



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3H1C
Title : Crystal structure of Polynucleotide Phosphorylase (PNPase) core bound to RNase E and Tungstate
Authors : Nurmohamed, S.
Deposited on : 2009-04-11
Resolution : 3.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

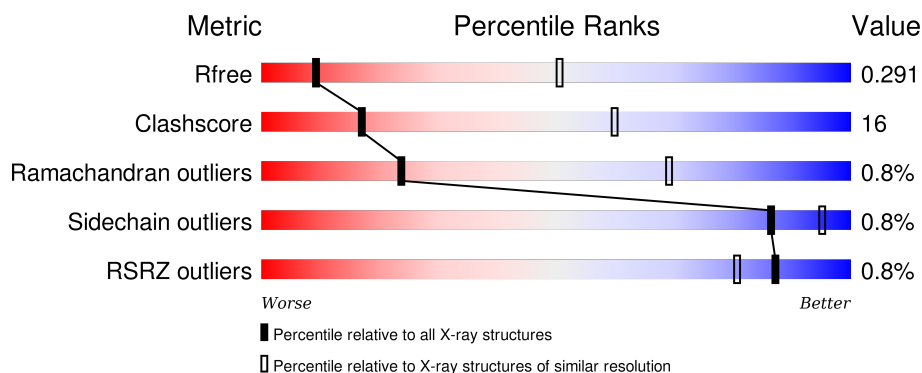
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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.





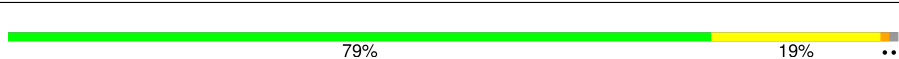
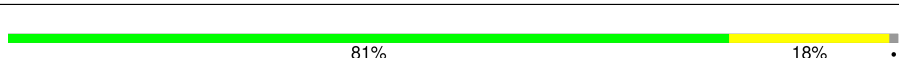
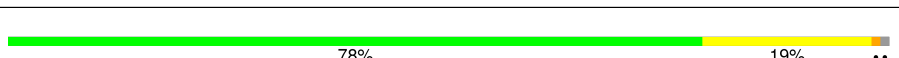
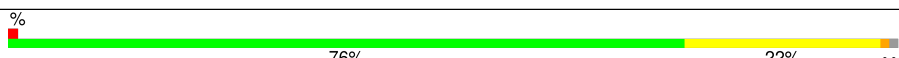
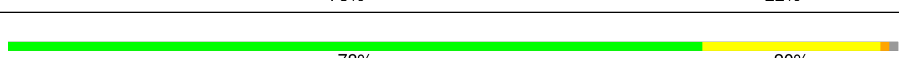
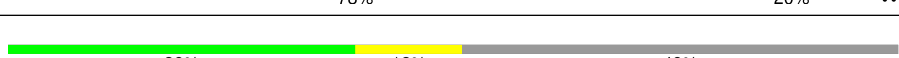
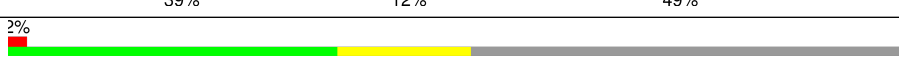
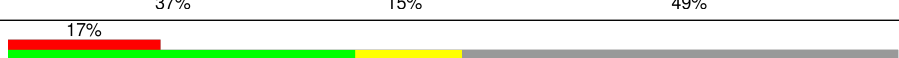
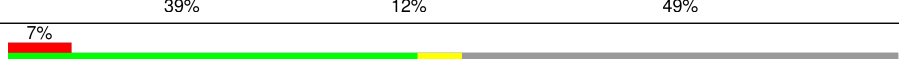
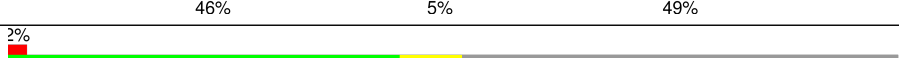
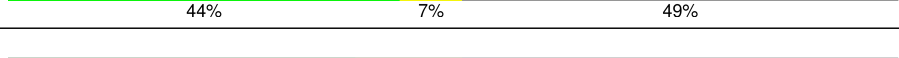
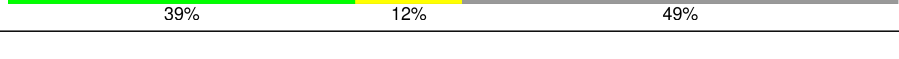



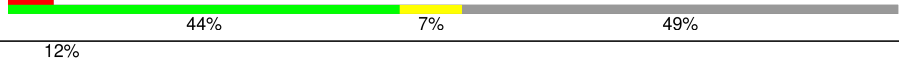

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1261 (3.76-3.40) |
| Clashscore | 102246 | 1026 (3.72-3.44) |
| Ramachandran outliers | 100387 | 1028 (3.74-3.42) |
| Sidechain outliers | 100360 | 1028 (3.74-3.42) |
| RSRZ outliers | 91569 | 1268 (3.76-3.40) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 549 | 77% 22% .. |
| 1 | B | 549 | 76% 23% .. |
| 1 | C | 549 | 75% 23% .. |
| 1 | G | 549 | 77% 21% .. |
| 1 | I | 549 | 77% 21% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | K | 549 |  |
| 1 | M | 549 |  |
| 1 | O | 549 |  |
| 1 | R | 549 |  |
| 1 | T | 549 |  |
| 1 | V | 549 |  |
| 1 | X | 549 |  |
| 2 | D | 41 |  |
| 2 | E | 41 |  |
| 2 | F | 41 |  |
| 2 | H | 41 |  |
| 2 | J | 41 |  |
| 2 | L | 41 |  |
| 2 | N | 41 |  |
| 2 | P | 41 |  |
| 2 | S | 41 |  |
| 2 | U | 41 |  |
| 2 | W | 41 |  |
| 2 | Y | 41 |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3 | WO4 | A | 551 | - | - | - | X |
| 3 | WO4 | K | 551 | - | - | - | X |
| 3 | WO4 | M | 551 | - | - | - | X |
| 3 | WO4 | X | 551 | - | - | - | X |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51109 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 Polyribonucleotide nucleotidyltransferase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4075 | 2559 | 704 | 792 | 20 | | | |
| 1 | B | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4107 | 2575 | 717 | 797 | 18 | | | |
| 1 | C | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4121 | 2583 | 720 | 798 | 20 | | | |
| 1 | G | 543 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4095 | 2571 | 715 | 789 | 20 | | | |
| 1 | I | 543 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4109 | 2576 | 716 | 797 | 20 | | | |
| 1 | K | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4127 | 2588 | 721 | 798 | 20 | | | |
| 1 | M | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4116 | 2581 | 718 | 797 | 20 | | | |
| 1 | O | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4124 | 2584 | 723 | 798 | 19 | | | |
| 1 | R | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4134 | 2590 | 724 | 800 | 20 | | | |
| 1 | T | 543 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4116 | 2582 | 720 | 795 | 19 | | | |
| 1 | V | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4118 | 2580 | 719 | 799 | 20 | | | |
| 1 | X | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4113 | 2581 | 717 | 795 | 20 | | | |

- Molecule 2 is a protein called Ribonuclease E.

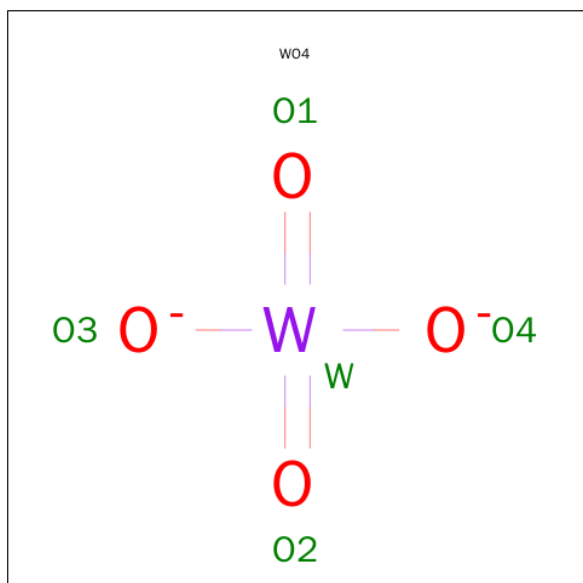
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2 | D | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | E | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2 | F | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | H | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | J | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | L | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | N | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | P | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | S | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | U | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |
| 2 | W | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 131 | 78 | 29 | 24 | | | |
| 2 | Y | 21 | Total | C | N | O | 0 | 0 | 0 |
| | | | 138 | 82 | 31 | 25 | | | |

- Molecule 3 is TUNGSTATE(VI)ION (three-letter code: WO4) (formula: O₄W).



| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3 | A | 1 | Total | O W | 0 | 0 |
| | | | 5 4 1 | | | |

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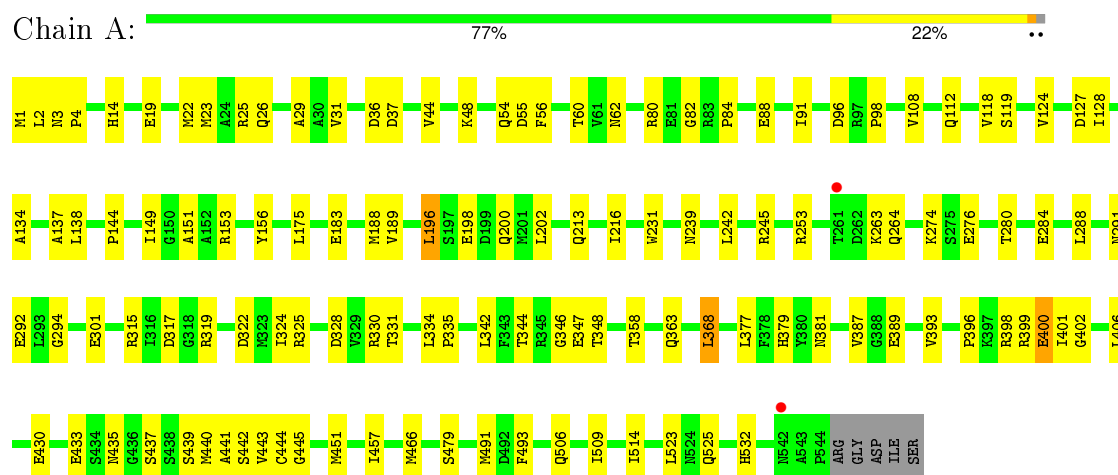
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 3 | A | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | B | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | B | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | C | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | G | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | I | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | K | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | K | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | M | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | M | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | O | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | O | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | R | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | R | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | T | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | T | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | V | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | V | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | X | 1 | Total 5 | O 4 | W 1 | 0 | 0 |
| 3 | X | 1 | Total 5 | O 4 | W 1 | 0 | 0 |

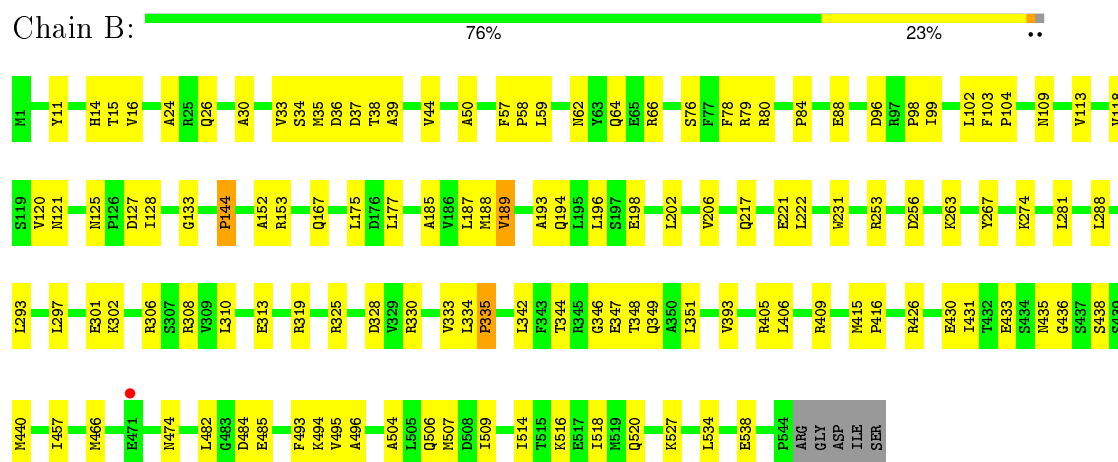
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

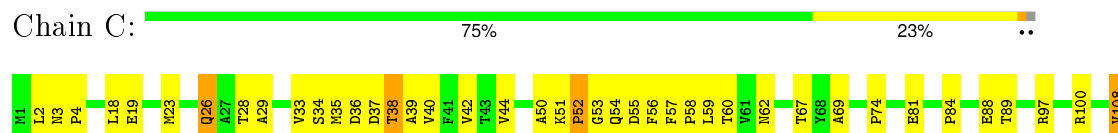
- Molecule 1: Polyribonucleotide nucleotidyltransferase

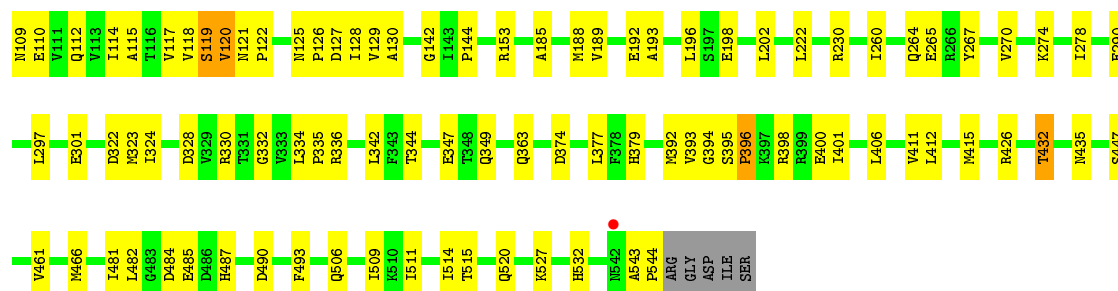


- Molecule 1: Polyribonucleotide nucleotidyltransferase

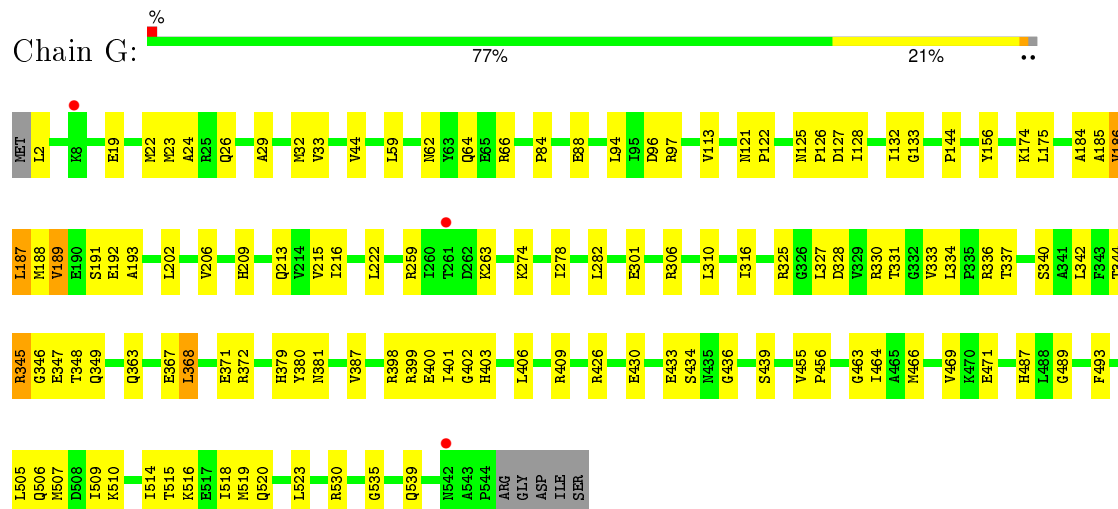


- Molecule 1: Polyribonucleotide nucleotidyltransferase

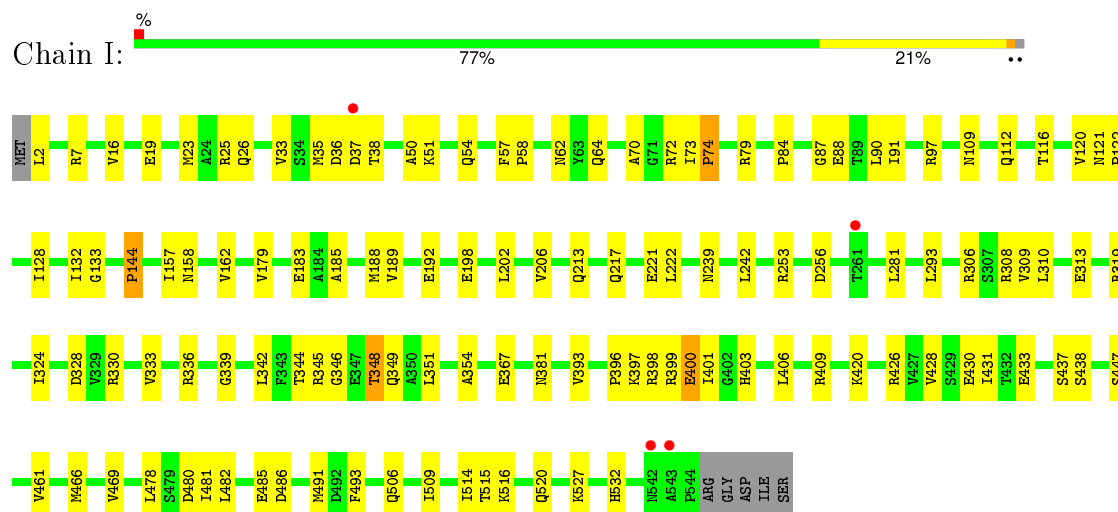




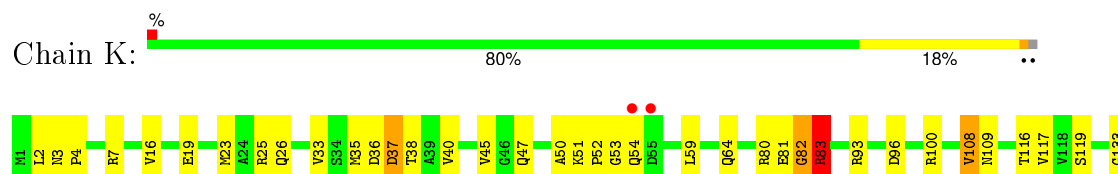
• Molecule 1: Polyribonucleotide nucleotidyltransferase

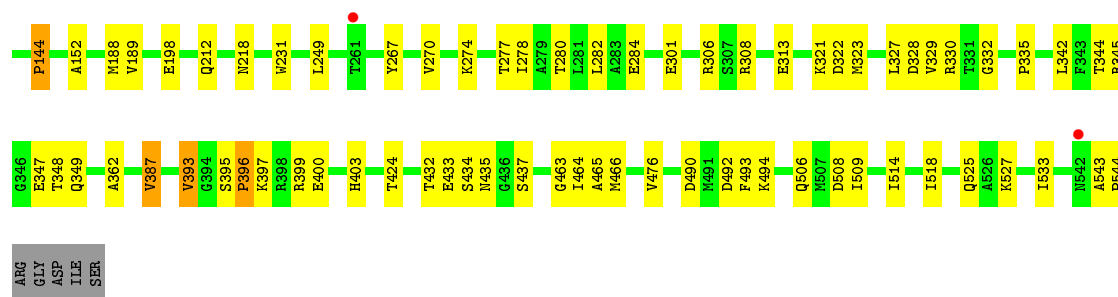


• Molecule 1: Polyribonucleotide nucleotidyltransferase

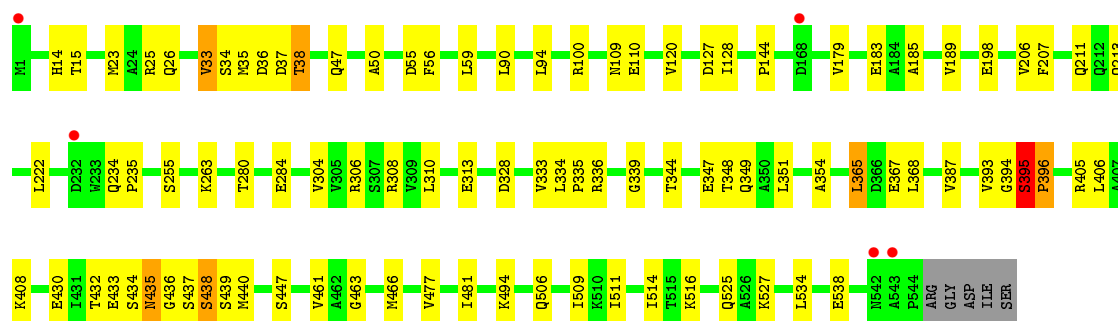
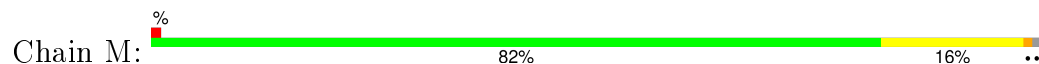


• Molecule 1: Polyribonucleotide nucleotidyltransferase

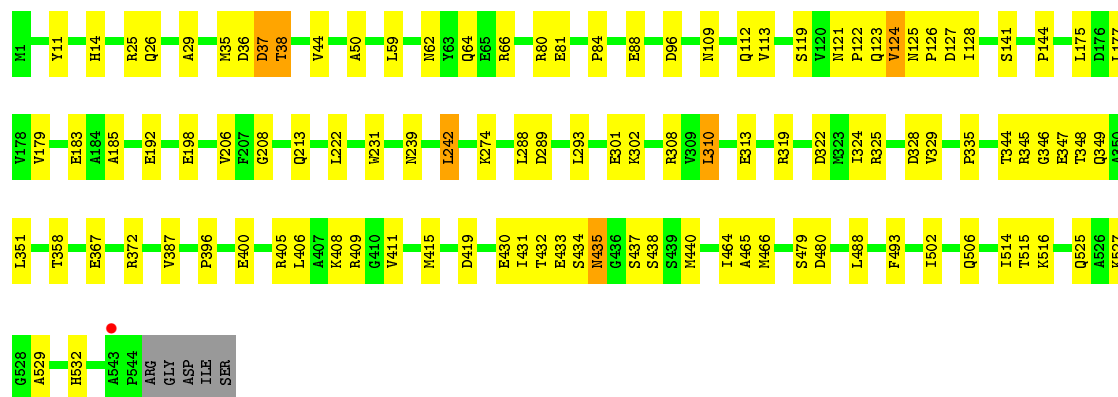
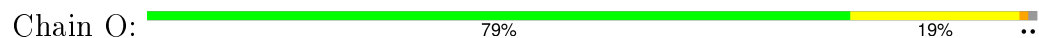




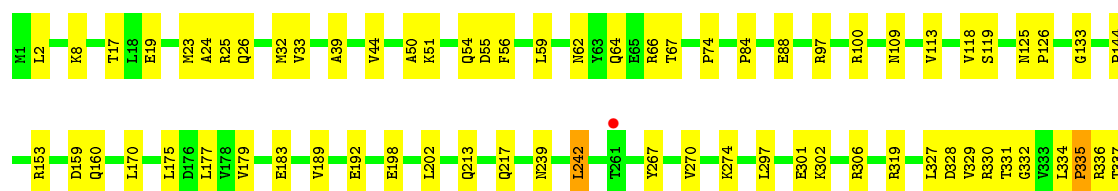
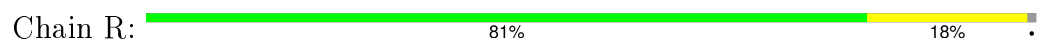
• Molecule 1: Polyribonucleotide nucleotidyltransferase

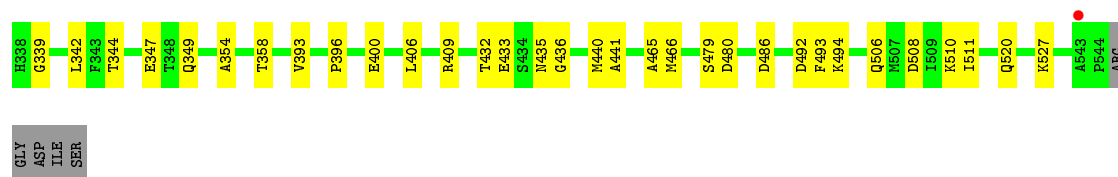


• Molecule 1: Polyribonucleotide nucleotidyltransferase

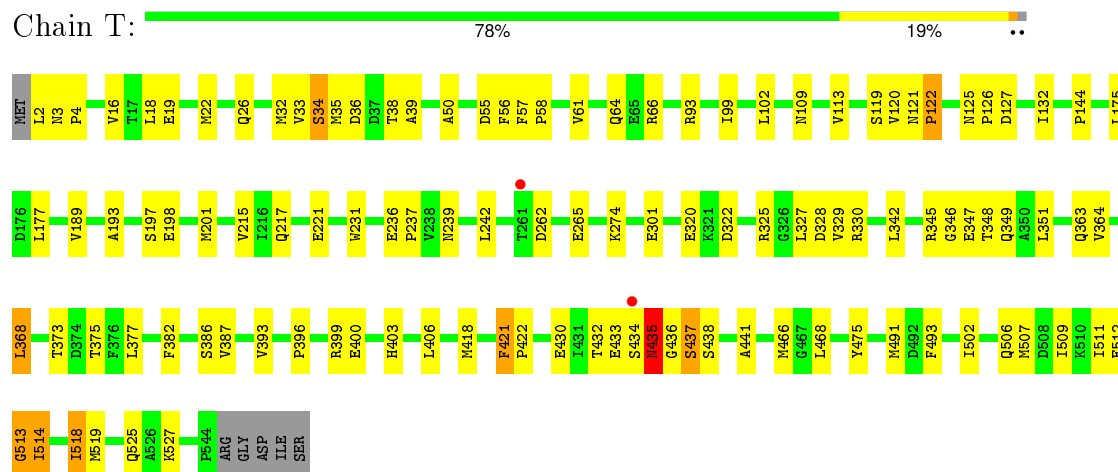


• Molecule 1: Polyribonucleotide nucleotidyltransferase

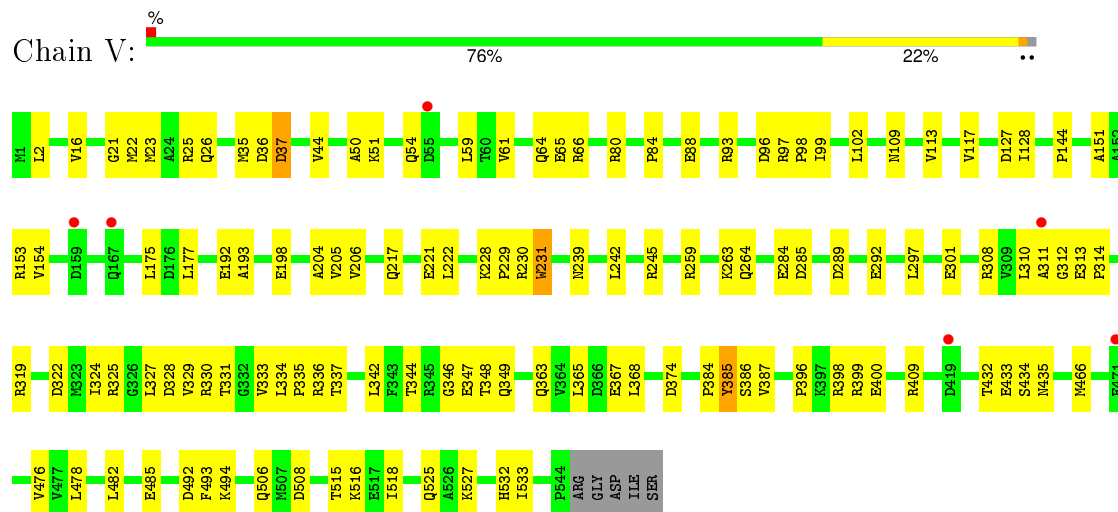




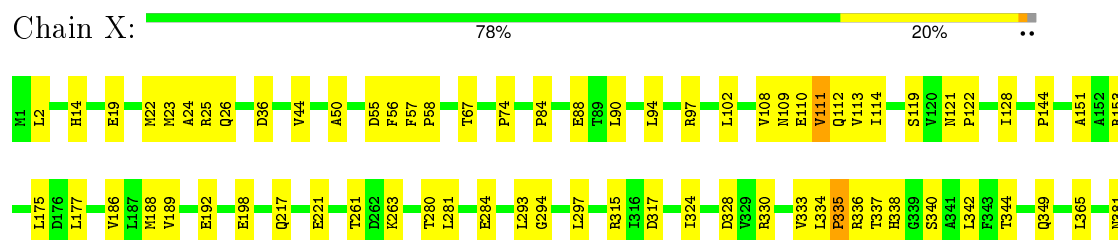
- Molecule 1: Polyribonucleotide nucleotidyltransferase

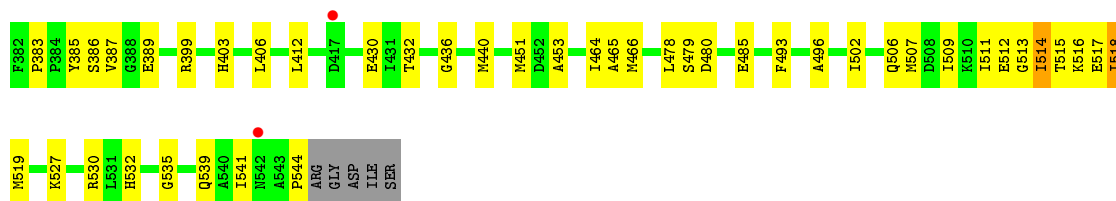


- Molecule 1: Polyribonucleotide nucleotidyltransferase



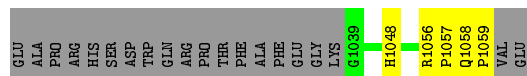
- Molecule 1: Polyribonucleotide nucleotidyltransferase





