395 | ARG | 2.2 |
| 1 | N | 242 | LYS | 2.2 |
| 1 | H | 319 | GLN | 2.2 |
| 1 | G | 263 | VAL | 2.2 |
| 1 | J | 376 | VAL | 2.2 |
| 1 | L | 190 | VAL | 2.2 |
| 1 | L | 236 | VAL | 2.2 |
| 1 | M | 281 | PHE | 2.2 |
| 1 | A | 339 | GLU | 2.2 |
| 1 | C | 216 | GLU | 2.2 |
| 1 | K | 186 | GLU | 2.2 |
| 1 | N | 391 | GLU | 2.2 |
| 1 | B | 181 | THR | 2.2 |
| 1 | B | 297 | GLY | 2.2 |
| 1 | J | 244 | GLY | 2.2 |
| 1 | M | 294 | THR | 2.2 |
| 1 | M | 306 | GLY | 2.2 |
| 1 | I | 228 | SER | 2.2 |
| 1 | J | 284 | ARG | 2.2 |
| 1 | J | 221 | LEU | 2.1 |
| 1 | A | 236 | VAL | 2.1 |
| 1 | A | 240 | VAL | 2.1 |
| 1 | J | 369 | VAL | 2.1 |
| 1 | C | 188 | ASP | 2.1 |
| 1 | D | 188 | ASP | 2.1 |
| 1 | A | 350 | ARG | 2.1 |
| 1 | C | 348 | GLN | 2.1 |
| 1 | C | 303 | GLU | 2.1 |
| 1 | L | 289 | LEU | 2.1 |
| 1 | L | 372 | LEU | 2.1 |
| 1 | A | 207 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | L | 245 | LYS | 2.1 |
| 1 | I | 236 | VAL | 2.1 |
| 1 | L | 213 | VAL | 2.1 |
| 1 | A | 267 | MET | 2.1 |
| 1 | E | 43 | SER | 2.1 |
| 1 | B | 331 | THR | 2.1 |
| 1 | C | 178 | GLU | 2.1 |
| 1 | E | 239 | ALA | 2.1 |
| 1 | I | 341 | ALA | 2.1 |
| 1 | J | 223 | ALA | 2.1 |
| 1 | L | 212 | ALA | 2.1 |
| 1 | E | 160 | LYS | 2.1 |
| 1 | K | 168 | LYS | 2.1 |
| 1 | G | 220 | ILE | 2.1 |
| 1 | I | 248 | LEU | 2.1 |
| 1 | J | 259 | LEU | 2.1 |
| 1 | H | 257 | GLU | 2.1 |
| 1 | N | 228 | SER | 2.1 |
| 1 | F | 364 | LYS | 2.1 |
| 1 | F | 316 | ASP | 2.1 |
| 1 | E | 366 | GLN | 2.1 |
| 1 | K | 292 | ILE | 2.1 |
| 1 | E | 372 | LEU | 2.1 |
| 1 | N | 134 | LEU | 2.1 |
| 1 | K | 254 | VAL | 2.1 |
| 1 | L | 369 | VAL | 2.1 |
| 1 | C | 210 | THR | 2.1 |
| 1 | F | 313 | THR | 2.1 |
| 1 | D | 253 | ASP | 2.1 |
| 1 | B | 290 | GLN | 2.1 |
| 1 | G | 255 | GLU | 2.1 |
| 1 | M | 252 | GLU | 2.1 |
| 1 | C | 134 | LEU | 2.1 |
| 1 | E | 259 | LEU | 2.1 |
| 1 | F | 247 | LEU | 2.1 |
| 1 | H | 222 | LEU | 2.1 |
| 1 | B | 324 | VAL | 2.1 |
| 1 | C | 252 | GLU | 2.1 |
| 1 | F | 308 | GLU | 2.1 |
| 1 | J | 206 | ASN | 2.1 |
| 1 | N | 355 | GLU | 2.1 |
| 1 | M | 278 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | M | 142 | LYS | 2.1 |
| 1 | E | 297 | GLY | 2.1 |
| 1 | B | 388 | GLU | 2.0 |
| 1 | K | 315 | GLU | 2.0 |
| 1 | M | 338 | GLU | 2.0 |
| 1 | C | 314 | LEU | 2.0 |
| 1 | D | 215 | LEU | 2.0 |
| 1 | G | 319 | GLN | 2.0 |
| 1 | E | 336 | VAL | 2.0 |
| 1 | G | 403 | THR | 2.0 |
| 1 | K | 401 | HIS | 2.0 |
| 1 | N | 223 | ALA | 2.0 |
| 1 | N | 271 | VAL | 2.0 |
| 1 | H | 281 | PHE | 2.0 |
| 1 | E | 306 | GLY | 2.0 |
| 1 | J | 201 | SER | 2.0 |
| 1 | M | 345 | ARG | 2.0 |
| 1 | F | 290 | GLN | 2.0 |
| 1 | I | 366 | GLN | 2.0 |
| 1 | E | 183 | LEU | 2.0 |
