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

Oct 31, 2023 – 12:13 PM JST

| | | |
|---|---|---|
| PDB ID | : | 5D4Z |
| Title | : | Crystal structure of Repressor from Salmonella-temperate phage |
| Authors | : | Kim, H.J.; Yoon, H.J.; Ryu, S.; Lee, H.H. |
| Deposited on | : | 2015-08-10 |
| Resolution | : | 2.98 Å(reported) |

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

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

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

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

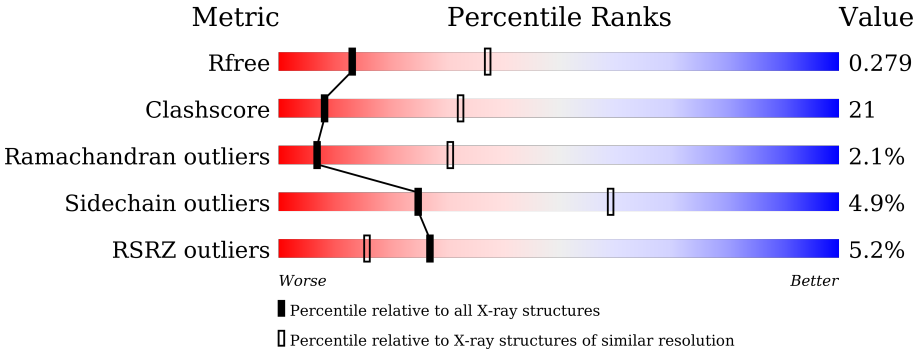
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.98 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2754 (3.00-2.96) |
| Clashscore | 141614 | 3103 (3.00-2.96) |
| Ramachandran outliers | 138981 | 2993 (3.00-2.96) |
| Sidechain outliers | 138945 | 2996 (3.00-2.96) |
| RSRZ outliers | 127900 | 2644 (3.00-2.96) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1 | 107 | 3%; 50%; 48%; • • |
| 1 | 2 | 107 | 8%; 57%; 34%; • • 6% |
| 1 | 3 | 107 | 2%; 50%; 38%; 5%; 7% |
| 1 | 4 | 107 | 17%; 48%; 45%; • 7% |
| 1 | 5 | 107 | 7%; 48%; 41%; • • 7% |
| 1 | 6 | 107 | 17%; 50%; 33%; 11%; • 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 7 | 107 | 14% 55% 36% 7% |
| 1 | A | 107 | 2% 73% 24% |
| 1 | B | 107 | % 69% 26% |
| 1 | C | 107 | 2% 60% 32% 7% |
| 1 | D | 107 | 72% 21% 6% |
| 1 | E | 107 | 66% 30% |
| 1 | F | 107 | 2% 64% 35% |
| 1 | G | 107 | % 56% 37% 5% |
| 1 | H | 107 | % 61% 32% 5% |
| 1 | I | 107 | 7% 64% 26% 7% |
| 1 | J | 107 | 2% 69% 23% |
| 1 | K | 107 | 10% 55% 36% 6% |
| 1 | L | 107 | 4% 65% 30% |
| 1 | M | 107 | 8% 61% 31% 7% |
| 1 | N | 107 | 7% 49% 40% 7% 5% |
| 1 | O | 107 | 13% 52% 38% 6% |
| 1 | P | 107 | 7% 42% 46% 7% |
| 1 | Q | 107 | 5% 69% 25% |
| 1 | R | 107 | % 70% 26% |
| 1 | T | 107 | 2% 71% 26% |
| 1 | U | 107 | 67% 28% |
| 1 | V | 107 | % 70% 27% |
| 1 | W | 107 | 2% 71% 25% |
| 1 | X | 107 | 2% 71% 24% |
| 1 | Y | 107 | 3% 70% 26% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | Z | 107 | 13% 47% 38% 8% 7% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25962 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 Repressor.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | B | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | C | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | D | 101 | 773 | 493 | 131 | 144 | 5 | 0 | 0 | 0 |
| 1 | E | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | F | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | G | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | H | 102 | 782 | 498 | 132 | 147 | 5 | 0 | 0 | 0 |
| 1 | I | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | J | 103 | 791 | 503 | 134 | 149 | 5 | 0 | 0 | 0 |
| 1 | K | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | L | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | M | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | N | 102 | 782 | 498 | 132 | 147 | 5 | 0 | 0 | 0 |
| 1 | O | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| 1 | P | 100 | 762 | 484 | 130 | 143 | 5 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | Q | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | R | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | T | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | U | 103 | 791 | 503 | 134 | 149 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | V | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | W | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | X | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | Y | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | Z | 100 | 762 | 484 | 130 | 143 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | 1 | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | 2 | 101 | 773 | 493 | 131 | 144 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | 3 | 100 | 762 | 484 | 130 | 143 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | 4 | 100 | 762 | 484 | 130 | 143 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | 5 | 100 | 762 | 484 | 130 | 143 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | 6 | 101 | 773 | 493 | 131 | 144 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | 7 | 105 | 808 | 513 | 138 | 152 | 5 | 0 | 0 | 0 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 2 | A | 21 | 21 | 21 | 0 | 0 |
| | | | Total | O | | |
| 2 | B | 24 | 24 | 24 | 0 | 0 |
| | | | Total | O | | |
| 2 | C | 25 | 25 | 25 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | D | 39 | Total O<br>39 39 | 0 | 0 |
| 2 | E | 21 | Total O<br>21 21 | 0 | 0 |
| 2 | F | 30 | Total O<br>30 30 | 0 | 0 |
| 2 | G | 19 | Total O<br>19 19 | 0 | 0 |
| 2 | H | 26 | Total O<br>26 26 | 0 | 0 |
| 2 | I | 3 | Total O<br>3 3 | 0 | 0 |
| 2 | J | 10 | Total O<br>10 10 | 0 | 0 |
| 2 | K | 5 | Total O<br>5 5 | 0 | 0 |
| 2 | L | 17 | Total O<br>17 17 | 0 | 0 |
| 2 | M | 5 | Total O<br>5 5 | 0 | 0 |
| 2 | N | 13 | Total O<br>13 13 | 0 | 0 |
| 2 | O | 3 | Total O<br>3 3 | 0 | 0 |
| 2 | P | 8 | Total O<br>8 8 | 0 | 0 |
| 2 | Q | 18 | Total O<br>18 18 | 0 | 0 |
| 2 | R | 33 | Total O<br>33 33 | 0 | 0 |
| 2 | T | 32 | Total O<br>32 32 | 0 | 0 |
| 2 | U | 27 | Total O<br>27 27 | 0 | 0 |
| 2 | V | 16 | Total O<br>16 16 | 0 | 0 |
| 2 | W | 27 | Total O<br>27 27 | 0 | 0 |
| 2 | X | 19 | Total O<br>19 19 | 0 | 0 |
| 2 | Y | 17 | Total O<br>17 17 | 0 | 0 |

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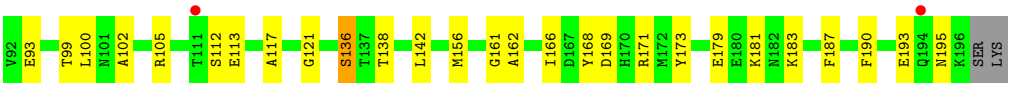
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | Z | 4 | Total O<br>4 4 | 0 | 0 |
| 2 | 1 | 8 | Total O<br>8 8 | 0 | 0 |
| 2 | 2 | 7 | Total O<br>7 7 | 0 | 0 |
| 2 | 3 | 18 | Total O<br>18 18 | 0 | 0 |
| 2 | 4 | 6 | Total O<br>6 6 | 0 | 0 |
| 2 | 5 | 14 | Total O<br>14 14 | 0 | 0 |
| 2 | 6 | 3 | Total O<br>3 3 | 0 | 0 |
| 2 | 7 | 9 | Total O<br>9 9 | 0 | 0 |

# 3 Residue-property plots (i)

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

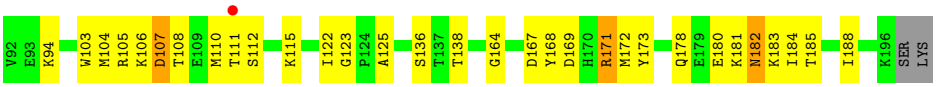
• Molecule 1: Repressor

Chain A:



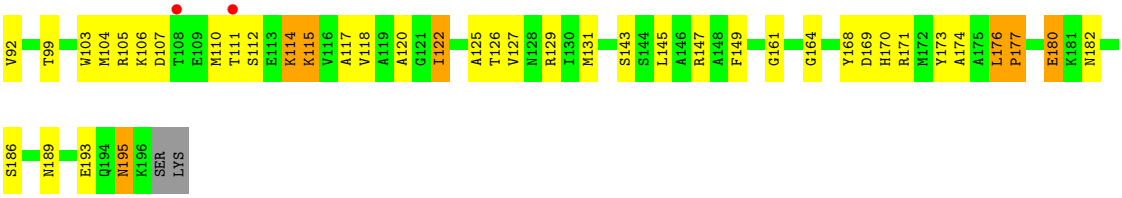

• Molecule 1: Repressor

Chain B:




• Molecule 1: Repressor

Chain C:




• Molecule 1: Repressor

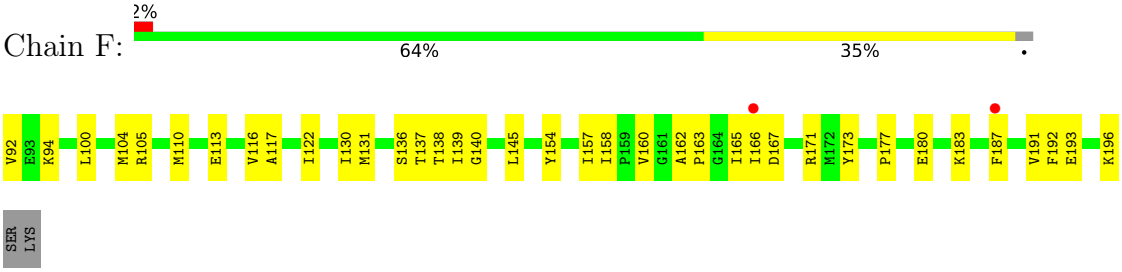
Chain D:

• Molecule 1: Repressor

Chain E:

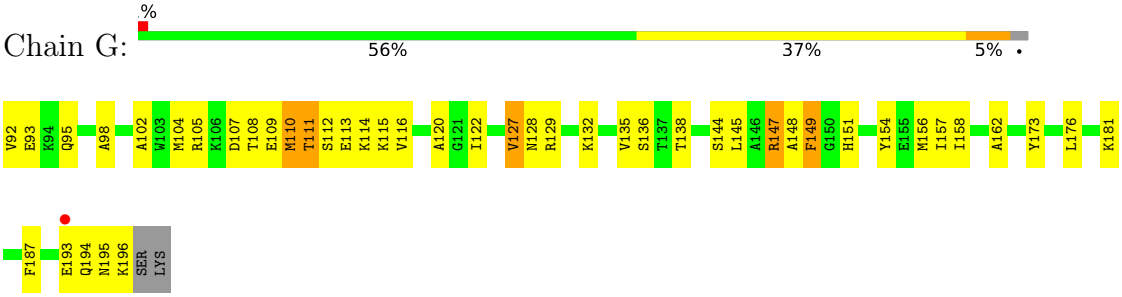
• Molecule 1: Repressor

Chain F:



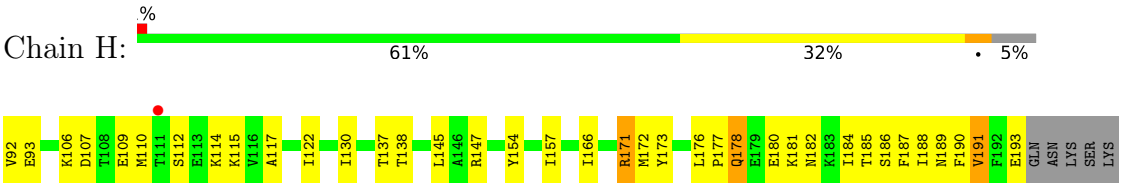

• Molecule 1: Repressor

Chain G:



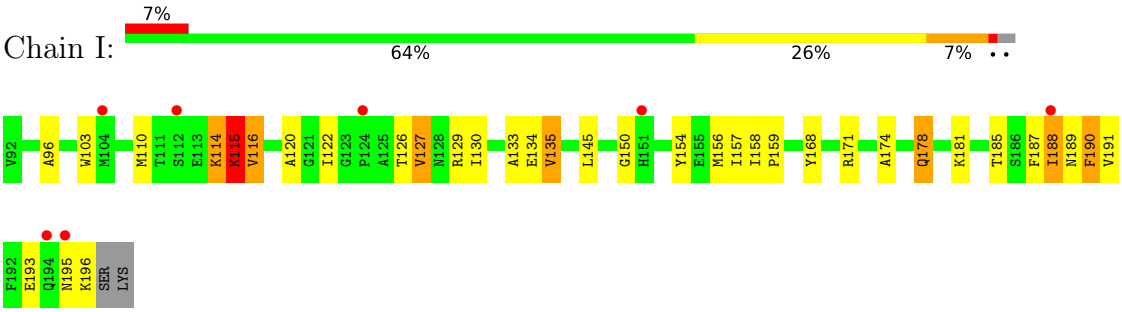

• Molecule 1: Repressor

Chain H:



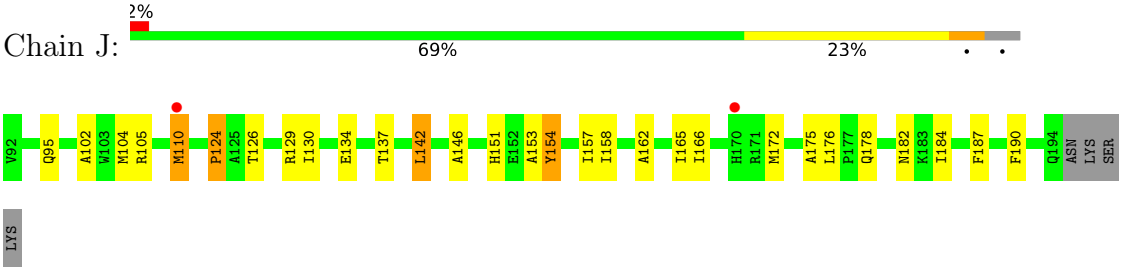

• Molecule 1: Repressor

Chain I:



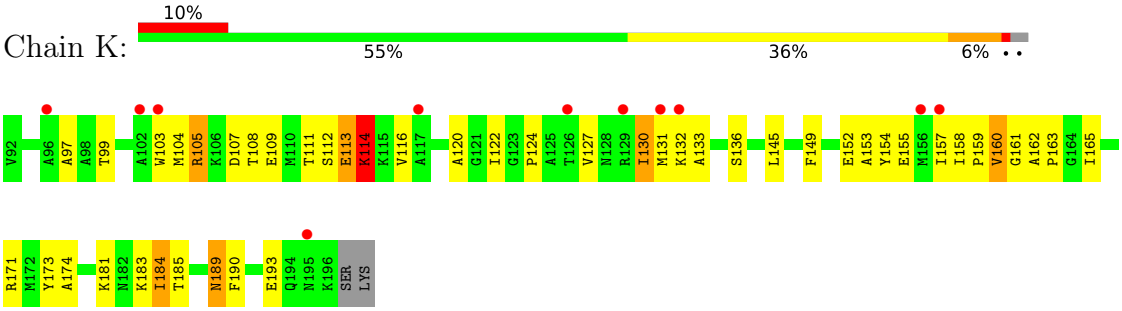

• Molecule 1: Repressor

Chain J:



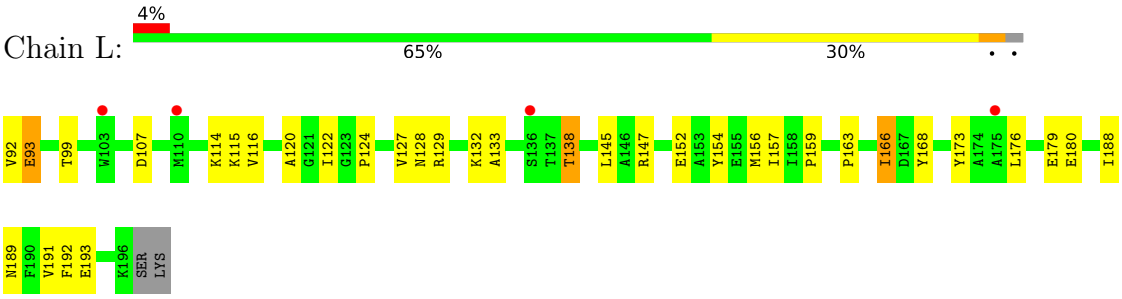

• Molecule 1: Repressor

Chain K:



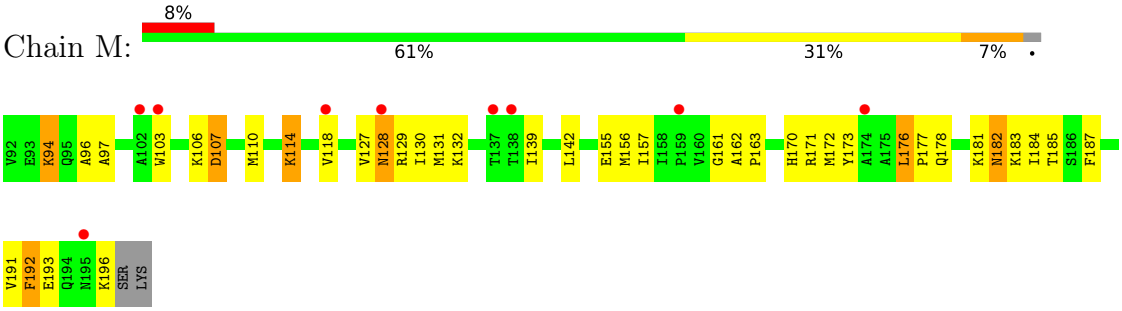

• Molecule 1: Repressor

Chain L:



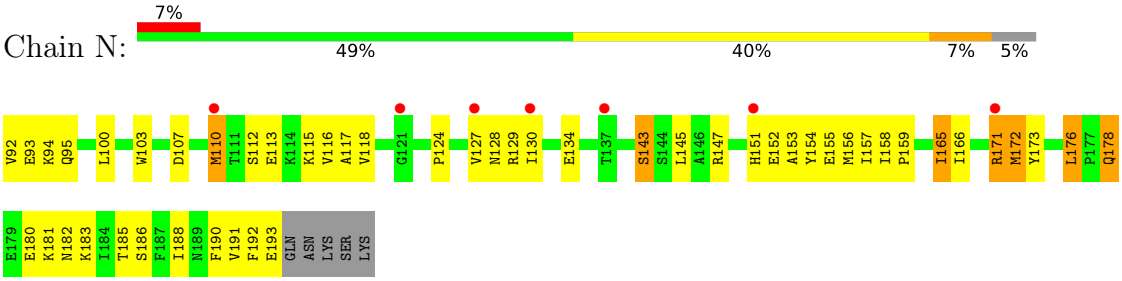

• Molecule 1: Repressor

Chain M:



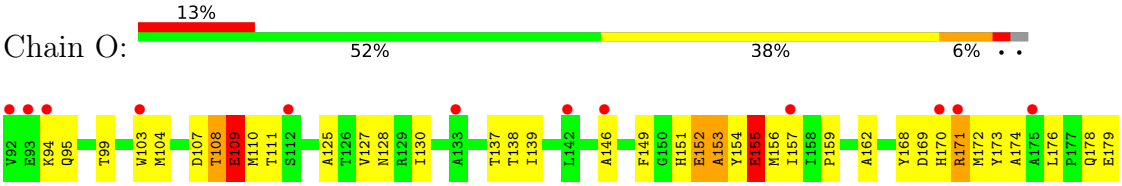

• Molecule 1: Repressor

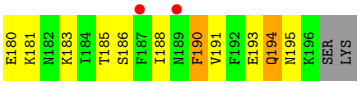
Chain N:




• Molecule 1: Repressor

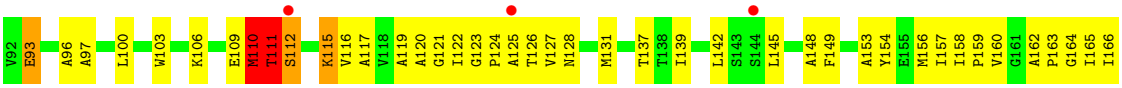
Chain O:

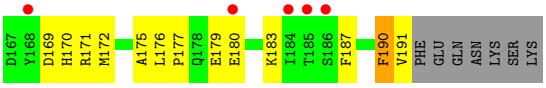





• Molecule 1: Repressor

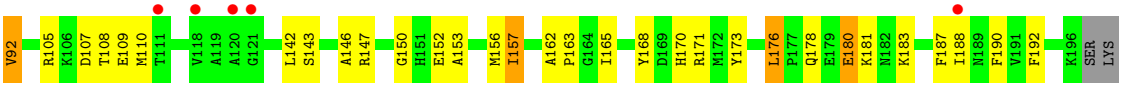
Chain P:



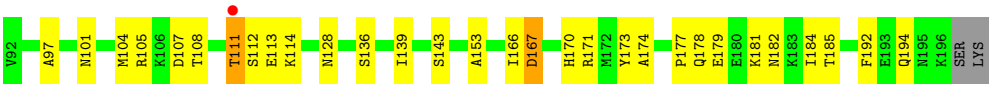

• Molecule 1: Repressor

Chain Q:




• Molecule 1: Repressor

Chain R:




• Molecule 1: Repressor

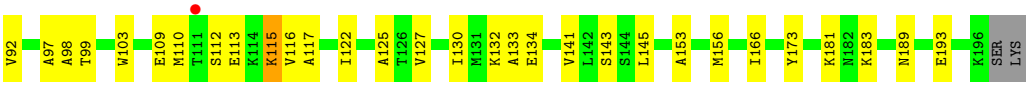
Chain T:

• Molecule 1: Repressor

Chain U:

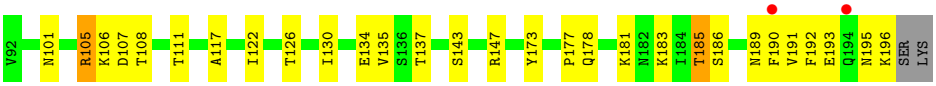
• Molecule 1: Repressor

Chain V:



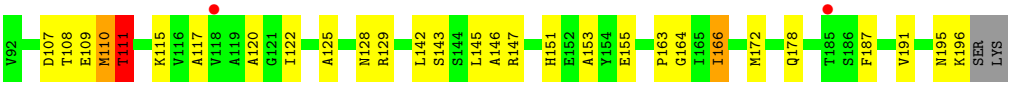

• Molecule 1: Repressor

Chain W:



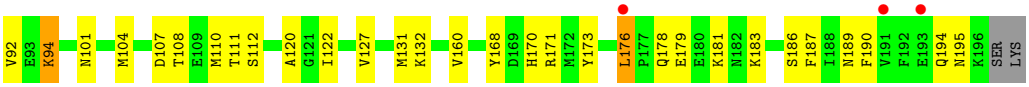

• Molecule 1: Repressor

Chain X:



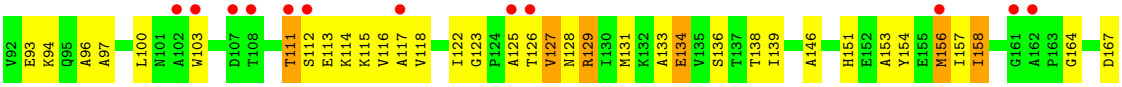

• Molecule 1: Repressor

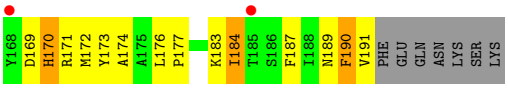
Chain Y:




• Molecule 1: Repressor

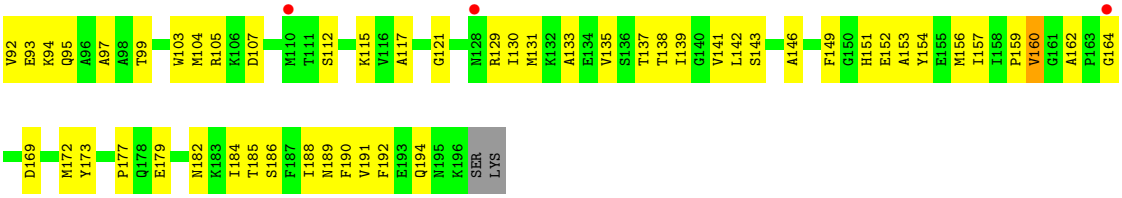
Chain Z:



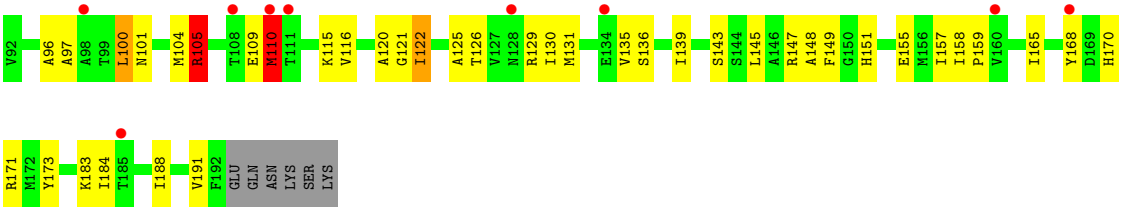

• Molecule 1: Repressor

Chain 1:



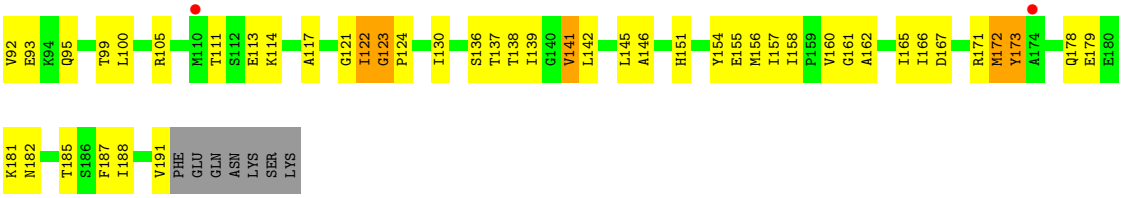

• Molecule 1: Repressor

Chain 2:



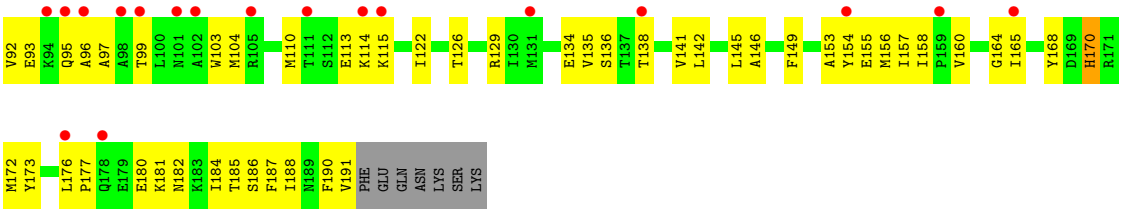

• Molecule 1: Repressor

Chain 3:



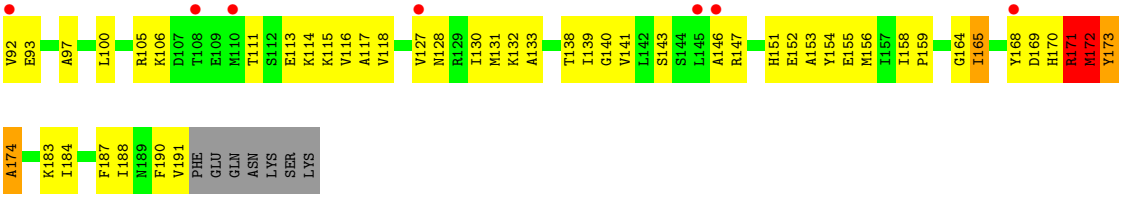

• Molecule 1: Repressor

Chain 4:



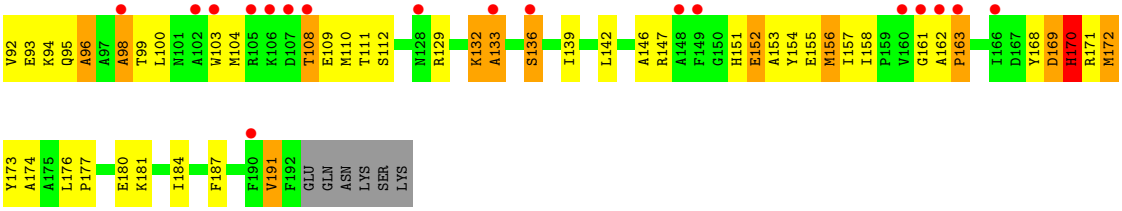

• Molecule 1: Repressor

Chain 5:



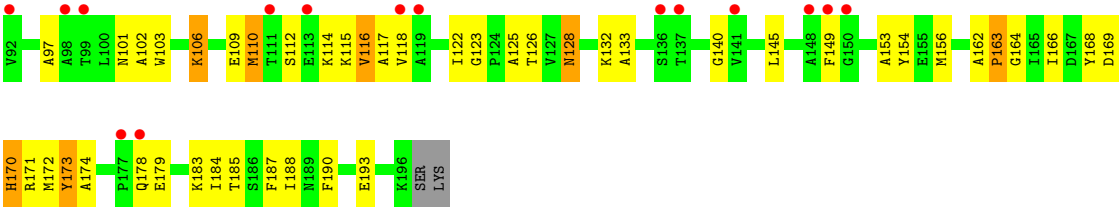

• Molecule 1: Repressor

Chain 6:



• Molecule 1: Repressor

Chain 7:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 61.60Å 62.50Å 267.90Å<br>89.99° 89.97° 72.70° | Depositor |
| Resolution (Å) | 49.13 – 2.98<br>49.13 – 2.98 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.5 (49.13-2.98)<br>98.8 (49.13-2.98) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.43 (at 2.96Å) | Xtriage |
| Refinement program | REFMAC 5.8.0049 | Depositor |
| R, $R_{free}$ | 0.216 , 0.273<br>0.228 , 0.279 | Depositor<br>DCC |
| $R_{free}$ test set | 3858 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 70.5 | Xtriage |
| Anisotropy | 0.028 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 97.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.53$, $< L^2 > = 0.36$ | Xtriage |
| Estimated twinning fraction | 0.069 for -h,-k,l<br>0.001 for k,h,-l<br>0.002 for -k,-h,-l | Xtriage |
| Reported twinning fraction | 0.509 for H, K, L<br>0.491 for -h,-k,l | Depositor |
| Outliers | 0 of 76987 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 25962 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 77.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | 1 | 0.38 | 0/822 | 0.61 | 0/1110 |
| 1 | 2 | 0.35 | 0/787 | 0.63 | 0/1064 |
| 1 | 3 | 0.34 | 0/775 | 0.62 | 0/1048 |
| 1 | 4 | 0.34 | 0/775 | 0.63 | 0/1048 |
| 1 | 5 | 0.37 | 0/775 | 0.62 | 0/1048 |
| 1 | 6 | 0.40 | 0/787 | 0.69 | 0/1064 |
| 1 | 7 | 0.42 | 0/822 | 0.73 | 0/1110 |
| 1 | A | 0.35 | 0/822 | 0.58 | 0/1110 |
| 1 | B | 0.38 | 0/822 | 0.59 | 0/1110 |
| 1 | C | 0.37 | 0/822 | 0.59 | 0/1110 |
| 1 | D | 0.38 | 0/787 | 0.60 | 0/1064 |
| 1 | E | 0.34 | 0/822 | 0.55 | 0/1110 |
| 1 | F | 0.38 | 0/822 | 0.58 | 0/1110 |
| 1 | G | 0.36 | 0/822 | 0.64 | 0/1110 |
| 1 | H | 0.40 | 0/796 | 0.61 | 0/1076 |
| 1 | I | 0.35 | 0/822 | 0.62 | 0/1110 |
| 1 | J | 0.35 | 0/805 | 0.56 | 0/1088 |
| 1 | K | 0.38 | 0/822 | 0.65 | 0/1110 |
| 1 | L | 0.36 | 0/822 | 0.65 | 0/1110 |
| 1 | M | 0.39 | 0/822 | 0.66 | 0/1110 |
| 1 | N | 0.38 | 0/796 | 0.64 | 0/1076 |
| 1 | O | 0.35 | 0/822 | 0.62 | 0/1110 |
| 1 | P | 0.39 | 0/775 | 0.65 | 0/1048 |
| 1 | Q | 0.37 | 0/822 | 0.57 | 0/1110 |
| 1 | R | 0.37 | 0/822 | 0.58 | 0/1110 |
| 1 | T | 0.35 | 0/822 | 0.62 | 0/1110 |
| 1 | U | 0.38 | 0/805 | 0.59 | 0/1088 |
| 1 | V | 0.37 | 0/822 | 0.59 | 0/1110 |
| 1 | W | 0.39 | 0/822 | 0.63 | 1/1110 (0.1%) |
| 1 | X | 0.38 | 0/822 | 0.63 | 0/1110 |
| 1 | Y | 0.38 | 0/822 | 0.62 | 0/1110 |
| 1 | Z | 0.38 | 0/775 | 0.70 | 0/1048 |
| All | All | 0.37 | 0/25878 | 0.62 | 1/34960 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | 2 | 0 | 2 |
| 1 | 5 | 0 | 1 |
| 1 | 6 | 0 | 2 |
| 1 | 7 | 0 | 1 |
| 1 | O | 0 | 1 |
| All | All | 0 | 7 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | W | 105 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | 2 | 105 | ARG | Peptide |
| 1 | 2 | 183 | LYS | Peptide |
| 1 | 5 | 171 | ARG | Peptide |
| 1 | 6 | 110 | MET | Peptide |
| 1 | 6 | 172 | MET | Peptide |
| 1 | 7 | 116 | VAL | Peptide |
| 1 | O | 155 | GLU | Peptide |

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 1 | 808 | 0 | 817 | 47 | 0 |
| 1 | 2 | 773 | 0 | 784 | 43 | 0 |
| 1 | 3 | 762 | 0 | 775 | 52 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 4 | 762 | 0 | 775 | 47 | 0 |
| 1 | 5 | 762 | 0 | 775 | 64 | 0 |
| 1 | 6 | 773 | 0 | 784 | 75 | 0 |
| 1 | 7 | 808 | 0 | 817 | 56 | 0 |
| 1 | A | 808 | 0 | 817 | 20 | 0 |
| 1 | B | 808 | 0 | 817 | 27 | 0 |
| 1 | C | 808 | 0 | 817 | 33 | 0 |
| 1 | D | 773 | 0 | 784 | 20 | 0 |
| 1 | E | 808 | 0 | 817 | 30 | 0 |
| 1 | F | 808 | 0 | 817 | 38 | 0 |
| 1 | G | 808 | 0 | 817 | 47 | 0 |
| 1 | H | 782 | 0 | 790 | 37 | 0 |
| 1 | I | 808 | 0 | 817 | 39 | 1 |
| 1 | J | 791 | 0 | 798 | 25 | 0 |
| 1 | K | 808 | 0 | 817 | 41 | 0 |
| 1 | L | 808 | 0 | 817 | 28 | 1 |
| 1 | M | 808 | 0 | 817 | 43 | 0 |
| 1 | N | 782 | 0 | 790 | 59 | 0 |
| 1 | O | 808 | 0 | 817 | 50 | 0 |
| 1 | P | 762 | 0 | 775 | 68 | 0 |
| 1 | Q | 808 | 0 | 817 | 35 | 0 |
| 1 | R | 808 | 0 | 817 | 24 | 1 |
| 1 | T | 808 | 0 | 817 | 22 | 0 |
| 1 | U | 791 | 0 | 798 | 24 | 0 |
| 1 | V | 808 | 0 | 817 | 32 | 0 |
| 1 | W | 808 | 0 | 817 | 37 | 0 |
| 1 | X | 808 | 0 | 817 | 28 | 0 |
| 1 | Y | 808 | 0 | 817 | 34 | 1 |
| 1 | Z | 762 | 0 | 775 | 53 | 0 |
| 2 | 1 | 8 | 0 | 0 | 3 | 0 |
| 2 | 2 | 7 | 0 | 0 | 0 | 0 |
| 2 | 3 | 18 | 0 | 0 | 2 | 0 |
| 2 | 4 | 6 | 0 | 0 | 0 | 0 |
| 2 | 5 | 14 | 0 | 0 | 2 | 0 |
| 2 | 6 | 3 | 0 | 0 | 0 | 0 |
| 2 | 7 | 9 | 0 | 0 | 2 | 0 |
| 2 | A | 21 | 0 | 0 | 4 | 0 |
| 2 | B | 24 | 0 | 0 | 4 | 0 |
| 2 | C | 25 | 0 | 0 | 4 | 0 |
| 2 | D | 39 | 0 | 0 | 2 | 0 |
| 2 | E | 21 | 0 | 0 | 2 | 0 |
| 2 | F | 30 | 0 | 0 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | G | 19 | 0 | 0 | 4 | 0 |
| 2 | H | 26 | 0 | 0 | 1 | 0 |
| 2 | I | 3 | 0 | 0 | 0 | 0 |
| 2 | J | 10 | 0 | 0 | 0 | 0 |
| 2 | K | 5 | 0 | 0 | 0 | 0 |
| 2 | L | 17 | 0 | 0 | 2 | 0 |
| 2 | M | 5 | 0 | 0 | 1 | 0 |
| 2 | N | 13 | 0 | 0 | 5 | 0 |
| 2 | O | 3 | 0 | 0 | 1 | 0 |
| 2 | P | 8 | 0 | 0 | 3 | 0 |
| 2 | Q | 18 | 0 | 0 | 2 | 0 |
| 2 | R | 33 | 0 | 0 | 2 | 0 |
| 2 | T | 32 | 0 | 0 | 4 | 0 |
| 2 | U | 27 | 0 | 0 | 2 | 0 |
| 2 | V | 16 | 0 | 0 | 2 | 0 |
| 2 | W | 27 | 0 | 0 | 4 | 0 |
| 2 | X | 19 | 0 | 0 | 3 | 0 |
| 2 | Y | 17 | 0 | 0 | 5 | 0 |
| 2 | Z | 4 | 0 | 0 | 2 | 0 |
| All | All | 25962 | 0 | 25743 | 1083 | 2 |

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 21.