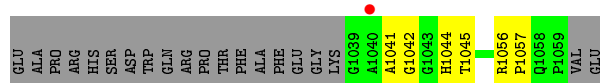
- Molecule 2: Ribonuclease E

Chain D: 39% 12% 49%



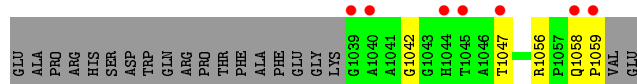
- Molecule 2: Ribonuclease E

Chain E: 2% 37% 15% 49%



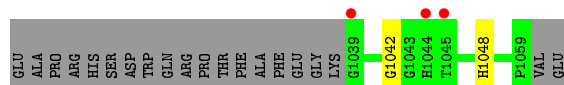
- Molecule 2: Ribonuclease E

Chain F: 17% 39% 12% 49%



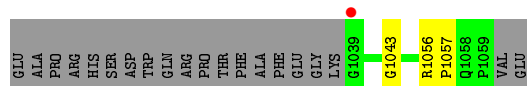
- Molecule 2: Ribonuclease E

Chain H: 7% 46% 5% 49%



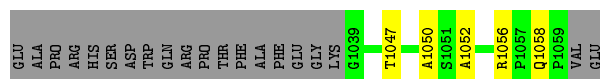
- Molecule 2: Ribonuclease E

Chain J: 2% 44% 7% 49%



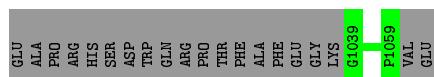
- Molecule 2: Ribonuclease E

Chain L: 39% 12% 49%



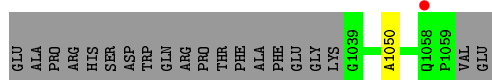
- Molecule 2: Ribonuclease E

Chain N:  51% 49%




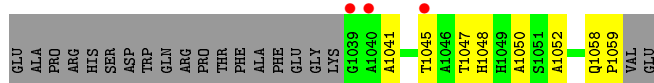
• Molecule 2: Ribonuclease E

Chain P:  2% 49% 49%




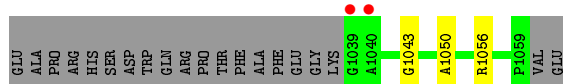
• Molecule 2: Ribonuclease E

Chain S:  7% 32% 20% 49%




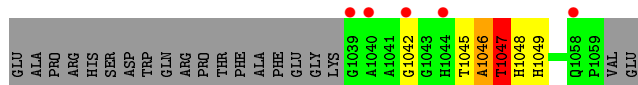
• Molecule 2: Ribonuclease E

Chain U:  5% 44% 7% 49%




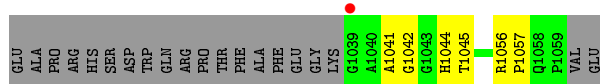
• Molecule 2: Ribonuclease E

Chain W:  12% 37% 10% 49%



• Molecule 2: Ribonuclease E

Chain Y:  2% 37% 15% 49%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 167.74Å 262.89Å 264.12Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 25.00 – 3.57 20.15 – 3.57 | Depositor EDS |
| % Data completeness (in resolution range) | 94.2 (25.00-3.57) 94.2 (20.15-3.57) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.57 (at 3.62Å) | Xtriage |
| Refinement program | REFMAC 5.0 | Depositor |
| R, R_{free} | 0.270 , 0.304 0.267 , 0.291 | Depositor DCC |
| R_{free} test set | 6514 reflections (5.28%) | DCC |
| Wilson B-factor (Å ²) | 79.4 | Xtriage |
| Anisotropy | 0.028 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 26.7 | EDS |
| Estimated twinning fraction | 0.038 for -h,l,k | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Outliers | 1 of 129939 reflections (0.001%) | Xtriage |
| F_o, F_c correlation | 0.85 | EDS |
| Total number of atoms | 51109 | wwPDB-VP |
| Average B, all atoms (Å ²) | 52.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WO4

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 | 0.35 | 0/4138 | 0.47 | 0/5621 |
| 1 | B | 0.30 | 0/4170 | 0.46 | 0/5660 |
| 1 | C | 0.37 | 0/4184 | 0.47 | 1/5675 (0.0%) |
| 1 | G | 0.41 | 0/4158 | 0.51 | 2/5643 (0.0%) |
| 1 | I | 0.38 | 0/4172 | 0.50 | 2/5660 (0.0%) |
| 1 | K | 0.37 | 0/4190 | 0.54 | 4/5681 (0.1%) |
| 1 | M | 0.33 | 0/4179 | 0.58 | 9/5668 (0.2%) |
| 1 | O | 0.34 | 0/4187 | 0.47 | 2/5679 (0.0%) |
| 1 | R | 0.30 | 0/4197 | 0.46 | 0/5690 |
| 1 | T | 0.32 | 0/4179 | 0.48 | 1/5667 (0.0%) |
| 1 | V | 0.36 | 0/4180 | 0.47 | 1/5671 (0.0%) |
| 1 | X | 0.30 | 0/4175 | 0.48 | 2/5661 (0.0%) |
| 2 | D | 0.34 | 0/143 | 0.47 | 0/196 |
| 2 | E | 0.31 | 0/143 | 0.38 | 0/196 |
| 2 | F | 0.32 | 0/143 | 0.49 | 0/196 |
| 2 | H | 0.32 | 0/143 | 0.39 | 0/196 |
| 2 | J | 0.33 | 0/143 | 0.48 | 0/196 |
| 2 | L | 0.36 | 0/143 | 0.47 | 0/196 |
| 2 | N | 0.33 | 0/143 | 0.38 | 0/196 |
| 2 | P | 0.33 | 0/143 | 0.39 | 0/196 |
| 2 | S | 0.32 | 0/143 | 0.38 | 0/196 |
| 2 | U | 0.32 | 0/143 | 0.40 | 0/196 |
| 2 | W | 0.49 | 0/135 | 0.68 | 0/185 |
| 2 | Y | 0.32 | 0/143 | 0.41 | 0/196 |
| All | All | 0.35 | 0/51817 | 0.49 | 24/70317 (0.0%) |

There are no bond length outliers.