| 1 | L | 323 | VAL | 2.0 |
| 1 | H | 298 | GLY | 2.0 |
| 1 | H | 184 | GLN | 2.0 |
| 1 | B | 235 | PRO | 2.0 |
| 1 | N | 397 | GLU | 2.0 |
| 1 | I | 249 | ILE | 2.0 |
| 1 | J | 230 | ILE | 2.0 |
| 1 | L | 243 | ALA | 2.0 |
| 1 | N | 372 | LEU | 2.0 |
| 1 | H | 323 | VAL | 2.0 |
| 1 | M | 352 | GLN | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | SO4 | K | 4021 | 5/5 | 0.55 | 0.44 | 137,138,139,139 | 0 |
| 2 | SO4 | H | 4017 | 5/5 | 0.68 | 0.33 | 145,146,146,146 | 0 |
| 2 | SO4 | C | 4012 | 5/5 | 0.70 | 0.27 | 141,141,141,142 | 0 |
| 2 | SO4 | M | 4014 | 5/5 | 0.74 | 0.24 | 142,142,143,143 | 0 |
| 2 | SO4 | J | 4020 | 5/5 | 0.75 | 0.47 | 160,160,160,160 | 0 |
| 2 | SO4 | E | 4006 | 5/5 | 0.75 | 0.33 | 118,119,119,120 | 0 |
| 2 | SO4 | L | 4003 | 5/5 | 0.75 | 0.25 | 130,131,132,132 | 0 |
| 2 | SO4 | H | 4018 | 5/5 | 0.75 | 0.33 | 125,125,126,126 | 0 |
| 2 | SO4 | A | 4008 | 5/5 | 0.77 | 0.36 | 150,150,150,150 | 0 |
| 2 | SO4 | M | 4013 | 5/5 | 0.81 | 0.23 | 126,126,127,127 | 0 |
| 2 | SO4 | G | 4002 | 5/5 | 0.82 | 0.27 | 128,128,129,129 | 0 |
| 2 | SO4 | C | 4011 | 5/5 | 0.83 | 0.29 | 137,137,137,138 | 0 |
| 2 | SO4 | N | 4016 | 5/5 | 0.83 | 0.26 | 137,137,137,138 | 0 |
| 2 | SO4 | F | 4004 | 5/5 | 0.84 | 0.31 | 137,138,138,138 | 0 |
| 2 | SO4 | B | 4010 | 5/5 | 0.84 | 0.29 | 137,137,137,138 | 0 |
| 2 | SO4 | A | 4007 | 5/5 | 0.84 | 0.27 | 128,129,129,129 | 0 |
| 2 | SO4 | K | 4022 | 5/5 | 0.84 | 0.27 | 145,146,146,146 | 0 |
| 2 | SO4 | N | 4015 | 5/5 | 0.85 | 0.27 | 132,133,133,133 | 0 |
| 2 | SO4 | A | 4001 | 5/5 | 0.86 | 0.24 | 119,120,120,120 | 0 |
| 2 | SO4 | B | 4009 | 5/5 | 0.86 | 0.28 | 118,119,119,120 | 0 |
| 2 | SO4 | E | 4005 | 5/5 | 0.87 | 0.35 | 140,141,141,141 | 0 |
| 2 | SO4 | J | 4019 | 5/5 | 0.89 | 0.23 | 123,124,124,124 | 0 |
| 3 | MG | L | 550 | 1/1 | 0.92 | 0.12 | 31,31,31,31 | 0 |
| 5 | AGS | D | 551 | 31/31 | 0.94 | 0.16 | 25,31,39,41 | 0 |
| 3 | MG | B | 550 | 1/1 | 0.95 | 0.14 | 31,31,31,31 | 0 |
| 5 | AGS | F | 1 | 31/31 | 0.95 | 0.14 | 34,37,44,45 | 0 |
| 5 | AGS | G | 1 | 31/31 | 0.95 | 0.14 | 25,32,40,41 | 0 |
| 5 | AGS | J | 1 | 31/31 | 0.95 | 0.13 | 39,42,53,54 | 0 |
| 5 | AGS | K | 1 | 31/31 | 0.95 | 0.13 | 37,40,51,54 | 0 |
| 5 | AGS | L | 1 | 31/31 | 0.95 | 0.14 | 34,37,45,48 | 0 |
| 5 | AGS | M | 1 | 31/31 | 0.95 | 0.14 | 38,42,50,52 | 0 |
| 4 | K | N | 549 | 1/1 | 0.96 | 0.13 | 41,41,41,41 | 0 |
| 5 | AGS | A | 1 | 31/31 | 0.96 | 0.12 | 35,38,42,44 | 0 |
| 5 | AGS | H | 1 | 31/31 | 0.96 | 0.13 | 30,34,38,42 | 0 |
| 5 | AGS | I | 1 | 31/31 | 0.96 | 0.14 | 37,41,48,51 | 0 |
| 5 | AGS | B | 1 | 31/31 | 0.96 | 0.12 | 31,37,48,50 | 0 |
| 5 | AGS | C | 1 | 31/31 | 0.96 | 0.14 | 37,41,49,52 | 0 |