All (1083) 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:P:111:THR:O | 1:P:115:LYS:HE2 | 1.42 | 1.18 |
| 1:P:109:GLU:CD | 1:P:115:LYS:HZ2 | 1.54 | 1.09 |
| 1:P:111:THR:O | 1:P:115:LYS:CE | 2.00 | 1.09 |
| 1:6:94:LYS:HD3 | 1:6:132:LYS:O | 1.53 | 1.09 |
| 1:M:114:LYS:NZ | 2:M:201:HOH:O | 1.89 | 1.06 |
| 1:6:156:MET:O | 1:6:156:MET:HG3 | 1.54 | 1.04 |
| 1:5:169:ASP:O | 1:5:173:TYR:OH | 1.76 | 1.04 |
| 1:P:109:GLU:CD | 1:P:115:LYS:NZ | 2.11 | 1.03 |
| 1:7:170:HIS:CD2 | 1:7:173:TYR:HE2 | 1.81 | 0.98 |
| 1:P:109:GLU:OE1 | 1:P:115:LYS:NZ | 1.98 | 0.96 |
| 1:M:176:LEU:HD23 | 1:M:177:PRO:O | 1.64 | 0.96 |
| 1:W:173:TYR:CZ | 1:W:181:LYS:HE2 | 2.03 | 0.93 |
| 1:2:158:ILE:HD11 | 1:2:165:ILE:HD13 | 1.50 | 0.93 |
| 1:I:185:THR:O | 1:I:188:ILE:HG23 | 1.67 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:187:PHE:HA | 1:Q:190:PHE:CD2 | 2.04 | 0.93 |
| 1:E:92:VAL:N | 2:E:201:HOH:O | 2.03 | 0.92 |
| 1:E:131:MET:O | 1:H:171:ARG:NH2 | 2.03 | 0.92 |
| 1:C:176:LEU:HB3 | 1:C:180:GLU:OE2 | 1.68 | 0.91 |
| 1:Z:171:ARG:HG3 | 1:1:164:GLY:HA2 | 1.51 | 0.90 |
| 1:P:120:ALA:HB1 | 1:P:122:ILE:HG12 | 1.51 | 0.89 |
| 1:7:170:HIS:CD2 | 1:7:173:TYR:CE2 | 2.60 | 0.89 |
| 1:B:103:TRP:O | 1:B:106:LYS:O | 1.90 | 0.89 |
| 1:P:109:GLU:OE2 | 1:P:115:LYS:NZ | 2.03 | 0.88 |
| 1:Y:107:ASP:O | 1:Y:110:MET:HB2 | 1.72 | 0.88 |
| 1:B:181:LYS:NZ | 2:B:201:HOH:O | 2.06 | 0.87 |
| 1:3:171:ARG:O | 1:3:173:TYR:N | 2.08 | 0.87 |
| 1:T:105:ARG:NH1 | 2:T:201:HOH:O | 2.07 | 0.86 |
| 1:W:173:TYR:CE2 | 1:W:181:LYS:HE2 | 2.11 | 0.85 |
| 1:3:142:LEU:HD21 | 1:3:157:ILE:HD11 | 1.57 | 0.85 |
| 1:1:146:ALA:HB1 | 1:1:152:GLU:HA | 1.58 | 0.85 |
| 1:P:123:GLY:O | 1:P:126:THR:O | 1.95 | 0.85 |
| 1:N:178:GLN:HB2 | 1:N:181:LYS:HB3 | 1.58 | 0.84 |
| 1:M:139:ILE:HD11 | 1:N:93:GLU:HG3 | 1.60 | 0.83 |
| 1:O:173:TYR:HB2 | 1:O:176:LEU:HD11 | 1.60 | 0.83 |
| 1:U:191:VAL:O | 1:U:193:GLU:HA | 1.77 | 0.83 |
| 1:K:154:TYR:HE1 | 1:L:157:ILE:C | 1.83 | 0.82 |
| 1:I:189:ASN:O | 1:I:191:VAL:N | 2.12 | 0.81 |
| 1:4:170:HIS:CE1 | 1:5:164:GLY:O | 2.33 | 0.81 |
| 1:7:162:ALA:HB1 | 1:7:163:PRO:HA | 1.62 | 0.81 |
| 1:Z:176:LEU:HG | 1:Z:177:PRO:HD2 | 1.62 | 0.81 |
| 1:Q:92:VAL:N | 2:Q:201:HOH:O | 2.12 | 0.81 |
| 1:Z:170:HIS:HB3 | 1:Z:172:MET:N | 1.95 | 0.81 |
| 1:6:169:ASP:OD1 | 1:6:172:MET:HA | 1.82 | 0.79 |
| 1:A:138:THR:OG1 | 1:B:136:SER:O | 2.00 | 0.79 |
| 1:6:170:HIS:CD2 | 1:7:164:GLY:O | 2.36 | 0.79 |
| 1:T:110:MET:HG2 | 1:T:115:LYS:HB3 | 1.62 | 0.79 |
| 1:3:173:TYR:O | 1:3:181:LYS:HE2 | 1.83 | 0.79 |
| 1:N:182:ASN:HB3 | 1:N:186:SER:HB3 | 1.64 | 0.78 |
| 1:4:96:ALA:O | 1:4:99:THR:HG22 | 1.83 | 0.78 |
| 1:O:190:PHE:CE1 | 1:O:191:VAL:HB | 2.18 | 0.78 |
| 1:R:113:GLU:OE1 | 1:R:128:ASN:ND2 | 2.17 | 0.78 |
| 1:O:194:GLN:NE2 | 1:P:172:MET:O | 2.16 | 0.78 |
| 1:6:129:ARG:CD | 1:6:132:LYS:HE2 | 2.11 | 0.78 |
| 1:H:187:PHE:O | 1:H:190:PHE:HD2 | 1.66 | 0.78 |
| 1:I:193:GLU:HA | 1:I:196:LYS:HB3 | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2:109:GLU:HG3 | 1:2:149:PHE:HE1 | 1.48 | 0.77 |
| 1:K:116:VAL:O | 1:K:127:VAL:HG11 | 1.85 | 0.77 |
| 1:N:143:SER:HA | 1:N:153:ALA:HB2 | 1.66 | 0.77 |
| 1:D:92:VAL:N | 2:D:202:HOH:O | 2.16 | 0.77 |
| 1:P:190:PHE:O | 1:P:191:VAL:HG22 | 1.83 | 0.77 |
| 1:F:193:GLU:O | 1:F:196:LYS:NZ | 2.12 | 0.77 |
| 1:O:171:ARG:CZ | 1:O:174:ALA:HB1 | 2.14 | 0.77 |
| 1:N:181:LYS:HG2 | 1:N:182:ASN:N | 1.97 | 0.76 |
| 1:N:173:TYR:CE2 | 1:N:183:LYS:HG3 | 2.21 | 0.76 |
| 1:7:97:ALA:HB2 | 1:7:133:ALA:HB2 | 1.65 | 0.76 |
| 1:M:155:GLU:OE2 | 1:M:170:HIS:ND1 | 2.18 | 0.76 |
| 1:Q:190:PHE:CE2 | 1:1:190:PHE:CE1 | 2.73 | 0.76 |
| 1:6:129:ARG:HD3 | 1:6:132:LYS:HE2 | 1.65 | 0.76 |
| 1:E:136:SER:HB3 | 1:F:138:THR:HG23 | 1.66 | 0.76 |
| 1:6:104:MET:CE | 1:6:111:THR:O | 2.34 | 0.76 |
| 1:2:96:ALA:HB1 | 1:2:100:LEU:HD23 | 1.67 | 0.75 |
| 1:M:155:GLU:CD | 1:M:170:HIS:HD1 | 1.89 | 0.75 |
| 1:Z:189:ASN:OD1 | 1:Z:190:PHE:CD2 | 2.38 | 0.75 |
| 1:Z:170:HIS:HB3 | 1:Z:171:ARG:C | 2.06 | 0.75 |
| 1:H:187:PHE:O | 1:H:190:PHE:CD2 | 2.40 | 0.75 |
| 1:6:104:MET:HE3 | 1:6:111:THR:O | 1.87 | 0.75 |
| 1:Q:150:GLY:O | 1:Q:171:ARG:HD3 | 1.86 | 0.74 |
| 1:P:117:ALA:O | 1:P:121:GLY:N | 2.19 | 0.74 |
| 1:7:112:SER:O | 1:7:115:LYS:HE2 | 1.86 | 0.74 |
| 1:F:171:ARG:HE | 1:G:132:LYS:HG3 | 1.53 | 0.74 |
| 1:A:156:MET:HE3 | 2:A:208:HOH:O | 1.86 | 0.73 |
| 1:4:93:GLU:O | 1:4:97:ALA:N | 2.20 | 0.73 |
| 1:A:169:ASP:OD1 | 1:A:171:ARG:HG2 | 1.88 | 0.73 |
| 1:O:173:TYR:CE2 | 1:P:191:VAL:HG23 | 2.23 | 0.73 |
| 1:D:108:THR:OG1 | 2:D:201:HOH:O | 2.06 | 0.73 |
| 1:O:108:THR:O | 1:O:109:GLU:HB3 | 1.89 | 0.73 |
| 1:I:116:VAL:HG21 | 1:I:127:VAL:HG21 | 1.70 | 0.73 |
| 1:P:176:LEU:HA | 1:P:177:PRO:C | 2.09 | 0.73 |
| 1:2:110:MET:HG3 | 1:2:149:PHE:CZ | 2.24 | 0.72 |
| 1:4:136:SER:OG | 1:5:140:GLY:N | 2.22 | 0.72 |
| 1:T:173:TYR:O | 1:T:181:LYS:NZ | 2.21 | 0.72 |
| 1:5:171:ARG:HG2 | 1:5:172:MET:N | 2.03 | 0.72 |
| 1:6:111:THR:HG23 | 1:6:112:SER:H | 1.55 | 0.72 |
| 1:I:157:ILE:HD11 | 1:J:154:TYR:N | 2.04 | 0.72 |
| 1:M:155:GLU:OE2 | 1:M:170:HIS:CE1 | 2.42 | 0.72 |
| 1:U:129:ARG:NH2 | 2:U:201:HOH:O | 2.22 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:6:99:THR:N | 1:6:156:MET:HE1 | 2.04 | 0.72 |
| 1:E:157:ILE:HD11 | 1:F:157:ILE:HD11 | 1.71 | 0.72 |
| 1:5:97:ALA:HB2 | 1:5:133:ALA:HB2 | 1.72 | 0.72 |
| 1:W:143:SER:O | 1:W:147:ARG:HG2 | 1.89 | 0.71 |
| 1:N:176:LEU:HD22 | 1:N:178:GLN:HE21 | 1.54 | 0.71 |
| 1:E:131:MET:O | 1:H:171:ARG:CZ | 2.38 | 0.71 |
| 1:6:154:TYR:CE2 | 1:6:170:HIS:HB3 | 2.25 | 0.71 |
| 1:T:92:VAL:HG12 | 2:T:220:HOH:O | 1.90 | 0.71 |
| 1:Z:153:ALA:HA | 2:Z:201:HOH:O | 1.90 | 0.70 |
| 1:Q:109:GLU:HG3 | 1:Q:110:MET:HG3 | 1.73 | 0.70 |
| 1:P:111:THR:C | 1:P:115:LYS:CE | 2.60 | 0.70 |
| 1:N:182:ASN:HB3 | 1:N:186:SER:CB | 2.21 | 0.70 |
| 1:K:99:THR:HG21 | 1:K:158:ILE:HD13 | 1.74 | 0.70 |
| 1:M:176:LEU:CD2 | 1:M:177:PRO:O | 2.39 | 0.70 |
| 1:N:192:PHE:O | 1:N:193:GLU:HB2 | 1.91 | 0.70 |
| 1:6:95:GLN:HG2 | 1:6:156:MET:HG2 | 1.74 | 0.69 |
| 1:6:169:ASP:O | 1:6:170:HIS:HB2 | 1.91 | 0.69 |
| 1:P:117:ALA:HB2 | 1:P:127:VAL:HG22 | 1.74 | 0.69 |
| 1:I:174:ALA:O | 1:I:178:GLN:NE2 | 2.25 | 0.69 |
| 1:P:190:PHE:O | 1:P:191:VAL:CG2 | 2.40 | 0.69 |
| 1:O:153:ALA:HB3 | 1:P:159:PRO:HD3 | 1.74 | 0.69 |
| 1:U:178:GLN:O | 1:U:182:ASN:ND2 | 2.26 | 0.69 |
| 1:G:111:THR:HG21 | 1:G:115:LYS:N | 2.07 | 0.69 |
| 1:Z:128:ASN:O | 1:Z:131:MET:HB3 | 1.93 | 0.69 |
| 1:J:158:ILE:HD11 | 1:J:165:ILE:HG21 | 1.73 | 0.69 |
| 1:6:156:MET:O | 1:6:156:MET:CG | 2.35 | 0.69 |
| 1:P:111:THR:N | 1:P:115:LYS:HZ3 | 1.91 | 0.69 |
| 1:A:173:TYR:O | 1:A:181:LYS:NZ | 2.25 | 0.68 |
| 1:7:116:VAL:HA | 1:7:118:VAL:HG12 | 1.75 | 0.68 |
| 1:K:113:GLU:OE1 | 1:K:130:ILE:N | 2.26 | 0.68 |
| 1:N:182:ASN:CB | 1:N:186:SER:HB3 | 2.24 | 0.68 |
| 1:U:147:ARG:NH1 | 1:U:152:GLU:OE2 | 2.26 | 0.68 |
| 1:Z:169:ASP:O | 1:Z:171:ARG:HA | 1.94 | 0.67 |
| 1:6:95:GLN:O | 1:6:156:MET:HE3 | 1.95 | 0.67 |
| 1:V:166:ILE:HG12 | 1:W:173:TYR:CZ | 2.29 | 0.67 |
| 1:5:114:LYS:HG2 | 1:5:128:ASN:OD1 | 1.94 | 0.67 |
| 1:Y:104:MET:O | 1:Y:110:MET:HA | 1.94 | 0.67 |
| 1:6:169:ASP:OD1 | 1:6:172:MET:CA | 2.42 | 0.67 |
| 1:O:157:ILE:HD12 | 1:P:154:TYR:HA | 1.77 | 0.67 |
| 1:T:149:PHE:O | 1:T:171:ARG:NH2 | 2.27 | 0.67 |
| 1:5:156:MET:SD | 2:5:209:HOH:O | 2.53 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:94:LYS:H | 1:B:94:LYS:HD2 | 1.59 | 0.66 |
| 1:6:109:GLU:O | 1:6:111:THR:HG22 | 1.95 | 0.66 |
| 1:V:166:ILE:HA | 1:W:173:TYR:OH | 1.95 | 0.66 |
| 1:2:168:TYR:CE2 | 1:3:166:ILE:HD11 | 2.30 | 0.66 |
| 1:G:110:MET:CE | 1:G:116:VAL:HG23 | 2.25 | 0.66 |
| 1:L:116:VAL:O | 1:L:120:ALA:O | 2.13 | 0.66 |
| 1:Q:142:LEU:HG | 1:Q:156:MET:HE3 | 1.77 | 0.66 |
| 1:Q:107:ASP:OD1 | 1:Q:108:THR:N | 2.29 | 0.66 |
| 1:2:158:ILE:HD12 | 1:2:159:PRO:HD2 | 1.78 | 0.65 |
| 1:O:173:TYR:CB | 1:O:176:LEU:HD11 | 2.26 | 0.65 |
| 1:K:154:TYR:CE1 | 1:L:157:ILE:C | 2.70 | 0.65 |
| 1:V:97:ALA:HB2 | 1:V:133:ALA:HB2 | 1.78 | 0.65 |
| 1:I:150:GLY:O | 1:I:171:ARG:NE | 2.29 | 0.65 |
| 1:O:139:ILE:HG22 | 1:P:139:ILE:HD13 | 1.77 | 0.65 |
| 1:P:169:ASP:OD1 | 1:P:171:ARG:HB2 | 1.95 | 0.65 |
| 1:V:110:MET:HE1 | 1:V:115:LYS:HG2 | 1.78 | 0.65 |
| 1:V:189:ASN:O | 1:V:193:GLU:OE1 | 2.13 | 0.65 |