All (24) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | M | 438 | SER | CB-CA-C | 13.85 | 136.42 | 110.10 |
| 1 | M | 434 | SER | CB-CA-C | -13.49 | 84.47 | 110.10 |
| 1 | K | 37 | ASP | CB-CA-C | -13.04 | 84.33 | 110.40 |
| 1 | M | 435 | ASN | N-CA-CB | -10.55 | 91.60 | 110.60 |
| 1 | M | 394 | GLY | N-CA-C | 8.54 | 134.46 | 113.10 |
| 1 | T | 34 | SER | CB-CA-C | 8.11 | 125.52 | 110.10 |
| 1 | X | 336 | ARG | N-CA-CB | -7.81 | 96.55 | 110.60 |
| 1 | K | 37 | ASP | N-CA-C | 7.50 | 131.26 | 111.00 |
| 1 | I | 70 | ALA | CB-CA-C | -7.08 | 99.48 | 110.10 |
| 1 | K | 38 | THR | N-CA-C | -6.85 | 92.49 | 111.00 |
| 1 | O | 434 | SER | CB-CA-C | -6.62 | 97.52 | 110.10 |
| 1 | C | 120 | VAL | CB-CA-C | -6.55 | 98.96 | 111.40 |
| 1 | G | 345 | ARG | N-CA-C | -6.49 | 93.49 | 111.00 |
| 1 | M | 395 | SER | N-CA-C | -6.45 | 93.60 | 111.00 |
| 1 | V | 37 | ASP | CB-CA-C | -6.04 | 98.32 | 110.40 |
| 1 | M | 434 | SER | N-CA-C | 5.88 | 126.89 | 111.00 |
| 1 | I | 437 | SER | N-CA-CB | 5.43 | 118.64 | 110.50 |
| 1 | G | 345 | ARG | CB-CA-C | 5.41 | 121.22 | 110.40 |
| 1 | K | 393 | VAL | N-CA-C | -5.40 | 96.42 | 111.00 |
| 1 | M | 395 | SER | N-CA-CB | 5.29 | 118.43 | 110.50 |
| 1 | O | 435 | ASN | N-CA-CB | -5.26 | 101.13 | 110.60 |
| 1 | X | 335 | PRO | N-CA-C | 5.20 | 125.63 | 112.10 |
| 1 | M | 438 | SER | N-CA-C | -5.10 | 97.23 | 111.00 |
| 1 | M | 33 | VAL | CB-CA-C | -5.09 | 101.74 | 111.40 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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 | 4075 | 0 | 4044 | 154 | 0 |
| 1 | B | 4107 | 0 | 4096 | 134 | 0 |
| 1 | C | 4121 | 0 | 4126 | 186 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | G | 4095 | 0 | 4087 | 168 | 0 |
| 1 | I | 4109 | 0 | 4108 | 138 | 0 |
| 1 | K | 4127 | 0 | 4141 | 148 | 0 |
| 1 | M | 4116 | 0 | 4116 | 98 | 0 |
| 1 | O | 4124 | 0 | 4130 | 119 | 0 |
| 1 | R | 4134 | 0 | 4150 | 101 | 0 |
| 1 | T | 4116 | 0 | 4127 | 160 | 0 |
| 1 | V | 4118 | 0 | 4115 | 173 | 0 |
| 1 | X | 4113 | 0 | 4117 | 176 | 0 |
| 2 | D | 138 | 0 | 125 | 5 | 0 |
| 2 | E | 138 | 0 | 125 | 8 | 0 |
| 2 | F | 138 | 0 | 125 | 16 | 0 |
| 2 | H | 138 | 0 | 125 | 2 | 0 |
| 2 | J | 138 | 0 | 125 | 2 | 0 |
| 2 | L | 138 | 0 | 125 | 8 | 0 |
| 2 | N | 138 | 0 | 125 | 0 | 0 |
| 2 | P | 138 | 0 | 125 | 1 | 0 |
| 2 | S | 138 | 0 | 125 | 9 | 0 |
| 2 | U | 138 | 0 | 125 | 4 | 0 |
| 2 | W | 131 | 0 | 115 | 21 | 0 |
| 2 | Y | 138 | 0 | 125 | 5 | 0 |
| 3 | A | 10 | 0 | 0 | 0 | 0 |
| 3 | B | 10 | 0 | 0 | 0 | 0 |
| 3 | C | 5 | 0 | 0 | 0 | 0 |
| 3 | G | 5 | 0 | 0 | 1 | 0 |
| 3 | I | 5 | 0 | 0 | 0 | 0 |
| 3 | K | 10 | 0 | 0 | 0 | 0 |
| 3 | M | 10 | 0 | 0 | 0 | 0 |
| 3 | O | 10 | 0 | 0 | 0 | 0 |
| 3 | R | 10 | 0 | 0 | 0 | 0 |
| 3 | T | 10 | 0 | 0 | 0 | 0 |
| 3 | V | 10 | 0 | 0 | 0 | 0 |
| 3 | X | 10 | 0 | 0 | 1 | 0 |
| All | All | 51109 | 0 | 50847 | 1659 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1659) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:310:LEU:HD21 | 1:I:469:VAL:CG1 | 1.47 | 1.44 |
| 1:G:26:GLN:NE2 | 1:K:387:VAL:HA | 1.36 | 1.40 |
| 1:R:51:LYS:HB3 | 1:R:54:GLN:CG | 1.52 | 1.36 |
| 1:O:239:ASN:ND2 | 1:O:242:LEU:HB2 | 1.40 | 1.35 |
| 1:V:342:LEU:HD11 | 1:V:349:GLN:NE2 | 1.40 | 1.32 |
| 1:R:239:ASN:ND2 | 1:R:242:LEU:HB2 | 1.44 | 1.31 |
| 1:T:347:GLU:HB3 | 1:T:435:ASN:ND2 | 1.43 | 1.30 |
| 1:M:120:VAL:CG1 | 1:M:368:LEU:HD11 | 1.59 | 1.30 |
| 1:C:34:SER:CB | 1:C:39:ALA:HB2 | 1.61 | 1.29 |
| 1:K:51:LYS:CG | 1:K:52:PRO:HD2 | 1.61 | 1.29 |
| 1:M:120:VAL:HG11 | 1:M:368:LEU:CD1 | 1.60 | 1.28 |
| 1:X:342:LEU:HD11 | 1:X:349:GLN:NE2 | 1.49 | 1.27 |
| 1:V:310:LEU:CD1 | 1:V:310:LEU:O | 1.81 | 1.26 |
| 1:X:509:ILE:CB | 1:X:514:ILE:HD11 | 1.65 | 1.26 |
| 1:V:342:LEU:CD1 | 1:V:349:GLN:HE21 | 1.47 | 1.26 |
| 1:A:196:LEU:CB | 1:A:200:GLN:HE21 | 1.47 | 1.25 |
| 1:C:323:MET:CG | 2:F:1056:ARG:HG3 | 1.67 | 1.25 |
| 1:T:491:MET:CE | 1:T:493:PHE:HD1 | 1.51 | 1.23 |
| 1:X:509:ILE:CD1 | 1:X:514:ILE:HG12 | 1.67 | 1.22 |
| 1:I:239:ASN:ND2 | 1:I:242:LEU:HB2 | 1.53 | 1.21 |
| 1:A:491:MET:CE | 1:A:493:PHE:HB2 | 1.69 | 1.21 |
| 1:K:464:ILE:HD11 | 1:K:533:ILE:CD1 | 1.69 | 1.21 |
| 1:T:491:MET:CE | 1:T:493:PHE:CD1 | 2.23 | 1.20 |
| 1:I:73:ILE:CG2 | 1:I:74:PRO:HD2 | 1.72 | 1.20 |
| 1:C:323:MET:CG | 2:F:1056:ARG:CG | 2.21 | 1.20 |
| 1:T:491:MET:HE1 | 1:T:493:PHE:CD1 | 1.76 | 1.19 |
| 1:I:310:LEU:CD2 | 1:I:469:VAL:CG1 | 2.20 | 1.18 |
| 1:C:323:MET:HG2 | 2:F:1056:ARG:HG3 | 1.19 | 1.17 |
| 1:O:14:HIS:HB3 | 1:O:36:ASP:HB2 | 1.21 | 1.16 |
| 1:C:67:THR:HG21 | 1:C:74:PRO:HD3 | 1.20 | 1.16 |
| 1:X:342:LEU:CD1 | 1:X:349:GLN:HE21 | 1.58 | 1.16 |
| 1:K:464:ILE:HD11 | 1:K:533:ILE:HD12 | 1.19 | 1.16 |
| 1:K:395:SER:CB | 1:K:396:PRO:HD2 | 1.73 | 1.16 |
| 1:T:342:LEU:HD11 | 1:T:349:GLN:NE2 | 1.59 | 1.16 |
| 1:X:509:ILE:HD13 | 1:X:514:ILE:HG12 | 1.19 | 1.15 |
| 1:X:509:ILE:CG2 | 1:X:514:ILE:HD11 | 1.75 | 1.15 |
| 1:M:406:LEU:HD11 | 1:M:506:GLN:OE1 | 1.45 | 1.14 |
| 1:K:59:LEU:HD23 | 1:K:100:ARG:HG2 | 1.17 | 1.14 |
| 1:T:239:ASN:ND2 | 1:T:242:LEU:HB2 | 1.60 | 1.14 |
| 1:T:491:MET:HE3 | 1:T:493:PHE:HD1 | 1.07 | 1.13 |
| 1:C:323:MET:HG2 | 2:F:1056:ARG:CG | 1.77 | 1.13 |
| 1:C:324:ILE:HD11 | 1:C:532:HIS:CD2 | 1.83 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:37:ASP:O | 1:C:121:ASN:HB2 | 1.48 | 1.12 |
| 1:G:310:LEU:CD1 | 1:G:469:VAL:HG12 | 1.78 | 1.12 |
| 1:I:420:LYS:HG3 | 1:O:123:GLN:HE22 | 1.12 | 1.12 |
| 1:O:349:GLN:HG3 | 1:O:432:THR:OG1 | 1.47 | 1.12 |
| 1:A:196:LEU:HB3 | 1:A:200:GLN:HE21 | 0.97 | 1.11 |
| 1:R:342:LEU:HD11 | 1:R:349:GLN:HE21 | 1.07 | 1.11 |
| 1:K:395:SER:HB3 | 1:K:396:PRO:HD2 | 1.27 | 1.11 |
| 1:C:342:LEU:HD11 | 1:C:349:GLN:HE21 | 1.14 | 1.11 |
| 1:I:426:ARG:NH1 | 1:I:428:VAL:HG21 | 1.66 | 1.11 |
| 1:T:491:MET:CE | 1:T:493:PHE:HB2 | 1.81 | 1.11 |
| 1:V:310:LEU:HD13 | 1:V:310:LEU:O | 0.93 | 1.10 |
| 1:T:50:ALA:HB2 | 1:T:109:ASN:OD1 | 1.49 | 1.10 |
| 1:K:51:LYS:CG | 1:K:52:PRO:CD | 2.30 | 1.10 |
| 1:A:44:VAL:HG11 | 1:A:138:LEU:HD23 | 1.32 | 1.10 |
| 1:V:177:LEU:HD22 | 1:V:204:ALA:CB | 1.81 | 1.09 |
| 1:A:196:LEU:HD22 | 1:A:200:GLN:NE2 | 1.65 | 1.09 |
| 1:I:319:ARG:HH21 | 1:I:482:LEU:HD11 | 1.05 | 1.09 |
| 1:A:440:MET:O | 1:A:443:VAL:HG22 | 1.51 | 1.09 |
| 1:I:310:LEU:CD2 | 1:I:469:VAL:HG11 | 1.81 | 1.08 |
| 1:C:342:LEU:HD11 | 1:C:349:GLN:NE2 | 1.67 | 1.08 |
| 1:V:311:ALA:HB3 | 1:V:312:GLY:CA | 1.83 | 1.08 |
| 1:K:274:LYS:HE3 | 1:K:301:GLU:OE2 | 1.51 | 1.08 |
| 1:V:313:GLU:HB3 | 1:V:314:PRO:HD2 | 1.12 | 1.07 |
| 1:G:26:GLN:CD | 1:K:387:VAL:HA | 1.75 | 1.06 |
| 1:K:59:LEU:HD23 | 1:K:100:ARG:CG | 1.85 | 1.06 |
| 1:C:323:MET:HG3 | 2:F:1056:ARG:CG | 1.86 | 1.06 |
| 1:V:311:ALA:HB3 | 1:V:312:GLY:HA2 | 1.10 | 1.06 |
| 1:X:515:THR:HB | 1:X:518:ILE:HG12 | 1.35 | 1.06 |
| 1:I:345:ARG:HG2 | 1:I:346:GLY:H | 1.15 | 1.06 |
| 1:G:310:LEU:HD21 | 1:G:471:GLU:HG2 | 1.36 | 1.05 |
| 1:X:509:ILE:HG21 | 1:X:514:ILE:CD1 | 1.85 | 1.05 |
| 1:I:198:GLU:OE2 | 1:I:527:LYS:HD2 | 1.56 | 1.05 |
| 1:C:54:GLN:HG3 | 1:C:108:VAL:HG12 | 1.34 | 1.05 |
| 1:T:342:LEU:CD1 | 1:T:349:GLN:HE21 | 1.68 | 1.05 |
| 1:K:349:GLN:HE21 | 1:K:432:THR:CG2 | 1.70 | 1.05 |
| 1:A:396:PRO:HA | 1:A:400:GLU:OE1 | 1.56 | 1.05 |
| 1:C:120:VAL:O | 1:C:120:VAL:HG13 | 1.55 | 1.04 |
| 1:G:328:ASP:OD2 | 1:I:2:LEU:HD23 | 1.55 | 1.04 |
| 1:B:198:GLU:OE2 | 1:B:527:LYS:HD2 | 1.56 | 1.04 |
| 1:A:128:ILE:HG23 | 1:A:151:ALA:HB1 | 1.37 | 1.04 |
| 1:C:324:ILE:HD11 | 1:C:532:HIS:HD2 | 1.14 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:175:LEU:HD13 | 1:V:193:ALA:HB2 | 1.38 | 1.04 |
| 1:K:50:ALA:HB2 | 1:K:109:ASN:OD1 | 1.56 | 1.04 |
| 1:V:313:GLU:HB3 | 1:V:314:PRO:CD | 1.89 | 1.03 |
| 1:I:342:LEU:HD11 | 1:I:349:GLN:HE21 | 1.16 | 1.03 |
| 1:R:51:LYS:HB3 | 1:R:54:GLN:HG2 | 1.05 | 1.03 |
| 1:I:37:ASP:HB3 | 1:I:121:ASN:HB2 | 1.41 | 1.03 |
| 1:C:198:GLU:OE2 | 1:C:527:LYS:HD2 | 1.59 | 1.03 |
| 1:V:50:ALA:HB2 | 1:V:109:ASN:OD1 | 1.59 | 1.02 |
| 1:A:451:MET:CE | 1:A:457:ILE:HD11 | 1.88 | 1.02 |
| 1:R:50:ALA:HB2 | 1:R:109:ASN:OD1 | 1.57 | 1.02 |
| 1:T:22:MET:HE2 | 1:X:330:ARG:NH1 | 1.73 | 1.02 |
| 1:X:342:LEU:HD11 | 1:X:349:GLN:HE21 | 0.87 | 1.02 |
| 1:X:509:ILE:HB | 1:X:514:ILE:HD11 | 1.36 | 1.02 |
| 1:A:196:LEU:HB3 | 1:A:200:GLN:NE2 | 1.73 | 1.02 |
| 1:I:319:ARG:HH21 | 1:I:482:LEU:CD1 | 1.72 | 1.02 |
| 1:A:91:ILE:HD12 | 1:A:127:ASP:OD1 | 1.60 | 1.02 |
| 1:G:26:GLN:NE2 | 1:K:387:VAL:CA | 2.21 | 1.02 |
| 1:T:342:LEU:HD11 | 1:T:349:GLN:HE21 | 0.85 | 1.02 |
| 1:I:73:ILE:HG23 | 1:I:74:PRO:CD | 1.89 | 1.01 |
| 1:M:395:SER:HB3 | 1:M:396:PRO:HD2 | 1.39 | 1.01 |
| 1:I:188:MET:HG2 | 1:I:189:VAL:N | 1.75 | 1.01 |
| 1:C:342:LEU:CD1 | 1:C:349:GLN:HE21 | 1.73 | 1.01 |
| 1:A:128:ILE:HG23 | 1:A:151:ALA:CB | 1.91 | 1.01 |
| 1:V:319:ARG:NH2 | 1:V:482:LEU:HD11 | 1.75 | 1.01 |
| 1:M:440:MET:HE3 | 1:M:494:LYS:NZ | 1.76 | 1.00 |
| 1:V:311:ALA:CB | 1:V:312:GLY:HA2 | 1.88 | 1.00 |
| 1:V:264:GLN:NE2 | 1:X:26:GLN:HA | 1.76 | 1.00 |
| 1:A:491:MET:HE1 | 1:A:493:PHE:HB2 | 1.38 | 1.00 |
| 1:C:34:SER:HB2 | 1:C:39:ALA:HB2 | 1.38 | 1.00 |
| 1:M:185:ALA:HB1 | 1:M:514:ILE:HG22 | 1.43 | 1.00 |
| 1:O:50:ALA:HB2 | 1:O:109:ASN:OD1 | 1.60 | 1.00 |
| 1:V:177:LEU:HD22 | 1:V:204:ALA:HB1 | 1.42 | 1.00 |
| 1:I:202:LEU:HD22 | 1:I:520:GLN:HB3 | 1.42 | 1.00 |
| 1:I:73:ILE:CG2 | 1:I:74:PRO:CD | 2.40 | 0.99 |
| 1:M:38:THR:HG23 | 1:M:120:VAL:HA | 1.44 | 0.99 |
| 1:T:2:LEU:HD21 | 1:X:328:ASP:OD2 | 1.60 | 0.99 |
| 1:V:319:ARG:HH21 | 1:V:482:LEU:HD11 | 1.23 | 0.99 |
| 1:I:308:ARG:HG2 | 1:I:313:GLU:OE1 | 1.63 | 0.99 |
| 1:B:202:LEU:CD2 | 1:B:520:GLN:HB3 | 1.93 | 0.99 |
| 1:R:51:LYS:HB3 | 1:R:54:GLN:HG3 | 1.44 | 0.98 |
| 1:I:202:LEU:CD2 | 1:I:520:GLN:HB3 | 1.93 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:73:ILE:HG23 | 1:I:74:PRO:HD2 | 0.98 | 0.98 |
| 1:A:491:MET:HE2 | 1:A:493:PHE:HB2 | 1.38 | 0.97 |
| 1:T:375:THR:HG21 | 1:T:418:MET:CE | 1.94 | 0.97 |
| 1:A:196:LEU:CD2 | 1:A:200:GLN:NE2 | 2.26 | 0.97 |
| 1:R:51:LYS:CB | 1:R:54:GLN:HG2 | 1.94 | 0.97 |
| 1:X:509:ILE:HG21 | 1:X:514:ILE:HD11 | 1.42 | 0.97 |
| 1:B:188:MET:O | 1:B:189:VAL:HG23 | 1.62 | 0.97 |
| 1:R:239:ASN:ND2 | 1:R:242:LEU:CB | 2.28 | 0.97 |
| 1:T:491:MET:HE1 | 1:T:493:PHE:CG | 1.99 | 0.97 |
| 1:V:342:LEU:HD11 | 1:V:349:GLN:HE21 | 0.83 | 0.97 |
| 1:B:319:ARG:HH21 | 1:B:482:LEU:HD11 | 1.26 | 0.97 |
| 1:G:310:LEU:HD12 | 1:G:469:VAL:HG12 | 1.45 | 0.97 |
| 1:K:387:VAL:HG23 | 1:K:434:SER:HB3 | 1.46 | 0.96 |
| 1:C:58:PRO:HG2 | 1:C:110:GLU:HG2 | 1.48 | 0.96 |
| 1:M:393:VAL:HG12 | 1:M:393:VAL:O | 1.66 | 0.96 |
| 1:X:509:ILE:HG12 | 1:X:514:ILE:HG13 | 1.48 | 0.96 |
| 1:O:328:ASP:OD2 | 1:R:2:LEU:HD12 | 1.65 | 0.96 |
| 1:O:239:ASN:ND2 | 1:O:242:LEU:CB | 2.29 | 0.96 |
| 1:C:54:GLN:HG3 | 1:C:108:VAL:CG1 | 1.95 | 0.95 |
| 1:I:213:GLN:O | 1:I:217:GLN:HG2 | 1.66 | 0.95 |
| 2:L:1058:GLN:O | 2:L:1058:GLN:HG2 | 1.65 | 0.95 |
| 1:I:426:ARG:NH1 | 1:I:428:VAL:CG2 | 2.29 | 0.95 |
| 1:G:188:MET:HG2 | 1:G:189:VAL:H | 1.29 | 0.95 |
| 1:A:196:LEU:CB | 1:A:200:GLN:NE2 | 2.26 | 0.95 |
| 1:X:509:ILE:HG12 | 1:X:514:ILE:CG1 | 1.96 | 0.95 |
| 1:A:322:ASP:HA | 1:A:525:GLN:HE21 | 1.30 | 0.95 |
| 1:K:59:LEU:CD2 | 1:K:100:ARG:HG2 | 1.96 | 0.95 |
| 1:A:491:MET:CE | 1:A:493:PHE:CD1 | 2.50 | 0.95 |
| 1:C:395:SER:HB2 | 1:C:396:PRO:HA | 1.47 | 0.94 |
| 1:R:342:LEU:HD11 | 1:R:349:GLN:NE2 | 1.82 | 0.94 |
| 1:G:310:LEU:CD1 | 1:G:469:VAL:CG1 | 2.46 | 0.94 |
| 1:A:44:VAL:HG11 | 1:A:138:LEU:CD2 | 1.97 | 0.94 |
| 1:I:310:LEU:CD2 | 1:I:469:VAL:HG12 | 1.87 | 0.94 |
| 1:I:426:ARG:HH12 | 1:I:428:VAL:HG21 | 1.28 | 0.94 |
| 1:G:188:MET:O | 1:G:189:VAL:HG23 | 1.68 | 0.94 |
| 1:B:302:LYS:HE2 | 1:B:306:ARG:HH11 | 1.31 | 0.94 |
| 1:X:315:ARG:HD3 | 1:X:478:LEU:HD23 | 1.50 | 0.94 |
| 1:T:22:MET:CE | 1:X:330:ARG:NH1 | 2.30 | 0.94 |
| 1:K:395:SER:HB3 | 1:K:396:PRO:CD | 1.98 | 0.94 |
| 1:V:175:LEU:CD1 | 1:V:193:ALA:HB2 | 1.97 | 0.93 |
| 1:C:54:GLN:CG | 1:C:108:VAL:HG12 | 1.98 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:440:MET:HE3 | 1:M:494:LYS:HZ3 | 1.26 | 0.93 |
| 2:E:1041:ALA:HB3 | 1:C:34:SER:OG | 1.69 | 0.93 |
| 1:G:310:LEU:HD11 | 1:G:469:VAL:HG12 | 1.50 | 0.93 |
| 1:G:403:HIS:CD2 | 1:G:439:SER:OG | 2.22 | 0.93 |
| 1:G:403:HIS:HD2 | 1:G:439:SER:OG | 1.52 | 0.93 |
| 1:I:239:ASN:HD22 | 1:I:242:LEU:HB2 | 1.30 | 0.93 |
| 1:T:514:ILE:HG23 | 1:T:518:ILE:HD11 | 1.50 | 0.93 |
| 1:X:466:MET:HE2 | 1:X:480:ASP:H | 1.30 | 0.93 |
| 1:I:239:ASN:ND2 | 1:I:242:LEU:CB | 2.32 | 0.92 |
| 1:A:509:ILE:HG21 | 1:A:514:ILE:HG13 | 1.49 | 0.92 |
| 1:I:306:ARG:O | 1:I:310:LEU:HD23 | 1.69 | 0.92 |
| 2:W:1046:ALA:CB | 2:W:1049:HIS:HD2 | 1.82 | 0.92 |
| 1:C:51:LYS:CG | 1:C:52:PRO:HD2 | 2.00 | 0.92 |
| 1:A:491:MET:HE3 | 1:A:493:PHE:HD1 | 1.34 | 0.92 |
| 1:C:50:ALA:HB2 | 1:C:109:ASN:OD1 | 1.69 | 0.91 |
| 1:T:327:LEU:HD23 | 1:T:345:ARG:HG3 | 1.52 | 0.91 |
| 1:C:323:MET:CG | 2:F:1056:ARG:HG2 | 1.97 | 0.91 |
| 1:I:319:ARG:NH2 | 1:I:482:LEU:HD11 | 1.86 | 0.91 |
| 1:X:110:GLU:O | 1:X:111:VAL:HG13 | 1.71 | 0.91 |
| 1:X:464:ILE:HD11 | 1:X:530:ARG:HA | 1.53 | 0.91 |
| 1:O:464:ILE:HD12 | 1:O:529:ALA:HB1 | 1.53 | 0.91 |
| 1:A:491:MET:HE1 | 1:A:493:PHE:CD1 | 2.05 | 0.91 |
| 1:T:491:MET:HE1 | 1:T:493:PHE:HB2 | 1.47 | 0.90 |
| 1:G:306:ARG:O | 1:G:310:LEU:HD13 | 1.70 | 0.90 |
| 1:T:491:MET:HE2 | 1:T:493:PHE:HB2 | 1.50 | 0.90 |
| 1:O:288:LEU:HD13 | 1:O:289:ASP:N | 1.87 | 0.90 |
| 1:I:319:ARG:NH2 | 1:I:482:LEU:CD1 | 2.34 | 0.90 |
| 1:C:395:SER:HB2 | 1:C:396:PRO:CA | 2.01 | 0.90 |
| 1:A:330:ARG:HD2 | 1:A:342:LEU:HD23 | 1.54 | 0.90 |
| 1:I:420:LYS:HG3 | 1:O:123:GLN:NE2 | 1.86 | 0.90 |
| 1:V:65:GLU:HB3 | 1:V:368:LEU:HD22 | 1.54 | 0.90 |
| 1:B:253:ARG:HD2 | 1:I:256:ASP:OD2 | 1.71 | 0.90 |
| 1:A:491:MET:HE1 | 1:A:493:PHE:CB | 2.02 | 0.89 |
| 1:X:509:ILE:HD13 | 1:X:514:ILE:CG1 | 2.03 | 0.89 |
| 1:X:186:VAL:O | 1:X:514:ILE:HD13 | 1.71 | 0.89 |
| 1:I:50:ALA:HB2 | 1:I:109:ASN:OD1 | 1.73 | 0.89 |
| 1:I:310:LEU:HD21 | 1:I:469:VAL:HG12 | 0.91 | 0.89 |
| 1:A:451:MET:HE2 | 1:A:457:ILE:HD11 | 1.52 | 0.89 |
| 1:A:188:MET:HG2 | 1:A:189:VAL:N | 1.85 | 0.89 |
| 1:X:509:ILE:CG1 | 1:X:514:ILE:CG1 | 2.50 | 0.89 |
| 1:X:466:MET:SD | 1:X:479:SER:HA | 2.13 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:324:ILE:HD11 | 1:V:532:HIS:CD2 | 2.07 | 0.89 |
| 1:G:23:MET:HE3 | 1:G:32:MET:HE2 | 1.54 | 0.89 |
| 1:C:34:SER:CB | 1:C:39:ALA:CB | 2.48 | 0.88 |
| 1:A:491:MET:CE | 1:A:493:PHE:CB | 2.50 | 0.88 |
| 1:M:368:LEU:HD13 | 1:M:368:LEU:O | 1.73 | 0.88 |
| 1:V:313:GLU:CB | 1:V:314:PRO:HD2 | 2.03 | 0.88 |
| 1:T:349:GLN:HB3 | 1:T:432:THR:OG1 | 1.73 | 0.88 |
| 1:M:406:LEU:CD1 | 1:M:506:GLN:OE1 | 2.21 | 0.88 |
| 1:K:349:GLN:NE2 | 1:K:432:THR:CG2 | 2.36 | 0.88 |
| 1:V:177:LEU:CD2 | 1:V:204:ALA:HB1 | 2.04 | 0.88 |
| 1:I:345:ARG:HG2 | 1:I:346:GLY:N | 1.88 | 0.88 |
| 1:T:347:GLU:HB3 | 1:T:435:ASN:HD22 | 1.37 | 0.88 |
| 1:G:23:MET:CE | 1:G:32:MET:HE2 | 2.04 | 0.88 |
| 1:O:302:LYS:HG2 | 1:O:488:LEU:HD22 | 1.55 | 0.88 |
| 1:C:188:MET:HG2 | 1:C:189:VAL:N | 1.88 | 0.88 |
| 1:I:73:ILE:HG22 | 1:I:74:PRO:N | 1.89 | 0.88 |
| 1:B:202:LEU:HD22 | 1:B:520:GLN:HB3 | 1.56 | 0.88 |
| 1:X:451:MET:HB3 | 1:X:541:ILE:HD13 | 1.55 | 0.87 |
| 1:T:491:MET:HE1 | 1:T:493:PHE:CB | 2.03 | 0.87 |
| 1:T:2:LEU:CD2 | 1:X:328:ASP:OD2 | 2.21 | 0.87 |
| 1:K:464:ILE:CD1 | 1:K:533:ILE:CD1 | 2.52 | 0.87 |
| 1:T:239:ASN:HD22 | 1:T:242:LEU:HB2 | 1.39 | 0.87 |
| 1:V:93:ARG:HG2 | 1:V:97:ARG:HH21 | 1.38 | 0.87 |
| 1:R:51:LYS:CB | 1:R:54:GLN:CG | 2.47 | 0.87 |
| 1:B:406:LEU:CD2 | 1:B:506:GLN:OE1 | 2.22 | 0.87 |
| 1:T:328:ASP:OD2 | 1:V:2:LEU:HD11 | 1.75 | 0.87 |
| 1:T:120:VAL:HG11 | 1:T:368:LEU:HD23 | 1.54 | 0.87 |
| 1:M:477:VAL:CG1 | 1:M:525:GLN:OE1 | 2.22 | 0.87 |
| 1:C:185:ALA:HB1 | 1:C:514:ILE:HG22 | 1.56 | 0.86 |
| 1:A:2:LEU:HD21 | 1:A:25:ARG:NH2 | 1.91 | 0.86 |
| 1:I:239:ASN:HD22 | 1:I:242:LEU:CB | 1.88 | 0.86 |
| 1:G:274:LYS:HE3 | 1:G:301:GLU:OE2 | 1.76 | 0.86 |
| 1:K:464:ILE:CD1 | 1:K:533:ILE:HD12 | 2.05 | 0.86 |
| 1:G:192:GLU:O | 1:G:192:GLU:OE1 | 1.94 | 0.86 |
| 1:M:367:GLU:HG2 | 1:M:368:LEU:H | 1.41 | 0.86 |
| 1:T:491:MET:HE3 | 1:T:493:PHE:CD1 | 1.99 | 0.85 |
| 1:A:491:MET:HE1 | 1:A:493:PHE:CG | 2.11 | 0.85 |
| 1:B:319:ARG:HH21 | 1:B:482:LEU:CD1 | 1.89 | 0.85 |
| 1:K:395:SER:CB | 1:K:396:PRO:CD | 2.52 | 0.85 |
| 1:C:192:GLU:OE2 | 1:C:412:LEU:HD23 | 1.77 | 0.85 |
| 2:E:1041:ALA:HB3 | 1:C:34:SER:CB | 2.06 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:280:THR:O | 1:M:284:GLU:HG2 | 1.75 | 0.85 |
| 1:G:469:VAL:O | 1:G:469:VAL:HG12 | 1.77 | 0.85 |
| 1:A:128:ILE:CD1 | 1:A:153:ARG:HB2 | 2.06 | 0.85 |
| 1:R:349:GLN:HB3 | 1:R:432:THR:OG1 | 1.77 | 0.85 |
| 1:A:440:MET:O | 1:A:443:VAL:CG2 | 2.25 | 0.85 |
| 1:G:26:GLN:HE22 | 1:K:387:VAL:HA | 1.39 | 0.85 |
| 1:T:491:MET:CE | 1:T:493:PHE:CB | 2.54 | 0.85 |
| 1:V:177:LEU:CD2 | 1:V:204:ALA:C | 2.45 | 0.85 |
| 1:X:464:ILE:CG2 | 1:X:466:MET:HE3 | 2.06 | 0.85 |
| 1:A:198:GLU:O | 1:A:523:LEU:HD21 | 1.77 | 0.85 |
| 1:C:34:SER:HB3 | 1:C:39:ALA:HB2 | 1.56 | 0.84 |
| 1:V:396:PRO:HA | 1:V:400:GLU:OE2 | 1.77 | 0.84 |
| 1:G:398:ARG:O | 1:G:401:ILE:HG22 | 1.75 | 0.84 |
| 1:T:347:GLU:HB3 | 1:T:435:ASN:HD21 | 1.39 | 0.84 |
| 1:O:302:LYS:CG | 1:O:488:LEU:HD22 | 2.07 | 0.84 |
| 1:X:515:THR:CB | 1:X:518:ILE:HG12 | 2.05 | 0.84 |
| 1:C:67:THR:HG21 | 1:C:74:PRO:CD | 2.06 | 0.84 |
| 1:B:319:ARG:NH2 | 1:B:482:LEU:HD11 | 1.91 | 0.84 |
| 1:G:186:VAL:O | 1:G:187:LEU:HD23 | 1.77 | 0.84 |
| 2:W:1042:GLY:HA2 | 1:X:19:GLU:OE1 | 1.78 | 0.84 |
| 1:T:102:LEU:HD23 | 1:T:512:GLU:OE2 | 1.76 | 0.84 |
| 1:G:188:MET:O | 1:G:189:VAL:CG2 | 2.25 | 0.84 |
| 1:R:466:MET:HE2 | 1:R:480:ASP:H | 1.42 | 0.84 |
| 1:V:177:LEU:HD21 | 1:V:204:ALA:C | 1.97 | 0.84 |
| 1:T:375:THR:HG21 | 1:T:418:MET:HE2 | 1.59 | 0.84 |
| 1:R:393:VAL:O | 1:R:393:VAL:HG12 | 1.75 | 0.84 |
| 1:X:509:ILE:CD1 | 1:X:514:ILE:CG1 | 2.53 | 0.84 |
| 1:O:37:ASP:CB | 1:O:121:ASN:HB2 | 2.06 | 0.84 |
| 1:V:93:ARG:NH2 | 1:V:399:ARG:HA | 1.93 | 0.84 |
| 1:A:491:MET:CE | 1:A:493:PHE:HD1 | 1.88 | 0.83 |
| 1:K:397:LYS:HG3 | 1:K:400:GLU:CD | 1.98 | 0.83 |
| 1:C:34:SER:CA | 1:C:39:ALA:HB2 | 2.07 | 0.83 |
| 1:R:342:LEU:CD1 | 1:R:349:GLN:HE21 | 1.90 | 0.83 |
| 1:G:349:GLN:HE22 | 1:I:23:MET:HA | 1.43 | 0.83 |
| 1:O:239:ASN:HD22 | 1:O:242:LEU:HB2 | 1.42 | 0.83 |
| 1:V:198:GLU:OE2 | 1:V:527:LYS:HB2 | 1.77 | 0.83 |
| 1:G:189:VAL:HG11 | 1:G:507:MET:CE | 2.08 | 0.83 |
| 1:I:188:MET:CG | 1:I:189:VAL:N | 2.38 | 0.83 |
| 1:I:482:LEU:HD13 | 1:I:485:GLU:OE1 | 1.78 | 0.83 |
| 1:C:125:ASN:OD1 | 1:C:126:PRO:HD2 | 1.77 | 0.83 |
| 1:G:330:ARG:HD2 | 1:G:342:LEU:HD23 | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:67:THR:CG2 | 1:C:74:PRO:HD3 | 2.06 | 0.83 |
| 1:V:324:ILE:HD12 | 1:V:533:ILE:HD11 | 1.59 | 0.83 |
| 1:C:323:MET:HG3 | 2:F:1056:ARG:HG2 | 1.55 | 0.83 |
| 1:B:319:ARG:NH2 | 1:B:482:LEU:CD1 | 2.42 | 0.83 |
| 1:O:464:ILE:CD1 | 1:O:529:ALA:HB1 | 2.09 | 0.83 |
| 1:X:451:MET:SD | 1:X:541:ILE:HG23 | 2.18 | 0.83 |
| 1:O:274:LYS:HE2 | 1:O:301:GLU:OE2 | 1.79 | 0.83 |
| 1:A:62:ASN:HD22 | 1:C:393:VAL:CG2 | 1.92 | 0.83 |
| 1:B:202:LEU:HD21 | 1:B:520:GLN:HB3 | 1.61 | 0.82 |
| 1:A:196:LEU:CA | 1:A:200:GLN:HE21 | 1.92 | 0.82 |
| 1:V:482:LEU:HD13 | 1:V:485:GLU:OE1 | 1.79 | 0.82 |
| 1:G:191:SER:CB | 1:G:505:LEU:HB3 | 2.10 | 0.82 |
| 1:V:310:LEU:HD13 | 1:V:310:LEU:C | 1.99 | 0.82 |
| 1:V:198:GLU:OE2 | 1:V:527:LYS:HD2 | 1.78 | 0.82 |
| 1:A:62:ASN:HD22 | 1:C:393:VAL:HG23 | 1.43 | 0.82 |
| 1:B:310:LEU:O | 1:B:310:LEU:HD13 | 1.80 | 0.82 |
| 1:M:395:SER:HB3 | 1:M:396:PRO:CD | 2.10 | 0.82 |
| 1:G:192:GLU:O | 1:G:192:GLU:CD | 2.17 | 0.82 |
| 1:G:398:ARG:C | 1:G:401:ILE:HG22 | 2.01 | 0.82 |
| 1:K:322:ASP:CB | 1:K:525:GLN:HE21 | 1.93 | 0.82 |
| 1:X:464:ILE:HG22 | 1:X:466:MET:HE3 | 1.61 | 0.82 |
| 2:W:1046:ALA:HB3 | 2:W:1049:HIS:HD2 | 1.43 | 0.81 |
| 1:M:437:SER:C | 1:M:439:SER:H | 1.83 | 0.81 |
| 1:A:22:MET:CE | 1:C:342:LEU:HD21 | 2.09 | 0.81 |
| 1:G:278:ILE:O | 1:G:282:LEU:HD13 | 1.79 | 0.81 |
| 1:V:177:LEU:HD22 | 1:V:204:ALA:HB3 | 1.62 | 0.81 |
| 1:A:451:MET:HE3 | 1:A:457:ILE:HD11 | 1.60 | 0.81 |
| 1:I:406:LEU:HD11 | 1:I:506:GLN:OE1 | 1.81 | 0.81 |
| 1:C:202:LEU:CD2 | 1:C:520:GLN:HB3 | 2.09 | 0.81 |
| 1:G:189:VAL:HB | 1:G:507:MET:HB2 | 1.62 | 0.81 |
| 1:K:322:ASP:HB3 | 1:K:525:GLN:NE2 | 1.96 | 0.81 |
| 1:G:188:MET:HG2 | 1:G:189:VAL:N | 1.96 | 0.81 |
| 1:A:196:LEU:HD22 | 1:A:200:GLN:HE22 | 1.41 | 0.81 |
| 1:K:464:ILE:HD11 | 1:K:533:ILE:HD11 | 1.58 | 0.81 |
| 1:C:37:ASP:O | 1:C:38:THR:HB | 1.80 | 0.81 |
| 1:I:202:LEU:HD22 | 1:I:520:GLN:CB | 2.10 | 0.81 |
| 1:T:22:MET:HE1 | 1:X:330:ARG:CZ | 2.09 | 0.80 |
| 1:V:177:LEU:CD2 | 1:V:204:ALA:CB | 2.58 | 0.80 |
| 1:R:465:ALA:O | 1:R:466:MET:HE2 | 1.81 | 0.80 |
| 1:O:239:ASN:HD21 | 1:O:242:LEU:HB2 | 1.46 | 0.80 |
| 1:C:120:VAL:O | 1:C:120:VAL:CG1 | 2.30 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:186:VAL:O | 1:G:187:LEU:CG | 2.29 | 0.80 |
| 1:C:37:ASP:O | 1:C:121:ASN:CB | 2.28 | 0.80 |
| 1:A:128:ILE:HD12 | 1:A:153:ARG:HB2 | 1.62 | 0.80 |
| 1:V:93:ARG:HH22 | 1:V:399:ARG:HA | 1.45 | 0.80 |
| 1:G:94:LEU:HG | 1:G:188:MET:HE1 | 1.63 | 0.80 |
| 1:B:256:ASP:OD2 | 1:I:253:ARG:HD2 | 1.82 | 0.80 |
| 2:W:1046:ALA:C | 2:W:1048:HIS:N | 2.33 | 0.80 |
| 1:X:509:ILE:CG1 | 1:X:514:ILE:HG12 | 2.12 | 0.80 |
| 1:I:37:ASP:CB | 1:I:121:ASN:HB2 | 2.11 | 0.80 |
| 2:W:1046:ALA:CB | 2:W:1049:HIS:CD2 | 2.65 | 0.79 |
| 1:G:192:GLU:HG3 | 1:G:409:ARG:HG2 | 1.64 | 0.79 |
| 1:C:97:ARG:NH2 | 1:C:506:GLN:NE2 | 2.28 | 0.79 |
| 1:O:14:HIS:CB | 1:O:36:ASP:HB2 | 2.09 | 0.79 |
| 1:C:406:LEU:HD11 | 1:C:506:GLN:OE1 | 1.82 | 0.79 |
| 1:C:34:SER:HB3 | 1:C:39:ALA:CB | 2.12 | 0.79 |
| 1:B:302:LYS:HE2 | 1:B:306:ARG:NH1 | 1.98 | 0.79 |
| 1:V:335:PRO:O | 1:V:335:PRO:CD | 2.29 | 0.79 |
| 1:K:349:GLN:HE21 | 1:K:432:THR:HG22 | 1.46 | 0.79 |
| 1:R:198:GLU:OE2 | 1:R:527:LYS:HE2 | 1.81 | 0.79 |
| 1:T:347:GLU:CB | 1:T:435:ASN:ND2 | 2.38 | 0.79 |
| 1:K:274:LYS:CE | 1:K:301:GLU:OE2 | 2.30 | 0.79 |
| 1:G:186:VAL:O | 1:G:187:LEU:HG | 1.83 | 0.79 |
| 1:C:188:MET:CG | 1:C:189:VAL:N | 2.46 | 0.78 |
| 1:C:84:PRO:HA | 1:C:88:GLU:OE1 | 1.83 | 0.78 |
| 1:I:309:VAL:HG11 | 1:I:478:LEU:HD11 | 1.66 | 0.78 |
| 1:A:322:ASP:HA | 1:A:525:GLN:NE2 | 1.98 | 0.78 |
| 1:A:22:MET:HE3 | 1:C:342:LEU:HD21 | 1.63 | 0.78 |
| 1:G:64:GLN:HE22 | 1:G:66:ARG:HH22 | 1.31 | 0.78 |
| 1:B:349:GLN:HG2 | 1:B:433:GLU:HG2 | 1.63 | 0.78 |
| 1:I:328:ASP:OD2 | 1:K:2:LEU:HD12 | 1.83 | 0.78 |
| 1:O:349:GLN:CG | 1:O:432:THR:OG1 | 2.29 | 0.78 |
| 1:V:239:ASN:HD22 | 1:V:242:LEU:HD12 | 1.49 | 0.78 |
| 1:C:38:THR:HB | 1:C:121:ASN:N | 1.99 | 0.78 |
| 1:R:202:LEU:CD2 | 1:R:520:GLN:HB3 | 2.14 | 0.78 |
| 1:T:342:LEU:HD21 | 1:V:22:MET:HE3 | 1.64 | 0.78 |
| 1:G:186:VAL:O | 1:G:187:LEU:CD2 | 2.30 | 0.78 |
| 1:C:330:ARG:HD2 | 1:C:342:LEU:HD23 | 1.66 | 0.78 |
| 1:C:198:GLU:OE2 | 1:C:527:LYS:CD | 2.31 | 0.77 |
| 1:B:50:ALA:HB2 | 1:B:109:ASN:OD1 | 1.84 | 0.77 |
| 1:V:36:ASP:O | 1:V:37:ASP:HB2 | 1.82 | 0.77 |
| 1:I:342:LEU:HD11 | 1:I:349:GLN:NE2 | 1.96 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:319:ARG:NH2 | 1:V:482:LEU:CD1 | 2.46 | 0.77 |
| 1:X:112:GLN:HE21 | 1:X:114:ILE:HD11 | 1.49 | 0.77 |
| 1:R:97:ARG:NH2 | 1:R:506:GLN:NE2 | 2.32 | 0.77 |
| 1:G:310:LEU:HD12 | 1:G:469:VAL:CG1 | 2.12 | 0.77 |
| 1:V:93:ARG:HG2 | 1:V:97:ARG:NH2 | 1.98 | 0.77 |
| 1:C:202:LEU:HD21 | 1:C:520:GLN:HB3 | 1.65 | 0.77 |
| 1:I:406:LEU:CD1 | 1:I:506:GLN:OE1 | 2.33 | 0.77 |
| 1:M:348:THR:OG1 | 1:M:435:ASN:HB3 | 1.85 | 0.77 |
| 1:G:23:MET:CE | 1:G:32:MET:CE | 2.63 | 0.76 |
| 1:G:188:MET:C | 1:G:189:VAL:HG23 | 2.05 | 0.76 |
| 1:M:90:LEU:O | 1:M:94:LEU:HD13 | 1.85 | 0.76 |
| 1:R:466:MET:SD | 1:R:479:SER:HA | 2.26 | 0.76 |
| 1:A:44:VAL:CG1 | 1:A:138:LEU:HD23 | 2.15 | 0.76 |
| 1:I:198:GLU:OE2 | 1:I:527:LYS:CD | 2.34 | 0.75 |
| 1:K:64:GLN:HE21 | 1:K:116:THR:HB | 1.51 | 0.75 |
| 1:A:274:LYS:HE3 | 1:A:301:GLU:OE2 | 1.87 | 0.75 |
| 1:B:349:GLN:HE22 | 1:C:23:MET:HA | 1.51 | 0.75 |
| 1:R:406:LEU:CD1 | 1:R:506:GLN:OE1 | 2.34 | 0.75 |
| 1:C:40:VAL:HG22 | 1:C:117:VAL:HG22 | 1.68 | 0.75 |
| 1:V:466:MET:HB2 | 1:V:493:PHE:HB3 | 1.66 | 0.75 |
| 1:T:349:GLN:HE22 | 1:V:23:MET:HG2 | 1.50 | 0.75 |
| 1:X:515:THR:H | 1:X:518:ILE:HD11 | 1.51 | 0.75 |
| 1:M:349:GLN:HB2 | 1:M:432:THR:OG1 | 1.84 | 0.75 |
| 1:C:69:ALA:O | 1:C:120:VAL:HG12 | 1.87 | 0.75 |
| 1:A:91:ILE:CD1 | 1:A:127:ASP:OD1 | 2.33 | 0.75 |
| 1:B:189:VAL:HB | 1:B:507:MET:HB3 | 1.68 | 0.75 |
| 1:V:515:THR:OG1 | 1:V:518:ILE:HG23 | 1.85 | 0.75 |
| 1:R:239:ASN:HD22 | 1:R:242:LEU:HB2 | 1.44 | 0.75 |
| 1:V:264:GLN:HE21 | 1:X:26:GLN:HA | 1.48 | 0.75 |
| 1:A:188:MET:CG | 1:A:189:VAL:N | 2.47 | 0.75 |
| 1:B:406:LEU:CD1 | 1:B:506:GLN:OE1 | 2.35 | 0.75 |
| 1:X:509:ILE:CB | 1:X:514:ILE:CD1 | 2.57 | 0.74 |
| 1:I:72:ARG:NH2 | 1:I:367:GLU:O | 2.20 | 0.74 |
| 1:R:51:LYS:CG | 1:R:54:GLN:HE21 | 2.00 | 0.74 |
| 1:X:315:ARG:HD2 | 1:X:485:GLU:OE2 | 1.87 | 0.74 |
| 1:A:188:MET:O | 1:A:189:VAL:HG23 | 1.87 | 0.74 |
| 1:A:19:GLU:OE1 | 2:F:1042:GLY:HA3 | 1.86 | 0.74 |
| 1:X:324:ILE:HD11 | 1:X:532:HIS:CD2 | 2.21 | 0.74 |
| 1:C:55:ASP:OD1 | 1:C:56:PHE:HD2 | 1.71 | 0.74 |
| 1:R:239:ASN:HD21 | 1:R:242:LEU:HB2 | 1.53 | 0.74 |
| 1:X:324:ILE:HD11 | 1:X:532:HIS:CG | 2.22 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:387:VAL:CG2 | 1:K:434:SER:HB3 | 2.17 | 0.74 |
| 1:T:382:PHE:HE1 | 1:T:434:SER:HG | 1.26 | 0.74 |
| 1:T:125:ASN:ND2 | 1:T:127:ASP:CG | 2.41 | 0.74 |
| 1:R:97:ARG:NH2 | 1:R:506:GLN:HE22 | 1.86 | 0.74 |
| 1:A:108:VAL:O | 1:A:108:VAL:HG12 | 1.87 | 0.74 |
| 1:K:349:GLN:HE21 | 1:K:432:THR:CB | 2.00 | 0.74 |
| 1:G:189:VAL:HG11 | 1:G:507:MET:HE3 | 1.67 | 0.74 |
| 1:B:406:LEU:HD22 | 1:B:506:GLN:OE1 | 1.86 | 0.73 |
| 1:K:395:SER:HB2 | 1:K:396:PRO:HD2 | 1.70 | 0.73 |
| 1:X:466:MET:CE | 1:X:480:ASP:H | 2.01 | 0.73 |
| 1:A:196:LEU:CD2 | 1:A:200:GLN:HE22 | 1.96 | 0.73 |
| 2:S:1045:THR:O | 2:S:1045:THR:HG22 | 1.88 | 0.73 |
| 1:R:239:ASN:HD22 | 1:R:242:LEU:CB | 1.96 | 0.73 |
| 1:R:406:LEU:HD11 | 1:R:506:GLN:OE1 | 1.88 | 0.73 |
| 1:V:198:GLU:OE2 | 1:V:527:LYS:CB | 2.36 | 0.73 |
| 1:V:65:GLU:CB | 1:V:368:LEU:HD22 | 2.19 | 0.73 |
| 1:K:198:GLU:OE2 | 1:K:527:LYS:HD2 | 1.89 | 0.73 |
| 1:B:198:GLU:OE2 | 1:B:527:LYS:CD | 2.35 | 0.73 |
| 1:C:274:LYS:HE2 | 1:C:301:GLU:OE2 | 1.86 | 0.73 |
| 1:V:335:PRO:O | 1:V:335:PRO:HD2 | 1.89 | 0.73 |
| 1:M:349:GLN:CB | 1:M:432:THR:OG1 | 2.37 | 0.73 |
| 1:T:342:LEU:HD21 | 1:V:22:MET:CE | 2.19 | 0.72 |
| 1:C:38:THR:HB | 1:C:121:ASN:H | 1.52 | 0.72 |
| 1:C:395:SER:CB | 1:C:396:PRO:HA | 2.13 | 0.72 |
| 1:K:93:ARG:HH12 | 1:K:399:ARG:HG2 | 1.54 | 0.72 |
| 1:X:406:LEU:CD1 | 1:X:506:GLN:OE1 | 2.37 | 0.72 |
| 1:X:315:ARG:HD3 | 1:X:478:LEU:CD2 | 2.19 | 0.72 |
| 1:T:93:ARG:HH12 | 1:T:399:ARG:HG2 | 1.54 | 0.72 |
| 1:T:93:ARG:NH1 | 1:T:399:ARG:HG2 | 2.04 | 0.72 |
| 1:A:347:GLU:OE2 | 1:A:435:ASN:ND2 | 2.22 | 0.72 |
| 2:W:1047:THR:O | 2:W:1048:HIS:CG | 2.43 | 0.72 |
| 1:G:64:GLN:NE2 | 1:G:66:ARG:NH2 | 2.38 | 0.72 |
| 1:C:37:ASP:O | 1:C:38:THR:CB | 2.38 | 0.71 |
| 1:V:117:VAL:HG11 | 1:V:368:LEU:HD21 | 1.72 | 0.71 |
| 1:K:322:ASP:CB | 1:K:525:GLN:NE2 | 2.52 | 0.71 |
| 1:B:328:ASP:OD2 | 1:C:2:LEU:HD12 | 1.89 | 0.71 |
| 1:B:302:LYS:CE | 1:B:306:ARG:HH11 | 2.02 | 0.71 |
| 1:O:349:GLN:HE22 | 1:R:23:MET:HA | 1.53 | 0.71 |
| 1:K:397:LYS:HG3 | 1:K:400:GLU:OE1 | 1.89 | 0.71 |
| 1:V:245:ARG:NH2 | 1:V:284:GLU:OE1 | 2.22 | 0.71 |
| 1:X:112:GLN:NE2 | 1:X:114:ILE:HD11 | 2.05 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:125:ASN:HD22 | 1:B:167:GLN:NE2 | 1.88 | 0.71 |
| 1:A:396:PRO:CA | 1:A:400:GLU:OE1 | 2.38 | 0.71 |
| 1:M:440:MET:CE | 1:M:494:LYS:NZ | 2.53 | 0.71 |
| 1:X:387:VAL:HG23 | 1:X:389:GLU:HG2 | 1.72 | 0.71 |
| 1:B:14:HIS:HB2 | 1:B:35:MET:HE2 | 1.71 | 0.71 |
| 1:T:93:ARG:HH12 | 1:T:399:ARG:CG | 2.03 | 0.71 |
| 1:B:34:SER:HB3 | 1:B:39:ALA:HA | 1.72 | 0.71 |
| 1:O:302:LYS:HG2 | 1:O:488:LEU:CD2 | 2.20 | 0.71 |
| 1:O:62:ASN:ND2 | 1:O:112:GLN:HE21 | 1.89 | 0.71 |
| 2:W:1046:ALA:C | 2:W:1048:HIS:H | 1.93 | 0.70 |
| 1:C:324:ILE:CD1 | 1:C:532:HIS:HD2 | 1.99 | 0.70 |
| 1:T:382:PHE:CE1 | 1:T:434:SER:OG | 2.42 | 0.70 |
| 1:M:25:ARG:HB2 | 1:R:433:GLU:OE2 | 1.91 | 0.70 |
| 1:K:36:ASP:O | 1:K:37:ASP:HB2 | 1.91 | 0.70 |
| 1:T:514:ILE:HG23 | 1:T:518:ILE:CD1 | 2.20 | 0.70 |
| 1:B:310:LEU:C | 1:B:310:LEU:HD13 | 2.11 | 0.70 |
| 1:T:435:ASN:OD1 | 1:T:435:ASN:C | 2.30 | 0.70 |
| 1:I:73:ILE:CG2 | 1:I:74:PRO:N | 2.49 | 0.70 |
| 1:O:344:THR:OG1 | 1:O:349:GLN:HB3 | 1.91 | 0.70 |
| 1:G:23:MET:HE1 | 1:G:32:MET:CE | 2.22 | 0.70 |
| 1:V:175:LEU:HD13 | 1:V:193:ALA:CB | 2.21 | 0.70 |
| 1:M:393:VAL:O | 1:M:393:VAL:CG1 | 2.40 | 0.70 |
| 1:G:23:MET:HE1 | 1:G:32:MET:HE3 | 1.73 | 0.70 |
| 1:K:33:VAL:HG21 | 1:K:133:GLY:HA2 | 1.73 | 0.70 |
| 1:T:198:GLU:OE2 | 1:T:527:LYS:HE2 | 1.91 | 0.70 |
| 1:X:509:ILE:HG21 | 1:X:514:ILE:HD12 | 1.72 | 0.70 |
| 1:V:330:ARG:NH1 | 2:W:1049:HIS:HB2 | 2.07 | 0.70 |
| 2:E:1041:ALA:CB | 1:C:34:SER:OG | 2.40 | 0.70 |
| 1:C:51:LYS:CB | 1:C:54:GLN:HB2 | 2.22 | 0.70 |
| 1:X:464:ILE:CD1 | 1:X:530:ARG:HA | 2.22 | 0.70 |
| 1:A:188:MET:CG | 1:A:189:VAL:H | 2.04 | 0.70 |
| 1:A:202:LEU:HD12 | 1:A:523:LEU:HD22 | 1.74 | 0.70 |
| 1:O:239:ASN:HD22 | 1:O:242:LEU:CB | 2.01 | 0.69 |
| 1:B:202:LEU:HD22 | 1:B:520:GLN:CB | 2.22 | 0.69 |
| 1:T:327:LEU:HD23 | 1:T:345:ARG:CG | 2.22 | 0.69 |
| 1:G:401:ILE:HG23 | 1:G:402:GLY:N | 2.08 | 0.69 |
| 1:K:93:ARG:NH1 | 1:K:399:ARG:HG2 | 2.06 | 0.69 |
| 1:I:319:ARG:NH2 | 1:I:482:LEU:HD12 | 2.07 | 0.69 |
| 1:T:342:LEU:CD2 | 1:V:22:MET:HE1 | 2.23 | 0.69 |
| 1:V:93:ARG:NH2 | 1:V:398:ARG:O | 2.24 | 0.69 |
| 1:T:274:LYS:HE3 | 1:T:301:GLU:OE2 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:437:SER:O | 1:M:439:SER:N | 2.24 | 0.69 |
| 1:R:302:LYS:O | 1:R:306:ARG:HG2 | 1.92 | 0.69 |
| 1:T:466:MET:HB2 | 1:T:493:PHE:HB3 | 1.75 | 0.69 |
| 1:K:349:GLN:NE2 | 1:K:432:THR:HG21 | 2.08 | 0.69 |
| 1:R:347:GLU:OE2 | 1:R:435:ASN:ND2 | 2.25 | 0.69 |
| 1:M:368:LEU:HD13 | 1:M:368:LEU:C | 2.13 | 0.69 |
| 1:K:47:GLN:O | 1:K:231:TRP:CH2 | 2.45 | 0.69 |
| 1:M:367:GLU:HG2 | 1:M:368:LEU:N | 2.07 | 0.69 |
| 1:G:493:PHE:CE2 | 1:G:523:LEU:HD23 | 2.28 | 0.69 |
| 1:G:175:LEU:HD12 | 1:G:193:ALA:HB2 | 1.75 | 0.69 |
| 1:X:464:ILE:CG2 | 1:X:466:MET:CE | 2.70 | 0.68 |
| 1:B:16:VAL:HG22 | 1:B:35:MET:HG2 | 1.75 | 0.68 |
| 1:X:44:VAL:HG22 | 1:X:113:VAL:HG22 | 1.75 | 0.68 |
| 1:O:288:LEU:CD1 | 1:O:289:ASP:O | 2.41 | 0.68 |
| 1:V:128:ILE:CD1 | 1:V:153:ARG:HB2 | 2.22 | 0.68 |
| 1:X:192:GLU:OE2 | 1:X:412:LEU:HD23 | 1.93 | 0.68 |
| 1:A:44:VAL:HG21 | 1:A:138:LEU:CD2 | 2.23 | 0.68 |
| 1:I:188:MET:O | 1:I:189:VAL:HG23 | 1.94 | 0.68 |
| 1:O:464:ILE:CD1 | 1:O:529:ALA:CB | 2.72 | 0.68 |
| 1:X:451:MET:SD | 1:X:541:ILE:CG2 | 2.82 | 0.68 |
| 2:H:1042:GLY:HA3 | 1:I:19:GLU:OE1 | 1.93 | 0.68 |
| 1:V:264:GLN:NE2 | 1:X:26:GLN:CA | 2.55 | 0.68 |
| 1:I:202:LEU:HD21 | 1:I:520:GLN:HB3 | 1.75 | 0.68 |
| 1:I:37:ASP:HB3 | 1:I:121:ASN:CB | 2.22 | 0.68 |
| 2:L:1058:GLN:CG | 2:L:1058:GLN:O | 2.40 | 0.68 |
| 1:V:324:ILE:CD1 | 1:V:533:ILE:HD11 | 2.24 | 0.68 |
| 1:O:198:GLU:OE2 | 1:O:527:LYS:HD2 | 1.93 | 0.68 |
| 1:A:264:GLN:NE2 | 1:B:26:GLN:O | 2.26 | 0.68 |
| 1:X:518:ILE:HG13 | 1:X:519:MET:N | 2.07 | 0.67 |
| 1:K:466:MET:HB2 | 1:K:493:PHE:HB3 | 1.76 | 0.67 |
| 1:R:239:ASN:ND2 | 1:R:242:LEU:CD1 | 2.57 | 0.67 |
| 1:V:65:GLU:CG | 1:V:368:LEU:HD22 | 2.24 | 0.67 |
| 1:G:192:GLU:HG3 | 1:G:409:ARG:CG | 2.24 | 0.67 |
| 1:R:202:LEU:HD21 | 1:R:520:GLN:HB3 | 1.74 | 0.67 |
| 1:X:517:GLU:HG2 | 1:X:518:ILE:N | 2.08 | 0.67 |
| 1:T:125:ASN:ND2 | 1:T:127:ASP:OD2 | 2.27 | 0.67 |
| 1:B:330:ARG:HD2 | 1:B:342:LEU:HD23 | 1.75 | 0.67 |
| 1:T:349:GLN:CB | 1:T:432:THR:OG1 | 2.43 | 0.67 |
| 1:R:239:ASN:HD22 | 1:R:242:LEU:CD1 | 2.06 | 0.67 |
| 1:T:342:LEU:CD2 | 1:V:22:MET:CE | 2.73 | 0.67 |
| 1:A:96:ASP:C | 1:A:96:ASP:OD1 | 2.30 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:509:ILE:CG1 | 1:X:514:ILE:HD11 | 2.25 | 0.67 |
| 1:X:515:THR:H | 1:X:518:ILE:CD1 | 2.07 | 0.67 |
| 1:G:189:VAL:HG11 | 1:G:507:MET:HE2 | 1.75 | 0.67 |
| 1:X:507:MET:SD | 1:X:509:ILE:HD11 | 2.35 | 0.66 |
| 1:V:324:ILE:HD12 | 1:V:533:ILE:CD1 | 2.24 | 0.66 |
| 1:T:22:MET:CE | 1:X:330:ARG:CZ | 2.71 | 0.66 |
| 1:O:349:GLN:HG3 | 1:O:432:THR:HG1 | 1.57 | 0.66 |
| 1:X:466:MET:CE | 1:X:479:SER:HA | 2.25 | 0.66 |
| 1:M:477:VAL:HG12 | 1:M:525:GLN:OE1 | 1.94 | 0.66 |
| 1:B:64:GLN:HE22 | 1:B:66:ARG:HH21 | 1.43 | 0.66 |
| 1:T:382:PHE:HE1 | 1:T:434:SER:OG | 1.78 | 0.66 |
| 1:B:127:ASP:OD2 | 1:B:153:ARG:NH1 | 2.29 | 0.66 |
| 1:G:310:LEU:HD21 | 1:G:471:GLU:CG | 2.22 | 0.66 |
| 1:V:324:ILE:CD1 | 1:V:533:ILE:CD1 | 2.74 | 0.66 |
| 1:R:84:PRO:HA | 1:R:88:GLU:OE1 | 1.95 | 0.66 |
| 1:K:387:VAL:O | 1:K:387:VAL:HG12 | 1.93 | 0.66 |
| 1:G:64:GLN:NE2 | 1:G:66:ARG:HH22 | 1.91 | 0.66 |
| 1:G:514:ILE:O | 1:G:514:ILE:HG23 | 1.96 | 0.66 |
| 1:V:333:VAL:O | 1:V:333:VAL:HG12 | 1.94 | 0.66 |
| 1:T:387:VAL:HG13 | 1:T:434:SER:HB3 | 1.77 | 0.66 |
| 1:B:33:VAL:O | 1:B:34:SER:HB3 | 1.96 | 0.66 |
| 1:T:396:PRO:HA | 1:T:400:GLU:OE1 | 1.95 | 0.66 |
| 1:T:34:SER:HB3 | 1:T:39:ALA:HB2 | 1.78 | 0.66 |
| 1:M:308:ARG:HG2 | 1:M:313:GLU:OE1 | 1.95 | 0.66 |
| 1:V:349:GLN:HE22 | 1:X:23:MET:HG2 | 1.61 | 0.66 |
| 1:G:466:MET:HB2 | 1:G:493:PHE:HB3 | 1.78 | 0.66 |
| 1:T:513:GLY:O | 1:T:514:ILE:C | 2.34 | 0.66 |
| 1:I:426:ARG:CZ | 1:I:428:VAL:HG21 | 2.26 | 0.65 |
| 1:X:387:VAL:HG21 | 1:X:389:GLU:OE2 | 1.96 | 0.65 |
| 1:G:121:ASN:OD1 | 1:G:122:PRO:HD2 | 1.96 | 0.65 |
| 2:E:1042:GLY:HA3 | 1:C:19:GLU:OE1 | 1.95 | 0.65 |
| 1:I:426:ARG:CZ | 1:I:428:VAL:CG2 | 2.74 | 0.65 |
| 1:I:188:MET:O | 1:I:189:VAL:CG2 | 2.43 | 0.65 |
| 1:O:464:ILE:HD13 | 1:O:529:ALA:CB | 2.25 | 0.65 |
| 1:V:128:ILE:HD11 | 1:V:153:ARG:HB2 | 1.78 | 0.65 |
| 1:X:334:LEU:HB2 | 1:X:340:SER:HB3 | 1.79 | 0.65 |
| 1:G:26:GLN:CD | 1:K:387:VAL:CA | 2.61 | 0.65 |
| 1:R:349:GLN:CB | 1:R:432:THR:OG1 | 2.43 | 0.65 |
| 1:O:64:GLN:HE22 | 1:O:66:ARG:HH21 | 1.43 | 0.65 |
| 1:V:284:GLU:O | 1:V:285:ASP:OD1 | 2.15 | 0.65 |
| 1:M:306:ARG:O | 1:M:310:LEU:HG | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:398:ARG:HA | 1:G:401:ILE:CG2 | 2.27 | 0.65 |
| 1:I:73:ILE:HG22 | 1:I:74:PRO:CD | 2.23 | 0.65 |
| 1:B:125:ASN:HD22 | 1:B:167:GLN:HE22 | 1.43 | 0.65 |
| 1:A:91:ILE:HD12 | 1:A:127:ASP:CG | 2.17 | 0.65 |
| 2:F:1058:GLN:N | 2:F:1058:GLN:OE1 | 2.30 | 0.65 |
| 1:V:177:LEU:CD2 | 1:V:204:ALA:O | 2.44 | 0.65 |
| 1:G:345:ARG:NH1 | 1:G:464:ILE:HG22 | 2.12 | 0.65 |
| 1:T:201:MET:HG3 | 1:T:502:ILE:HD12 | 1.77 | 0.65 |
| 1:T:435:ASN:OD1 | 1:T:436:GLY:N | 2.30 | 0.65 |
| 1:C:406:LEU:CD1 | 1:C:506:GLN:OE1 | 2.44 | 0.65 |
| 1:R:202:LEU:HD22 | 1:R:520:GLN:HB3 | 1.79 | 0.65 |
| 1:G:368:LEU:HD12 | 1:G:368:LEU:O | 1.97 | 0.64 |
| 1:G:493:PHE:HE2 | 1:G:523:LEU:HD23 | 1.61 | 0.64 |
| 1:V:330:ARG:HH11 | 2:W:1049:HIS:HB2 | 1.62 | 0.64 |
| 1:A:44:VAL:CG1 | 1:A:138:LEU:CD2 | 2.75 | 0.64 |
| 1:V:324:ILE:HD11 | 1:V:532:HIS:HD2 | 1.59 | 0.64 |
| 1:V:432:THR:HG22 | 1:X:24:ALA:H | 1.63 | 0.64 |
| 1:C:188:MET:CG | 1:C:189:VAL:H | 2.09 | 0.64 |
| 1:V:64:GLN:HE22 | 1:V:66:ARG:NH2 | 1.95 | 0.64 |
| 1:M:437:SER:C | 1:M:439:SER:N | 2.50 | 0.64 |
| 1:X:315:ARG:CD | 1:X:478:LEU:HD23 | 2.23 | 0.64 |
| 1:C:347:GLU:OE1 | 1:C:435:ASN:ND2 | 2.30 | 0.64 |
| 1:X:515:THR:O | 1:X:518:ILE:HG13 | 1.98 | 0.64 |
| 1:G:184:ALA:O | 1:G:185:ALA:HB2 | 1.96 | 0.64 |
| 1:B:440:MET:CE | 1:B:496:ALA:HB2 | 2.28 | 0.64 |
| 1:A:128:ILE:HG23 | 1:A:151:ALA:HB3 | 1.79 | 0.64 |
| 1:C:58:PRO:HG2 | 1:C:110:GLU:CG | 2.27 | 0.64 |
| 1:V:64:GLN:NE2 | 1:V:66:ARG:NH2 | 2.46 | 0.64 |
| 1:C:38:THR:CB | 1:C:120:VAL:HA | 2.27 | 0.64 |
| 1:C:55:ASP:OD1 | 1:C:56:PHE:N | 2.30 | 0.64 |
| 1:I:64:GLN:HA | 1:I:88:GLU:OE2 | 1.98 | 0.64 |
| 1:B:263:LYS:HB2 | 1:B:347:GLU:OE2 | 1.98 | 0.64 |
| 1:T:436:GLY:O | 1:T:437:SER:C | 2.34 | 0.64 |
| 1:O:288:LEU:HD13 | 1:O:289:ASP:O | 1.98 | 0.64 |
| 1:C:509:ILE:HD13 | 1:C:514:ILE:HD13 | 1.79 | 0.64 |
| 1:T:197:SER:O | 1:T:201:MET:HG2 | 1.98 | 0.64 |
| 1:T:406:LEU:CD1 | 1:T:506:GLN:OE1 | 2.46 | 0.64 |
| 1:O:406:LEU:CD1 | 1:O:506:GLN:OE1 | 2.46 | 0.64 |
| 1:M:395:SER:CB | 1:M:396:PRO:HD2 | 2.23 | 0.63 |
| 1:X:315:ARG:HH11 | 1:X:478:LEU:HD23 | 1.62 | 0.63 |
| 1:A:406:LEU:HD23 | 1:A:439:SER:HB2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:W:1046:ALA:HB1 | 2:W:1049:HIS:CD2 | 2.32 | 0.63 |
| 1:O:36:ASP:O | 1:O:37:ASP:CB | 2.46 | 0.63 |
| 1:I:188:MET:CG | 1:I:189:VAL:H | 2.09 | 0.63 |
| 1:G:189:VAL:O | 1:G:506:GLN:HA | 1.98 | 0.63 |
| 1:G:327:LEU:HD23 | 1:G:345:ARG:HG3 | 1.79 | 0.63 |
| 1:M:511:ILE:HD12 | 1:M:511:ILE:O | 1.97 | 0.63 |
| 1:K:52:PRO:HD2 | 1:K:53:GLY:H | 1.63 | 0.63 |
| 1:A:491:MET:HE2 | 1:A:493:PHE:CB | 2.22 | 0.63 |
| 1:K:188:MET:HG2 | 1:K:189:VAL:N | 2.12 | 0.63 |
| 1:M:50:ALA:HB2 | 1:M:109:ASN:OD1 | 1.98 | 0.63 |
| 1:C:127:ASP:OD2 | 1:C:153:ARG:NH2 | 2.31 | 0.63 |
| 1:T:518:ILE:HG13 | 1:T:519:MET:N | 2.11 | 0.63 |
| 1:X:128:ILE:CD1 | 1:X:153:ARG:HB2 | 2.29 | 0.63 |
| 1:M:367:GLU:CG | 1:M:368:LEU:H | 2.10 | 0.63 |
| 1:R:349:GLN:CG | 1:R:432:THR:OG1 | 2.46 | 0.63 |
| 1:O:288:LEU:HD13 | 1:O:288:LEU:C | 2.19 | 0.63 |
| 1:R:198:GLU:OE2 | 1:R:527:LYS:CE | 2.46 | 0.63 |
| 1:K:50:ALA:HB2 | 1:K:109:ASN:CG | 2.19 | 0.63 |
| 1:A:196:LEU:CA | 1:A:200:GLN:NE2 | 2.59 | 0.63 |
| 1:M:395:SER:CB | 1:M:396:PRO:CD | 2.73 | 0.63 |
| 1:K:397:LYS:HD2 | 1:K:400:GLU:OE2 | 1.98 | 0.63 |
| 1:C:3:ASN:ND2 | 1:K:3:ASN:ND2 | 2.46 | 0.63 |
| 1:T:349:GLN:NE2 | 1:V:23:MET:HG2 | 2.13 | 0.63 |
| 1:G:185:ALA:O | 1:G:209:HIS:NE2 | 2.32 | 0.63 |
| 1:K:327:LEU:HB2 | 2:L:1052:ALA:HB3 | 1.80 | 0.63 |
| 1:R:62:ASN:O | 1:R:62:ASN:OD1 | 2.16 | 0.63 |
| 1:C:38:THR:OG1 | 1:C:120:VAL:HA | 1.99 | 0.62 |
| 1:M:477:VAL:HG11 | 1:M:525:GLN:OE1 | 1.98 | 0.62 |
| 1:G:64:GLN:HE22 | 1:G:66:ARG:NH2 | 1.97 | 0.62 |
| 1:B:514:ILE:HG13 | 1:B:518:ILE:HD11 | 1.79 | 0.62 |
| 1:A:317:ASP:OD2 | 1:A:319:ARG:NE | 2.30 | 0.62 |
| 1:C:38:THR:HA | 1:C:119:SER:O | 1.99 | 0.62 |
| 1:A:399:ARG:O | 1:A:402:GLY:N | 2.32 | 0.62 |
| 1:T:406:LEU:HD12 | 1:T:506:GLN:OE1 | 2.00 | 0.62 |
| 1:X:55:ASP:OD1 | 1:X:56:PHE:N | 2.32 | 0.62 |
| 1:M:387:VAL:HA | 1:O:26:GLN:NE2 | 2.14 | 0.62 |
| 1:C:34:SER:HA | 1:C:39:ALA:HB2 | 1.79 | 0.62 |
| 1:K:52:PRO:CD | 1:K:53:GLY:H | 2.12 | 0.62 |
| 1:T:491:MET:CE | 1:T:493:PHE:CG | 2.71 | 0.62 |
| 1:X:464:ILE:HD11 | 1:X:530:ARG:CA | 2.28 | 0.62 |
| 1:B:64:GLN:NE2 | 1:B:66:ARG:HH21 | 1.97 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:263:LYS:NZ | 1:I:26:GLN:HE22 | 1.96 | 0.62 |
| 1:C:466:MET:HB2 | 1:C:493:PHE:HB3 | 1.81 | 0.62 |
| 1:V:59:LEU:HD23 | 1:V:96:ASP:OD1 | 1.98 | 0.62 |
| 1:K:7:ARG:NE | 1:K:218:ASN:OD1 | 2.32 | 0.62 |
| 1:A:315:ARG:HD3 | 1:A:319:ARG:O | 1.99 | 0.62 |
| 1:O:348:THR:HG21 | 1:O:437:SER:O | 2.00 | 0.62 |
| 1:O:50:ALA:CB | 1:O:109:ASN:OD1 | 2.41 | 0.62 |
| 1:T:93:ARG:NH1 | 1:T:399:ARG:CG | 2.61 | 0.62 |
| 1:G:306:ARG:NH2 | 1:G:471:GLU:OE2 | 2.33 | 0.62 |
| 1:K:349:GLN:HE21 | 1:K:432:THR:HB | 1.63 | 0.62 |
| 1:T:375:THR:HG21 | 1:T:418:MET:HE1 | 1.80 | 0.62 |
| 1:A:188:MET:O | 1:A:189:VAL:CG2 | 2.47 | 0.62 |
| 1:T:18:LEU:HG | 1:T:33:VAL:HG22 | 1.81 | 0.62 |
| 1:T:102:LEU:CD2 | 1:T:512:GLU:OE2 | 2.48 | 0.62 |
| 1:V:239:ASN:ND2 | 1:V:242:LEU:HG | 2.15 | 0.62 |
| 1:X:406:LEU:HD11 | 1:X:506:GLN:OE1 | 2.00 | 0.62 |
| 1:I:64:GLN:HE21 | 1:I:116:THR:HB | 1.64 | 0.62 |
| 1:C:260:ILE:HG21 | 1:C:265:GLU:HG2 | 1.82 | 0.62 |
| 1:M:387:VAL:O | 1:O:26:GLN:NE2 | 2.33 | 0.61 |
| 1:M:90:LEU:O | 1:M:94:LEU:CD1 | 2.48 | 0.61 |
| 1:G:387:VAL:HA | 1:I:26:GLN:NE2 | 2.15 | 0.61 |
| 1:K:464:ILE:CD1 | 1:K:533:ILE:HD11 | 2.25 | 0.61 |
| 1:R:492:ASP:HB3 | 1:R:508:ASP:HB2 | 1.82 | 0.61 |
| 1:B:76:SER:O | 1:B:79:ARG:NH1 | 2.34 | 0.61 |
| 1:X:97:ARG:HB3 | 1:X:188:MET:SD | 2.39 | 0.61 |
| 1:A:62:ASN:HB2 | 1:C:393:VAL:HG21 | 1.81 | 0.61 |
| 1:O:387:VAL:O | 1:R:26:GLN:NE2 | 2.33 | 0.61 |
| 1:R:239:ASN:ND2 | 1:R:242:LEU:HD12 | 2.16 | 0.61 |
| 1:T:491:MET:HE2 | 1:T:493:PHE:CB | 2.25 | 0.61 |
| 1:X:515:THR:CA | 1:X:518:ILE:HG12 | 2.31 | 0.61 |
| 1:T:34:SER:CB | 1:T:39:ALA:HB2 | 2.31 | 0.61 |
| 1:B:59:LEU:HD23 | 1:B:96:ASP:OD1 | 2.01 | 0.61 |
| 1:V:21:GLY:O | 1:V:25:ARG:HG2 | 2.01 | 0.61 |
| 1:K:349:GLN:HG3 | 1:K:432:THR:HB | 1.81 | 0.61 |
| 1:G:398:ARG:O | 1:G:401:ILE:CG2 | 2.47 | 0.61 |
| 1:K:399:ARG:O | 1:K:403:HIS:CD2 | 2.54 | 0.61 |
| 1:T:19:GLU:OE1 | 2:Y:1042:GLY:HA3 | 2.01 | 0.61 |
| 1:O:11:TYR:HD2 | 1:O:35:MET:HE2 | 1.65 | 0.60 |
| 1:B:466:MET:HB2 | 1:B:493:PHE:HB3 | 1.82 | 0.60 |
| 1:I:466:MET:HB2 | 1:I:493:PHE:HB3 | 1.82 | 0.60 |
| 1:A:466:MET:HB2 | 1:A:493:PHE:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:381:ASN:ND2 | 1:A:430:GLU:OE2 | 2.32 | 0.60 |
| 2:F:1058:GLN:H | 2:F:1058:GLN:CD | 2.05 | 0.60 |
| 1:K:393:VAL:O | 1:K:393:VAL:HG13 | 2.01 | 0.60 |
| 1:K:397:LYS:CG | 1:K:400:GLU:CD | 2.68 | 0.60 |
| 1:R:334:LEU:HD12 | 1:R:337:THR:HG21 | 1.83 | 0.60 |
| 1:T:348:THR:HG23 | 1:T:435:ASN:OD1 | 2.01 | 0.60 |
| 1:T:239:ASN:ND2 | 1:T:242:LEU:CB | 2.53 | 0.60 |
| 1:C:51:LYS:HB2 | 1:C:54:GLN:HB2 | 1.82 | 0.60 |
| 1:R:51:LYS:CB | 1:R:54:GLN:HG3 | 2.24 | 0.60 |
| 1:C:51:LYS:HB3 | 1:C:54:GLN:HB2 | 1.82 | 0.60 |
| 1:G:398:ARG:HA | 1:G:401:ILE:HG21 | 1.82 | 0.60 |
| 1:I:38:THR:HG23 | 1:I:120:VAL:HA | 1.84 | 0.60 |
| 1:O:308:ARG:HG3 | 1:O:313:GLU:OE1 | 2.01 | 0.60 |
| 1:I:239:ASN:HD21 | 1:I:242:LEU:HB2 | 1.58 | 0.60 |
| 1:R:466:MET:CE | 1:R:480:ASP:H | 2.12 | 0.60 |
| 1:O:64:GLN:HE22 | 1:O:66:ARG:NH2 | 2.00 | 0.60 |
| 1:V:16:VAL:HG22 | 1:V:35:MET:HG3 | 1.84 | 0.60 |
| 1:O:239:ASN:HD22 | 1:O:242:LEU:CD1 | 2.15 | 0.60 |
| 1:I:36:ASP:O | 1:I:37:ASP:HB2 | 2.00 | 0.60 |
| 1:A:393:VAL:CG1 | 1:B:62:ASN:ND2 | 2.65 | 0.60 |
| 1:I:345:ARG:CG | 1:I:346:GLY:N | 2.56 | 0.59 |
| 2:F:1058:GLN:O | 2:F:1059:PRO:C | 2.40 | 0.59 |
| 1:G:310:LEU:HD11 | 1:G:469:VAL:CG1 | 2.20 | 0.59 |
| 1:C:89:THR:HG22 | 1:C:398:ARG:HG3 | 1.83 | 0.59 |
| 1:C:58:PRO:CG | 1:C:110:GLU:HG2 | 2.29 | 0.59 |
| 1:K:198:GLU:OE2 | 1:K:527:LYS:CD | 2.50 | 0.59 |
| 1:I:399:ARG:HG2 | 1:I:403:HIS:CE1 | 2.38 | 0.59 |
| 1:B:274:LYS:HE3 | 1:B:301:GLU:OE2 | 2.02 | 0.59 |
| 1:X:509:ILE:CG1 | 1:X:514:ILE:CD1 | 2.79 | 0.59 |
| 1:V:198:GLU:OE2 | 1:V:527:LYS:CD | 2.49 | 0.59 |
| 1:M:14:HIS:CG | 1:M:35:MET:HE2 | 2.37 | 0.59 |
| 1:T:342:LEU:HD23 | 1:V:22:MET:HE1 | 1.84 | 0.59 |
| 1:O:62:ASN:HD22 | 1:O:112:GLN:HE21 | 1.48 | 0.59 |
| 1:O:239:ASN:ND2 | 1:O:242:LEU:HD12 | 2.17 | 0.59 |
| 1:K:96:ASP:OD1 | 1:K:100:ARG:HD2 | 2.01 | 0.59 |
| 1:X:464:ILE:CD1 | 1:X:530:ARG:CA | 2.81 | 0.59 |
| 1:T:327:LEU:CD2 | 1:T:345:ARG:HG3 | 2.30 | 0.59 |
| 1:T:386:SER:HB2 | 1:T:434:SER:HB2 | 1.84 | 0.59 |
| 1:K:51:LYS:CG | 1:K:52:PRO:HD3 | 2.28 | 0.59 |
| 1:G:263:LYS:NZ | 1:I:26:GLN:NE2 | 2.50 | 0.59 |
| 1:A:196:LEU:HA | 1:A:200:GLN:NE2 | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:22:MET:HE1 | 1:C:342:LEU:HD21 | 1.84 | 0.59 |
| 1:G:403:HIS:CD2 | 1:G:439:SER:HG | 2.17 | 0.59 |
| 1:T:34:SER:HA | 1:T:38:THR:O | 2.03 | 0.59 |
| 1:M:365:LEU:CD1 | 1:M:365:LEU:H | 2.15 | 0.59 |
| 1:X:464:ILE:HG22 | 1:X:465:ALA:N | 2.16 | 0.59 |
| 1:G:509:ILE:HD13 | 1:G:514:ILE:CD1 | 2.33 | 0.59 |
| 1:K:64:GLN:O | 1:K:64:GLN:HG3 | 2.03 | 0.59 |
| 1:X:334:LEU:HB2 | 1:X:337:THR:HG22 | 1.85 | 0.59 |
| 1:A:22:MET:HE1 | 1:C:342:LEU:CD2 | 2.33 | 0.58 |
| 1:X:440:MET:SD | 1:X:496:ALA:HB2 | 2.43 | 0.58 |
| 1:X:97:ARG:CZ | 1:X:188:MET:SD | 2.91 | 0.58 |
| 1:T:348:THR:HA | 1:T:433:GLU:O | 2.02 | 0.58 |
| 1:X:334:LEU:HD12 | 1:X:337:THR:HG21 | 1.83 | 0.58 |
| 1:K:51:LYS:HB3 | 1:K:54:GLN:HG3 | 1.83 | 0.58 |
| 1:K:347:GLU:OE1 | 1:K:435:ASN:ND2 | 2.24 | 0.58 |
| 1:X:464:ILE:CG2 | 1:X:465:ALA:N | 2.66 | 0.58 |
| 1:V:335:PRO:O | 1:V:335:PRO:CG | 2.50 | 0.58 |
| 1:B:14:HIS:CG | 1:B:35:MET:HE2 | 2.39 | 0.58 |
| 1:O:349:GLN:NE2 | 1:R:24:ALA:H | 2.00 | 0.58 |
| 1:X:324:ILE:HD11 | 1:X:532:HIS:HB3 | 1.85 | 0.58 |
| 1:O:64:GLN:NE2 | 1:O:66:ARG:NH2 | 2.51 | 0.58 |
| 1:A:239:ASN:HD22 | 1:A:242:LEU:HD12 | 1.68 | 0.58 |
| 1:O:322:ASP:HA | 1:O:525:GLN:HE21 | 1.68 | 0.58 |
| 1:X:509:ILE:HB | 1:X:514:ILE:CD1 | 2.23 | 0.58 |
| 1:B:14:HIS:CD2 | 1:B:35:MET:HE2 | 2.38 | 0.58 |
| 1:T:348:THR:CG2 | 1:T:436:GLY:H | 2.16 | 0.58 |
| 1:V:264:GLN:HE21 | 1:X:26:GLN:CA | 2.13 | 0.58 |
| 1:G:403:HIS:HD2 | 1:G:439:SER:HG | 1.49 | 0.58 |
| 1:M:348:THR:HG21 | 1:M:438:SER:H | 1.68 | 0.58 |
| 1:K:330:ARG:HD2 | 1:K:342:LEU:HD23 | 1.86 | 0.58 |
| 2:S:1058:GLN:NE2 | 2:S:1059:PRO:HD2 | 2.19 | 0.58 |
| 1:T:349:GLN:CG | 1:T:432:THR:OG1 | 2.52 | 0.58 |
| 1:A:188:MET:HG2 | 1:A:189:VAL:H | 1.56 | 0.58 |
| 1:G:349:GLN:NE2 | 1:I:23:MET:HA | 2.17 | 0.58 |
| 1:I:185:ALA:HB1 | 1:I:514:ILE:HG22 | 1.86 | 0.58 |
| 1:B:482:LEU:HD13 | 1:B:485:GLU:OE1 | 2.04 | 0.58 |
| 1:X:110:GLU:O | 1:X:111:VAL:CG1 | 2.48 | 0.58 |
| 1:O:288:LEU:HD11 | 1:O:293:LEU:HG | 1.86 | 0.58 |
| 1:X:14:HIS:ND1 | 1:X:36:ASP:OD2 | 2.35 | 0.58 |
| 1:B:406:LEU:HD21 | 1:B:506:GLN:OE1 | 2.02 | 0.58 |
| 1:C:89:THR:CG2 | 1:C:398:ARG:HG3 | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:64:GLN:HE22 | 1:R:66:ARG:HH21 | 1.52 | 0.58 |
| 1:T:368:LEU:H | 1:T:368:LEU:CD1 | 2.17 | 0.58 |
| 1:B:62:ASN:O | 1:B:62:ASN:OD1 | 2.21 | 0.58 |
| 1:V:347:GLU:OE2 | 1:V:435:ASN:ND2 | 2.37 | 0.58 |
| 1:A:196:LEU:CG | 1:A:200:GLN:NE2 | 2.66 | 0.57 |
| 1:X:465:ALA:O | 1:X:466:MET:HE2 | 2.04 | 0.57 |
| 1:B:406:LEU:HD13 | 1:B:506:GLN:OE1 | 2.03 | 0.57 |
| 1:G:186:VAL:HG23 | 1:G:514:ILE:HG21 | 1.84 | 0.57 |
| 1:C:125:ASN:HD22 | 1:C:153:ARG:HH22 | 1.51 | 0.57 |
| 1:T:22:MET:HE2 | 1:X:330:ARG:HH11 | 1.66 | 0.57 |
| 1:G:306:ARG:HH21 | 1:G:471:GLU:CD | 2.07 | 0.57 |
| 1:G:399:ARG:NH2 | 3:G:550:WO4:O4 | 2.37 | 0.57 |
| 1:T:386:SER:CB | 1:T:434:SER:HB2 | 2.34 | 0.57 |
| 2:W:1046:ALA:O | 2:W:1048:HIS:N | 2.37 | 0.57 |
| 1:X:514:ILE:H | 1:X:514:ILE:HD12 | 1.70 | 0.57 |
| 1:V:432:THR:CG2 | 1:X:24:ALA:H | 2.18 | 0.57 |
| 1:M:14:HIS:CD2 | 1:M:35:MET:CE | 2.87 | 0.57 |
| 1:B:308:ARG:HG2 | 1:B:313:GLU:OE1 | 2.04 | 0.57 |
| 1:K:464:ILE:HG22 | 1:K:465:ALA:N | 2.20 | 0.57 |
| 1:V:177:LEU:HD21 | 1:V:205:VAL:N | 2.19 | 0.57 |
| 1:A:322:ASP:OD1 | 2:D:1056:ARG:HG2 | 2.04 | 0.57 |
| 1:M:263:LYS:HB2 | 1:M:347:GLU:OE2 | 2.05 | 0.57 |
| 1:A:291:ASN:O | 1:A:294:GLY:N | 2.37 | 0.57 |
| 1:X:436:GLY:O | 3:X:550:WO4:O2 | 2.21 | 0.57 |
| 1:K:47:GLN:O | 1:K:231:TRP:HH2 | 1.85 | 0.57 |
| 1:X:515:THR:HG22 | 1:X:516:LYS:N | 2.18 | 0.57 |
| 1:K:399:ARG:HB3 | 1:K:403:HIS:CD2 | 2.40 | 0.57 |
| 1:A:128:ILE:HD11 | 1:A:153:ARG:HB2 | 1.86 | 0.57 |
| 1:R:97:ARG:CZ | 1:R:506:GLN:NE2 | 2.67 | 0.57 |
| 1:T:19:GLU:HB3 | 1:T:32:MET:HB3 | 1.85 | 0.57 |
| 1:I:447:SER:HB2 | 1:I:461:VAL:HG12 | 1.87 | 0.57 |
| 1:I:16:VAL:HG22 | 1:I:35:MET:HG2 | 1.85 | 0.57 |
| 1:V:239:ASN:HD22 | 1:V:242:LEU:CD1 | 2.17 | 0.57 |
| 1:T:125:ASN:OD1 | 1:T:126:PRO:HD2 | 2.05 | 0.57 |
| 1:X:128:ILE:HD11 | 1:X:153:ARG:HB2 | 1.86 | 0.57 |
| 1:B:84:PRO:HA | 1:B:88:GLU:OE1 | 2.04 | 0.57 |
| 1:O:347:GLU:HB2 | 1:O:435:ASN:HD22 | 1.70 | 0.57 |
| 1:K:348:THR:HG22 | 1:K:435:ASN:H | 1.69 | 0.57 |
| 1:B:188:MET:O | 1:B:189:VAL:CG2 | 2.47 | 0.57 |
| 1:G:188:MET:C | 1:G:189:VAL:CG2 | 2.73 | 0.57 |
| 1:A:322:ASP:CA | 1:A:525:GLN:HE21 | 2.12 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:97:ARG:NH2 | 1:C:506:GLN:HE21 | 2.02 | 0.56 |
| 1:M:440:MET:HE3 | 1:M:494:LYS:HG2 | 1.87 | 0.56 |
| 1:A:44:VAL:HG21 | 1:A:138:LEU:HD23 | 1.85 | 0.56 |
| 1:G:399:ARG:O | 1:G:403:HIS:ND1 | 2.37 | 0.56 |
| 1:I:62:ASN:ND2 | 1:I:112:GLN:HE21 | 2.02 | 0.56 |
| 1:I:310:LEU:HD23 | 1:I:469:VAL:HG11 | 1.79 | 0.56 |
| 1:G:328:ASP:OD2 | 1:I:2:LEU:CD2 | 2.44 | 0.56 |
| 1:G:401:ILE:HG23 | 1:G:402:GLY:H | 1.69 | 0.56 |
| 1:B:310:LEU:HD21 | 1:B:474:ASN:OD1 | 2.06 | 0.56 |
| 1:X:324:ILE:HD11 | 1:X:532:HIS:CB | 2.35 | 0.56 |
| 1:T:399:ARG:O | 1:T:403:HIS:CD2 | 2.58 | 0.56 |
| 1:X:128:ILE:HG23 | 1:X:151:ALA:CB | 2.35 | 0.56 |
| 1:O:175:LEU:HD11 | 1:O:177:LEU:HD23 | 1.86 | 0.56 |
| 1:X:381:ASN:ND2 | 1:X:430:GLU:OE2 | 2.38 | 0.56 |
| 1:X:385:TYR:HE2 | 1:X:432:THR:HA | 1.69 | 0.56 |
| 1:R:297:LEU:O | 1:R:301:GLU:HG3 | 2.06 | 0.56 |
| 1:B:328:ASP:HB3 | 1:B:344:THR:HB | 1.86 | 0.56 |
| 1:M:14:HIS:CG | 1:M:35:MET:CE | 2.88 | 0.56 |
| 1:B:33:VAL:HG12 | 1:B:34:SER:N | 2.20 | 0.56 |
| 1:A:37:ASP:OD1 | 1:C:336:ARG:HG2 | 2.06 | 0.56 |
| 1:K:397:LYS:CD | 1:K:400:GLU:OE2 | 2.53 | 0.56 |
| 1:V:335:PRO:O | 1:V:336:ARG:HB2 | 2.05 | 0.56 |
| 1:A:406:LEU:HD23 | 1:A:439:SER:CB | 2.36 | 0.56 |
| 1:C:3:ASN:O | 1:C:3:ASN:OD1 | 2.23 | 0.56 |
| 2:D:1058:GLN:HG3 | 2:D:1059:PRO:C | 2.26 | 0.56 |
| 1:T:175:LEU:HD11 | 1:T:177:LEU:HD23 | 1.87 | 0.56 |
| 2:W:1046:ALA:HB3 | 2:W:1049:HIS:CD2 | 2.33 | 0.56 |
| 1:C:34:SER:CA | 1:C:39:ALA:CB | 2.81 | 0.56 |
| 1:A:442:SER:O | 1:A:445:GLY:N | 2.39 | 0.56 |
| 1:V:263:LYS:HD2 | 1:V:435:ASN:CG | 2.25 | 0.56 |
| 1:T:320:GLU:OE1 | 2:U:1056:ARG:NH2 | 2.39 | 0.56 |
| 1:O:310:LEU:O | 1:O:310:LEU:HD12 | 2.06 | 0.56 |
| 1:I:121:ASN:OD1 | 1:I:122:PRO:HD2 | 2.06 | 0.56 |
| 1:V:50:ALA:CB | 1:V:109:ASN:OD1 | 2.44 | 0.56 |
| 1:C:395:SER:HB2 | 1:C:396:PRO:CB | 2.35 | 0.56 |
| 1:C:51:LYS:CG | 1:C:52:PRO:CD | 2.81 | 0.56 |
| 1:T:387:VAL:CG1 | 1:T:434:SER:HB3 | 2.35 | 0.56 |
| 1:G:535:GLY:O | 1:G:539:GLN:HG3 | 2.06 | 0.56 |
| 1:X:515:THR:CG2 | 1:X:516:LYS:N | 2.69 | 0.56 |
| 1:R:50:ALA:CB | 1:R:109:ASN:OD1 | 2.43 | 0.56 |
| 1:R:465:ALA:O | 1:R:466:MET:CE | 2.54 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:R:393:VAL:O | 1:R:393:VAL:CG1 | 2.48 | 0.55 |
| 1:K:349:GLN:NE2 | 1:K:432:THR:HG22 | 2.12 | 0.55 |
| 1:T:198:GLU:OE2 | 1:T:527:LYS:CE | 2.54 | 0.55 |
| 1:M:333:VAL:HG13 | 1:M:334:LEU:HG | 1.87 | 0.55 |
| 1:O:302:LYS:HG3 | 1:O:488:LEU:HD22 | 1.86 | 0.55 |
| 1:O:64:GLN:NE2 | 1:O:66:ARG:HH21 | 2.04 | 0.55 |
| 1:O:322:ASP:HA | 1:O:525:GLN:NE2 | 2.21 | 0.55 |
| 1:C:332:GLY:HA3 | 2:F:1047:THR:HG22 | 1.88 | 0.55 |
| 1:O:239:ASN:ND2 | 1:O:242:LEU:CD1 | 2.69 | 0.55 |
| 1:M:440:MET:CE | 1:M:494:LYS:HZ3 | 2.11 | 0.55 |
| 1:M:23:MET:HG2 | 1:R:349:GLN:HE22 | 1.72 | 0.55 |
| 1:A:108:VAL:CG1 | 1:A:108:VAL:O | 2.54 | 0.55 |
| 1:V:128:ILE:HG23 | 1:V:151:ALA:CB | 2.36 | 0.55 |
| 1:X:507:MET:HG2 | 1:X:509:ILE:HD12 | 1.89 | 0.55 |
| 1:K:328:ASP:HB3 | 1:K:344:THR:HB | 1.87 | 0.55 |
| 1:V:322:ASP:HA | 1:V:525:GLN:HE21 | 1.71 | 0.55 |
| 1:X:102:LEU:HD23 | 1:X:512:GLU:OE2 | 2.06 | 0.55 |
| 1:C:396:PRO:HA | 1:C:400:GLU:OE1 | 2.06 | 0.55 |
| 1:R:466:MET:HB2 | 1:R:493:PHE:HB3 | 1.89 | 0.55 |
| 1:G:191:SER:N | 1:G:505:LEU:O | 2.32 | 0.55 |
| 1:T:363:GLN:OE1 | 1:T:377:LEU:CD2 | 2.55 | 0.55 |
| 1:T:514:ILE:CG2 | 1:T:518:ILE:HD11 | 2.31 | 0.55 |
| 1:R:466:MET:CE | 1:R:479:SER:HA | 2.37 | 0.55 |
| 1:B:125:ASN:ND2 | 1:B:167:GLN:NE2 | 2.55 | 0.55 |
| 1:B:14:HIS:CB | 1:B:35:MET:HE2 | 2.37 | 0.55 |
| 1:T:421:PHE:HB3 | 1:T:422:PRO:HA | 1.88 | 0.55 |
| 1:A:368:LEU:O | 1:A:368:LEU:HD12 | 2.07 | 0.55 |
| 1:X:464:ILE:HG21 | 1:X:466:MET:CE | 2.37 | 0.55 |
| 1:B:34:SER:HB2 | 1:B:38:THR:O | 2.07 | 0.55 |
| 1:R:33:VAL:HG21 | 1:R:133:GLY:HA2 | 1.88 | 0.55 |
| 1:A:31:VAL:HG22 | 1:A:137:ALA:HB2 | 1.89 | 0.55 |
| 1:K:47:GLN:O | 1:K:231:TRP:CZ3 | 2.60 | 0.54 |
| 1:M:328:ASP:HB3 | 1:M:344:THR:HB | 1.89 | 0.54 |
| 1:V:217:GLN:O | 1:V:221:GLU:HG2 | 2.07 | 0.54 |
| 1:A:451:MET:HE3 | 1:A:457:ILE:CD1 | 2.35 | 0.54 |
| 1:K:188:MET:CG | 1:K:189:VAL:N | 2.69 | 0.54 |
| 1:A:334:LEU:HD11 | 1:B:118:VAL:HG22 | 1.89 | 0.54 |
| 1:O:345:ARG:O | 1:O:345:ARG:HG2 | 2.06 | 0.54 |
| 1:C:34:SER:HA | 1:C:39:ALA:CB | 2.37 | 0.54 |
| 1:X:330:ARG:HD2 | 1:X:342:LEU:HD23 | 1.89 | 0.54 |
| 1:G:310:LEU:CD2 | 1:G:471:GLU:HG2 | 2.24 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:441:ALA:O | 1:A:444:CYS:N | 2.41 | 0.54 |
| 1:B:34:SER:CB | 1:B:39:ALA:HA | 2.37 | 0.54 |
| 1:I:84:PRO:HA | 1:I:88:GLU:OE1 | 2.08 | 0.54 |
| 1:B:98:PRO:O | 1:B:187:LEU:HD13 | 2.07 | 0.54 |
| 1:K:59:LEU:CD2 | 1:K:100:ARG:CG | 2.68 | 0.54 |
| 1:C:54:GLN:HG2 | 1:C:108:VAL:HG12 | 1.89 | 0.54 |
| 1:V:175:LEU:HD12 | 1:V:193:ALA:HB2 | 1.86 | 0.54 |
| 1:A:406:LEU:HD22 | 1:A:506:GLN:OE1 | 2.07 | 0.54 |
| 1:R:153:ARG:HH21 | 1:R:170:LEU:CD1 | 2.21 | 0.54 |
| 1:K:274:LYS:CE | 1:K:301:GLU:CD | 2.75 | 0.54 |
| 1:R:153:ARG:HH21 | 1:R:170:LEU:HD13 | 1.72 | 0.54 |
| 1:O:349:GLN:NE2 | 1:O:432:THR:OG1 | 2.40 | 0.54 |
| 1:M:365:LEU:H | 1:M:365:LEU:HD13 | 1.71 | 0.54 |
| 1:A:328:ASP:HB3 | 1:A:344:THR:HB | 1.90 | 0.54 |
| 1:T:239:ASN:HD22 | 1:T:242:LEU:CB | 2.13 | 0.54 |
| 1:C:97:ARG:HH22 | 1:C:506:GLN:NE2 | 2.03 | 0.54 |
| 1:K:349:GLN:HG2 | 1:K:433:GLU:HB2 | 1.89 | 0.54 |
| 1:M:183:GLU:HG3 | 1:M:213:GLN:HE22 | 1.73 | 0.54 |
| 1:K:308:ARG:HG2 | 1:K:313:GLU:OE1 | 2.08 | 0.54 |
| 1:M:440:MET:CE | 1:M:494:LYS:HZ2 | 2.21 | 0.54 |
| 1:B:440:MET:HE3 | 1:B:496:ALA:HB2 | 1.89 | 0.54 |
| 1:X:509:ILE:CG2 | 1:X:514:ILE:CD1 | 2.51 | 0.54 |
| 1:G:398:ARG:CA | 1:G:401:ILE:HG22 | 2.37 | 0.54 |
| 1:C:40:VAL:O | 1:C:42:VAL:HG23 | 2.08 | 0.54 |
| 1:A:263:LYS:NZ | 1:B:26:GLN:HE22 | 2.06 | 0.54 |
| 1:I:158:ASN:HD22 | 1:O:419:ASP:HB3 | 1.72 | 0.54 |
| 1:O:387:VAL:HA | 1:R:26:GLN:NE2 | 2.23 | 0.53 |
| 1:G:333:VAL:H | 1:G:340:SER:HB2 | 1.73 | 0.53 |
| 2:E:1044:HIS:CD2 | 2:E:1045:THR:HG23 | 2.43 | 0.53 |
| 1:K:387:VAL:CG1 | 1:K:387:VAL:O | 2.56 | 0.53 |
| 1:X:128:ILE:HG23 | 1:X:151:ALA:HB3 | 1.90 | 0.53 |
| 1:G:433:GLU:OE2 | 1:I:25:ARG:HB2 | 2.07 | 0.53 |
| 1:G:24:ALA:H | 1:K:432:THR:CG2 | 2.22 | 0.53 |
| 1:G:514:ILE:CG2 | 1:G:514:ILE:O | 2.57 | 0.53 |
| 1:B:14:HIS:HB2 | 1:B:35:MET:CE | 2.39 | 0.53 |
| 1:V:177:LEU:HD21 | 1:V:204:ALA:O | 2.06 | 0.53 |
| 1:A:1:MET:C | 1:A:2:LEU:HD12 | 2.29 | 0.53 |
| 1:V:336:ARG:HB2 | 1:X:119:SER:OG | 2.09 | 0.53 |
| 1:G:306:ARG:O | 1:G:310:LEU:CD1 | 2.51 | 0.53 |
| 1:A:437:SER:OG | 1:A:440:MET:CG | 2.57 | 0.53 |
| 1:T:38:THR:HG23 | 1:T:119:SER:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:406:LEU:HD11 | 1:O:506:GLN:OE1 | 2.07 | 0.53 |
| 1:G:84:PRO:HA | 1:G:88:GLU:OE1 | 2.09 | 0.53 |
| 1:R:153:ARG:NH2 | 1:R:170:LEU:HD13 | 2.24 | 0.53 |
| 1:X:50:ALA:HA | 1:X:109:ASN:OD1 | 2.09 | 0.53 |
| 1:K:82:GLY:O | 1:K:83:ARG:C | 2.47 | 0.53 |
| 1:V:259:ARG:HE | 1:V:308:ARG:HH21 | 1.57 | 0.53 |
| 1:V:363:GLN:NE2 | 1:V:365:LEU:HD21 | 2.24 | 0.53 |
| 1:V:330:ARG:HB2 | 1:V:342:LEU:HB3 | 1.91 | 0.53 |
| 1:M:336:ARG:HB2 | 1:O:119:SER:HB2 | 1.90 | 0.53 |
| 1:T:38:THR:HG23 | 1:T:120:VAL:HA | 1.91 | 0.53 |
| 1:B:333:VAL:HG13 | 1:B:334:LEU:HG | 1.89 | 0.53 |
| 1:G:263:LYS:HZ3 | 1:I:26:GLN:HE22 | 1.56 | 0.52 |
| 2:W:1042:GLY:CA | 1:X:19:GLU:OE1 | 2.55 | 0.52 |
| 1:B:440:MET:CE | 1:B:495:VAL:O | 2.57 | 0.52 |
| 1:G:62:ASN:ND2 | 1:K:393:VAL:HG12 | 2.24 | 0.52 |
| 1:O:351:LEU:HB3 | 1:O:430:GLU:HB2 | 1.91 | 0.52 |
| 1:K:393:VAL:O | 1:K:393:VAL:CG1 | 2.57 | 0.52 |
| 1:C:51:LYS:CB | 1:C:52:PRO:HD2 | 2.39 | 0.52 |
| 1:G:514:ILE:HG13 | 1:G:518:ILE:HD11 | 1.90 | 0.52 |
| 1:X:387:VAL:CG2 | 1:X:389:GLU:OE2 | 2.57 | 0.52 |
| 1:V:492:ASP:HB3 | 1:V:508:ASP:HB2 | 1.90 | 0.52 |
| 1:A:437:SER:OG | 1:A:440:MET:HG2 | 2.09 | 0.52 |
| 1:R:486:ASP:O | 1:R:510:LYS:HE3 | 2.10 | 0.52 |
| 1:M:349:GLN:HB3 | 1:M:432:THR:OG1 | 2.08 | 0.52 |
| 1:X:188:MET:HG2 | 1:X:189:VAL:N | 2.23 | 0.52 |
| 1:X:2:LEU:HD11 | 1:X:22:MET:HG3 | 1.92 | 0.52 |
| 1:K:50:ALA:O | 1:K:51:LYS:C | 2.48 | 0.52 |
| 1:V:177:LEU:HD23 | 1:V:204:ALA:O | 2.08 | 0.52 |
| 1:B:302:LYS:CE | 1:B:306:ARG:NH1 | 2.69 | 0.52 |
| 1:G:202:LEU:CD2 | 1:G:520:GLN:OE1 | 2.58 | 0.52 |
| 1:V:230:ARG:O | 1:V:231:TRP:C | 2.48 | 0.52 |
| 1:A:80:ARG:HB2 | 1:C:379:HIS:CE1 | 2.45 | 0.52 |
| 1:K:322:ASP:HB2 | 1:K:525:GLN:HE21 | 1.71 | 0.52 |
| 1:M:349:GLN:HB2 | 1:M:432:THR:HG1 | 1.74 | 0.52 |
| 1:X:383:PRO:HB2 | 1:X:385:TYR:CE1 | 2.45 | 0.52 |
| 1:V:384:PRO:C | 1:V:386:SER:H | 2.12 | 0.52 |
| 1:A:491:MET:HE3 | 1:A:493:PHE:CD1 | 2.20 | 0.52 |
| 1:O:37:ASP:O | 1:O:38:THR:C | 2.48 | 0.52 |
| 1:X:515:THR:O | 1:X:518:ILE:CG1 | 2.58 | 0.52 |
| 1:I:481:ILE:HD12 | 1:I:486:ASP:CA | 2.40 | 0.52 |
| 1:V:329:VAL:O | 2:W:1049:HIS:HA | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:322:ASP:OD1 | 2:F:1056:ARG:HD2 | 2.10 | 0.52 |
| 1:G:487:HIS:O | 1:G:510:LYS:NZ | 2.43 | 0.52 |
| 1:G:33:VAL:HG21 | 1:G:133:GLY:HA2 | 1.92 | 0.52 |
| 1:M:336:ARG:NH1 | 1:O:121:ASN:OD1 | 2.41 | 0.51 |
| 1:G:24:ALA:H | 1:K:349:GLN:HE22 | 1.58 | 0.51 |
| 1:I:349:GLN:NE2 | 1:K:23:MET:HG2 | 2.26 | 0.51 |
| 1:T:509:ILE:HG12 | 1:T:514:ILE:HG13 | 1.92 | 0.51 |
| 1:R:406:LEU:HD12 | 1:R:506:GLN:OE1 | 2.08 | 0.51 |
| 1:X:14:HIS:HB3 | 1:X:36:ASP:OD2 | 2.10 | 0.51 |
| 1:B:37:ASP:HB2 | 1:B:121:ASN:HB2 | 1.92 | 0.51 |
| 1:M:198:GLU:OE2 | 1:M:527:LYS:HE2 | 2.10 | 0.51 |
| 1:A:348:THR:HA | 1:A:433:GLU:HG3 | 1.92 | 0.51 |
| 1:A:253:ARG:NH1 | 1:A:276:GLU:OE2 | 2.36 | 0.51 |
| 1:V:331:THR:HB | 2:W:1048:HIS:HB2 | 1.91 | 0.51 |
| 1:M:120:VAL:HG21 | 1:M:368:LEU:HD12 | 1.92 | 0.51 |
| 1:B:189:VAL:HB | 1:B:507:MET:CB | 2.40 | 0.51 |
| 1:T:34:SER:HB3 | 1:T:39:ALA:CB | 2.40 | 0.51 |
| 1:A:112:GLN:NE2 | 1:C:393:VAL:HG23 | 2.25 | 0.51 |
| 1:X:509:ILE:CG2 | 1:X:511:ILE:O | 2.59 | 0.51 |
| 1:V:64:GLN:NE2 | 1:V:66:ARG:HH21 | 2.08 | 0.51 |
| 1:T:144:PRO:HD3 | 1:T:231:TRP:HB2 | 1.91 | 0.51 |
| 1:B:267:TYR:OH | 1:B:484:ASP:OD1 | 2.20 | 0.51 |
| 1:T:330:ARG:HD2 | 1:T:342:LEU:HD23 | 1.92 | 0.51 |
| 1:I:481:ILE:HD12 | 1:I:486:ASP:HA | 1.91 | 0.51 |
| 2:Y:1044:HIS:CD2 | 2:Y:1045:THR:HG23 | 2.44 | 0.51 |
| 1:M:34:SER:CB | 2:S:1041:ALA:HB3 | 2.41 | 0.51 |
| 1:M:47:GLN:OE1 | 1:M:110:GLU:HB3 | 2.11 | 0.51 |
| 1:I:330:ARG:HD2 | 1:I:342:LEU:HD23 | 1.92 | 0.51 |
| 1:X:383:PRO:CB | 1:X:385:TYR:CE1 | 2.93 | 0.51 |
| 1:A:324:ILE:HD11 | 1:A:532:HIS:HD2 | 1.76 | 0.51 |
| 1:C:74:PRO:HB3 | 1:C:81:GLU:OE2 | 2.11 | 0.51 |
| 1:C:192:GLU:OE2 | 1:C:412:LEU:CD2 | 2.55 | 0.51 |
| 1:K:387:VAL:HG22 | 1:K:434:SER:O | 2.11 | 0.51 |
| 1:R:239:ASN:HD22 | 1:R:242:LEU:HD13 | 1.74 | 0.51 |
| 1:X:464:ILE:HG21 | 1:X:466:MET:HE3 | 1.91 | 0.51 |
| 1:X:466:MET:HB2 | 1:X:493:PHE:HB3 | 1.93 | 0.51 |
| 1:X:334:LEU:HB2 | 1:X:337:THR:CG2 | 2.40 | 0.51 |
| 1:V:433:GLU:OE2 | 1:X:25:ARG:HB2 | 2.10 | 0.51 |
| 1:G:202:LEU:HD22 | 1:G:520:GLN:OE1 | 2.10 | 0.51 |
| 1:I:51:LYS:HB3 | 1:I:54:GLN:HB2 | 1.91 | 0.51 |
| 1:K:52:PRO:CG | 1:K:53:GLY:N | 2.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:125:ASN:ND2 | 1:C:127:ASP:CG | 2.64 | 0.51 |
| 1:O:406:LEU:CD2 | 1:O:440:MET:CE | 2.89 | 0.51 |
| 1:I:158:ASN:ND2 | 1:O:419:ASP:HB3 | 2.25 | 0.51 |
| 1:K:323:MET:HB3 | 2:L:1056:ARG:HG2 | 1.93 | 0.51 |
| 1:O:464:ILE:HG12 | 1:O:465:ALA:N | 2.26 | 0.51 |
| 1:B:34:SER:HB3 | 1:B:39:ALA:CA | 2.40 | 0.51 |
| 1:X:509:ILE:HG22 | 1:X:511:ILE:H | 1.75 | 0.51 |
| 1:T:509:ILE:HG21 | 1:T:514:ILE:CG1 | 2.41 | 0.51 |
| 1:B:187:LEU:O | 1:B:509:ILE:HD12 | 2.11 | 0.51 |
| 1:T:262:ASP:HB3 | 1:T:265:GLU:HG2 | 1.92 | 0.51 |
| 1:I:339:GLY:HA3 | 1:I:354:ALA:HB3 | 1.92 | 0.51 |
| 1:V:324:ILE:CD1 | 1:V:533:ILE:HD12 | 2.40 | 0.50 |
| 1:B:310:LEU:CD1 | 1:B:310:LEU:C | 2.78 | 0.50 |
| 1:G:278:ILE:O | 1:G:282:LEU:CD1 | 2.56 | 0.50 |
| 1:I:328:ASP:HB3 | 1:I:344:THR:HB | 1.93 | 0.50 |
| 1:O:325:ARG:HD2 | 1:O:346:GLY:HA3 | 1.92 | 0.50 |
| 1:V:325:ARG:HD2 | 1:V:346:GLY:HA3 | 1.93 | 0.50 |
| 1:T:35:MET:O | 1:T:36:ASP:C | 2.47 | 0.50 |
| 1:I:431:ILE:HG12 | 1:I:438:SER:HB2 | 1.93 | 0.50 |
| 1:O:288:LEU:HD12 | 1:O:293:LEU:HD11 | 1.92 | 0.50 |
| 1:T:99:ILE:HA | 1:T:102:LEU:HD12 | 1.93 | 0.50 |
| 1:B:440:MET:HE1 | 1:B:496:ALA:HB2 | 1.91 | 0.50 |
| 1:B:496:ALA:HB3 | 1:B:504:ALA:HB3 | 1.93 | 0.50 |
| 1:T:26:GLN:NE2 | 1:X:263:LYS:HD3 | 2.26 | 0.50 |
| 1:A:2:LEU:CD2 | 1:A:25:ARG:NH2 | 2.68 | 0.50 |
| 1:G:192:GLU:CG | 1:G:409:ARG:HB3 | 2.41 | 0.50 |
| 1:M:348:THR:OG1 | 1:M:435:ASN:CB | 2.59 | 0.50 |
| 1:X:406:LEU:CD2 | 1:X:440:MET:CE | 2.89 | 0.50 |
| 1:A:119:SER:HB2 | 1:C:336:ARG:HB2 | 1.93 | 0.50 |
| 1:R:328:ASP:HB3 | 1:R:344:THR:HB | 1.92 | 0.50 |
| 1:X:507:MET:HG2 | 1:X:509:ILE:CD1 | 2.41 | 0.50 |
| 1:K:35:MET:HG3 | 1:K:35:MET:O | 2.12 | 0.50 |
| 1:X:333:VAL:O | 1:X:335:PRO:HD3 | 2.12 | 0.50 |
| 1:V:331:THR:HB | 2:W:1047:THR:HG22 | 1.92 | 0.50 |
| 1:C:121:ASN:OD1 | 1:C:122:PRO:HD2 | 2.12 | 0.50 |
| 1:C:330:ARG:HB3 | 1:C:342:LEU:HB3 | 1.92 | 0.50 |
| 1:G:387:VAL:O | 1:I:26:GLN:NE2 | 2.45 | 0.50 |
| 1:K:82:GLY:O | 1:K:83:ARG:O | 2.30 | 0.50 |
| 1:T:132:ILE:HD12 | 1:T:215:VAL:HG11 | 1.94 | 0.50 |
| 1:I:381:ASN:ND2 | 1:I:430:GLU:OE2 | 2.36 | 0.50 |
| 1:M:440:MET:HE3 | 1:M:494:LYS:CD | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:519:MET:O | 1:G:523:LEU:HG | 2.12 | 0.50 |
| 1:I:351:LEU:HB3 | 1:I:430:GLU:HB2 | 1.92 | 0.50 |
| 1:O:192:GLU:OE1 | 1:O:409:ARG:HG2 | 2.12 | 0.50 |
| 1:T:347:GLU:CB | 1:T:435:ASN:HD21 | 2.17 | 0.50 |
| 1:M:509:ILE:HG12 | 1:M:514:ILE:HD12 | 1.94 | 0.50 |
| 1:M:365:LEU:O | 1:M:365:LEU:HD22 | 2.11 | 0.50 |
| 1:K:52:PRO:CD | 1:K:53:GLY:N | 2.73 | 0.50 |
| 1:C:330:ARG:CD | 1:C:342:LEU:HD23 | 2.40 | 0.49 |
| 1:I:345:ARG:HB3 | 1:I:348:THR:OG1 | 2.12 | 0.49 |
| 1:B:494:LYS:HB2 | 1:B:506:GLN:HB3 | 1.94 | 0.49 |
| 1:G:345:ARG:O | 1:G:346:GLY:C | 2.48 | 0.49 |
| 1:M:437:SER:CB | 1:M:440:MET:HB2 | 2.42 | 0.49 |
| 1:T:513:GLY:O | 1:T:514:ILE:O | 2.30 | 0.49 |
| 1:K:36:ASP:O | 1:K:37:ASP:CB | 2.58 | 0.49 |
| 1:T:217:GLN:O | 1:T:221:GLU:HG2 | 2.11 | 0.49 |
| 1:O:302:LYS:CG | 1:O:488:LEU:CD2 | 2.82 | 0.49 |
| 1:G:380:TYR:CE2 | 1:G:400:GLU:HA | 2.48 | 0.49 |
| 1:O:329:VAL:HB | 2:P:1050:ALA:HB3 | 1.94 | 0.49 |
| 1:V:432:THR:HG22 | 1:X:24:ALA:N | 2.28 | 0.49 |
| 1:V:319:ARG:HH21 | 1:V:482:LEU:CD1 | 2.08 | 0.49 |
| 1:C:188:MET:O | 1:C:189:VAL:HG23 | 2.12 | 0.49 |
| 1:G:185:ALA:HB1 | 1:G:514:ILE:HG22 | 1.94 | 0.49 |
| 1:B:78:PHE:O | 1:B:79:ARG:HB2 | 2.13 | 0.49 |
| 1:M:433:GLU:OE2 | 1:O:25:ARG:HB2 | 2.13 | 0.49 |
| 1:V:61:VAL:HG22 | 1:V:113:VAL:HB | 1.94 | 0.49 |
| 1:K:464:ILE:CG2 | 1:K:465:ALA:N | 2.75 | 0.49 |
| 1:V:154:VAL:HB | 1:V:177:LEU:HB3 | 1.95 | 0.49 |
| 1:G:186:VAL:HG23 | 1:G:514:ILE:HD13 | 1.94 | 0.49 |
| 1:R:319:ARG:HH12 | 1:R:480:ASP:HB3 | 1.78 | 0.49 |
| 1:V:59:LEU:CD2 | 1:V:96:ASP:OD1 | 2.60 | 0.49 |
| 1:M:36:ASP:O | 1:M:37:ASP:OD1 | 2.30 | 0.49 |
| 1:T:438:SER:O | 1:T:441:ALA:N | 2.46 | 0.49 |
| 1:X:509:ILE:HG22 | 1:X:511:ILE:O | 2.12 | 0.49 |
| 1:G:263:LYS:HZ1 | 1:I:26:GLN:NE2 | 2.09 | 0.49 |
| 1:X:50:ALA:CA | 1:X:109:ASN:OD1 | 2.61 | 0.49 |
| 1:A:324:ILE:HD11 | 1:A:532:HIS:CD2 | 2.47 | 0.49 |
| 1:M:207:PHE:O | 1:M:211:GLN:HG2 | 2.12 | 0.49 |
| 1:M:368:LEU:C | 1:M:368:LEU:CD1 | 2.80 | 0.49 |
| 1:K:347:GLU:O | 1:K:433:GLU:HB3 | 2.12 | 0.49 |
| 1:A:118:VAL:HG11 | 1:C:334:LEU:HD22 | 1.95 | 0.49 |
| 1:B:188:MET:HA | 1:B:507:MET:O | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:217:GLN:O | 1:I:221:GLU:HG2 | 2.13 | 0.49 |
| 1:C:395:SER:HB2 | 1:C:396:PRO:HB3 | 1.93 | 0.49 |
| 1:G:192:GLU:HG2 | 1:G:409:ARG:HB3 | 1.93 | 0.49 |
| 1:V:64:GLN:HE22 | 1:V:66:ARG:HH21 | 1.59 | 0.49 |
| 1:I:333:VAL:HG23 | 2:J:1043:GLY:HA2 | 1.94 | 0.49 |
| 1:G:371:GLU:O | 1:G:372:ARG:HB2 | 2.12 | 0.49 |
| 1:R:336:ARG:O | 1:R:336:ARG:HG3 | 2.13 | 0.49 |
| 2:W:1045:THR:O | 2:W:1047:THR:N | 2.43 | 0.48 |
| 1:A:322:ASP:CA | 1:A:525:GLN:NE2 | 2.71 | 0.48 |
| 1:G:19:GLU:HB3 | 1:G:32:MET:HB3 | 1.94 | 0.48 |
| 1:A:54:GLN:HB3 | 1:A:108:VAL:CG1 | 2.43 | 0.48 |
| 1:M:14:HIS:CD2 | 1:M:35:MET:HE3 | 2.47 | 0.48 |
| 1:M:447:SER:HB2 | 1:M:461:VAL:HG12 | 1.95 | 0.48 |
| 1:O:411:VAL:HG12 | 1:O:415:MET:HG2 | 1.95 | 0.48 |
| 1:B:175:LEU:HD11 | 1:B:177:LEU:HD23 | 1.94 | 0.48 |
| 1:O:37:ASP:O | 1:O:38:THR:O | 2.30 | 0.48 |
| 1:V:482:LEU:N | 1:V:482:LEU:HD12 | 2.27 | 0.48 |
| 1:R:274:LYS:HG2 | 1:R:297:LEU:HD13 | 1.94 | 0.48 |
| 1:A:26:GLN:OE1 | 1:C:264:GLN:HG3 | 2.13 | 0.48 |
| 1:V:99:ILE:HA | 1:V:102:LEU:HD12 | 1.93 | 0.48 |
| 1:K:395:SER:O | 1:K:396:PRO:C | 2.50 | 0.48 |
| 1:V:93:ARG:CG | 1:V:97:ARG:HH21 | 2.18 | 0.48 |
| 1:G:401:ILE:CG2 | 1:G:402:GLY:N | 2.73 | 0.48 |
| 1:O:406:LEU:HD22 | 1:O:440:MET:CE | 2.43 | 0.48 |
| 1:I:397:LYS:O | 1:I:398:ARG:C | 2.52 | 0.48 |
| 1:T:363:GLN:OE1 | 1:T:377:LEU:HD21 | 2.13 | 0.48 |
| 1:I:128:ILE:O | 1:I:132:ILE:HD12 | 2.13 | 0.48 |
| 1:O:29:ALA:HB2 | 1:O:141:SER:HA | 1.95 | 0.48 |
| 1:G:132:ILE:HD12 | 1:G:215:VAL:HG11 | 1.95 | 0.48 |
| 1:B:125:ASN:ND2 | 1:B:167:GLN:HE22 | 2.11 | 0.48 |
| 1:V:44:VAL:HG22 | 1:V:113:VAL:HG22 | 1.96 | 0.48 |
| 1:B:193:ALA:HB1 | 1:B:196:LEU:HD12 | 1.96 | 0.48 |
| 1:I:33:VAL:HG21 | 1:I:133:GLY:HA2 | 1.95 | 0.48 |
| 1:K:332:GLY:HA3 | 2:L:1047:THR:HG22 | 1.95 | 0.48 |
| 1:B:206:VAL:HG21 | 1:B:516:LYS:HE3 | 1.95 | 0.48 |
| 1:R:349:GLN:HG2 | 1:R:432:THR:OG1 | 2.12 | 0.48 |
| 1:G:94:LEU:HG | 1:G:188:MET:CE | 2.37 | 0.48 |
| 1:A:330:ARG:HB2 | 1:A:342:LEU:HB3 | 1.95 | 0.48 |
| 1:I:87:GLY:HA2 | 1:I:90:LEU:HD12 | 1.96 | 0.48 |
| 1:A:183:GLU:HG3 | 1:A:213:GLN:HE22 | 1.77 | 0.48 |
| 1:I:482:LEU:N | 1:I:482:LEU:HD12 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:263:LYS:HD2 | 1:V:435:ASN:HB2 | 1.95 | 0.48 |
| 1:C:193:ALA:HB1 | 1:C:196:LEU:HD13 | 1.95 | 0.48 |
| 1:B:416:PRO:HD3 | 1:B:457:ILE:HA | 1.96 | 0.48 |
| 1:G:59:LEU:HD23 | 1:G:96:ASP:OD1 | 2.14 | 0.48 |
| 1:I:188:MET:C | 1:I:189:VAL:HG23 | 2.34 | 0.48 |
| 1:V:198:GLU:CD | 1:V:527:LYS:HD2 | 2.34 | 0.48 |
| 1:C:202:LEU:HD22 | 1:C:520:GLN:HB3 | 1.94 | 0.48 |
| 1:B:14:HIS:HB3 | 1:B:36:ASP:OD1 | 2.13 | 0.48 |
| 1:V:263:LYS:HE2 | 1:V:435:ASN:OD1 | 2.14 | 0.48 |
| 1:A:156:TYR:HB2 | 1:A:175:LEU:HB3 | 1.95 | 0.48 |
| 1:T:329:VAL:HB | 2:U:1050:ALA:HB3 | 1.95 | 0.48 |
| 1:X:399:ARG:O | 1:X:403:HIS:CD2 | 2.67 | 0.48 |
| 1:G:336:ARG:NE | 1:I:37:ASP:OD2 | 2.45 | 0.48 |
| 1:A:479:SER:OG | 1:A:525:GLN:NE2 | 2.47 | 0.48 |
| 1:V:206:VAL:HG21 | 1:V:516:LYS:HE2 | 1.94 | 0.48 |
| 1:R:329:VAL:HB | 2:S:1050:ALA:HB3 | 1.96 | 0.48 |
| 1:K:349:GLN:NE2 | 1:K:432:THR:HB | 2.27 | 0.48 |
| 1:X:466:MET:HE2 | 1:X:480:ASP:N | 2.12 | 0.48 |
| 1:A:509:ILE:HG21 | 1:A:514:ILE:CG1 | 2.32 | 0.48 |
| 1:K:399:ARG:O | 1:K:403:HIS:HD2 | 1.96 | 0.48 |
| 1:M:15:THR:O | 1:M:35:MET:HA | 2.13 | 0.48 |
| 1:V:365:LEU:HD11 | 1:V:374:ASP:OD2 | 2.14 | 0.48 |
| 1:G:406:LEU:HD11 | 1:G:506:GLN:OE1 | 2.14 | 0.47 |
| 1:K:397:LYS:CD | 1:K:400:GLU:CD | 2.83 | 0.47 |
| 1:V:432:THR:CG2 | 1:X:24:ALA:N | 2.77 | 0.47 |
| 1:B:99:ILE:HA | 1:B:102:LEU:HD12 | 1.95 | 0.47 |
| 1:G:26:GLN:NE2 | 1:K:387:VAL:C | 2.67 | 0.47 |
| 1:V:177:LEU:HD23 | 1:V:204:ALA:HB1 | 1.95 | 0.47 |
| 1:G:64:GLN:CD | 1:G:66:ARG:HH12 | 2.17 | 0.47 |
| 1:O:84:PRO:HA | 1:O:88:GLU:OE1 | 2.14 | 0.47 |
| 1:A:363:GLN:OE1 | 1:A:377:LEU:CD2 | 2.62 | 0.47 |
| 1:K:45:VAL:HG13 | 1:K:45:VAL:O | 2.13 | 0.47 |
| 1:C:33:VAL:O | 1:C:39:ALA:HB1 | 2.13 | 0.47 |
| 1:C:38:THR:HA | 1:C:119:SER:C | 2.35 | 0.47 |
| 1:T:93:ARG:HH12 | 1:T:399:ARG:HG3 | 1.78 | 0.47 |
| 1:B:15:THR:O | 1:B:35:MET:O | 2.32 | 0.47 |
| 1:T:19:GLU:OE1 | 2:Y:1042:GLY:CA | 2.61 | 0.47 |
| 1:B:274:LYS:HG2 | 1:B:297:LEU:HD13 | 1.96 | 0.47 |
| 1:K:81:GLU:O | 1:K:82:GLY:O | 2.32 | 0.47 |
| 1:G:206:VAL:HG21 | 1:G:516:LYS:HE3 | 1.96 | 0.47 |
| 1:A:399:ARG:O | 1:A:400:GLU:C | 2.51 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:51:LYS:HB2 | 1:V:54:GLN:HB2 | 1.97 | 0.47 |
| 1:G:381:ASN:ND2 | 1:G:430:GLU:OE2 | 2.47 | 0.47 |
| 1:T:393:VAL:O | 1:T:393:VAL:HG12 | 2.13 | 0.47 |
| 1:B:426:ARG:HH12 | 1:C:67:THR:HG22 | 1.79 | 0.47 |
| 1:C:342:LEU:HD12 | 1:C:349:GLN:HE21 | 1.73 | 0.47 |
| 1:A:202:LEU:HB2 | 1:A:523:LEU:HD22 | 1.97 | 0.47 |
| 2:D:1058:GLN:N | 2:D:1059:PRO:HA | 2.29 | 0.47 |
| 1:R:125:ASN:OD1 | 1:R:126:PRO:HD2 | 2.15 | 0.47 |
| 1:B:482:LEU:HD12 | 1:B:482:LEU:N | 2.29 | 0.47 |
| 1:V:336:ARG:HB2 | 1:X:119:SER:HG | 1.80 | 0.47 |
| 1:T:386:SER:OG | 1:T:434:SER:HB2 | 2.14 | 0.47 |
| 1:V:494:LYS:HB2 | 1:V:506:GLN:HB3 | 1.96 | 0.47 |
| 1:V:342:LEU:CD1 | 1:V:349:GLN:NE2 | 2.25 | 0.47 |
| 2:E:1041:ALA:N | 1:C:34:SER:OG | 2.48 | 0.47 |
| 1:B:406:LEU:HD11 | 1:B:506:GLN:OE1 | 2.15 | 0.47 |
| 1:G:509:ILE:HD13 | 1:G:514:ILE:HD13 | 1.97 | 0.47 |
| 1:I:192:GLU:OE1 | 1:I:409:ARG:HG2 | 2.15 | 0.47 |
| 1:O:324:ILE:HD11 | 1:O:532:HIS:CD2 | 2.49 | 0.47 |
| 1:G:24:ALA:H | 1:K:349:GLN:NE2 | 2.13 | 0.47 |
| 1:O:464:ILE:HD13 | 1:O:529:ALA:HB3 | 1.96 | 0.47 |
| 1:G:515:THR:OG1 | 1:G:518:ILE:HG12 | 2.14 | 0.47 |
| 1:G:278:ILE:HG22 | 1:G:282:LEU:HD13 | 1.97 | 0.47 |
| 1:B:185:ALA:HB1 | 1:B:514:ILE:HG22 | 1.97 | 0.47 |
| 1:I:399:ARG:O | 1:I:401:ILE:N | 2.48 | 0.47 |
| 1:T:16:VAL:HG22 | 1:T:35:MET:HG3 | 1.97 | 0.47 |
| 1:M:405:ARG:HD3 | 1:M:408:LYS:HD3 | 1.96 | 0.47 |
| 1:B:34:SER:HB3 | 1:B:39:ALA:CB | 2.44 | 0.47 |
| 1:M:34:SER:HB3 | 2:S:1041:ALA:HB3 | 1.96 | 0.47 |
| 1:O:206:VAL:HG21 | 1:O:516:LYS:HE3 | 1.97 | 0.47 |
| 1:A:440:MET:O | 1:A:441:ALA:C | 2.53 | 0.47 |
| 1:C:188:MET:O | 1:C:189:VAL:CG2 | 2.63 | 0.47 |
| 1:B:33:VAL:HG21 | 1:B:133:GLY:HA2 | 1.97 | 0.47 |
| 1:K:16:VAL:HG22 | 1:K:35:MET:HB3 | 1.97 | 0.47 |
| 1:R:339:GLY:HA3 | 1:R:354:ALA:HB3 | 1.97 | 0.47 |
| 1:R:175:LEU:HD11 | 1:R:177:LEU:HD23 | 1.97 | 0.47 |
| 1:C:328:ASP:HB3 | 1:C:344:THR:HB | 1.96 | 0.47 |
| 1:I:206:VAL:HG21 | 1:I:516:LYS:HE3 | 1.96 | 0.47 |
| 1:V:328:ASP:HB2 | 1:V:344:THR:HB | 1.96 | 0.47 |
| 1:X:217:GLN:O | 1:X:221:GLU:HG2 | 2.15 | 0.47 |
| 1:K:509:ILE:HD13 | 1:K:514:ILE:HG13 | 1.96 | 0.47 |
| 1:C:323:MET:HG3 | 2:F:1056:ARG:CD | 2.41 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:349:GLN:CB | 1:M:432:THR:HG1 | 2.26 | 0.46 |
| 1:O:466:MET:HB2 | 1:O:493:PHE:HB3 | 1.97 | 0.46 |
| 1:X:198:GLU:OE2 | 1:X:527:LYS:HE2 | 2.15 | 0.46 |
| 1:T:175:LEU:HD13 | 1:T:193:ALA:HB2 | 1.97 | 0.46 |
| 1:G:2:LEU:HD22 | 1:K:328:ASP:OD2 | 2.15 | 0.46 |
| 1:C:543:ALA:HA | 1:C:544:PRO:HD3 | 1.62 | 0.46 |
| 1:R:198:GLU:CD | 1:R:527:LYS:HE2 | 2.36 | 0.46 |
| 1:V:36:ASP:O | 1:V:37:ASP:CB | 2.54 | 0.46 |
| 1:V:128:ILE:HG23 | 1:V:151:ALA:HB1 | 1.96 | 0.46 |
| 1:K:249:LEU:HD23 | 1:K:277:THR:HG23 | 1.97 | 0.46 |
| 1:R:183:GLU:HG3 | 1:R:213:GLN:HE22 | 1.80 | 0.46 |
| 1:B:349:GLN:NE2 | 1:C:23:MET:HA | 2.26 | 0.46 |
| 1:K:144:PRO:HD3 | 1:K:231:TRP:HB2 | 1.98 | 0.46 |
| 1:O:406:LEU:CD2 | 1:O:440:MET:HE1 | 2.45 | 0.46 |
| 1:X:14:HIS:CB | 1:X:36:ASP:OD2 | 2.64 | 0.46 |
| 1:R:179:VAL:HG23 | 1:R:189:VAL:HG22 | 1.97 | 0.46 |
| 1:T:322:ASP:HA | 1:T:525:GLN:HE21 | 1.80 | 0.46 |
| 1:X:67:THR:HG21 | 1:X:74:PRO:HB3 | 1.98 | 0.46 |
| 2:W:1046:ALA:O | 2:W:1047:THR:C | 2.53 | 0.46 |
| 1:C:323:MET:SD | 2:F:1056:ARG:HG3 | 2.54 | 0.46 |
| 1:M:440:MET:HB3 | 1:M:463:GLY:O | 2.16 | 0.46 |
| 1:B:440:MET:HE2 | 1:B:495:VAL:O | 2.16 | 0.46 |
| 1:K:280:THR:O | 1:K:284:GLU:HG3 | 2.16 | 0.46 |
| 1:G:44:VAL:HG22 | 1:G:113:VAL:HG22 | 1.98 | 0.46 |
| 1:R:332:GLY:HA3 | 2:S:1047:THR:HG22 | 1.96 | 0.46 |
| 2:E:1041:ALA:HB3 | 1:C:34:SER:HB3 | 1.93 | 0.46 |
| 1:R:465:ALA:HA | 1:R:494:LYS:HA | 1.98 | 0.46 |
| 1:B:34:SER:HA | 1:B:38:THR:O | 2.16 | 0.46 |
| 1:I:87:GLY:O | 1:I:91:ILE:HD12 | 2.15 | 0.46 |
| 1:M:179:VAL:HG23 | 1:M:189:VAL:HG22 | 1.98 | 0.46 |
| 1:M:494:LYS:HB2 | 1:M:506:GLN:HB3 | 1.98 | 0.46 |
| 1:V:333:VAL:HG13 | 2:W:1042:GLY:O | 2.16 | 0.46 |
| 1:A:393:VAL:HG11 | 1:B:62:ASN:ND2 | 2.30 | 0.46 |
| 1:G:348:THR:HG23 | 1:G:434:SER:HA | 1.97 | 0.46 |
| 1:O:144:PRO:HD3 | 1:O:231:TRP:HB2 | 1.97 | 0.46 |
| 1:A:196:LEU:HB3 | 1:A:200:GLN:HG3 | 1.98 | 0.46 |
| 1:C:120:VAL:HG22 | 1:C:121:ASN:N | 2.30 | 0.46 |
| 1:C:53:GLY:O | 1:C:54:GLN:C | 2.54 | 0.46 |
| 1:I:128:ILE:HG13 | 1:I:128:ILE:H | 1.63 | 0.46 |
| 1:V:228:LYS:HB3 | 1:V:229:PRO:HD2 | 1.97 | 0.46 |
| 1:X:515:THR:HB | 1:X:518:ILE:CG1 | 2.25 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:518:ILE:HG13 | 1:X:519:MET:H | 1.81 | 0.46 |
| 1:G:330:ARG:HB2 | 1:G:342:LEU:HB3 | 1.97 | 0.46 |
| 1:I:406:LEU:CG | 1:I:506:GLN:OE1 | 2.64 | 0.46 |
| 1:G:379:HIS:HD2 | 1:G:426:ARG:HE | 1.62 | 0.46 |
| 1:V:385:TYR:C | 1:V:385:TYR:CD2 | 2.90 | 0.46 |
| 1:C:54:GLN:HG3 | 1:C:108:VAL:HG11 | 1.89 | 0.46 |
| 1:V:367:GLU:HG2 | 1:V:368:LEU:N | 2.30 | 0.46 |
| 1:B:14:HIS:CD2 | 1:B:35:MET:CE | 2.99 | 0.46 |
| 1:G:156:TYR:HB2 | 1:G:175:LEU:HB3 | 1.98 | 0.46 |
| 1:V:127:ASP:OD2 | 1:V:153:ARG:NH2 | 2.49 | 0.46 |
| 1:C:435:ASN:HD21 | 1:C:482:LEU:HD23 | 1.81 | 0.46 |
| 1:T:509:ILE:HG21 | 1:T:514:ILE:HG13 | 1.97 | 0.45 |
| 1:G:398:ARG:HA | 1:G:401:ILE:HG22 | 1.94 | 0.45 |
| 1:C:3:ASN:ND2 | 1:K:3:ASN:CB | 2.79 | 0.45 |
| 1:G:401:ILE:CG2 | 1:G:402:GLY:H | 2.28 | 0.45 |
| 1:C:398:ARG:O | 1:C:401:ILE:N | 2.50 | 0.45 |
| 1:G:125:ASN:HA | 1:G:126:PRO:HD3 | 1.85 | 0.45 |
| 1:X:280:THR:O | 1:X:284:GLU:HG2 | 2.16 | 0.45 |
| 1:R:59:LEU:HD23 | 1:R:100:ARG:HE | 1.80 | 0.45 |
| 1:O:431:ILE:HG12 | 1:O:438:SER:HB2 | 1.98 | 0.45 |
| 1:T:330:ARG:HD3 | 2:U:1043:GLY:O | 2.16 | 0.45 |
| 1:K:96:ASP:OD1 | 1:K:100:ARG:CD | 2.64 | 0.45 |
| 1:B:348:THR:HG22 | 1:B:435:ASN:H | 1.82 | 0.45 |
| 1:I:399:ARG:CG | 1:I:403:HIS:CE1 | 2.99 | 0.45 |
| 1:A:325:ARG:HD2 | 1:A:346:GLY:HA3 | 1.99 | 0.45 |
| 1:O:185:ALA:HB1 | 1:O:514:ILE:HG22 | 1.98 | 0.45 |
| 1:T:239:ASN:HD22 | 1:T:242:LEU:CD1 | 2.30 | 0.45 |
| 1:I:342:LEU:CD1 | 1:I:349:GLN:HE21 | 2.06 | 0.45 |
| 1:K:397:LYS:HD3 | 1:K:400:GLU:HG3 | 1.97 | 0.45 |
| 1:G:64:GLN:NE2 | 1:G:66:ARG:CZ | 2.79 | 0.45 |
| 1:G:62:ASN:HD22 | 1:K:393:VAL:HG12 | 1.81 | 0.45 |
| 1:V:177:LEU:HD11 | 1:V:205:VAL:HG22 | 1.99 | 0.45 |
| 1:A:322:ASP:OD1 | 1:A:322:ASP:C | 2.53 | 0.45 |
| 1:X:509:ILE:HD13 | 1:X:514:ILE:CD1 | 2.45 | 0.45 |
| 1:V:264:GLN:NE2 | 1:X:26:GLN:O | 2.50 | 0.45 |
| 1:G:325:ARG:HH22 | 1:G:436:GLY:HA3 | 1.81 | 0.45 |
| 1:R:440:MET:O | 1:R:441:ALA:HB3 | 2.16 | 0.45 |
| 1:I:345:ARG:HD3 | 1:I:480:ASP:OD2 | 2.17 | 0.45 |
| 1:A:48:LYS:HA | 1:A:231:TRP:CZ3 | 2.52 | 0.45 |
| 1:X:535:GLY:O | 1:X:539:GLN:HG3 | 2.16 | 0.45 |
| 1:X:513:GLY:O | 1:X:514:ILE:C | 2.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:188:MET:O | 1:G:189:VAL:HG22 | 2.14 | 0.45 |
| 1:G:406:LEU:CD1 | 1:G:506:GLN:OE1 | 2.64 | 0.45 |
| 1:V:396:PRO:CA | 1:V:400:GLU:OE2 | 2.56 | 0.45 |
| 1:X:192:GLU:OE2 | 1:X:412:LEU:CD2 | 2.63 | 0.45 |
| 1:B:347:GLU:OE2 | 1:B:435:ASN:ND2 | 2.50 | 0.45 |
| 1:X:188:MET:CG | 1:X:189:VAL:N | 2.79 | 0.45 |
| 1:B:175:LEU:HD13 | 1:B:193:ALA:HB2 | 1.99 | 0.45 |
| 1:G:463:GLY:HA2 | 1:G:530:ARG:HG2 | 1.96 | 0.45 |
| 1:V:349:GLN:NE2 | 1:X:23:MET:HG2 | 2.29 | 0.45 |
| 1:X:517:GLU:HG2 | 1:X:518:ILE:H | 1.77 | 0.45 |
| 1:V:319:ARG:HH22 | 1:V:482:LEU:CD1 | 2.29 | 0.45 |
| 1:O:464:ILE:CG1 | 1:O:465:ALA:N | 2.79 | 0.45 |
| 1:M:466:MET:CE | 1:M:477:VAL:HG12 | 2.47 | 0.45 |
| 1:V:239:ASN:ND2 | 1:V:242:LEU:CG | 2.79 | 0.45 |
| 1:G:345:ARG:NH1 | 1:G:464:ILE:CG2 | 2.79 | 0.45 |
| 1:T:421:PHE:HB3 | 1:T:422:PRO:CA | 2.46 | 0.45 |
| 1:G:489:GLY:O | 1:G:510:LYS:CE | 2.65 | 0.45 |
| 1:G:29:ALA:HB3 | 1:G:44:VAL:HB | 1.99 | 0.45 |
| 1:B:288:LEU:HD13 | 1:B:293:LEU:HD21 | 1.99 | 0.45 |
| 1:M:440:MET:HE3 | 1:M:494:LYS:CG | 2.47 | 0.45 |
| 1:K:349:GLN:NE2 | 1:K:432:THR:CB | 2.76 | 0.45 |
| 1:A:55:ASP:OD1 | 1:A:56:PHE:HD1 | 2.00 | 0.45 |
| 1:M:120:VAL:HG21 | 1:M:368:LEU:CD1 | 2.47 | 0.44 |
| 1:K:54:GLN:OE1 | 1:K:108:VAL:O | 2.35 | 0.44 |
| 1:O:288:LEU:CD1 | 1:O:288:LEU:C | 2.85 | 0.44 |
| 1:C:35:MET:SD | 1:C:129:VAL:HG22 | 2.56 | 0.44 |
| 1:B:325:ARG:HD2 | 1:B:346:GLY:HA3 | 1.99 | 0.44 |
| 1:B:24:ALA:HB3 | 1:B:30:ALA:CB | 2.47 | 0.44 |
| 2:E:1056:ARG:HB3 | 2:E:1057:PRO:HD2 | 1.98 | 0.44 |
| 1:I:393:VAL:HG12 | 1:I:393:VAL:O | 2.16 | 0.44 |
| 1:A:19:GLU:OE1 | 2:F:1042:GLY:CA | 2.63 | 0.44 |
| 1:I:396:PRO:HA | 1:I:400:GLU:OE1 | 2.17 | 0.44 |
| 1:A:14:HIS:HB3 | 1:A:36:ASP:HB2 | 1.99 | 0.44 |
| 1:B:11:TYR:OH | 1:B:152:ALA:HB2 | 2.17 | 0.44 |
| 1:X:315:ARG:HD2 | 1:X:485:GLU:CD | 2.38 | 0.44 |
| 1:A:363:GLN:OE1 | 1:A:377:LEU:HD21 | 2.17 | 0.44 |
| 1:O:367:GLU:OE1 | 1:O:372:ARG:NH2 | 2.50 | 0.44 |
| 1:G:259:ARG:O | 1:G:259:ARG:HG2 | 2.17 | 0.44 |
| 1:K:52:PRO:HG2 | 1:K:53:GLY:N | 2.33 | 0.44 |
| 1:O:14:HIS:ND1 | 1:O:36:ASP:CG | 2.71 | 0.44 |
| 1:A:23:MET:HB3 | 1:C:432:THR:HG21 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:3:ASN:HD22 | 1:K:3:ASN:CB | 2.31 | 0.44 |
| 1:V:327:LEU:O | 1:V:328:ASP:OD1 | 2.36 | 0.44 |
| 1:K:514:ILE:HA | 1:K:518:ILE:HD11 | 2.00 | 0.44 |
| 1:O:59:LEU:HD23 | 1:O:96:ASP:OD1 | 2.18 | 0.44 |
| 1:T:61:VAL:HG22 | 1:T:113:VAL:HB | 1.99 | 0.44 |
| 1:X:515:THR:HB | 1:X:518:ILE:CG2 | 2.47 | 0.44 |
| 1:I:183:GLU:HG3 | 1:I:213:GLN:HE22 | 1.82 | 0.44 |
| 1:C:396:PRO:CA | 1:C:400:GLU:OE1 | 2.65 | 0.44 |
| 1:B:344:THR:HG23 | 1:B:349:GLN:HB3 | 1.98 | 0.44 |
| 1:B:328:ASP:OD2 | 1:C:2:LEU:HB2 | 2.18 | 0.44 |
| 1:V:239:ASN:ND2 | 1:V:242:LEU:CD1 | 2.81 | 0.44 |
| 1:B:405:ARG:O | 1:B:409:ARG:HG2 | 2.18 | 0.44 |
| 1:C:142:GLY:HA2 | 1:C:230:ARG:HD3 | 1.99 | 0.44 |
| 1:K:152:ALA:HB2 | 1:K:212:GLN:HB3 | 2.00 | 0.44 |
| 1:T:330:ARG:NH1 | 2:U:1043:GLY:O | 2.51 | 0.44 |
| 1:I:158:ASN:OD1 | 1:I:158:ASN:O | 2.35 | 0.44 |
| 1:X:57:PHE:HA | 1:X:58:PRO:HD3 | 1.88 | 0.44 |
| 1:A:331:THR:HB | 2:D:1048:HIS:HB2 | 1.98 | 0.44 |
| 1:C:363:GLN:HB3 | 1:C:374:ASP:HB3 | 1.99 | 0.44 |
| 1:X:328:ASP:HB3 | 1:X:344:THR:HB | 2.00 | 0.44 |
| 1:K:347:GLU:O | 1:K:433:GLU:OE1 | 2.36 | 0.44 |
| 2:S:1045:THR:CG2 | 2:S:1045:THR:O | 2.60 | 0.44 |
| 1:T:468:LEU:HD11 | 1:T:475:TYR:HB2 | 1.99 | 0.44 |
| 1:A:134:ALA:O | 1:A:138:LEU:HD12 | 2.18 | 0.44 |
| 1:C:51:LYS:CB | 1:C:52:PRO:CD | 2.96 | 0.44 |
| 1:V:482:LEU:N | 1:V:482:LEU:CD1 | 2.81 | 0.44 |
| 1:G:97:ARG:NH1 | 1:G:188:MET:HE2 | 2.32 | 0.44 |
| 1:G:509:ILE:HD13 | 1:G:514:ILE:HD12 | 1.98 | 0.44 |
| 1:V:128:ILE:HG23 | 1:V:151:ALA:HB3 | 1.99 | 0.44 |
| 1:V:365:LEU:CD1 | 1:V:374:ASP:OD2 | 2.65 | 0.44 |
| 1:O:351:LEU:HD21 | 1:R:118:VAL:HG21 | 2.00 | 0.44 |
| 1:M:436:GLY:HA3 | 1:M:481:ILE:O | 2.18 | 0.44 |
| 1:R:239:ASN:HD21 | 1:R:242:LEU:HD12 | 1.83 | 0.44 |
| 1:O:14:HIS:ND1 | 1:O:36:ASP:OD2 | 2.50 | 0.44 |
| 1:C:3:ASN:ND2 | 1:K:3:ASN:HB2 | 2.33 | 0.44 |
| 1:I:324:ILE:HD11 | 1:I:532:HIS:HD2 | 1.83 | 0.44 |
| 1:M:127:ASP:OD1 | 1:M:128:ILE:N | 2.51 | 0.44 |
| 1:G:2:LEU:HD21 | 1:G:22:MET:HG3 | 2.01 | 0.43 |
| 1:X:338:HIS:O | 1:X:453:ALA:HA | 2.18 | 0.43 |
| 1:B:57:PHE:HA | 1:B:58:PRO:HD3 | 1.88 | 0.43 |
| 1:M:120:VAL:CB | 1:M:368:LEU:HD11 | 2.42 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:188:MET:HG2 | 1:C:189:VAL:H | 1.70 | 0.43 |
| 1:T:368:LEU:H | 1:T:368:LEU:HD13 | 1.83 | 0.43 |
| 1:A:347:GLU:CG | 1:A:435:ASN:HD22 | 2.30 | 0.43 |
| 1:O:11:TYR:CD2 | 1:O:35:MET:HE2 | 2.49 | 0.43 |
| 1:V:289:ASP:OD2 | 1:V:292:GLU:HG3 | 2.18 | 0.43 |
| 1:C:377:LEU:HB2 | 1:C:426:ARG:HA | 2.00 | 0.43 |
| 1:T:3:ASN:HA | 1:T:4:PRO:HD3 | 1.86 | 0.43 |
| 1:A:196:LEU:HB3 | 1:A:200:GLN:CG | 2.49 | 0.43 |
| 1:O:14:HIS:HB3 | 1:O:36:ASP:CB | 2.16 | 0.43 |
| 1:I:319:ARG:HH22 | 1:I:482:LEU:HD12 | 1.80 | 0.43 |
| 1:A:441:ALA:O | 1:A:444:CYS:HB2 | 2.19 | 0.43 |
| 1:X:315:ARG:NH1 | 1:X:478:LEU:HB3 | 2.33 | 0.43 |
| 1:G:192:GLU:HB2 | 1:G:409:ARG:HD3 | 2.00 | 0.43 |
| 1:B:38:THR:HA | 1:B:120:VAL:HA | 1.99 | 0.43 |
| 1:X:334:LEU:CB | 1:X:337:THR:HG22 | 2.48 | 0.43 |
| 1:B:263:LYS:NZ | 1:C:26:GLN:HE22 | 2.17 | 0.43 |
| 1:B:351:LEU:HB3 | 1:B:430:GLU:HB2 | 2.00 | 0.43 |
| 1:I:7:ARG:HB2 | 1:I:222:LEU:HD12 | 2.00 | 0.43 |
| 1:C:18:LEU:HD23 | 1:C:33:VAL:HG22 | 2.00 | 0.43 |
| 1:A:2:LEU:HD12 | 1:A:2:LEU:N | 2.34 | 0.43 |
| 1:V:263:LYS:HD2 | 1:V:435:ASN:CB | 2.49 | 0.43 |
| 1:V:230:ARG:O | 1:V:231:TRP:O | 2.37 | 0.43 |
| 1:X:175:LEU:HD11 | 1:X:177:LEU:HD23 | 2.00 | 0.43 |
| 1:A:245:ARG:HH12 | 1:A:288:LEU:HD11 | 1.83 | 0.43 |
| 1:A:441:ALA:O | 1:A:442:SER:C | 2.56 | 0.43 |
| 1:T:387:VAL:O | 1:V:26:GLN:NE2 | 2.51 | 0.43 |
| 1:R:335:PRO:HG2 | 1:R:336:ARG:H | 1.83 | 0.43 |
| 1:V:297:LEU:O | 1:V:301:GLU:HG3 | 2.18 | 0.43 |
| 1:R:44:VAL:HG22 | 1:R:113:VAL:HG22 | 1.99 | 0.43 |
| 1:O:344:THR:OG1 | 1:O:349:GLN:CB | 2.61 | 0.43 |
| 1:I:97:ARG:NH2 | 1:I:188:MET:SD | 2.91 | 0.43 |
| 1:C:50:ALA:CB | 1:C:109:ASN:OD1 | 2.54 | 0.43 |
| 1:B:33:VAL:CG1 | 1:B:34:SER:N | 2.82 | 0.43 |
| 1:O:62:ASN:ND2 | 1:O:112:GLN:NE2 | 2.64 | 0.43 |
| 1:B:348:THR:HG21 | 1:B:436:GLY:H | 1.83 | 0.43 |
| 1:C:62:ASN:HB2 | 1:C:114:ILE:HG22 | 2.00 | 0.43 |
| 1:O:396:PRO:HA | 1:O:400:GLU:OE1 | 2.18 | 0.43 |
| 1:R:55:ASP:OD1 | 1:R:56:PHE:N | 2.51 | 0.43 |
| 1:X:90:LEU:O | 1:X:94:LEU:HG | 2.19 | 0.43 |
| 1:K:463:GLY:O | 1:K:464:ILE:HD13 | 2.19 | 0.43 |
| 1:O:433:GLU:OE2 | 1:R:25:ARG:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:288:LEU:HD12 | 1:O:293:LEU:CD1 | 2.49 | 0.43 |
| 1:T:386:SER:C | 1:T:434:SER:H | 2.21 | 0.43 |
| 1:C:484:ASP:O | 1:C:487:HIS:N | 2.52 | 0.43 |
| 1:M:339:GLY:HA3 | 1:M:354:ALA:HB3 | 2.00 | 0.43 |
| 1:M:59:LEU:HB3 | 1:M:100:ARG:HH21 | 1.84 | 0.43 |
| 1:I:482:LEU:N | 1:I:482:LEU:CD1 | 2.82 | 0.43 |
| 1:C:57:PHE:HA | 1:C:58:PRO:HD3 | 1.88 | 0.43 |
| 1:O:198:GLU:HG3 | 1:O:502:ILE:HD11 | 2.01 | 0.43 |
| 1:C:3:ASN:HA | 1:C:4:PRO:HD3 | 1.94 | 0.43 |
| 1:X:97:ARG:NE | 1:X:188:MET:SD | 2.92 | 0.43 |
| 1:C:481:ILE:HA | 1:C:485:GLU:OE1 | 2.18 | 0.43 |
| 1:B:534:LEU:O | 1:B:538:GLU:HG3 | 2.19 | 0.43 |
| 1:G:316:ILE:HD12 | 1:G:316:ILE:H | 1.84 | 0.43 |
| 2:Y:1056:ARG:HA | 2:Y:1057:PRO:HD3 | 1.91 | 0.43 |
| 1:C:37:ASP:O | 1:C:38:THR:CG2 | 2.66 | 0.43 |
| 1:A:23:MET:O | 1:C:349:GLN:OE1 | 2.37 | 0.43 |
| 1:G:185:ALA:HB1 | 1:G:514:ILE:CG2 | 2.49 | 0.43 |
| 1:C:127:ASP:OD1 | 1:C:128:ILE:N | 2.51 | 0.43 |
| 1:C:202:LEU:HD22 | 1:C:520:GLN:CB | 2.49 | 0.43 |
| 1:X:324:ILE:CD1 | 1:X:532:HIS:HB3 | 2.49 | 0.43 |
| 1:X:198:GLU:OE2 | 1:X:527:LYS:CE | 2.67 | 0.43 |
| 1:C:392:MET:C | 1:C:394:GLY:N | 2.72 | 0.43 |
| 1:B:144:PRO:HD3 | 1:B:231:TRP:HB2 | 1.99 | 0.43 |
| 1:C:411:VAL:HG12 | 1:C:415:MET:HG2 | 2.00 | 0.43 |
| 1:I:281:LEU:HD13 | 1:I:293:LEU:HD22 | 2.01 | 0.43 |
| 1:A:188:MET:C | 1:A:189:VAL:HG23 | 2.38 | 0.43 |
| 1:C:509:ILE:CD1 | 1:C:514:ILE:HD13 | 2.45 | 0.43 |
| 1:T:399:ARG:O | 1:T:403:HIS:HD2 | 2.02 | 0.43 |
| 1:R:331:THR:HB | 2:S:1048:HIS:HB2 | 2.01 | 0.43 |
| 1:C:274:LYS:CE | 1:C:301:GLU:OE2 | 2.61 | 0.42 |
| 1:R:64:GLN:NE2 | 1:R:66:ARG:HH21 | 2.13 | 0.42 |
| 1:A:291:ASN:O | 1:A:292:GLU:C | 2.57 | 0.42 |
| 1:T:322:ASP:HA | 1:T:525:GLN:NE2 | 2.34 | 0.42 |
| 1:X:261:THR:HG23 | 1:X:317:ASP:HA | 2.00 | 0.42 |
| 1:X:281:LEU:HD13 | 1:X:293:LEU:HD22 | 2.00 | 0.42 |
| 1:A:322:ASP:O | 2:D:1057:PRO:HD3 | 2.18 | 0.42 |
| 1:T:93:ARG:NH1 | 1:T:399:ARG:HG3 | 2.34 | 0.42 |
| 1:R:213:GLN:O | 1:R:217:GLN:HG3 | 2.18 | 0.42 |
| 1:M:351:LEU:HB3 | 1:M:430:GLU:HB2 | 2.00 | 0.42 |
| 1:K:494:LYS:HB2 | 1:K:506:GLN:HB3 | 2.01 | 0.42 |
| 1:T:437:SER:OG | 1:T:437:SER:O | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:121:ASN:OD1 | 1:O:122:PRO:HD2 | 2.20 | 0.42 |
| 1:B:482:LEU:N | 1:B:482:LEU:CD1 | 2.82 | 0.42 |
| 1:K:64:GLN:CG | 1:K:64:GLN:O | 2.67 | 0.42 |
| 1:C:3:ASN:ND2 | 1:K:3:ASN:CG | 2.72 | 0.42 |
| 1:O:308:ARG:CG | 1:O:313:GLU:OE1 | 2.66 | 0.42 |
| 1:G:489:GLY:O | 1:G:510:LYS:HE3 | 2.19 | 0.42 |
| 1:M:534:LEU:O | 1:M:538:GLU:HG3 | 2.19 | 0.42 |
| 1:K:50:ALA:CB | 1:K:109:ASN:OD1 | 2.47 | 0.42 |
| 1:A:44:VAL:CG2 | 1:A:138:LEU:CD2 | 2.95 | 0.42 |
| 1:C:202:LEU:CD2 | 1:C:520:GLN:CB | 2.90 | 0.42 |
| 1:M:511:ILE:HD12 | 1:M:511:ILE:C | 2.39 | 0.42 |
| 1:I:157:ILE:O | 1:I:158:ASN:OD1 | 2.36 | 0.42 |
| 1:O:179:VAL:HG11 | 1:O:208:GLY:HA3 | 2.02 | 0.42 |
| 1:K:329:VAL:HB | 2:L:1050:ALA:HB3 | 2.01 | 0.42 |
| 1:V:84:PRO:HA | 1:V:88:GLU:OE1 | 2.19 | 0.42 |
| 1:B:431:ILE:HD12 | 1:B:438:SER:HB3 | 2.01 | 0.42 |
| 1:O:349:GLN:HG2 | 1:O:433:GLU:HB2 | 2.00 | 0.42 |
| 1:V:264:GLN:NE2 | 1:X:26:GLN:C | 2.72 | 0.42 |
| 1:X:451:MET:HG2 | 1:X:544:PRO:HG3 | 2.01 | 0.42 |
| 1:V:97:ARG:N | 1:V:98:PRO:HD2 | 2.35 | 0.42 |
| 1:T:34:SER:HA | 1:T:39:ALA:HA | 2.02 | 0.42 |
| 1:C:40:VAL:CG1 | 1:C:115:ALA:HB1 | 2.50 | 0.42 |
| 1:C:40:VAL:HG11 | 1:C:130:ALA:HB2 | 2.00 | 0.42 |
| 1:V:476:VAL:HG12 | 1:V:478:LEU:HD12 | 1.99 | 0.42 |
| 1:C:37:ASP:O | 1:C:121:ASN:N | 2.53 | 0.42 |
| 1:A:4:PRO:HB3 | 1:A:22:MET:HB2 | 2.01 | 0.42 |
| 1:G:213:GLN:HA | 1:G:216:ILE:HD12 | 2.01 | 0.42 |
| 1:O:44:VAL:HG22 | 1:O:113:VAL:HG22 | 2.01 | 0.42 |
| 1:K:278:ILE:O | 1:K:282:LEU:HG | 2.19 | 0.42 |
| 1:G:278:ILE:CG2 | 1:G:282:LEU:HD13 | 2.50 | 0.42 |
| 1:T:189:VAL:HB | 1:T:507:MET:HB3 | 2.01 | 0.42 |
| 1:V:192:GLU:HB3 | 1:V:409:ARG:HD3 | 2.02 | 0.42 |
| 1:G:24:ALA:H | 1:K:432:THR:HG22 | 1.83 | 0.42 |
| 1:K:347:GLU:O | 1:K:433:GLU:CB | 2.68 | 0.42 |
| 1:K:47:GLN:C | 1:K:231:TRP:HH2 | 2.23 | 0.42 |
| 1:R:125:ASN:HA | 1:R:126:PRO:HD3 | 1.88 | 0.42 |
| 1:O:183:GLU:HG3 | 1:O:213:GLN:HE22 | 1.85 | 0.42 |
| 1:X:121:ASN:OD1 | 1:X:122:PRO:HD2 | 2.20 | 0.42 |
| 1:G:328:ASP:HB3 | 1:G:344:THR:HB | 2.01 | 0.42 |
| 1:T:509:ILE:HG22 | 1:T:511:ILE:H | 1.85 | 0.42 |
| 1:T:368:LEU:HD13 | 1:T:368:LEU:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:239:ASN:HD21 | 1:V:242:LEU:HG | 1.84 | 0.42 |
| 1:C:297:LEU:O | 1:C:301:GLU:HG3 | 2.20 | 0.42 |
| 1:G:367:GLU:HG2 | 1:G:368:LEU:N | 2.34 | 0.42 |
| 1:V:348:THR:HB | 1:V:435:ASN:H | 1.84 | 0.42 |
| 1:T:363:GLN:OE1 | 1:T:377:LEU:HD22 | 2.19 | 0.42 |
| 1:V:385:TYR:O | 1:V:385:TYR:HD2 | 2.03 | 0.42 |
| 1:K:40:VAL:HG22 | 1:K:117:VAL:HG22 | 2.02 | 0.42 |
| 1:C:198:GLU:CD | 1:C:527:LYS:HD2 | 2.33 | 0.42 |
| 1:B:263:LYS:HD3 | 1:C:26:GLN:NE2 | 2.34 | 0.42 |
| 1:R:159:ASP:O | 1:R:160:GLN:OE1 | 2.38 | 0.42 |
| 1:T:121:ASN:HA | 1:T:122:PRO:HD3 | 1.93 | 0.42 |
| 1:T:348:THR:CG2 | 1:T:436:GLY:N | 2.83 | 0.41 |
| 1:B:319:ARG:NH2 | 1:B:482:LEU:HD12 | 2.32 | 0.41 |
| 1:O:479:SER:OG | 1:O:525:GLN:NE2 | 2.52 | 0.41 |
| 1:B:281:LEU:HD13 | 1:B:293:LEU:HD22 | 2.02 | 0.41 |
| 1:M:481:ILE:HG13 | 1:M:481:ILE:H | 1.65 | 0.41 |
| 1:K:543:ALA:HA | 1:K:544:PRO:HD3 | 1.94 | 0.41 |
| 1:T:364:VAL:HG22 | 1:T:373:THR:HG22 | 2.02 | 0.41 |
| 1:O:37:ASP:CB | 1:O:121:ASN:CB | 2.91 | 0.41 |
| 1:I:426:ARG:NH1 | 1:I:428:VAL:HG23 | 2.28 | 0.41 |
| 1:C:3:ASN:HD22 | 1:K:3:ASN:HB2 | 1.83 | 0.41 |
| 1:I:157:ILE:HD12 | 1:I:162:VAL:HG21 | 2.02 | 0.41 |
| 1:V:230:ARG:C | 1:V:231:TRP:O | 2.55 | 0.41 |
| 1:K:323:MET:HB3 | 2:L:1056:ARG:CG | 2.50 | 0.41 |
| 1:X:198:GLU:HG3 | 1:X:502:ILE:HD11 | 2.02 | 0.41 |
| 1:O:405:ARG:HD3 | 1:O:408:LYS:HD3 | 2.02 | 0.41 |
| 1:C:29:ALA:HB3 | 1:C:44:VAL:HB | 2.01 | 0.41 |
| 1:A:379:HIS:CD2 | 1:B:80:ARG:HE | 2.38 | 0.41 |
| 1:M:55:ASP:OD1 | 1:M:56:PHE:N | 2.53 | 0.41 |
| 1:G:24:ALA:N | 1:K:432:THR:CG2 | 2.82 | 0.41 |
| 1:M:234:GLN:HA | 1:M:235:PRO:HD3 | 1.95 | 0.41 |
| 1:G:128:ILE:HG13 | 1:G:128:ILE:H | 1.67 | 0.41 |
| 1:K:4:PRO:HB3 | 1:K:19:GLU:OE2 | 2.20 | 0.41 |
| 1:R:39:ALA:HB3 | 1:R:119:SER:HB3 | 2.02 | 0.41 |
| 1:I:433:GLU:OE2 | 1:K:25:ARG:HB2 | 2.19 | 0.41 |
| 1:M:439:SER:HB3 | 1:M:494:LYS:NZ | 2.35 | 0.41 |
| 1:V:324:ILE:HD13 | 1:V:533:ILE:CD1 | 2.48 | 0.41 |
| 1:X:128:ILE:HG23 | 1:X:151:ALA:HB1 | 2.02 | 0.41 |
| 1:C:490:ASP:HB3 | 1:C:511:ILE:HG12 | 2.03 | 0.41 |
| 1:G:363:GLN:HB3 | 1:I:79:ARG:HG3 | 2.03 | 0.41 |
| 1:O:127:ASP:OD1 | 1:O:128:ILE:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:80:ARG:HG2 | 1:O:81:GLU:N | 2.35 | 0.41 |
| 1:T:2:LEU:HD11 | 1:T:22:MET:SD | 2.60 | 0.41 |
| 1:V:310:LEU:C | 1:V:310:LEU:CD1 | 2.68 | 0.41 |
| 1:T:349:GLN:HG2 | 1:T:432:THR:OG1 | 2.21 | 0.41 |
| 1:X:315:ARG:NH1 | 1:X:478:LEU:HD23 | 2.32 | 0.41 |
| 1:A:213:GLN:HA | 1:A:216:ILE:HD12 | 2.02 | 0.41 |
| 1:C:60:THR:HG23 | 1:C:112:GLN:HG3 | 2.02 | 0.41 |
| 1:G:334:LEU:HB2 | 1:G:337:THR:HG22 | 2.03 | 0.41 |
| 1:K:345:ARG:HH21 | 1:K:437:SER:HB3 | 1.85 | 0.41 |
| 1:R:67:THR:OG1 | 1:R:74:PRO:HD3 | 2.20 | 0.41 |
| 1:X:84:PRO:HA | 1:X:88:GLU:OE1 | 2.20 | 0.41 |
| 1:K:267:TYR:HA | 1:K:270:VAL:HG12 | 2.03 | 0.41 |
| 1:O:319:ARG:HH12 | 1:O:480:ASP:HB3 | 1.86 | 0.41 |
| 1:B:426:ARG:NH1 | 1:C:67:THR:CG2 | 2.84 | 0.41 |
| 1:T:38:THR:HG22 | 1:T:39:ALA:N | 2.35 | 0.41 |
| 1:G:174:LYS:O | 1:G:193:ALA:HB1 | 2.21 | 0.41 |
| 1:I:399:ARG:C | 1:I:401:ILE:N | 2.72 | 0.41 |
| 1:M:14:HIS:CG | 1:M:35:MET:HE3 | 2.55 | 0.41 |
| 1:T:26:GLN:OE1 | 1:X:386:SER:O | 2.38 | 0.41 |
| 1:T:325:ARG:HD2 | 1:T:346:GLY:HA3 | 2.03 | 0.41 |
| 1:T:351:LEU:HB3 | 1:T:430:GLU:HB2 | 2.02 | 0.41 |
| 2:J:1056:ARG:HA | 2:J:1057:PRO:HD3 | 1.95 | 0.41 |
| 1:V:334:LEU:HA | 1:V:334:LEU:HD23 | 1.84 | 0.41 |
| 1:A:84:PRO:HA | 1:A:88:GLU:OE1 | 2.21 | 0.41 |
| 1:C:447:SER:HB2 | 1:C:461:VAL:HG12 | 2.02 | 0.41 |
| 1:A:280:THR:O | 1:A:284:GLU:HG2 | 2.21 | 0.41 |
| 1:T:64:GLN:NE2 | 1:T:66:ARG:NH2 | 2.69 | 0.41 |
| 1:T:2:LEU:HD23 | 1:X:328:ASP:OD2 | 2.14 | 0.41 |
| 1:O:38:THR:OG1 | 1:O:124:VAL:HG23 | 2.20 | 0.41 |
| 1:O:14:HIS:ND1 | 1:O:36:ASP:CB | 2.83 | 0.41 |
| 1:A:29:ALA:HB3 | 1:A:44:VAL:HB | 2.02 | 0.41 |
| 1:O:464:ILE:CG1 | 1:O:465:ALA:H | 2.34 | 0.41 |
| 1:V:65:GLU:OE2 | 1:V:368:LEU:HD23 | 2.21 | 0.41 |
| 1:R:202:LEU:HD22 | 1:R:520:GLN:CB | 2.50 | 0.41 |
| 1:B:440:MET:HE1 | 1:B:495:VAL:C | 2.41 | 0.41 |
| 1:A:98:PRO:HB2 | 1:A:149:ILE:HD13 | 2.03 | 0.41 |
| 1:T:236:GLU:HA | 1:T:237:PRO:HD3 | 1.96 | 0.41 |
| 1:K:306:ARG:NH2 | 1:K:490:ASP:OD2 | 2.54 | 0.41 |
| 2:W:1047:THR:O | 2:W:1048:HIS:ND1 | 2.54 | 0.41 |
| 1:I:179:VAL:HG23 | 1:I:189:VAL:HG22 | 2.03 | 0.41 |
| 2:L:1058:GLN:CD | 2:L:1058:GLN:H | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:288:LEU:HD13 | 1:O:289:ASP:C | 2.41 | 0.41 |
| 1:A:387:VAL:O | 1:B:26:GLN:NE2 | 2.54 | 0.41 |
| 1:T:396:PRO:HG3 | 1:V:80:ARG:NH1 | 2.36 | 0.41 |
| 1:I:491:MET:HB3 | 1:I:509:ILE:HG23 | 2.03 | 0.41 |
| 1:T:57:PHE:HA | 1:T:58:PRO:HD3 | 1.89 | 0.41 |
| 1:B:44:VAL:HG22 | 1:B:113:VAL:HG22 | 2.02 | 0.41 |
| 1:I:57:PHE:HA | 1:I:58:PRO:HD3 | 1.90 | 0.41 |
| 1:X:294:GLY:HA2 | 1:X:297:LEU:HD12 | 2.02 | 0.41 |
| 1:G:455:VAL:HA | 1:G:456:PRO:HD3 | 1.87 | 0.41 |
| 1:K:492:ASP:HB3 | 1:K:508:ASP:HB2 | 2.03 | 0.41 |
| 1:K:362:ALA:HB2 | 1:K:424:THR:HG21 | 2.03 | 0.41 |
| 1:B:393:VAL:O | 1:B:393:VAL:HG13 | 2.21 | 0.41 |
| 1:R:330:ARG:HB2 | 1:R:342:LEU:HB3 | 2.02 | 0.41 |
| 1:A:37:ASP:OD1 | 1:A:37:ASP:O | 2.39 | 0.41 |
| 1:R:19:GLU:HB3 | 1:R:32:MET:HB3 | 2.02 | 0.41 |
| 1:K:321:LYS:HE3 | 1:K:476:VAL:HG13 | 2.03 | 0.41 |
| 1:R:396:PRO:HA | 1:R:400:GLU:OE1 | 2.21 | 0.41 |
| 1:C:69:ALA:HA | 1:C:119:SER:HA | 2.03 | 0.40 |
| 1:A:399:ARG:O | 1:A:401:ILE:N | 2.53 | 0.40 |
| 1:C:509:ILE:HD13 | 1:C:514:ILE:CD1 | 2.47 | 0.40 |
| 1:C:55:ASP:OD1 | 1:C:56:PHE:CD2 | 2.61 | 0.40 |
| 1:B:128:ILE:H | 1:B:128:ILE:HG13 | 1.77 | 0.40 |
| 1:B:334:LEU:HA | 1:B:335:PRO:HD3 | 1.94 | 0.40 |
| 1:C:28:THR:OG1 | 1:C:44:VAL:O | 2.37 | 0.40 |
| 1:O:125:ASN:HA | 1:O:126:PRO:HD3 | 1.89 | 0.40 |
| 1:R:192:GLU:HB3 | 1:R:409:ARG:HD3 | 2.01 | 0.40 |
| 1:T:55:ASP:OD1 | 1:T:56:PHE:N | 2.54 | 0.40 |
| 1:V:330:ARG:HD3 | 2:W:1049:HIS:HB3 | 2.03 | 0.40 |
| 1:X:515:THR:C | 1:X:518:ILE:HG12 | 2.41 | 0.40 |
| 1:A:387:VAL:HG23 | 1:A:389:GLU:HG2 | 2.03 | 0.40 |
| 1:V:384:PRO:C | 1:V:386:SER:N | 2.74 | 0.40 |
| 1:X:335:PRO:CG | 2:Y:1041:ALA:HB2 | 2.52 | 0.40 |
| 1:G:127:ASP:OD1 | 1:G:128:ILE:N | 2.53 | 0.40 |
| 1:I:345:ARG:O | 1:I:346:GLY:C | 2.58 | 0.40 |
| 1:T:368:LEU:N | 1:T:368:LEU:CD1 | 2.82 | 0.40 |
| 1:G:398:ARG:CA | 1:G:401:ILE:CG2 | 2.97 | 0.40 |
| 1:T:26:GLN:NE2 | 1:X:263:LYS:CD | 2.84 | 0.40 |
| 1:G:331:THR:HB | 2:H:1048:HIS:HB2 | 2.03 | 0.40 |
| 1:R:267:TYR:HA | 1:R:270:VAL:HG12 | 2.03 | 0.40 |
| 1:C:278:ILE:HG21 | 1:C:290:GLU:HG3 | 2.04 | 0.40 |
| 1:M:440:MET:HE3 | 1:M:494:LYS:CE | 2.50 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:309:VAL:HG13 | 1:I:478:LEU:HD21 | 2.04 | 0.40 |
| 1:B:127:ASP:OD1 | 1:B:128:ILE:N | 2.54 | 0.40 |
| 1:G:346:GLY:O | 1:G:347:GLU:CB | 2.70 | 0.40 |
| 1:X:2:LEU:HD22 | 1:X:25:ARG:NE | 2.36 | 0.40 |
| 1:V:334:LEU:O | 1:V:337:THR:HG22 | 2.21 | 0.40 |
| 1:B:217:GLN:O | 1:B:221:GLU:HG2 | 2.22 | 0.40 |
| 1:M:206:VAL:HG21 | 1:M:516:LYS:HE3 | 2.04 | 0.40 |
| 1:I:336:ARG:HB3 | 1:K:119:SER:HB2 | 2.04 | 0.40 |
| 1:R:8:LYS:HB3 | 1:R:17:THR:HG23 | 2.02 | 0.40 |
| 1:M:255:SER:HA | 1:M:304:VAL:HG11 | 2.03 | 0.40 |
| 1:V:387:VAL:CG1 | 1:V:434:SER:HB3 | 2.52 | 0.40 |
| 1:V:387:VAL:HA | 1:X:26:GLN:CD | 2.41 | 0.40 |
| 1:C:188:MET:HB3 | 1:C:188:MET:HE2 | 1.93 | 0.40 |
| 1:A:60:THR:HG23 | 1:A:112:GLN:HG3 | 2.02 | 0.40 |
| 1:B:103:PHE:HA | 1:B:104:PRO:HD3 | 1.95 | 0.40 |
| 1:C:267:TYR:HA | 1:C:270:VAL:HG12 | 2.04 | 0.40 |
| 1:R:327:LEU:HB2 | 2:S:1052:ALA:HB3 | 2.03 | 0.40 |
| 1:C:59:LEU:HD23 | 1:C:100:ARG:HE | 1.87 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 542/549 (99%) | 496 (92%) | 40 (7%) | 6 (1%) | 17 | 64 |
| 1 | B | 542/549 (99%) | 508 (94%) | 30 (6%) | 4 (1%) | 26 | 72 |
| 1 | C | 542/549 (99%) | 497 (92%) | 39 (7%) | 6 (1%) | 17 | 64 |
| 1 | G | 541/549 (98%) | 500 (92%) | 38 (7%) | 3 (1%) | 30 | 74 |
| 1 | I | 541/549 (98%) | 502 (93%) | 36 (7%) | 3 (1%) | 30 | 74 |
| 1 | K | 542/549 (99%) | 502 (93%) | 34 (6%) | 6 (1%) | 17 | 64 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | M | 542/549 (99%) | 501 (92%) | 37 (7%) | 4 (1%) | 26 | 72 |
| 1 | O | 542/549 (99%) | 507 (94%) | 32 (6%) | 3 (1%) | 30 | 74 |
| 1 | R | 542/549 (99%) | 505 (93%) | 33 (6%) | 4 (1%) | 26 | 72 |
| 1 | T | 541/549 (98%) | 499 (92%) | 36 (7%) | 6 (1%) | 17 | 64 |
| 1 | V | 542/549 (99%) | 506 (93%) | 33 (6%) | 3 (1%) | 30 | 74 |
| 1 | X | 542/549 (99%) | 510 (94%) | 29 (5%) | 3 (1%) | 30 | 74 |
| 2 | D | 19/41 (46%) | 19 (100%) | 0 | 0 | 100 | 100 |
| 2 | E | 19/41 (46%) | 19 (100%) | 0 | 0 | 100 | 100 |
| 2 | F | 19/41 (46%) | 17 (90%) | 2 (10%) | 0 | 100 | 100 |
| 2 | H | 19/41 (46%) | 19 (100%) | 0 | 0 | 100 | 100 |
| 2 | J | 19/41 (46%) | 18 (95%) | 1 (5%) | 0 | 100 | 100 |
| 2 | L | 19/41 (46%) | 19 (100%) | 0 | 0 | 100 | 100 |
| 2 | N | 19/41 (46%) | 17 (90%) | 2 (10%) | 0 | 100 | 100 |
| 2 | P | 19/41 (46%) | 18 (95%) | 1 (5%) | 0 | 100 | 100 |
| 2 | S | 19/41 (46%) | 19 (100%) | 0 | 0 | 100 | 100 |
| 2 | U | 19/41 (46%) | 18 (95%) | 1 (5%) | 0 | 100 | 100 |
| 2 | W | 19/41 (46%) | 13 (68%) | 4 (21%) | 2 (10%) | 1 | 10 |
| 2 | Y | 19/41 (46%) | 19 (100%) | 0 | 0 | 100 | 100 |
| All | All | 6729/7080 (95%) | 6248 (93%) | 428 (6%) | 53 (1%) | 24 | 69 |