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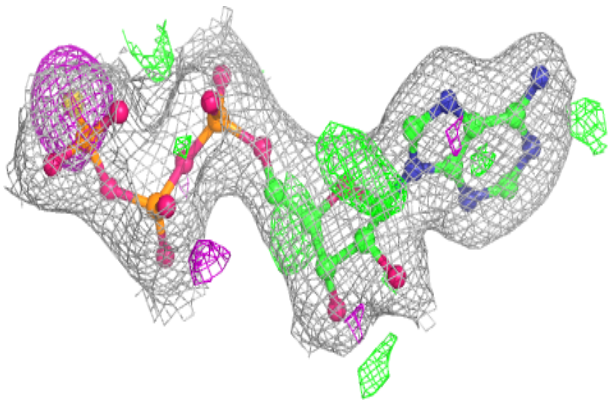
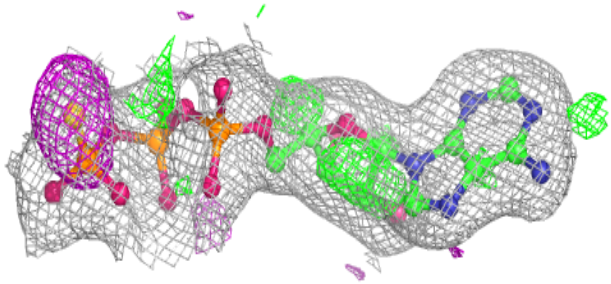
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | MG | A | 550 | 1/1 | 0.96 | 0.18 | 31,31,31,31 | 0 |
| 5 | AGS | E | 1 | 31/31 | 0.96 | 0.12 | 27,30,34,37 | 0 |
| 5 | AGS | N | 1 | 31/31 | 0.96 | 0.14 | 35,39,47,48 | 0 |
| 3 | MG | G | 550 | 1/1 | 0.97 | 0.19 | 29,29,29,29 | 0 |
| 3 | MG | K | 550 | 1/1 | 0.97 | 0.12 | 35,35,35,35 | 0 |
| 3 | MG | D | 550 | 1/1 | 0.97 | 0.14 | 29,29,29,29 | 0 |
| 3 | MG | N | 550 | 1/1 | 0.97 | 0.20 | 34,34,34,34 | 0 |
| 4 | K | C | 549 | 1/1 | 0.97 | 0.12 | 45,45,45,45 | 0 |
| 4 | K | K | 549 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 3 | MG | F | 550 | 1/1 | 0.97 | 0.13 | 30,30,30,30 | 0 |
| 4 | K | G | 549 | 1/1 | 0.98 | 0.15 | 39,39,39,39 | 0 |
| 4 | K | H | 549 | 1/1 | 0.98 | 0.15 | 41,41,41,41 | 0 |
| 3 | MG | E | 550 | 1/1 | 0.98 | 0.10 | 24,24,24,24 | 0 |
| 3 | MG | H | 550 | 1/1 | 0.98 | 0.15 | 26,26,26,26 | 0 |
| 3 | MG | M | 550 | 1/1 | 0.98 | 0.19 | 38,38,38,38 | 0 |
| 3 | MG | I | 550 | 1/1 | 0.98 | 0.17 | 34,34,34,34 | 0 |
| 4 | K | B | 549 | 1/1 | 0.98 | 0.12 | 38,38,38,38 | 0 |
| 3 | MG | J | 550 | 1/1 | 0.98 | 0.13 | 37,37,37,37 | 0 |
| 4 | K | D | 549 | 1/1 | 0.98 | 0.14 | 34,34,34,34 | 0 |
| 4 | K | I | 549 | 1/1 | 0.99 | 0.18 | 43,43,43,43 | 0 |
| 4 | K | J | 549 | 1/1 | 0.99 | 0.14 | 47,47,47,47 | 0 |
| 3 | MG | C | 550 | 1/1 | 0.99 | 0.15 | 36,36,36,36 | 0 |
| 4 | K | L | 549 | 1/1 | 0.99 | 0.15 | 39,39,39,39 | 0 |
| 4 | K | M | 549 | 1/1 | 0.99 | 0.14 | 45,45,45,45 | 0 |
| 4 | K | E | 549 | 1/1 | 0.99 | 0.08 | 31,31,31,31 | 0 |
| 4 | K | E | 4007 | 1/1 | 0.99 | 0.11 | 36,36,36,36 | 0 |
| 4 | K | F | 549 | 1/1 | 0.99 | 0.11 | 41,41,41,41 | 0 |
| 4 | K | A | 549 | 1/1 | 0.99 | 0.12 | 40,40,40,40 | 0 |
| 4 | K | D | 1 | 1/1 | 0.99 | 0.12 | 30,30,30,30 | 0 |