| 1:W:122:ILE:HG12 | 1:W:126:THR:OG1 | 1.97 | 0.65 |
| 1:N:182:ASN:HA | 1:N:185:THR:HB | 1.78 | 0.65 |
| 1:P:103:TRP:O | 1:P:106:LYS:HG2 | 1.96 | 0.65 |
| 1:6:93:GLU:C | 1:6:133:ALA:HB2 | 2.17 | 0.65 |
| 1:W:130:ILE:HG12 | 1:W:137:THR:OG1 | 1.96 | 0.64 |
| 1:L:128:ASN:OD1 | 1:L:132:LYS:NZ | 2.30 | 0.64 |
| 1:P:111:THR:O | 1:P:115:LYS:HE3 | 1.92 | 0.64 |
| 1:Y:189:ASN:OD1 | 1:Y:190:PHE:N | 2.30 | 0.64 |
| 1:Z:125:ALA:C | 1:Z:127:VAL:HG22 | 2.17 | 0.64 |
| 1:Z:171:ARG:HB3 | 1:Z:173:TYR:HB3 | 1.79 | 0.64 |
| 1:T:122:ILE:HD13 | 1:T:141:VAL:HG13 | 1.80 | 0.64 |
| 1:A:138:THR:HA | 1:B:138:THR:HA | 1.78 | 0.64 |
| 1:G:128:ASN:ND2 | 2:G:201:HOH:O | 2.30 | 0.64 |
| 1:6:146:ALA:HB1 | 1:6:151:HIS:O | 1.98 | 0.64 |
| 1:2:126:THR:O | 1:2:130:ILE:HG13 | 1.97 | 0.64 |
| 1:X:178:GLN:O | 2:X:201:HOH:O | 2.15 | 0.63 |
| 1:5:171:ARG:HG2 | 1:5:172:MET:H | 1.62 | 0.63 |
| 1:6:168:TYR:CZ | 1:6:170:HIS:CD2 | 2.85 | 0.63 |
| 1:X:108:THR:N | 1:X:109:GLU:HA | 2.13 | 0.63 |
| 1:Z:189:ASN:OD1 | 1:Z:190:PHE:CG | 2.51 | 0.63 |
| 1:7:103:TRP:HB3 | 1:7:149:PHE:CZ | 2.33 | 0.63 |
| 1:1:186:SER:HA | 1:1:189:ASN:HB2 | 1.80 | 0.63 |
| 1:I:159:PRO:HD3 | 1:J:154:TYR:CE1 | 2.34 | 0.63 |
| 1:K:103:TRP:HE1 | 1:K:158:ILE:HD11 | 1.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:155:GLU:CD | 1:M:170:HIS:ND1 | 2.51 | 0.63 |
| 1:N:95:GLN:NE2 | 2:N:202:HOH:O | 2.31 | 0.63 |
| 1:O:107:ASP:O | 1:O:109:GLU:N | 2.32 | 0.63 |
| 1:I:126:THR:O | 1:I:130:ILE:N | 2.24 | 0.63 |
| 1:Q:142:LEU:O | 1:Q:156:MET:HE1 | 1.98 | 0.63 |
| 1:F:171:ARG:O | 1:F:171:ARG:NH1 | 2.32 | 0.63 |
| 1:Q:105:ARG:NH1 | 1:U:175:ALA:O | 2.32 | 0.63 |
| 1:V:166:ILE:HG12 | 1:W:173:TYR:CE2 | 2.34 | 0.63 |
| 1:D:158:ILE:O | 1:F:105:ARG:NH2 | 2.32 | 0.63 |
| 1:G:110:MET:HE2 | 1:G:116:VAL:HA | 1.80 | 0.63 |
| 1:I:190:PHE:CE1 | 1:J:184:ILE:HD11 | 2.34 | 0.63 |
| 1:7:103:TRP:HB3 | 1:7:149:PHE:HZ | 1.64 | 0.63 |
| 1:5:97:ALA:CB | 1:5:133:ALA:HB2 | 2.29 | 0.62 |
| 1:U:179:GLU:HG3 | 1:3:179:GLU:CD | 2.18 | 0.62 |
| 1:N:171:ARG:HG2 | 1:N:172:MET:N | 2.15 | 0.62 |
| 1:4:92:VAL:N | 1:4:95:GLN:OE1 | 2.32 | 0.62 |
| 1:W:173:TYR:CZ | 1:W:181:LYS:CE | 2.81 | 0.62 |
| 1:W:135:VAL:N | 2:W:201:HOH:O | 2.31 | 0.62 |
| 1:I:189:ASN:C | 1:I:191:VAL:H | 2.02 | 0.62 |
| 1:X:110:MET:HG3 | 1:X:111:THR:N | 2.14 | 0.62 |
| 1:6:99:THR:H | 1:6:156:MET:HE1 | 1.63 | 0.62 |
| 1:O:176:LEU:HD13 | 1:O:180:GLU:CD | 2.20 | 0.62 |
| 1:G:111:THR:HG21 | 1:G:116:VAL:N | 2.14 | 0.62 |
| 1:O:190:PHE:CE1 | 1:Y:189:ASN:ND2 | 2.68 | 0.62 |
| 1:R:104:MET:SD | 1:R:112:SER:N | 2.72 | 0.62 |
| 1:1:142:LEU:HD13 | 1:1:153:ALA:HB2 | 1.82 | 0.62 |
| 1:N:117:ALA:HB2 | 1:N:127:VAL:HG11 | 1.81 | 0.61 |
| 1:N:178:GLN:OE1 | 1:N:181:LYS:CB | 2.47 | 0.61 |
| 1:B:106:LYS:O | 1:B:107:ASP:CB | 2.48 | 0.61 |
| 1:L:116:VAL:HG11 | 1:L:127:VAL:HG21 | 1.82 | 0.61 |
| 1:1:162:ALA:HB3 | 1:7:132:LYS:NZ | 2.15 | 0.61 |
| 1:3:178:GLN:HA | 1:3:181:LYS:HE3 | 1.83 | 0.61 |
| 1:4:158:ILE:HG12 | 1:4:165:ILE:HG21 | 1.82 | 0.61 |
| 1:C:106:LYS:O | 1:C:110:MET:SD | 2.58 | 0.61 |
| 1:I:191:VAL:HB | 1:I:195:ASN:HB2 | 1.83 | 0.61 |
| 1:P:109:GLU:O | 1:P:110:MET:HB2 | 2.00 | 0.61 |
| 1:T:127:VAL:O | 1:T:131:MET:HG3 | 2.01 | 0.61 |
| 1:5:117:ALA:HB2 | 1:5:127:VAL:HG21 | 1.83 | 0.61 |
| 1:P:111:THR:C | 1:P:115:LYS:HE3 | 2.21 | 0.61 |
| 1:7:109:GLU:OE2 | 1:7:149:PHE:HA | 2.01 | 0.61 |
| 1:O:168:TYR:OH | 1:P:164:GLY:O | 2.17 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:110:MET:C | 1:P:115:LYS:HZ3 | 2.04 | 0.60 |
| 1:1:99:THR:HG23 | 1:7:102:ALA:HB2 | 1.82 | 0.60 |
| 1:6:191:VAL:HG12 | 1:6:191:VAL:O | 2.02 | 0.60 |
| 1:P:126:THR:HG22 | 1:P:128:ASN:H | 1.65 | 0.60 |
| 1:5:170:HIS:O | 1:5:173:TYR:CE2 | 2.53 | 0.60 |
| 1:5:170:HIS:C | 1:5:173:TYR:CE2 | 2.74 | 0.60 |
| 1:3:93:GLU:HG2 | 1:3:136:SER:HA | 1.84 | 0.60 |
| 1:6:95:GLN:O | 1:6:156:MET:CE | 2.50 | 0.60 |
| 1:6:111:THR:HG23 | 1:6:112:SER:N | 2.17 | 0.60 |
| 1:C:117:ALA:HB2 | 1:C:127:VAL:HG11 | 1.83 | 0.60 |
| 1:J:142:LEU:HD13 | 1:J:153:ALA:HB1 | 1.84 | 0.60 |
| 1:J:172:MET:HG3 | 1:J:175:ALA:HB3 | 1.84 | 0.60 |
| 1:R:113:GLU:HB3 | 1:R:128:ASN:OD1 | 2.02 | 0.60 |
| 1:O:190:PHE:HB2 | 1:Y:190:PHE:HA | 1.84 | 0.60 |
| 1:3:138:THR:HG22 | 1:3:141:VAL:HG22 | 1.83 | 0.60 |
| 1:H:188:ILE:O | 1:H:191:VAL:N | 2.34 | 0.60 |
| 1:M:182:ASN:HA | 1:M:185:THR:HB | 1.83 | 0.60 |
| 1:2:126:THR:HA | 1:2:129:ARG:HB2 | 1.83 | 0.60 |
| 1:L:114:LYS:HA | 1:L:124:PRO:HB3 | 1.83 | 0.59 |
| 1:Y:173:TYR:HA | 1:Y:176:LEU:HD22 | 1.82 | 0.59 |
| 1:L:115:LYS:NZ | 2:L:201:HOH:O | 2.35 | 0.59 |
| 1:F:138:THR:HG22 | 1:F:140:GLY:H | 1.67 | 0.59 |
| 1:5:171:ARG:HG2 | 1:5:173:TYR:N | 2.16 | 0.59 |
| 1:I:189:ASN:O | 1:I:190:PHE:CD1 | 2.56 | 0.59 |
| 1:I:134:GLU:O | 1:I:135:VAL:HG13 | 2.02 | 0.59 |
| 1:Y:94:LYS:H | 1:Y:94:LYS:HD2 | 1.67 | 0.59 |
| 1:B:104:MET:HB3 | 1:B:111:THR:HG23 | 1.82 | 0.59 |
| 1:U:130:ILE:HG12 | 1:U:137:THR:OG1 | 2.03 | 0.59 |
| 1:O:139:ILE:HD11 | 1:P:93:GLU:HB3 | 1.83 | 0.59 |
| 1:6:129:ARG:HD2 | 1:6:132:LYS:HE2 | 1.85 | 0.59 |
| 1:A:166:ILE:HG12 | 1:B:173:TYR:CZ | 2.37 | 0.59 |
| 1:L:129:ARG:O | 1:L:133:ALA:N | 2.36 | 0.59 |
| 1:Q:142:LEU:HG | 1:Q:156:MET:CE | 2.33 | 0.58 |
| 1:2:100:LEU:HD11 | 1:2:131:MET:HA | 1.85 | 0.58 |
| 1:H:190:PHE:CD1 | 1:H:191:VAL:N | 2.71 | 0.58 |
| 1:A:142:LEU:HD12 | 2:A:208:HOH:O | 2.03 | 0.58 |
| 1:Z:158:ILE:N | 1:1:154:TYR:OH | 2.36 | 0.58 |
| 1:5:170:HIS:O | 1:5:170:HIS:CD2 | 2.56 | 0.58 |
| 1:5:171:ARG:HG3 | 1:5:174:ALA:H | 1.68 | 0.58 |
| 1:J:126:THR:HG23 | 1:J:129:ARG:CZ | 2.34 | 0.58 |
| 1:5:143:SER:O | 1:5:147:ARG:HG3 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:188:ILE:O | 1:5:191:VAL:HG22 | 2.03 | 0.58 |
| 1:O:185:THR:HG22 | 1:P:166:ILE:HG23 | 1.86 | 0.58 |
| 1:L:189:ASN:O | 1:L:192:PHE:CD1 | 2.57 | 0.58 |
| 1:U:185:THR:O | 1:U:189:ASN:ND2 | 2.32 | 0.58 |
| 1:O:108:THR:O | 1:O:109:GLU:CB | 2.51 | 0.58 |
| 1:3:142:LEU:HD21 | 1:3:157:ILE:CD1 | 2.33 | 0.58 |
| 1:G:158:ILE:HG22 | 1:H:154:TYR:CG | 2.39 | 0.58 |
| 1:M:157:ILE:HG13 | 1:M:157:ILE:O | 2.03 | 0.58 |
| 1:X:110:MET:SD | 1:X:111:THR:OG1 | 2.61 | 0.58 |
| 1:W:173:TYR:CE2 | 1:W:181:LYS:CE | 2.87 | 0.58 |
| 1:N:181:LYS:CG | 1:N:182:ASN:N | 2.67 | 0.57 |
| 1:N:182:ASN:HB2 | 1:W:183:LYS:NZ | 2.19 | 0.57 |
| 1:6:132:LYS:O | 1:6:133:ALA:HB3 | 2.04 | 0.57 |
| 1:O:99:THR:OG1 | 1:O:156:MET:HG3 | 2.04 | 0.57 |
| 1:W:191:VAL:O | 1:W:195:ASN:ND2 | 2.36 | 0.57 |
| 1:P:109:GLU:OE2 | 1:P:115:LYS:CD | 2.52 | 0.57 |
| 1:T:93:GLU:H | 1:T:93:GLU:CD | 2.08 | 0.57 |
| 1:Z:158:ILE:HD12 | 1:1:154:TYR:CZ | 2.40 | 0.57 |
| 1:7:187:PHE:HA | 1:7:190:PHE:CE2 | 2.39 | 0.57 |
| 1:H:92:VAL:HG13 | 1:H:93:GLU:H | 1.70 | 0.57 |
| 1:T:129:ARG:NH2 | 2:T:202:HOH:O | 2.36 | 0.57 |
| 1:1:129:ARG:O | 1:1:133:ALA:O | 2.22 | 0.57 |
| 1:4:154:TYR:CE2 | 1:5:158:ILE:HD13 | 2.39 | 0.57 |
| 1:6:171:ARG:O | 1:6:174:ALA:N | 2.37 | 0.57 |
| 1:A:168:TYR:OH | 1:B:164:GLY:O | 2.14 | 0.57 |
| 1:K:190:PHE:O | 1:K:193:GLU:HG3 | 2.05 | 0.57 |
| 1:2:104:MET:HG3 | 1:2:105:ARG:N | 2.20 | 0.57 |
| 1:4:99:THR:HG21 | 1:4:156:MET:CA | 2.35 | 0.57 |
| 1:X:166:ILE:HG22 | 1:Y:173:TYR:CZ | 2.40 | 0.57 |
| 1:3:114:LYS:HE3 | 1:3:124:PRO:HB2 | 1.85 | 0.57 |
| 1:5:171:ARG:HG3 | 1:5:174:ALA:N | 2.20 | 0.57 |
| 1:E:131:MET:O | 1:H:171:ARG:NH1 | 2.38 | 0.57 |
| 1:P:111:THR:N | 1:P:115:LYS:NZ | 2.52 | 0.57 |
| 1:X:151:HIS:ND1 | 1:X:155:GLU:OE1 | 2.33 | 0.57 |
| 1:4:170:HIS:ND1 | 1:5:164:GLY:O | 2.37 | 0.57 |
| 1:F:113:GLU:HG2 | 1:F:131:MET:SD | 2.45 | 0.56 |
| 1:N:178:GLN:OE1 | 1:N:181:LYS:HB2 | 2.05 | 0.56 |
| 1:V:110:MET:SD | 1:V:115:LYS:HG2 | 2.44 | 0.56 |
| 1:Z:128:ASN:OD1 | 1:Z:131:MET:SD | 2.63 | 0.56 |
| 1:F:130:ILE:HG12 | 1:F:137:THR:CG2 | 2.35 | 0.56 |
| 1:G:111:THR:HG21 | 1:G:116:VAL:H | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:192:PHE:HZ | 1:W:186:SER:CB | 2.18 | 0.56 |
| 1:N:100:LEU:HD13 | 1:N:145:LEU:HD21 | 1.85 | 0.56 |
| 1:P:117:ALA:HB2 | 1:P:127:VAL:CG2 | 2.35 | 0.56 |
| 1:W:193:GLU:HA | 1:W:196:LYS:HG2 | 1.87 | 0.56 |
| 1:X:143:SER:HB2 | 1:Y:92:VAL:HG21 | 1.87 | 0.56 |
| 1:1:151:HIS:HE2 | 1:7:106:LYS:HG2 | 1.70 | 0.56 |
| 1:2:122:ILE:HD11 | 1:2:145:LEU:CD2 | 2.35 | 0.56 |
| 1:3:137:THR:HG22 | 1:3:141:VAL:HG23 | 1.86 | 0.56 |
| 1:6:94:LYS:N | 1:6:133:ALA:HB2 | 2.19 | 0.56 |