All (53) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 38 | THR |
| 1 | G | 187 | LEU |
| 1 | G | 189 | VAL |
| 1 | O | 37 | ASP |
| 1 | O | 38 | THR |
| 1 | R | 335 | PRO |
| 1 | T | 514 | ILE |
| 1 | A | 196 | LEU |
| 1 | B | 189 | VAL |
| 1 | K | 82 | GLY |
| 1 | K | 387 | VAL |
| 1 | M | 395 | SER |
| 1 | T | 437 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 398 | ARG |
| 1 | C | 335 | PRO |
| 1 | I | 400 | GLU |
| 1 | M | 396 | PRO |
| 1 | T | 421 | PHE |
| 2 | W | 1047 | THR |
| 1 | A | 335 | PRO |
| 1 | B | 335 | PRO |
| 1 | G | 144 | PRO |
| 1 | K | 396 | PRO |
| 1 | T | 435 | ASN |
| 1 | A | 400 | GLU |
| 1 | B | 194 | GLN |
| 1 | C | 52 | PRO |
| 1 | K | 83 | ARG |
| 1 | V | 231 | TRP |
| 1 | V | 385 | TYR |
| 2 | W | 1046 | ALA |
| 1 | X | 144 | PRO |
| 1 | C | 36 | ASP |
| 1 | C | 144 | PRO |
| 1 | C | 396 | PRO |
| 1 | R | 144 | PRO |
| 1 | O | 335 | PRO |
| 1 | X | 111 | VAL |
| 1 | X | 514 | ILE |
| 1 | I | 74 | PRO |
| 1 | M | 144 | PRO |
| 1 | R | 436 | GLY |
| 1 | A | 82 | GLY |
| 1 | I | 144 | PRO |
| 1 | R | 511 | ILE |
| 1 | T | 122 | PRO |
| 1 | T | 513 | GLY |
| 1 | V | 144 | PRO |
| 1 | A | 144 | PRO |
| 1 | B | 144 | PRO |
| 1 | K | 335 | PRO |
| 1 | M | 335 | PRO |
| 1 | K | 144 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | A | 426/446 (96%) | 422 (99%) | 4 (1%) | 84 | 94 |
| 1 | B | 432/446 (97%) | 430 (100%) | 2 (0%) | 92 | 97 |
| 1 | C | 436/446 (98%) | 429 (98%) | 7 (2%) | 70 | 90 |
| 1 | G | 429/446 (96%) | 426 (99%) | 3 (1%) | 88 | 96 |
| 1 | I | 435/446 (98%) | 432 (99%) | 3 (1%) | 88 | 96 |
| 1 | K | 437/446 (98%) | 433 (99%) | 4 (1%) | 84 | 94 |
| 1 | M | 434/446 (97%) | 429 (99%) | 5 (1%) | 78 | 92 |
| 1 | O | 436/446 (98%) | 430 (99%) | 6 (1%) | 74 | 91 |
| 1 | R | 439/446 (98%) | 437 (100%) | 2 (0%) | 92 | 97 |
| 1 | T | 435/446 (98%) | 432 (99%) | 3 (1%) | 88 | 96 |
| 1 | V | 435/446 (98%) | 434 (100%) | 1 (0%) | 95 | 99 |
| 1 | X | 433/446 (97%) | 430 (99%) | 3 (1%) | 88 | 96 |
| 2 | D | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | E | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | F | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | H | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | J | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | L | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | N | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | P | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | S | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | U | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| 2 | W | 9/28 (32%) | 8 (89%) | 1 (11%) | 8 | 38 |
| 2 | Y | 11/28 (39%) | 11 (100%) | 0 | 100 | 100 |
| All | All | 5337/5688 (94%) | 5293 (99%) | 44 (1%) | 86 | 95 |