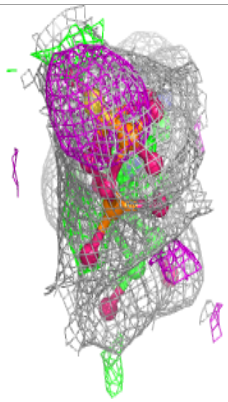
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around AGS D 551:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

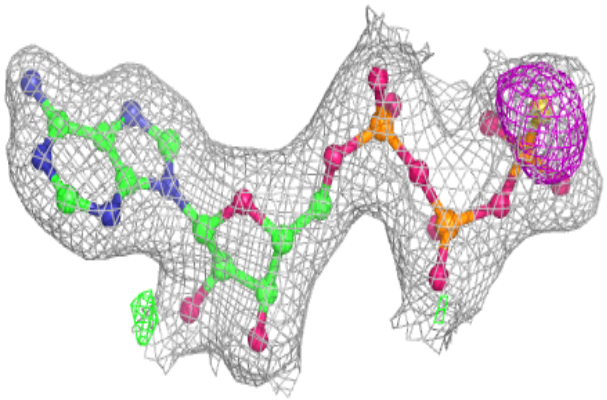


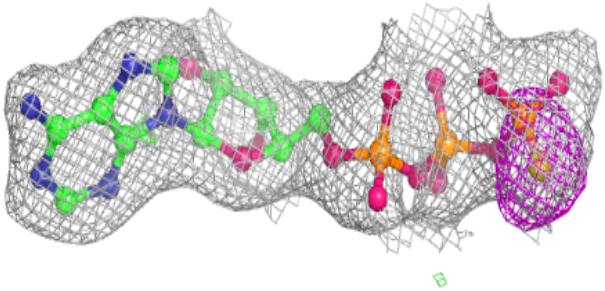


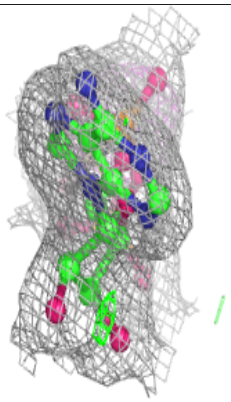


**Electron density around AGS F 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

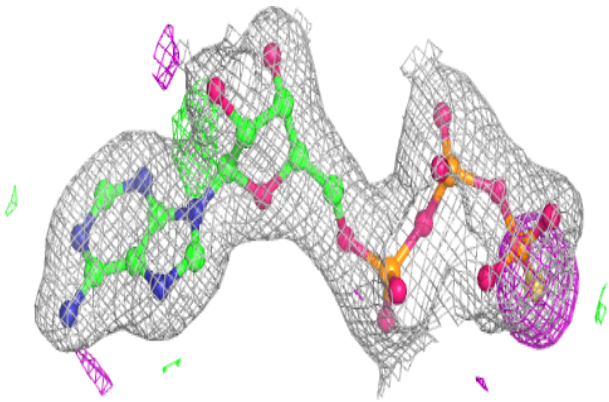


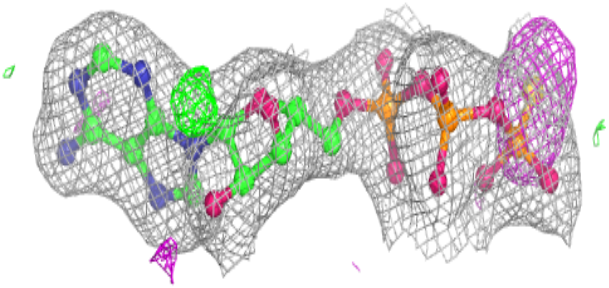


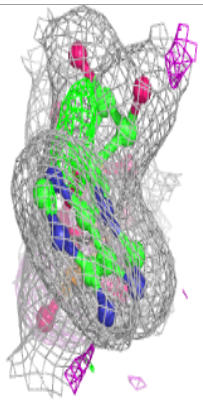


**Electron density around AGS G 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

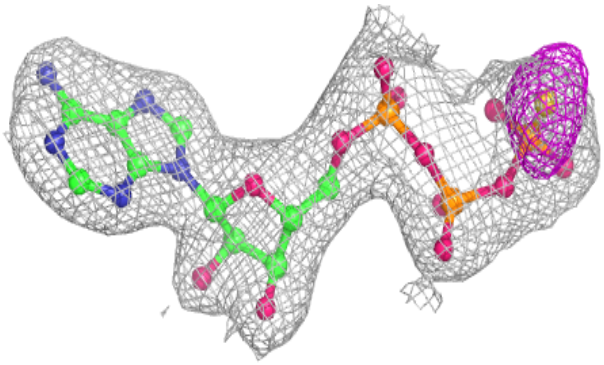