| 1:H:189:ASN:HA | 1:H:191:VAL:HG23 | 1.86 | 0.56 |
| 1:K:173:TYR:O | 1:K:181:LYS:NZ | 2.39 | 0.56 |
| 1:M:94:LYS:HA | 1:M:132:LYS:HA | 1.87 | 0.56 |
| 1:M:97:ALA:HA | 1:M:131:MET:HB3 | 1.87 | 0.56 |
| 1:N:94:LYS:H | 1:N:94:LYS:HD2 | 1.69 | 0.56 |
| 1:A:93:GLU:OE2 | 1:A:136:SER:OG | 2.24 | 0.56 |
| 1:Q:187:PHE:HE2 | 1:R:184:ILE:HA | 1.71 | 0.56 |
| 1:6:187:PHE:HE2 | 1:7:183:LYS:HE2 | 1.70 | 0.56 |
| 1:O:139:ILE:HG23 | 1:P:137:THR:O | 2.06 | 0.56 |
| 1:O:190:PHE:CD1 | 1:O:191:VAL:HB | 2.40 | 0.56 |
| 1:Q:176:LEU:HD21 | 1:R:192:PHE:HA | 1.87 | 0.56 |
| 1:Q:190:PHE:CE2 | 1:1:190:PHE:CD1 | 2.94 | 0.56 |
| 1:W:105:ARG:HG2 | 1:W:105:ARG:HH11 | 1.70 | 0.56 |
| 1:J:187:PHE:O | 1:J:190:PHE:HB3 | 2.06 | 0.56 |
| 1:O:127:VAL:O | 1:O:130:ILE:HG22 | 2.05 | 0.56 |
| 1:I:114:LYS:O | 1:I:115:LYS:O | 2.22 | 0.56 |
| 1:O:174:ALA:O | 1:O:181:LYS:NZ | 2.39 | 0.56 |
| 1:Q:188:ILE:HG22 | 1:Q:192:PHE:CE2 | 2.40 | 0.56 |
| 1:1:169:ASP:HB3 | 1:1:172:MET:HG2 | 1.88 | 0.56 |
| 1:M:184:ILE:HG21 | 1:N:188:ILE:HD11 | 1.88 | 0.56 |
| 1:N:92:VAL:N | 2:N:203:HOH:O | 2.38 | 0.56 |
| 1:N:171:ARG:CG | 1:N:172:MET:N | 2.69 | 0.56 |
| 1:2:143:SER:O | 1:2:147:ARG:HG2 | 2.05 | 0.56 |
| 1:D:191:VAL:HG12 | 1:D:191:VAL:O | 2.07 | 0.55 |
| 1:K:158:ILE:HD12 | 1:K:158:ILE:N | 2.21 | 0.55 |
| 1:U:183:LYS:O | 1:U:186:SER:OG | 2.21 | 0.55 |
| 1:K:154:TYR:CE1 | 1:L:157:ILE:HB | 2.40 | 0.55 |
| 1:2:100:LEU:HD22 | 1:2:130:ILE:HG22 | 1.87 | 0.55 |
| 1:K:154:TYR:CE1 | 1:L:157:ILE:O | 2.60 | 0.55 |
| 1:2:136:SER:C | 1:3:138:THR:OG1 | 2.44 | 0.55 |
| 1:O:171:ARG:NH1 | 1:O:174:ALA:HB1 | 2.21 | 0.55 |
| 1:Q:147:ARG:NH1 | 1:Q:152:GLU:OE2 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:95:GLN:NE2 | 1:G:158:ILE:O | 2.40 | 0.55 |
| 1:3:99:THR:HG21 | 1:3:156:MET:HA | 1.88 | 0.55 |
| 1:R:179:GLU:HA | 1:R:182:ASN:HB2 | 1.88 | 0.55 |
| 1:6:99:THR:HG22 | 1:6:103:TRP:NE1 | 2.22 | 0.55 |
| 1:4:187:PHE:CE2 | 1:5:187:PHE:HB3 | 2.42 | 0.55 |
| 1:7:170:HIS:CD2 | 1:7:170:HIS:C | 2.80 | 0.55 |
| 1:K:160:VAL:HG22 | 1:K:161:GLY:H | 1.71 | 0.55 |
| 1:M:178:GLN:HB2 | 1:M:182:ASN:OD1 | 2.06 | 0.55 |
| 1:1:129:ARG:HB3 | 1:1:135:VAL:HG11 | 1.88 | 0.55 |
| 1:6:100:LEU:HA | 1:6:103:TRP:CE3 | 2.41 | 0.55 |
| 1:Z:138:THR:HA | 1:1:138:THR:HA | 1.89 | 0.55 |
| 1:7:110:MET:O | 1:7:115:LYS:NZ | 2.22 | 0.55 |
| 1:N:92:VAL:O | 2:N:201:HOH:O | 2.18 | 0.54 |
| 1:6:129:ARG:HD3 | 1:6:132:LYS:CE | 2.36 | 0.54 |
| 1:C:177:PRO:O | 1:C:180:GLU:OE2 | 2.25 | 0.54 |
| 1:M:96:ALA:HA | 1:M:156:MET:O | 2.07 | 0.54 |
| 1:O:139:ILE:N | 1:P:137:THR:O | 2.35 | 0.54 |
| 1:7:169:ASP:OD1 | 1:7:170:HIS:N | 2.40 | 0.54 |
| 1:G:108:THR:N | 1:G:109:GLU:HA | 2.23 | 0.54 |
| 1:G:111:THR:CG2 | 1:G:116:VAL:N | 2.71 | 0.54 |
| 1:K:152:GLU:O | 1:K:154:TYR:N | 2.40 | 0.54 |
| 1:U:162:ALA:HB2 | 1:W:105:ARG:NH2 | 2.23 | 0.54 |
| 1:4:99:THR:HG21 | 1:4:156:MET:HA | 1.90 | 0.54 |
| 1:5:97:ALA:HB2 | 1:5:133:ALA:CB | 2.36 | 0.54 |
| 1:C:110:MET:HB2 | 1:C:115:LYS:HE3 | 1.88 | 0.54 |
| 1:C:195:ASN:N | 1:C:195:ASN:HD22 | 2.05 | 0.54 |
| 1:2:110:MET:O | 1:2:115:LYS:HD3 | 2.07 | 0.54 |
| 1:6:94:LYS:HA | 1:6:132:LYS:O | 2.07 | 0.54 |
| 1:7:103:TRP:CE3 | 1:7:149:PHE:CE1 | 2.96 | 0.54 |
| 1:2:136:SER:HA | 1:3:139:ILE:HG13 | 1.90 | 0.54 |
| 1:4:110:MET:SD | 1:4:115:LYS:HG2 | 2.47 | 0.54 |
| 1:C:105:ARG:NH2 | 2:C:201:HOH:O | 2.22 | 0.54 |
| 1:O:157:ILE:HD13 | 1:P:157:ILE:HD11 | 1.90 | 0.54 |
| 1:G:144:SER:HA | 1:G:147:ARG:NH1 | 2.22 | 0.54 |
| 1:H:112:SER:OG | 1:H:114:LYS:HB3 | 2.07 | 0.54 |
| 1:I:116:VAL:HG21 | 1:I:127:VAL:CG2 | 2.38 | 0.54 |
| 1:G:111:THR:HG23 | 1:G:116:VAL:HG12 | 1.88 | 0.54 |
| 1:5:152:GLU:HB2 | 1:5:154:TYR:CE2 | 2.43 | 0.54 |
| 1:C:114:LYS:HA | 1:C:117:ALA:HB3 | 1.89 | 0.54 |
| 1:H:173:TYR:CE1 | 1:H:184:ILE:HD11 | 2.43 | 0.53 |
| 1:W:101:ASN:HD21 | 1:W:105:ARG:NH2 | 2.06 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:147:ARG:NH1 | 2:T:203:HOH:O | 2.39 | 0.53 |
| 1:1:104:MET:SD | 1:1:131:MET:SD | 3.07 | 0.53 |
| 1:4:134:GLU:HG3 | 1:4:135:VAL:HG23 | 1.91 | 0.53 |
| 1:D:117:ALA:HB2 | 1:D:127:VAL:HG21 | 1.91 | 0.53 |
| 1:H:190:PHE:CG | 1:H:191:VAL:N | 2.76 | 0.53 |
| 1:O:110:MET:SD | 1:O:149:PHE:CE1 | 3.02 | 0.53 |
| 1:P:180:GLU:N | 1:Y:179:GLU:HG2 | 2.24 | 0.53 |
| 1:W:193:GLU:O | 1:W:196:LYS:HG3 | 2.08 | 0.53 |
| 1:Y:101:ASN:OD1 | 1:Y:131:MET:HG3 | 2.09 | 0.53 |
| 1:L:189:ASN:O | 1:L:192:PHE:HD1 | 1.91 | 0.53 |
| 1:N:182:ASN:HB3 | 1:N:186:SER:N | 2.24 | 0.53 |
| 1:5:171:ARG:HG2 | 1:5:173:TYR:H | 1.74 | 0.53 |
| 1:7:190:PHE:HA | 1:7:193:GLU:OE2 | 2.08 | 0.53 |
| 1:K:136:SER:HB3 | 1:L:138:THR:HG21 | 1.89 | 0.53 |
| 1:V:110:MET:CG | 1:V:116:VAL:HG13 | 2.38 | 0.53 |
| 1:X:143:SER:O | 1:X:147:ARG:HB2 | 2.09 | 0.53 |
| 1:B:106:LYS:O | 1:B:107:ASP:HB3 | 2.07 | 0.53 |
| 1:G:114:LYS:C | 1:G:116:VAL:H | 2.11 | 0.53 |
| 1:O:172:MET:HE1 | 2:O:203:HOH:O | 2.08 | 0.53 |
| 1:3:146:ALA:HB1 | 1:3:151:HIS:O | 2.08 | 0.53 |
| 1:4:99:THR:HG21 | 1:4:156:MET:CB | 2.38 | 0.53 |
| 1:6:157:ILE:HG23 | 1:7:154:TYR:CB | 2.39 | 0.53 |
| 1:6:169:ASP:OD1 | 1:6:172:MET:N | 2.40 | 0.53 |
| 1:F:196:LYS:NZ | 2:F:202:HOH:O | 2.39 | 0.53 |
| 1:Z:184:ILE:HA | 1:Z:187:PHE:CZ | 2.44 | 0.53 |
| 1:1:94:LYS:H | 1:1:94:LYS:HD2 | 1.72 | 0.53 |
| 1:4:187:PHE:HE2 | 1:5:184:ILE:HA | 1.73 | 0.53 |
| 1:N:165:ILE:HG22 | 1:N:166:ILE:N | 2.24 | 0.53 |
| 1:N:182:ASN:HB2 | 1:W:183:LYS:HZ1 | 1.74 | 0.53 |
| 1:P:120:ALA:CB | 1:P:122:ILE:HG12 | 2.32 | 0.53 |
| 1:V:116:VAL:HG21 | 1:V:127:VAL:HG11 | 1.90 | 0.53 |
| 1:C:168:TYR:CZ | 1:D:166:ILE:HD12 | 2.43 | 0.52 |
| 1:P:109:GLU:OE2 | 1:P:115:LYS:CE | 2.57 | 0.52 |
| 1:M:157:ILE:HD11 | 1:N:154:TYR:HB3 | 1.91 | 0.52 |
| 1:6:184:ILE:HD11 | 1:7:188:ILE:HG23 | 1.90 | 0.52 |
| 1:E:103:TRP:CH2 | 1:E:151:HIS:HB2 | 2.45 | 0.52 |
| 1:6:132:LYS:H | 1:6:132:LYS:HZ2 | 1.57 | 0.52 |
| 1:F:138:THR:HG22 | 1:F:140:GLY:N | 2.25 | 0.52 |
| 1:L:92:VAL:HG23 | 1:L:93:GLU:HG3 | 1.91 | 0.52 |
| 1:L:180:GLU:HG2 | 2:L:213:HOH:O | 2.10 | 0.52 |
| 1:P:109:GLU:OE2 | 1:P:115:LYS:HD2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:178:GLN:HA | 1:Q:181:LYS:HG3 | 1.92 | 0.52 |
| 1:Z:158:ILE:HD12 | 1:1:154:TYR:CE2 | 2.44 | 0.52 |
| 1:6:100:LEU:O | 1:6:104:MET:HG2 | 2.09 | 0.52 |
| 1:6:187:PHE:CE2 | 1:7:183:LYS:HE2 | 2.45 | 0.52 |
| 1:N:178:GLN:OE1 | 1:N:181:LYS:HD2 | 2.09 | 0.52 |
| 1:P:100:LEU:HD13 | 1:P:156:MET:HE3 | 1.92 | 0.52 |
| 1:V:109:GLU:OE1 | 1:V:109:GLU:N | 2.42 | 0.52 |
| 1:2:122:ILE:HD11 | 1:2:145:LEU:HD22 | 1.90 | 0.52 |
| 1:C:173:TYR:CZ | 1:D:166:ILE:HG13 | 2.44 | 0.52 |
| 1:H:188:ILE:O | 1:H:191:VAL:CG2 | 2.57 | 0.52 |
| 1:X:110:MET:O | 1:X:111:THR:HG23 | 2.10 | 0.52 |
| 1:1:162:ALA:HB3 | 1:7:132:LYS:HZ3 | 1.74 | 0.52 |
| 1:I:178:GLN:HG3 | 1:I:181:LYS:HD2 | 1.92 | 0.52 |
| 1:P:162:ALA:HB3 | 1:P:165:ILE:CG2 | 2.40 | 0.52 |
| 1:R:105:ARG:HD2 | 1:R:111:THR:HG21 | 1.91 | 0.52 |
| 1:2:188:ILE:O | 1:2:191:VAL:HG12 | 2.09 | 0.52 |
| 1:6:176:LEU:HG | 1:6:180:GLU:CG | 2.39 | 0.52 |
| 1:C:182:ASN:O | 1:C:186:SER:N | 2.41 | 0.52 |
| 1:E:162:ALA:HB3 | 1:E:165:ILE:HD12 | 1.91 | 0.52 |
| 1:K:120:ALA:HB2 | 1:K:127:VAL:CG1 | 2.40 | 0.52 |
| 1:V:92:VAL:N | 2:V:201:HOH:O | 2.41 | 0.52 |
| 1:X:166:ILE:HG22 | 1:Y:173:TYR:CE1 | 2.44 | 0.52 |
| 1:Z:151:HIS:CD2 | 1:Z:170:HIS:O | 2.62 | 0.52 |
| 1:G:102:ALA:HA | 1:G:105:ARG:HD3 | 1.91 | 0.52 |
| 1:6:176:LEU:HG | 1:6:180:GLU:HG2 | 1.91 | 0.52 |
| 1:G:110:MET:HE1 | 1:G:116:VAL:HG23 | 1.92 | 0.52 |
| 1:G:195:ASN:OD1 | 1:G:196:LYS:N | 2.43 | 0.52 |
| 1:1:189:ASN:HA | 1:1:192:PHE:CD2 | 2.45 | 0.52 |
| 1:6:99:THR:OG1 | 1:6:156:MET:HB2 | 2.10 | 0.52 |
| 1:4:157:ILE:HG23 | 1:5:154:TYR:HB3 | 1.92 | 0.51 |
| 1:M:161:GLY:O | 1:M:162:ALA:HB3 | 2.10 | 0.51 |
| 1:Z:136:SER:OG | 1:1:139:ILE:HG13 | 2.10 | 0.51 |
| 1:M:162:ALA:HB1 | 1:M:163:PRO:HD2 | 1.93 | 0.51 |
| 1:3:105:ARG:HH12 | 1:5:151:HIS:HA | 1.75 | 0.51 |
| 1:M:196:LYS:O | 1:O:195:ASN:ND2 | 2.43 | 0.51 |
| 1:R:143:SER:HA | 1:R:153:ALA:HB2 | 1.92 | 0.51 |
| 1:Z:176:LEU:O | 1:Z:177:PRO:C | 2.47 | 0.51 |
| 1:1:182:ASN:HA | 1:1:185:THR:HB | 1.93 | 0.51 |
| 1:7:114:LYS:HA | 1:7:117:ALA:HB3 | 1.92 | 0.51 |
| 1:1:97:ALA:HB1 | 1:1:131:MET:O | 2.11 | 0.51 |
| 1:H:122:ILE:HD11 | 1:H:145:LEU:HD21 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:162:ALA:HB3 | 1:P:165:ILE:HG23 | 1.92 | 0.51 |