All (44) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 3 | ASN |
| 1 | A | 124 | VAL |
| 1 | A | 358 | THR |
| 1 | A | 368 | LEU |
| 1 | B | 222 | LEU |
| 1 | B | 415 | MET |
| 1 | C | 26 | GLN |
| 1 | C | 108 | VAL |
| 1 | C | 118 | VAL |
| 1 | C | 119 | SER |
| 1 | C | 222 | LEU |
| 1 | C | 432 | THR |
| 1 | C | 515 | THR |
| 1 | G | 186 | VAL |
| 1 | G | 222 | LEU |
| 1 | G | 368 | LEU |
| 1 | I | 144 | PRO |
| 1 | I | 348 | THR |
| 1 | I | 515 | THR |
| 1 | K | 26 | GLN |
| 1 | K | 80 | ARG |
| 1 | K | 83 | ARG |
| 1 | K | 108 | VAL |
| 1 | M | 26 | GLN |
| 1 | M | 33 | VAL |
| 1 | M | 38 | THR |
| 1 | M | 222 | LEU |
| 1 | M | 365 | LEU |
| 1 | O | 124 | VAL |
| 1 | O | 222 | LEU |
| 1 | O | 242 | LEU |
| 1 | O | 310 | LEU |
| 1 | O | 358 | THR |
| 1 | O | 515 | THR |
| 1 | R | 242 | LEU |
| 1 | R | 358 | THR |
| 1 | T | 368 | LEU |
| 1 | T | 435 | ASN |
| 1 | T | 518 | ILE |
| 1 | V | 222 | LEU |
| 2 | W | 1047 | THR |
| 1 | X | 108 | VAL |
| 1 | X | 365 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 518 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 54 | GLN |
| 1 | A | 62 | ASN |
| 1 | A | 200 | GLN |
| 1 | A | 239 | ASN |
| 1 | A | 379 | HIS |
| 1 | A | 435 | ASN |
| 1 | A | 525 | GLN |
| 1 | A | 532 | HIS |
| 1 | B | 26 | GLN |
| 1 | B | 62 | ASN |
| 1 | B | 64 | GLN |
| 1 | B | 167 | GLN |
| 1 | B | 234 | GLN |
| 1 | B | 264 | GLN |
| 1 | B | 349 | GLN |
| 1 | B | 525 | GLN |
| 1 | C | 3 | ASN |
| 1 | C | 26 | GLN |
| 1 | C | 125 | ASN |
| 1 | C | 167 | GLN |
| 1 | C | 349 | GLN |
| 1 | C | 532 | HIS |
| 1 | G | 62 | ASN |
| 1 | G | 64 | GLN |
| 1 | G | 167 | GLN |
| 1 | G | 349 | GLN |
| 1 | G | 403 | HIS |
| 1 | G | 532 | HIS |
| 1 | I | 26 | GLN |
| 1 | I | 62 | ASN |
| 1 | I | 64 | GLN |
| 1 | I | 158 | ASN |
| 1 | I | 239 | ASN |
| 1 | I | 264 | GLN |
| 1 | I | 349 | GLN |
| 1 | I | 379 | HIS |
| 1 | I | 403 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | I | 532 | HIS |
| 2 | J | 1044 | HIS |
| 1 | K | 3 | ASN |
| 1 | K | 62 | ASN |
| 1 | K | 64 | GLN |
| 1 | K | 349 | GLN |
| 1 | K | 525 | GLN |
| 1 | K | 532 | HIS |
| 1 | M | 14 | HIS |
| 1 | M | 167 | GLN |
| 1 | M | 213 | GLN |
| 1 | M | 403 | HIS |
| 1 | M | 532 | HIS |
| 1 | O | 26 | GLN |
| 1 | O | 62 | ASN |
| 1 | O | 64 | GLN |
| 1 | O | 123 | GLN |
| 1 | O | 209 | HIS |
| 1 | O | 239 | ASN |
| 1 | O | 298 | HIS |
| 1 | O | 349 | GLN |
| 1 | O | 435 | ASN |
| 1 | O | 525 | GLN |
| 1 | O | 532 | HIS |
| 1 | R | 26 | GLN |
| 1 | R | 54 | GLN |
| 1 | R | 64 | GLN |
| 1 | R | 160 | GLN |
| 1 | R | 213 | GLN |
| 1 | R | 239 | ASN |
| 1 | R | 349 | GLN |
| 1 | R | 435 | ASN |
| 1 | R | 525 | GLN |
| 1 | R | 532 | HIS |
| 2 | S | 1058 | GLN |
| 1 | T | 10 | GLN |
| 1 | T | 62 | ASN |
| 1 | T | 64 | GLN |
| 1 | T | 160 | GLN |
| 1 | T | 200 | GLN |
| 1 | T | 239 | ASN |
| 1 | T | 349 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | T | 403 | HIS |
| 1 | T | 525 | GLN |
| 1 | T | 532 | HIS |
| 1 | V | 62 | ASN |
| 1 | V | 64 | GLN |
| 1 | V | 167 | GLN |
| 1 | V | 239 | ASN |
| 1 | V | 264 | GLN |
| 1 | V | 349 | GLN |
| 1 | V | 525 | GLN |
| 1 | V | 532 | HIS |
| 2 | W | 1049 | HIS |
| 1 | X | 112 | GLN |
| 1 | X | 209 | HIS |
| 1 | X | 349 | GLN |
| 1 | X | 532 | HIS |