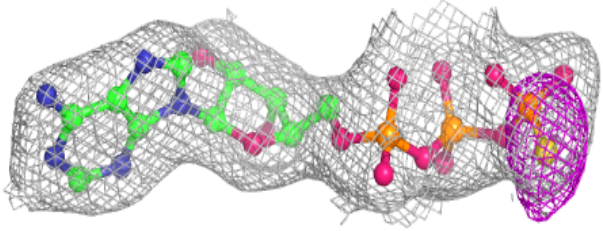


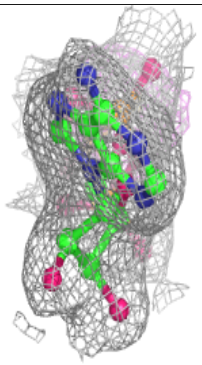


**Electron density around AGS J 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

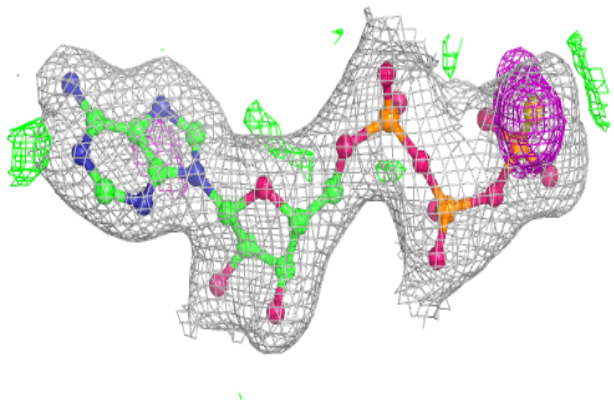


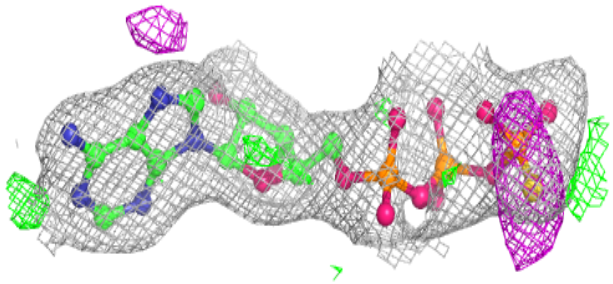


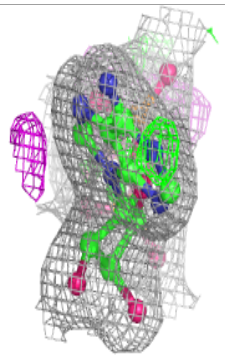


**Electron density around AGS K 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

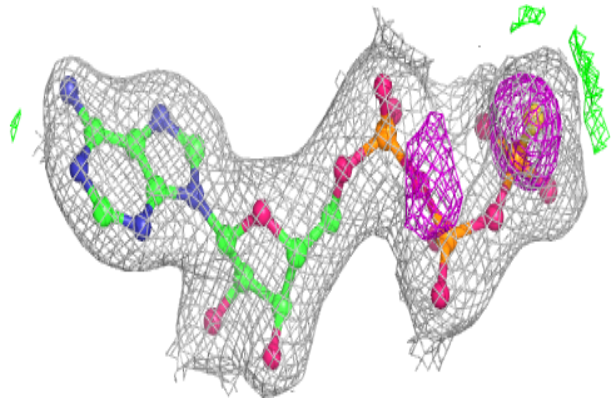


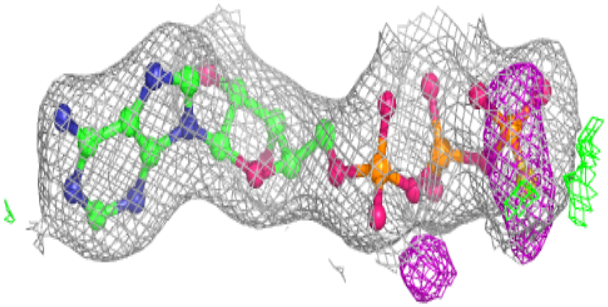


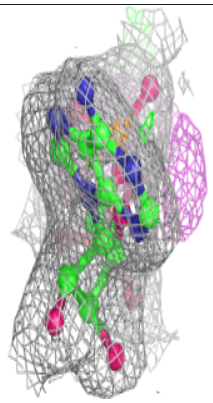