| 1:L:116:VAL:HG23 | 1:L:122:ILE:O | 2.10 | 0.51 |
| 1:Y:120:ALA:O | 2:Y:201:HOH:O | 2.19 | 0.51 |
| 1:4:184:ILE:O | 1:4:188:ILE:HG12 | 2.09 | 0.51 |
| 1:H:172:MET:HE3 | 1:H:176:LEU:HD21 | 1.92 | 0.51 |
| 1:Q:92:VAL:CG1 | 1:R:139:ILE:HG22 | 2.41 | 0.51 |
| 1:V:110:MET:HE3 | 1:V:112:SER:H | 1.76 | 0.51 |
| 1:3:113:GLU:HG2 | 1:3:114:LYS:HD3 | 1.93 | 0.51 |
| 1:N:171:ARG:O | 1:N:172:MET:HB2 | 2.10 | 0.50 |
| 1:T:100:LEU:HD13 | 1:T:145:LEU:HD21 | 1.92 | 0.50 |
| 1:Z:154:TYR:HA | 1:1:157:ILE:HD11 | 1.93 | 0.50 |
| 1:6:156:MET:O | 1:6:158:ILE:O | 2.29 | 0.50 |
| 1:6:184:ILE:CD1 | 1:7:188:ILE:HG23 | 2.42 | 0.50 |
| 1:E:104:MET:HG2 | 1:E:116:VAL:HG21 | 1.92 | 0.50 |
| 1:W:105:ARG:HH11 | 1:W:105:ARG:CG | 2.23 | 0.50 |
| 1:Y:176:LEU:HD21 | 1:Y:181:LYS:HG2 | 1.92 | 0.50 |
| 1:4:164:GLY:O | 1:5:170:HIS:CE1 | 2.64 | 0.50 |
| 1:C:176:LEU:HG | 1:C:180:GLU:OE1 | 2.11 | 0.50 |
| 1:D:117:ALA:O | 1:D:120:ALA:O | 2.29 | 0.50 |
| 1:E:191:VAL:O | 1:E:195:ASN:ND2 | 2.45 | 0.50 |
| 1:J:178:GLN:O | 1:J:182:ASN:ND2 | 2.44 | 0.50 |
| 1:V:110:MET:CE | 1:V:115:LYS:HG2 | 2.41 | 0.50 |
| 1:Y:186:SER:O | 1:Y:189:ASN:ND2 | 2.44 | 0.50 |
| 1:Z:184:ILE:HA | 1:Z:187:PHE:CE2 | 2.46 | 0.50 |
| 1:7:184:ILE:O | 1:7:185:THR:OG1 | 2.22 | 0.50 |
| 1:A:187:PHE:O | 1:A:190:PHE:HB3 | 2.12 | 0.50 |
| 1:G:138:THR:HA | 1:H:138:THR:HA | 1.93 | 0.50 |
| 1:O:146:ALA:HB1 | 1:O:155:GLU:HG2 | 1.94 | 0.50 |
| 1:P:124:PRO:O | 1:P:125:ALA:HB3 | 2.11 | 0.50 |
| 1:T:103:TRP:CZ3 | 1:T:156:MET:HG2 | 2.47 | 0.50 |
| 1:2:145:LEU:HD23 | 1:2:145:LEU:N | 2.26 | 0.50 |
| 1:H:178:GLN:CD | 1:H:178:GLN:H | 2.15 | 0.50 |
| 1:Z:114:LYS:O | 1:Z:117:ALA:HB3 | 2.11 | 0.50 |
| 1:X:125:ALA:N | 2:X:202:HOH:O | 2.39 | 0.50 |
| 1:3:105:ARG:NH2 | 1:5:154:TYR:OH | 2.40 | 0.50 |
| 1:6:111:THR:CG2 | 1:6:112:SER:H | 2.21 | 0.50 |
| 1:B:178:GLN:O | 1:B:182:ASN:OD1 | 2.29 | 0.50 |
| 1:E:106:LYS:HG2 | 1:E:107:ASP:H | 1.76 | 0.50 |
| 1:G:104:MET:HA | 1:G:107:ASP:HB2 | 1.93 | 0.50 |
| 1:H:188:ILE:O | 1:H:191:VAL:HG22 | 2.11 | 0.50 |
| 1:I:157:ILE:HD11 | 1:J:154:TYR:CA | 2.40 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:100:LEU:HD11 | 1:Z:156:MET:CE | 2.42 | 0.50 |
| 1:2:110:MET:HG3 | 1:2:149:PHE:CE1 | 2.47 | 0.50 |
| 1:2:136:SER:HA | 1:3:139:ILE:CG1 | 2.42 | 0.50 |
| 1:B:180:GLU:HB3 | 2:B:201:HOH:O | 2.11 | 0.50 |
| 1:F:100:LEU:O | 1:F:104:MET:HG3 | 2.11 | 0.50 |
| 1:Q:187:PHE:CE2 | 1:R:184:ILE:HA | 2.47 | 0.50 |
| 1:C:169:ASP:OD2 | 1:C:171:ARG:NH2 | 2.40 | 0.50 |
| 1:I:157:ILE:HD13 | 1:J:153:ALA:HB3 | 1.93 | 0.50 |
| 1:U:179:GLU:HA | 1:U:182:ASN:HB2 | 1.94 | 0.50 |
| 1:V:130:ILE:HD13 | 1:V:145:LEU:HD11 | 1.94 | 0.50 |
| 1:1:99:THR:HG21 | 1:1:156:MET:HA | 1.93 | 0.50 |
| 1:3:165:ILE:HD11 | 1:5:105:ARG:NH2 | 2.27 | 0.50 |
| 1:C:174:ALA:HB3 | 2:C:208:HOH:O | 2.12 | 0.49 |
| 1:I:126:THR:HG22 | 1:I:130:ILE:HG23 | 1.92 | 0.49 |
| 1:K:185:THR:O | 1:K:189:ASN:HB2 | 2.12 | 0.49 |
| 1:M:187:PHE:O | 1:M:191:VAL:HG23 | 2.12 | 0.49 |
| 1:P:162:ALA:HB1 | 1:P:163:PRO:HD2 | 1.92 | 0.49 |
| 1:T:120:ALA:HB3 | 1:T:122:ILE:HG22 | 1.94 | 0.49 |
| 1:1:142:LEU:HD13 | 1:1:153:ALA:CB | 2.41 | 0.49 |
| 1:7:126:THR:OG1 | 1:7:128:ASN:OD1 | 2.24 | 0.49 |
| 1:D:173:TYR:O | 1:D:181:LYS:NZ | 2.45 | 0.49 |
| 1:H:147:ARG:NH1 | 2:H:203:HOH:O | 2.44 | 0.49 |
| 1:N:176:LEU:HD22 | 1:N:178:GLN:NE2 | 2.23 | 0.49 |
| 1:Y:104:MET:CG | 2:Y:202:HOH:O | 2.59 | 0.49 |
| 1:Z:146:ALA:HB2 | 2:Z:201:HOH:O | 2.11 | 0.49 |
| 1:6:108:THR:O | 1:6:109:GLU:HG2 | 2.12 | 0.49 |
| 1:K:184:ILE:HG13 | 1:K:185:THR:H | 1.76 | 0.49 |
| 1:A:112:SER:O | 2:A:201:HOH:O | 2.20 | 0.49 |
| 1:Q:109:GLU:HG3 | 1:Q:110:MET:N | 2.27 | 0.49 |
| 1:4:142:LEU:HA | 1:4:145:LEU:HG | 1.93 | 0.49 |
| 1:7:126:THR:CB | 1:7:128:ASN:OD1 | 2.61 | 0.49 |
| 1:F:180:GLU:HA | 1:F:183:LYS:HE2 | 1.93 | 0.49 |
| 1:P:149:PHE:HA | 2:P:205:HOH:O | 2.11 | 0.49 |
| 1:Y:110:MET:HG2 | 1:Y:111:THR:HG23 | 1.95 | 0.49 |
| 1:2:157:ILE:CD1 | 1:3:154:TYR:HA | 2.43 | 0.49 |
| 1:3:92:VAL:N | 2:3:202:HOH:O | 2.46 | 0.49 |
| 1:6:168:TYR:CE2 | 1:6:170:HIS:HD2 | 2.30 | 0.49 |
| 1:E:166:ILE:HG12 | 1:F:173:TYR:CZ | 2.48 | 0.49 |
| 1:E:181:LYS:NZ | 2:E:203:HOH:O | 2.45 | 0.49 |
| 1:O:95:GLN:HE22 | 1:O:159:PRO:HA | 1.77 | 0.49 |
| 1:3:117:ALA:O | 1:3:121:GLY:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:120:ALA:HB2 | 1:C:145:LEU:HD23 | 1.95 | 0.49 |
| 1:E:136:SER:HB3 | 1:F:138:THR:CG2 | 2.39 | 0.49 |
| 1:K:122:ILE:HG22 | 1:K:124:PRO:HD2 | 1.95 | 0.49 |
| 1:K:184:ILE:CG2 | 1:L:166:ILE:HG23 | 2.43 | 0.49 |
| 1:3:151:HIS:CE1 | 1:5:106:LYS:HA | 2.47 | 0.49 |
| 1:4:168:TYR:CE2 | 1:5:165:ILE:HG13 | 2.46 | 0.49 |
| 1:H:190:PHE:O | 1:H:193:GLU:HG3 | 2.13 | 0.49 |
| 1:F:110:MET:HB3 | 1:F:116:VAL:HG22 | 1.95 | 0.49 |
| 1:M:130:ILE:O | 1:M:131:MET:C | 2.51 | 0.49 |
| 1:U:101:ASN:OD1 | 1:U:105:ARG:NH2 | 2.46 | 0.49 |
| 1:2:136:SER:C | 1:3:138:THR:HG1 | 2.15 | 0.49 |
| 1:7:123:GLY:O | 1:7:125:ALA:N | 2.41 | 0.49 |
| 1:B:122:ILE:HG22 | 1:B:123:GLY:H | 1.77 | 0.49 |
| 1:E:117:ALA:HB2 | 1:E:127:VAL:HG21 | 1.95 | 0.49 |
| 1:J:130:ILE:HG12 | 1:J:137:THR:OG1 | 2.13 | 0.49 |
| 1:N:180:GLU:O | 1:W:183:LYS:NZ | 2.42 | 0.49 |
| 1:Q:168:TYR:CE2 | 1:Q:170:HIS:CD2 | 3.01 | 0.49 |
| 1:R:177:PRO:HA | 1:T:105:ARG:HH12 | 1.76 | 0.49 |
| 1:V:173:TYR:O | 1:V:181:LYS:NZ | 2.45 | 0.49 |
| 1:Z:139:ILE:HG12 | 1:1:137:THR:O | 2.13 | 0.49 |
| 1:3:161:GLY:HA2 | 1:5:132:LYS:HG3 | 1.95 | 0.48 |
| 1:A:179:GLU:O | 1:A:183:LYS:HG2 | 2.13 | 0.48 |
| 1:C:110:MET:SD | 1:C:115:LYS:NZ | 2.77 | 0.48 |
| 1:F:165:ILE:HD12 | 1:F:165:ILE:N | 2.28 | 0.48 |
| 1:K:158:ILE:HG22 | 1:K:158:ILE:O | 2.12 | 0.48 |
| 1:6:168:TYR:CZ | 1:6:170:HIS:HD2 | 2.30 | 0.48 |
| 1:F:183:LYS:HG2 | 1:5:183:LYS:HG2 | 1.95 | 0.48 |
| 1:I:126:THR:O | 1:I:130:ILE:HG23 | 2.13 | 0.48 |
| 1:K:159:PRO:O | 1:K:165:ILE:HD11 | 2.13 | 0.48 |
| 1:O:125:ALA:O | 1:O:128:ASN:ND2 | 2.46 | 0.48 |
| 1:6:157:ILE:HG12 | 1:7:154:TYR:HB3 | 1.94 | 0.48 |
| 1:M:187:PHE:HE2 | 1:N:183:LYS:O | 1.96 | 0.48 |
| 1:X:107:ASP:CG | 1:X:110:MET:H | 2.16 | 0.48 |
| 1:4:110:MET:HE1 | 1:4:115:LYS:HB3 | 1.96 | 0.48 |
| 1:N:190:PHE:O | 1:N:191:VAL:C | 2.52 | 0.48 |
| 1:Q:92:VAL:HG13 | 1:Q:157:ILE:CG2 | 2.44 | 0.48 |
| 1:J:146:ALA:HB1 | 1:J:151:HIS:O | 2.12 | 0.48 |
| 1:W:106:LYS:NZ | 2:W:202:HOH:O | 2.34 | 0.48 |
| 1:Y:112:SER:N | 2:Y:202:HOH:O | 2.22 | 0.48 |
| 1:7:172:MET:O | 1:7:174:ALA:N | 2.47 | 0.48 |
| 1:F:94:LYS:NZ | 2:F:205:HOH:O | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:187:PHE:O | 1:I:190:PHE:HB3 | 2.14 | 0.48 |
| 1:J:104:MET:O | 1:J:110:MET:HA | 2.13 | 0.48 |
| 1:N:173:TYR:CE2 | 1:N:181:LYS:HD2 | 2.49 | 0.48 |
| 1:N:173:TYR:CE2 | 1:N:183:LYS:CG | 2.93 | 0.48 |
| 1:Q:176:LEU:HG | 1:Q:180:GLU:OE2 | 2.13 | 0.48 |
| 1:V:99:THR:HG22 | 1:V:103:TRP:CE2 | 2.48 | 0.48 |
| 1:3:154:TYR:CE2 | 1:3:155:GLU:HG2 | 2.49 | 0.48 |
| 1:5:100:LEU:HB2 | 2:5:209:HOH:O | 2.13 | 0.48 |
| 1:5:155:GLU:O | 1:5:155:GLU:HG3 | 2.13 | 0.48 |
| 1:6:151:HIS:CD2 | 1:6:152:GLU:N | 2.82 | 0.48 |
| 1:P:190:PHE:C | 1:P:191:VAL:HG22 | 2.33 | 0.48 |
| 1:3:165:ILE:HD11 | 1:5:105:ARG:HH22 | 1.79 | 0.48 |
| 1:E:163:PRO:HB3 | 1:G:98:ALA:HB2 | 1.96 | 0.48 |
| 1:K:116:VAL:O | 1:K:116:VAL:HG23 | 2.14 | 0.48 |
| 1:M:187:PHE:HA | 1:W:190:PHE:CE1 | 2.48 | 0.48 |
| 1:O:99:THR:HG21 | 1:O:156:MET:HA | 1.96 | 0.48 |
| 1:O:104:MET:O | 1:O:111:THR:HG23 | 2.13 | 0.48 |
| 1:P:96:ALA:N | 2:P:201:HOH:O | 2.46 | 0.48 |
| 1:U:162:ALA:HB2 | 1:W:105:ARG:CZ | 2.44 | 0.48 |
| 1:X:125:ALA:O | 1:X:128:ASN:HB3 | 2.14 | 0.48 |
| 1:C:111:THR:OG1 | 1:C:112:SER:N | 2.47 | 0.47 |
| 1:C:125:ALA:O | 1:C:129:ARG:N | 2.37 | 0.47 |
| 1:E:167:ASP:OD1 | 1:E:167:ASP:N | 2.47 | 0.47 |
| 1:N:124:PRO:HA | 1:N:127:VAL:HG12 | 1.96 | 0.47 |
| 1:Q:188:ILE:HG22 | 1:Q:192:PHE:CZ | 2.49 | 0.47 |
| 1:T:174:ALA:HA | 1:T:181:LYS:HZ1 | 1.77 | 0.47 |
| 1:Z:164:GLY:HA2 | 1:1:173:TYR:CD1 | 2.48 | 0.47 |
| 1:1:151:HIS:NE2 | 1:7:106:LYS:HG2 | 2.29 | 0.47 |
| 1:1:160:VAL:HG11 | 1:7:97:ALA:HB3 | 1.95 | 0.47 |
| 1:4:157:ILE:HG21 | 1:5:153:ALA:HB3 | 1.96 | 0.47 |
| 1:5:170:HIS:O | 1:5:170:HIS:CG | 2.66 | 0.47 |
| 1:E:172:MET:SD | 1:F:192:PHE:CE2 | 3.07 | 0.47 |
| 1:V:99:THR:HG21 | 1:V:156:MET:HA | 1.96 | 0.47 |