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|-------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | WO4 | A | 550 | - | 2,4,4 | 11.39 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | A | 551 | - | 2,4,4 | 11.38 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | B | 550 | - | 2,4,4 | 11.40 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | B | 551 | - | 2,4,4 | 11.38 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | C | 550 | - | 2,4,4 | 11.37 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | G | 550 | - | 2,4,4 | 11.37 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | I | 550 | - | 2,4,4 | 11.36 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | K | 550 | - | 2,4,4 | 11.36 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | K | 551 | - | 2,4,4 | 11.37 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | M | 550 | - | 2,4,4 | 10.45 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | M | 551 | - | 2,4,4 | 11.38 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | O | 550 | - | 2,4,4 | 11.40 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | O | 551 | - | 2,4,4 | 11.39 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | R | 550 | - | 2,4,4 | 11.38 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | R | 551 | - | 2,4,4 | 11.39 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | T | 550 | - | 2,4,4 | 11.37 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | T | 551 | - | 2,4,4 | 11.40 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | V | 550 | - | 2,4,4 | 11.39 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | V | 551 | - | 2,4,4 | 11.37 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | X | 550 | - | 2,4,4 | 11.37 | 2 (100%) | 0,6,6 | 0.00 | - |
| 3 | WO4 | X | 551 | - | 2,4,4 | 11.40 | 2 (100%) | 0,6,6 | 0.00 | - |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 3 | WO4 | A | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | A | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | B | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | B | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | C | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | G | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | I | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | K | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | K | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | M | 550 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 3 | WO4 | M | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | O | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | O | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | R | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | R | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | T | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | T | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | V | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | V | 551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | X | 550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | WO4 | X | 551 | - | - | 0/0/0/0 | 0/0/0/0 |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | M | 550 | WO4 | W-O1 | 10.45 | 2.02 | 1.74 |
| 3 | M | 550 | WO4 | W-O2 | 10.45 | 2.02 | 1.74 |
| 3 | K | 550 | WO4 | W-O2 | 11.34 | 2.04 | 1.74 |
| 3 | I | 550 | WO4 | W-O2 | 11.34 | 2.04 | 1.74 |
| 3 | R | 550 | WO4 | W-O2 | 11.36 | 2.04 | 1.74 |
| 3 | V | 551 | WO4 | W-O2 | 11.36 | 2.04 | 1.74 |
| 3 | B | 551 | WO4 | W-O2 | 11.36 | 2.04 | 1.74 |
| 3 | G | 550 | WO4 | W-O2 | 11.36 | 2.04 | 1.74 |
| 3 | C | 550 | WO4 | W-O2 | 11.37 | 2.04 | 1.74 |
| 3 | X | 550 | WO4 | W-O2 | 11.37 | 2.04 | 1.74 |
| 3 | A | 551 | WO4 | W-O1 | 11.37 | 2.04 | 1.74 |
| 3 | A | 550 | WO4 | W-O1 | 11.37 | 2.04 | 1.74 |
| 3 | K | 551 | WO4 | W-O1 | 11.37 | 2.04 | 1.74 |
| 3 | G | 550 | WO4 | W-O1 | 11.37 | 2.04 | 1.74 |
| 3 | K | 550 | WO4 | W-O1 | 11.37 | 2.04 | 1.74 |
| 3 | T | 550 | WO4 | W-O1 | 11.37 | 2.04 | 1.74 |
| 3 | M | 551 | WO4 | W-O2 | 11.37 | 2.04 | 1.74 |
| 3 | C | 550 | WO4 | W-O1 | 11.37 | 2.04 | 1.74 |
| 3 | T | 550 | WO4 | W-O2 | 11.38 | 2.04 | 1.74 |
| 3 | O | 551 | WO4 | W-O1 | 11.38 | 2.04 | 1.74 |
| 3 | K | 551 | WO4 | W-O2 | 11.38 | 2.04 | 1.74 |
| 3 | M | 551 | WO4 | W-O1 | 11.38 | 2.04 | 1.74 |
| 3 | X | 550 | WO4 | W-O1 | 11.38 | 2.04 | 1.74 |
| 3 | V | 551 | WO4 | W-O1 | 11.38 | 2.04 | 1.74 |
| 3 | R | 551 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | I | 550 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | V | 550 | WO4 | W-O2 | 11.39 | 2.04 | 1.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | R | 551 | WO4 | W-O2 | 11.39 | 2.04 | 1.74 |
| 3 | B | 551 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | X | 551 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | V | 550 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | B | 550 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | O | 550 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | T | 551 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | R | 550 | WO4 | W-O1 | 11.39 | 2.04 | 1.74 |
| 3 | A | 551 | WO4 | W-O2 | 11.40 | 2.04 | 1.74 |
| 3 | O | 551 | WO4 | W-O2 | 11.40 | 2.04 | 1.74 |
| 3 | O | 550 | WO4 | W-O2 | 11.40 | 2.04 | 1.74 |
| 3 | T | 551 | WO4 | W-O2 | 11.40 | 2.04 | 1.74 |
| 3 | A | 550 | WO4 | W-O2 | 11.40 | 2.04 | 1.74 |
| 3 | X | 551 | WO4 | W-O2 | 11.41 | 2.04 | 1.74 |
| 3 | B | 550 | WO4 | W-O2 | 11.41 | 2.04 | 1.74 |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | G | 550 | WO4 | 1 | 0 |
| 3 | X | 550 | WO4 | 1 | 0 |