**Electron density around AGS L 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

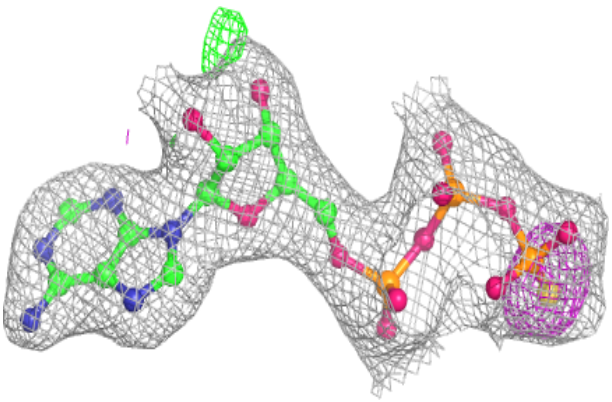


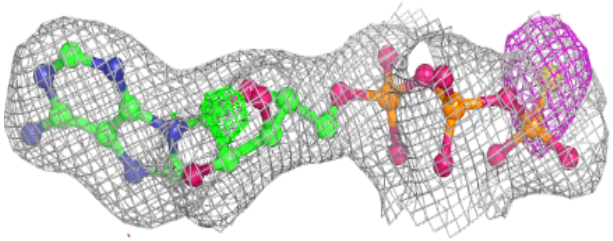


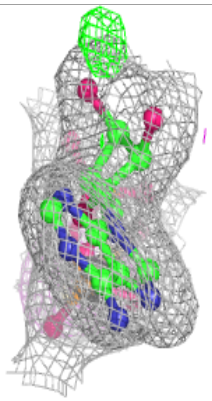


**Electron density around AGS M 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

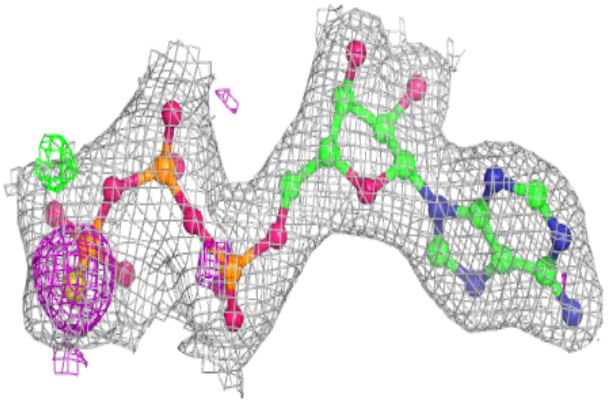


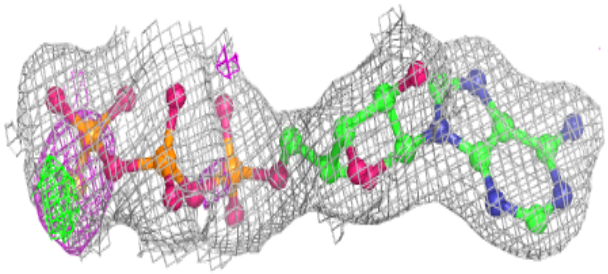


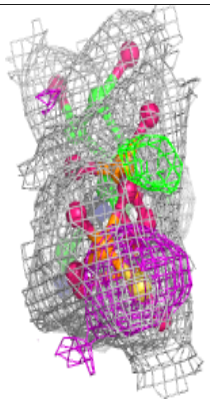


**Electron density around AGS A 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

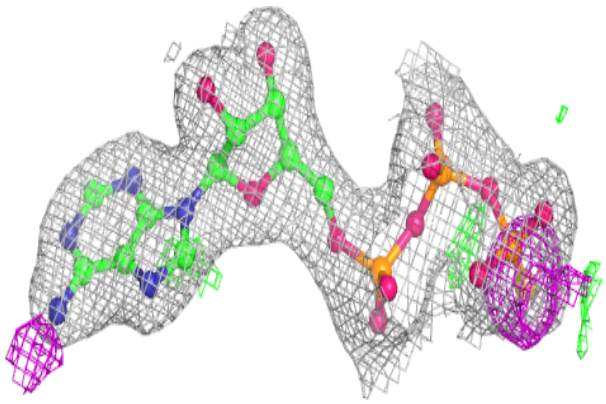


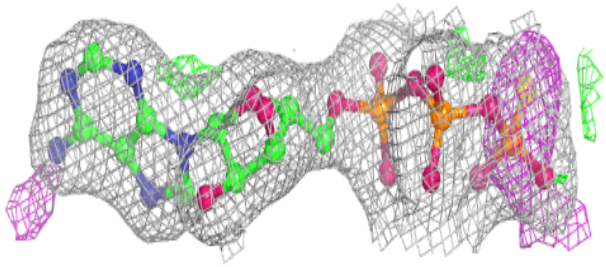


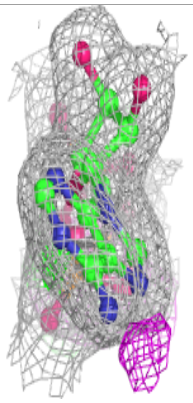


**Electron density around AGS H 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

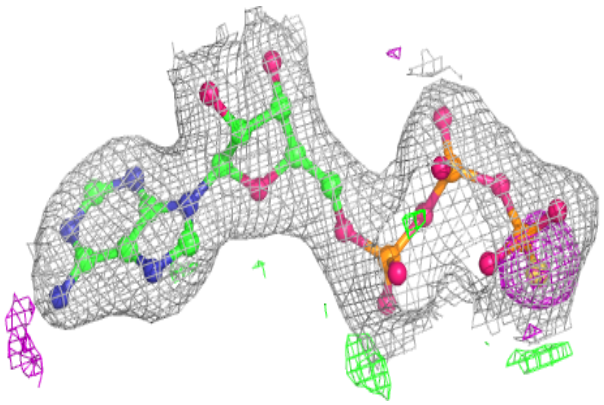


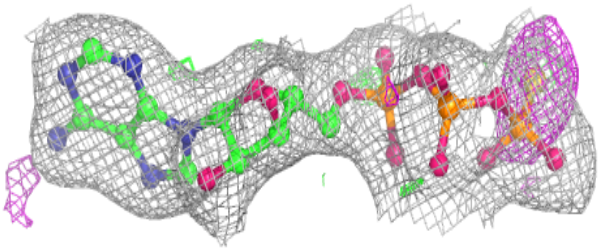


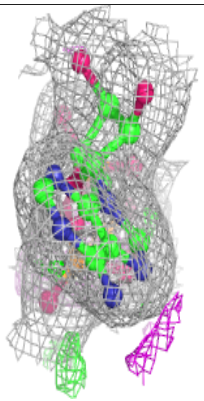


**Electron density around AGS I 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

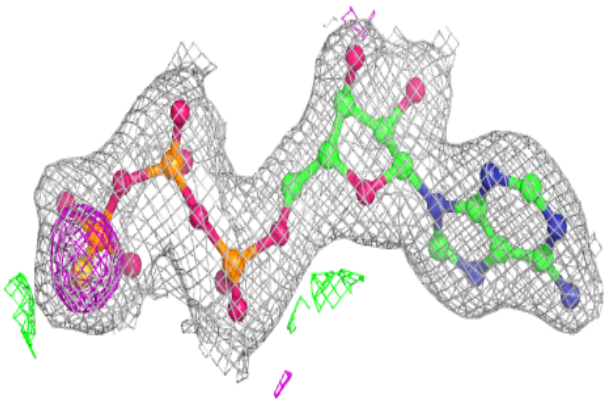


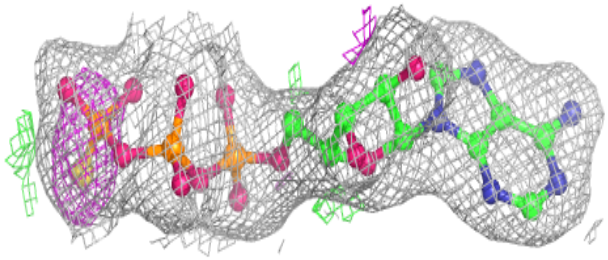


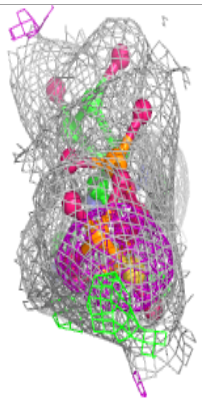


**Electron density around AGS B 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

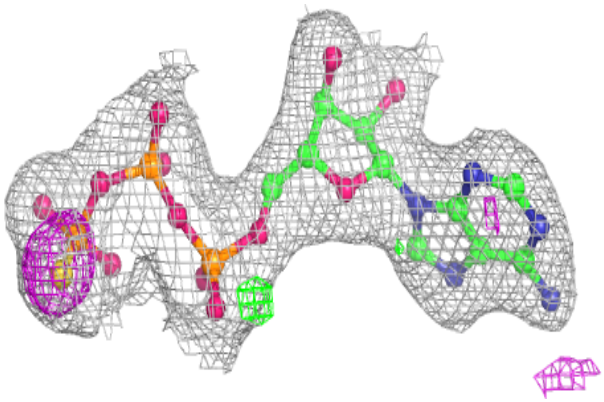


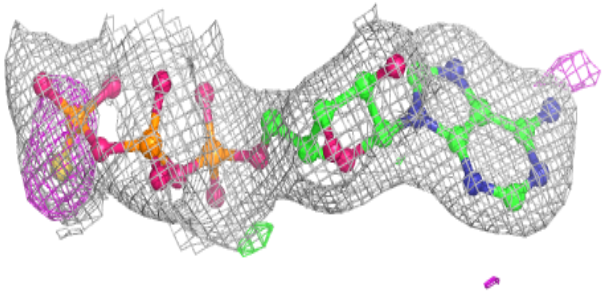


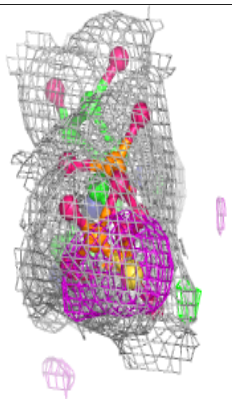