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|--------|
| 1 | A | 544/549 (99%) | -0.25 | 2 (0%) 93 90 | 15, 50, 83, 103 | 1 (0%) |
| 1 | B | 544/549 (99%) | -0.32 | 1 (0%) 95 93 | 9, 39, 76, 101 | 1 (0%) |
| 1 | C | 544/549 (99%) | -0.27 | 1 (0%) 95 93 | 14, 48, 83, 106 | 1 (0%) |
| 1 | G | 543/549 (98%) | -0.26 | 3 (0%) 90 85 | 20, 51, 83, 111 | 1 (0%) |
| 1 | I | 543/549 (98%) | -0.30 | 4 (0%) 89 83 | 14, 40, 76, 98 | 1 (0%) |
| 1 | K | 544/549 (99%) | -0.30 | 4 (0%) 89 83 | 13, 43, 82, 115 | 1 (0%) |
| 1 | M | 544/549 (99%) | -0.18 | 5 (0%) 85 79 | 20, 54, 89, 110 | 1 (0%) |
| 1 | O | 544/549 (99%) | -0.30 | 1 (0%) 95 93 | 8, 41, 79, 97 | 1 (0%) |
| 1 | R | 544/549 (99%) | -0.24 | 2 (0%) 93 90 | 13, 46, 83, 101 | 1 (0%) |
| 1 | T | 543/549 (98%) | -0.25 | 2 (0%) 93 90 | 20, 53, 84, 108 | 1 (0%) |
| 1 | V | 544/549 (99%) | -0.17 | 6 (1%) 82 74 | 19, 62, 92, 105 | 1 (0%) |
| 1 | X | 544/549 (99%) | -0.19 | 2 (0%) 93 90 | 20, 52, 85, 100 | 1 (0%) |
| 2 | D | 21/41 (51%) | 0.56 | 0 100 100 | 44, 80, 95, 96 | 0 |
| 2 | E | 21/41 (51%) | 0.52 | 1 (4%) 34 27 | 34, 69, 98, 104 | 0 |
| 2 | F | 21/41 (51%) | 1.19 | 7 (33%) 0 1 | 70, 92, 111, 117 | 0 |
| 2 | H | 21/41 (51%) | 0.65 | 3 (14%) 4 3 | 62, 95, 107, 109 | 0 |
| 2 | J | 21/41 (51%) | 0.33 | 1 (4%) 34 27 | 43, 70, 85, 91 | 0 |
| 2 | L | 21/41 (51%) | 0.32 | 0 100 100 | 49, 78, 103, 107 | 0 |
| 2 | N | 21/41 (51%) | 0.34 | 0 100 100 | 64, 84, 97, 97 | 0 |
| 2 | P | 21/41 (51%) | 0.28 | 1 (4%) 34 27 | 33, 73, 93, 98 | 0 |
| 2 | S | 21/41 (51%) | 0.82 | 3 (14%) 4 3 | 64, 96, 117, 121 | 0 |
| 2 | U | 21/41 (51%) | 0.64 | 2 (9%) 10 9 | 49, 91, 107, 111 | 0 |
| 2 | W | 21/41 (51%) | 1.42 | 5 (23%) 1 1 | 78, 111, 130, 134 | 0 |
| 2 | Y | 21/41 (51%) | 0.41 | 1 (4%) 34 27 | 62, 90, 101, 103 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| All | All | 6777/7080 (95%) | -0.22 | 57 (0%) 87 81 | 8, 49, 88, 134 | 12 (0%) |