**Electron density around AGS C 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

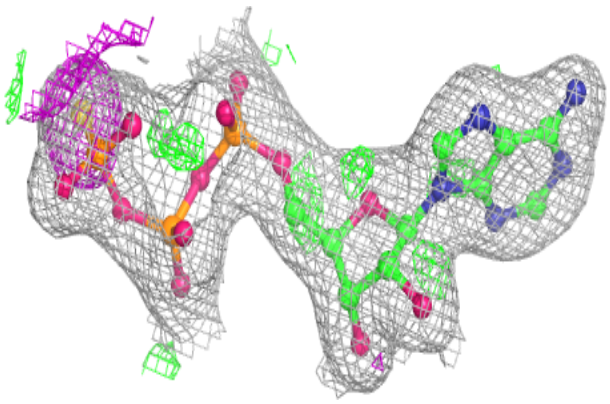


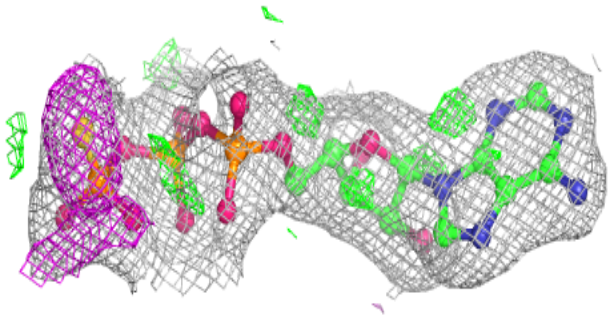


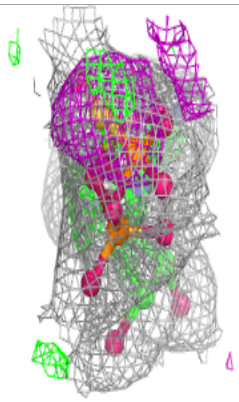


**Electron density around AGS E 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

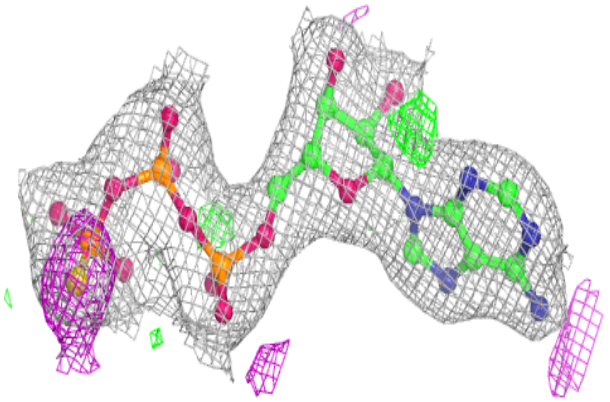


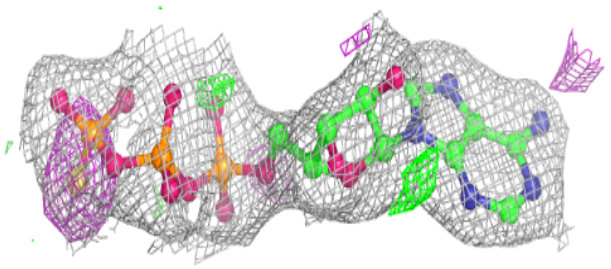


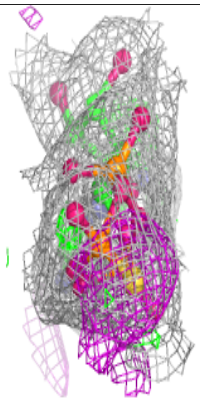


**Electron density around AGS N 1:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)







## 6.5 Other polymers (i)

There are no such residues in this entry.