All (57) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | W | 1044 | HIS | 4.6 |
| 1 | C | 542 | ASN | 4.0 |
| 2 | U | 1039 | GLY | 3.6 |
| 2 | H | 1045 | THR | 3.5 |
| 2 | W | 1039 | GLY | 3.2 |
| 1 | V | 311 | ALA | 3.1 |
| 2 | F | 1045 | THR | 3.1 |
| 1 | K | 261 | THR | 3.0 |
| 2 | F | 1059 | PRO | 3.0 |
| 1 | T | 261 | THR | 2.9 |
| 2 | H | 1039 | GLY | 2.9 |
| 2 | S | 1039 | GLY | 2.9 |
| 2 | W | 1058 | GLN | 2.9 |
| 1 | T | 434 | SER | 2.8 |
| 2 | P | 1058 | GLN | 2.7 |
| 1 | A | 542 | ASN | 2.7 |
| 2 | J | 1039 | GLY | 2.7 |
| 1 | K | 55 | ASP | 2.7 |
| 2 | F | 1040 | ALA | 2.6 |
| 1 | G | 542 | ASN | 2.6 |
| 1 | I | 37 | ASP | 2.6 |
| 2 | F | 1039 | GLY | 2.6 |
| 2 | E | 1040 | ALA | 2.6 |
| 1 | R | 261 | THR | 2.5 |
| 2 | Y | 1039 | GLY | 2.5 |
| 1 | X | 542 | ASN | 2.5 |
| 2 | S | 1045 | THR | 2.5 |
| 1 | I | 542 | ASN | 2.5 |
| 1 | R | 543 | ALA | 2.4 |
| 2 | S | 1040 | ALA | 2.4 |
| 2 | U | 1040 | ALA | 2.4 |
| 1 | M | 1 | MET | 2.3 |
| 2 | F | 1044 | HIS | 2.3 |
| 1 | M | 542 | ASN | 2.3 |
| 1 | M | 543 | ALA | 2.3 |
| 1 | X | 417 | ASP | 2.3 |
| 2 | H | 1044 | HIS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | M | 232 | ASP | 2.2 |
| 2 | W | 1042 | GLY | 2.2 |
| 1 | V | 471 | GLU | 2.2 |
| 1 | M | 168 | ASP | 2.2 |
| 1 | V | 55 | ASP | 2.2 |
| 1 | I | 543 | ALA | 2.2 |
| 1 | V | 167 | GLN | 2.1 |
| 2 | W | 1040 | ALA | 2.1 |
| 2 | F | 1047 | THR | 2.1 |
| 1 | V | 159 | ASP | 2.1 |
| 1 | G | 261 | THR | 2.0 |
| 1 | B | 471 | GLU | 2.0 |
| 1 | G | 8 | LYS | 2.0 |
| 1 | O | 543 | ALA | 2.0 |
| 1 | K | 542 | ASN | 2.0 |
| 1 | V | 419 | ASP | 2.0 |
| 1 | K | 54 | GLN | 2.0 |
| 1 | A | 261 | THR | 2.0 |
| 1 | I | 261 | THR | 2.0 |
| 2 | F | 1058 | 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 3 | WO4 | M | 551 | 5/5 | 0.74 | 0.52 | 4.40 | 131,133,133,137 | 5 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 3 | WO4 | X | 551 | 5/5 | 0.94 | 0.43 | 3.77 | 88,90,91,93 | 5 |
| 3 | WO4 | A | 551 | 5/5 | 0.87 | 0.36 | 2.29 | 103,105,108,113 | 5 |
| 3 | WO4 | K | 551 | 5/5 | 0.89 | 0.32 | 2.07 | 96,97,101,108 | 5 |
| 3 | WO4 | B | 551 | 5/5 | 0.92 | 0.32 | 1.80 | 88,89,93,97 | 5 |
| 3 | WO4 | M | 550 | 5/5 | 0.78 | 0.38 | 1.79 | 112,113,118,118 | 5 |
| 3 | WO4 | V | 550 | 5/5 | 0.79 | 0.36 | 1.77 | 107,108,112,113 | 5 |
| 3 | WO4 | K | 550 | 5/5 | 0.84 | 0.33 | 1.58 | 78,79,82,88 | 5 |
| 3 | WO4 | T | 550 | 5/5 | 0.90 | 0.37 | 1.54 | 103,104,113,115 | 5 |
| 3 | WO4 | R | 551 | 5/5 | 0.92 | 0.34 | 1.40 | 86,88,95,98 | 5 |
| 3 | WO4 | V | 551 | 5/5 | 0.91 | 0.33 | 1.37 | 102,102,105,109 | 5 |
| 3 | WO4 | O | 550 | 5/5 | 0.91 | 0.25 | 0.76 | 100,100,105,109 | 5 |
| 3 | WO4 | G | 550 | 5/5 | 0.87 | 0.30 | 0.75 | 79,79,88,93 | 5 |
| 3 | WO4 | T | 551 | 5/5 | 0.81 | 0.35 | 0.50 | 113,114,117,119 | 5 |
| 3 | WO4 | C | 550 | 5/5 | 0.89 | 0.28 | 0.32 | 80,84,89,90 | 5 |
| 3 | WO4 | O | 551 | 5/5 | 0.93 | 0.25 | 0.20 | 71,75,80,87 | 5 |
| 3 | WO4 | X | 550 | 5/5 | 0.92 | 0.24 | 0.07 | 94,99,99,100 | 5 |
| 3 | WO4 | R | 550 | 5/5 | 0.93 | 0.26 | -0.10 | 106,107,111,116 | 5 |
| 3 | WO4 | B | 550 | 5/5 | 0.91 | 0.23 | -0.15 | 72,73,77,82 | 5 |
| 3 | WO4 | A | 550 | 5/5 | 0.93 | 0.23 | -0.36 | 84,86,88,93 | 5 |
| 3 | WO4 | I | 550 | 5/5 | 0.95 | 0.22 | -0.71 | 89,90,91,91 | 5 |

6.5 Other polymers [i](#)

There are no such residues in this entry.