| 1:Z:96:ALA:C | 1:Z:100:LEU:HD13 | 2.35 | 0.47 |
| 1:Z:115:LYS:O | 1:Z:118:VAL:HG12 | 2.15 | 0.47 |
| 1:G:113:GLU:O | 1:G:114:LYS:HG3 | 2.15 | 0.47 |
| 1:N:157:ILE:O | 1:N:159:PRO:HD3 | 2.14 | 0.47 |
| 1:O:159:PRO:HB2 | 1:O:162:ALA:HA | 1.95 | 0.47 |
| 1:U:128:ASN:OD1 | 1:U:132:LYS:HD3 | 2.14 | 0.47 |
| 1:G:173:TYR:O | 1:G:181:LYS:HE2 | 2.15 | 0.47 |
| 1:W:107:ASP:OD1 | 1:W:108:THR:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:103:TRP:CE2 | 1:Z:151:HIS:CD2 | 3.02 | 0.47 |
| 1:K:184:ILE:HG13 | 1:K:185:THR:N | 2.29 | 0.47 |
| 1:N:171:ARG:CG | 1:N:172:MET:H | 2.27 | 0.47 |
| 1:P:110:MET:O | 1:P:111:THR:HG22 | 2.13 | 0.47 |
| 1:T:126:THR:HA | 1:T:129:ARG:HE | 1.79 | 0.47 |
| 1:V:110:MET:HG3 | 1:V:116:VAL:HG13 | 1.96 | 0.47 |
| 1:1:142:LEU:HD12 | 1:1:143:SER:N | 2.28 | 0.47 |
| 1:3:137:THR:CG2 | 1:3:141:VAL:HG23 | 2.45 | 0.47 |
| 1:G:116:VAL:O | 1:G:120:ALA:N | 2.42 | 0.47 |
| 1:O:193:GLU:OE1 | 1:O:193:GLU:N | 2.47 | 0.47 |
| 1:6:184:ILE:HG12 | 1:7:188:ILE:HG13 | 1.97 | 0.47 |
| 1:C:104:MET:HE3 | 1:C:131:MET:SD | 2.55 | 0.47 |
| 1:K:184:ILE:HG22 | 1:L:166:ILE:HG23 | 1.95 | 0.47 |
| 1:P:111:THR:O | 1:P:112:SER:CB | 2.62 | 0.47 |
| 1:Q:162:ALA:HB1 | 1:Q:163:PRO:HD2 | 1.96 | 0.47 |
| 1:Y:194:GLN:HG2 | 1:Y:195:ASN:ND2 | 2.30 | 0.47 |
| 1:3:92:VAL:HB | 1:3:93:GLU:OE1 | 2.14 | 0.47 |
| 1:5:111:THR:OG1 | 1:5:116:VAL:HG13 | 2.14 | 0.47 |
| 1:5:114:LYS:CG | 1:5:128:ASN:OD1 | 2.63 | 0.47 |
| 1:5:172:MET:HG2 | 1:5:173:TYR:CD1 | 2.50 | 0.47 |
| 1:M:193:GLU:O | 1:M:196:LYS:HB3 | 2.15 | 0.47 |
| 1:X:143:SER:CB | 1:Y:92:VAL:HG21 | 2.45 | 0.47 |
| 1:D:191:VAL:O | 1:D:191:VAL:CG1 | 2.63 | 0.47 |
| 1:I:126:THR:HA | 1:I:129:ARG:HB2 | 1.96 | 0.47 |
| 1:L:99:THR:HG21 | 1:L:156:MET:HA | 1.97 | 0.47 |
| 1:P:119:ALA:HB2 | 1:P:148:ALA:HB2 | 1.97 | 0.47 |
| 1:P:177:PRO:HB2 | 1:Y:179:GLU:OE1 | 2.15 | 0.47 |
| 1:T:102:ALA:O | 1:T:105:ARG:HG2 | 2.15 | 0.47 |
| 1:Y:122:ILE:HD11 | 1:Y:127:VAL:HG22 | 1.97 | 0.47 |
| 1:5:170:HIS:O | 1:5:173:TYR:CD2 | 2.68 | 0.47 |
| 1:6:157:ILE:HD11 | 1:7:153:ALA:HB1 | 1.97 | 0.47 |
| 1:I:110:MET:HE2 | 1:I:114:LYS:HG3 | 1.97 | 0.47 |
| 1:K:157:ILE:HG21 | 1:L:154:TYR:CD1 | 2.50 | 0.47 |
| 1:Q:180:GLU:O | 1:Q:183:LYS:HB2 | 2.15 | 0.47 |
| 1:W:117:ALA:HA | 1:W:122:ILE:HG22 | 1.97 | 0.47 |
| 1:X:146:ALA:O | 1:X:151:HIS:N | 2.44 | 0.47 |
| 1:Y:187:PHE:O | 1:Y:190:PHE:HD1 | 1.98 | 0.47 |
| 1:4:182:ASN:O | 1:4:186:SER:OG | 2.31 | 0.47 |
| 1:5:113:GLU:HB3 | 1:5:128:ASN:CG | 2.34 | 0.47 |
| 1:C:168:TYR:CZ | 1:C:170:HIS:CE1 | 3.03 | 0.46 |
| 1:D:112:SER:HB3 | 1:D:115:LYS:HG3 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:143:SER:HA | 1:D:153:ALA:HB2 | 1.96 | 0.46 |
| 1:R:170:HIS:O | 1:R:174:ALA:N | 2.44 | 0.46 |
| 1:U:192:PHE:HA | 1:U:193:GLU:CG | 2.44 | 0.46 |
| 1:1:194:GLN:NE2 | 2:1:202:HOH:O | 2.47 | 0.46 |
| 1:5:114:LYS:O | 1:5:118:VAL:N | 2.43 | 0.46 |
| 1:F:154:TYR:O | 1:F:158:ILE:HG13 | 2.14 | 0.46 |
| 1:G:154:TYR:O | 1:G:158:ILE:HG23 | 2.15 | 0.46 |
| 1:G:194:GLN:NE2 | 1:7:179:GLU:O | 2.48 | 0.46 |
| 1:H:182:ASN:HA | 1:H:185:THR:OG1 | 2.15 | 0.46 |
| 1:U:92:VAL:N | 2:U:208:HOH:O | 2.47 | 0.46 |
| 1:6:98:ALA:N | 1:6:156:MET:CE | 2.79 | 0.46 |
| 1:7:183:LYS:NZ | 1:7:184:ILE:HG22 | 2.30 | 0.46 |
| 1:A:100:LEU:C | 1:A:100:LEU:HD23 | 2.35 | 0.46 |
| 1:M:139:ILE:HA | 1:M:142:LEU:HD12 | 1.97 | 0.46 |
| 1:O:190:PHE:CG | 1:O:191:VAL:N | 2.84 | 0.46 |
| 1:P:187:PHE:CE1 | 1:P:190:PHE:CD2 | 3.03 | 0.46 |
| 1:R:185:THR:CB | 2:R:201:HOH:O | 2.61 | 0.46 |
| 1:U:113:GLU:OE2 | 1:U:128:ASN:HB2 | 2.15 | 0.46 |
| 1:6:96:ALA:HA | 1:6:156:MET:HB3 | 1.96 | 0.46 |
| 1:E:173:TYR:CZ | 1:F:166:ILE:HG12 | 2.50 | 0.46 |
| 1:K:155:GLU:O | 1:K:158:ILE:HD12 | 2.14 | 0.46 |
| 1:N:129:ARG:NH2 | 1:N:134:GLU:OE1 | 2.49 | 0.46 |
| 1:Q:92:VAL:CG1 | 1:R:139:ILE:CG2 | 2.94 | 0.46 |
| 1:2:125:ALA:O | 1:2:129:ARG:N | 2.47 | 0.46 |
| 1:4:103:TRP:HB3 | 1:4:149:PHE:CD2 | 2.51 | 0.46 |
| 1:4:155:GLU:OE1 | 1:4:170:HIS:CG | 2.69 | 0.46 |
| 1:5:138:THR:HG23 | 1:5:141:VAL:H | 1.80 | 0.46 |
| 1:K:171:ARG:O | 1:K:174:ALA:HB3 | 2.16 | 0.46 |
| 1:P:179:GLU:O | 1:Y:183:LYS:NZ | 2.48 | 0.46 |
| 1:R:178:GLN:O | 1:R:182:ASN:OD1 | 2.34 | 0.46 |
| 1:1:149:PHE:HD1 | 1:7:106:LYS:HZ2 | 1.62 | 0.46 |
| 1:A:117:ALA:O | 1:A:121:GLY:N | 2.48 | 0.46 |
| 1:C:112:SER:O | 1:C:115:LYS:HB3 | 2.15 | 0.46 |
| 1:K:154:TYR:CE1 | 1:L:159:PRO:HD3 | 2.51 | 0.46 |
| 1:5:170:HIS:O | 1:5:171:ARG:HB2 | 2.16 | 0.46 |
| 1:G:114:LYS:C | 1:G:116:VAL:N | 2.69 | 0.46 |
| 1:I:191:VAL:HG23 | 1:I:196:LYS:HB2 | 1.97 | 0.46 |
| 1:K:154:TYR:CZ | 1:L:159:PRO:HD3 | 2.50 | 0.46 |
| 1:N:112:SER:O | 1:N:116:VAL:HG13 | 2.16 | 0.46 |
| 1:N:158:ILE:HG23 | 1:N:158:ILE:O | 2.16 | 0.46 |
| 1:X:191:VAL:O | 1:X:195:ASN:OD1 | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:188:ILE:HA | 1:1:191:VAL:HG22 | 1.97 | 0.46 |
| 1:2:122:ILE:N | 1:2:122:ILE:HD12 | 2.30 | 0.46 |
| 1:5:92:VAL:HB | 1:5:93:GLU:OE1 | 2.16 | 0.46 |
| 1:7:126:THR:HB | 1:7:128:ASN:OD1 | 2.15 | 0.46 |
| 1:C:161:GLY:N | 2:C:203:HOH:O | 2.38 | 0.46 |
| 1:D:125:ALA:O | 1:D:129:ARG:HG3 | 2.16 | 0.46 |
| 1:N:115:LYS:HA | 1:N:118:VAL:HG22 | 1.96 | 0.46 |
| 1:N:127:VAL:HA | 1:N:130:ILE:HD13 | 1.97 | 0.46 |
| 1:O:185:THR:O | 1:O:188:ILE:HG12 | 2.15 | 0.46 |
| 1:2:104:MET:HG3 | 1:2:105:ARG:HG2 | 1.98 | 0.46 |
| 1:3:122:ILE:HG22 | 1:3:123:GLY:N | 2.31 | 0.46 |
| 1:6:98:ALA:N | 1:6:156:MET:HE3 | 2.30 | 0.46 |
| 1:7:103:TRP:CZ3 | 1:7:156:MET:SD | 3.09 | 0.46 |
| 1:H:117:ALA:HB1 | 1:H:122:ILE:O | 2.16 | 0.46 |
| 1:T:117:ALA:HA | 1:T:122:ILE:HG23 | 1.98 | 0.46 |
| 1:T:136:SER:HB3 | 1:U:138:THR:HB | 1.98 | 0.46 |
| 1:6:139:ILE:HD13 | 2:7:201:HOH:O | 2.15 | 0.46 |
| 1:C:114:LYS:O | 1:C:118:VAL:HG23 | 2.16 | 0.46 |
| 1:E:138:THR:HG23 | 1:F:136:SER:OG | 2.16 | 0.46 |
| 1:G:193:GLU:HA | 1:G:195:ASN:OD1 | 2.15 | 0.46 |
| 1:K:97:ALA:HB1 | 1:K:131:MET:SD | 2.56 | 0.46 |
| 1:K:120:ALA:HB2 | 1:K:127:VAL:HG12 | 1.97 | 0.46 |
| 1:2:168:TYR:CZ | 1:3:166:ILE:HD11 | 2.51 | 0.46 |
| 1:6:152:GLU:CG | 1:6:153:ALA:H | 2.29 | 0.46 |
| 1:L:116:VAL:HG21 | 1:L:127:VAL:HG21 | 1.98 | 0.45 |
| 1:Y:173:TYR:O | 1:Y:181:LYS:HE2 | 2.16 | 0.45 |
| 1:3:167:ASP:OD2 | 1:5:113:GLU:OE1 | 2.34 | 0.45 |
| 1:6:94:LYS:N | 1:6:133:ALA:CB | 2.78 | 0.45 |
| 1:G:149:PHE:HB2 | 1:G:151:HIS:HD2 | 1.81 | 0.45 |
| 1:M:157:ILE:CD1 | 1:N:154:TYR:HB3 | 2.46 | 0.45 |
| 1:G:93:GLU:HG2 | 1:G:136:SER:HA | 1.99 | 0.45 |
| 1:G:129:ARG:HB2 | 1:G:135:VAL:HG22 | 1.99 | 0.45 |
| 1:P:119:ALA:CB | 1:P:148:ALA:HB2 | 2.47 | 0.45 |
| 1:1:103:TRP:CD1 | 1:7:102:ALA:HB1 | 2.51 | 0.45 |
| 1:7:170:HIS:CD2 | 1:7:173:TYR:CD2 | 3.04 | 0.45 |
| 1:E:104:MET:HA | 1:E:110:MET:O | 2.16 | 0.45 |
| 1:P:157:ILE:HA | 2:P:201:HOH:O | 2.15 | 0.45 |
| 1:Q:92:VAL:N | 2:Q:202:HOH:O | 2.48 | 0.45 |
| 1:R:171:ARG:NH1 | 1:T:132:LYS:O | 2.50 | 0.45 |
| 1:4:187:PHE:CE2 | 1:5:184:ILE:HA | 2.50 | 0.45 |
| 1:5:146:ALA:HB1 | 1:5:151:HIS:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:6:163:PRO:HB2 | 1:7:178:GLN:OE1 | 2.16 | 0.45 |
| 1:F:162:ALA:HB1 | 1:F:165:ILE:HB | 1.99 | 0.45 |
| 1:J:129:ARG:HG2 | 1:J:134:GLU:HB2 | 1.98 | 0.45 |
| 1:Z:129:ARG:NH2 | 1:Z:134:GLU:CD | 2.70 | 0.45 |
| 1:H:190:PHE:CD1 | 1:H:190:PHE:C | 2.90 | 0.45 |
| 1:R:107:ASP:OD1 | 1:R:108:THR:N | 2.49 | 0.45 |
| 1:Y:108:THR:C | 1:Y:110:MET:H | 2.19 | 0.45 |
| 1:1:112:SER:CB | 1:1:115:LYS:HE2 | 2.46 | 0.45 |
| 1:2:110:MET:CE | 1:2:148:ALA:HB1 | 2.47 | 0.45 |
| 1:G:173:TYR:CE2 | 1:H:166:ILE:HG12 | 2.52 | 0.45 |
| 1:I:103:TRP:HH2 | 1:I:156:MET:SD | 2.39 | 0.45 |
| 1:Z:103:TRP:CZ2 | 1:Z:151:HIS:CD2 | 3.05 | 0.45 |
| 1:3:178:GLN:HA | 1:3:181:LYS:CE | 2.45 | 0.45 |
| 1:4:92:VAL:O | 1:5:139:ILE:HD13 | 2.17 | 0.45 |
| 1:6:132:LYS:H | 1:6:132:LYS:NZ | 2.15 | 0.45 |
| 1:D:101:ASN:HD21 | 1:F:160:VAL:HA | 1.81 | 0.45 |
| 1:L:116:VAL:HG11 | 1:L:127:VAL:CG2 | 2.47 | 0.45 |
| 1:W:177:PRO:O | 1:W:181:LYS:N | 2.49 | 0.45 |
| 1:Y:178:GLN:O | 1:Y:181:LYS:HB2 | 2.16 | 0.45 |
| 1:3:111:THR:HG21 | 1:5:168:TYR:HA | 1.99 | 0.45 |
| 1:3:138:THR:CG2 | 1:3:141:VAL:HG22 | 2.45 | 0.45 |
| 1:4:99:THR:HG21 | 1:4:156:MET:HB3 | 1.98 | 0.45 |
| 1:G:176:LEU:O | 1:G:181:LYS:HE3 | 2.17 | 0.45 |
| 1:H:177:PRO:O | 1:H:181:LYS:HG3 | 2.17 | 0.45 |
| 1:M:128:ASN:C | 1:M:128:ASN:OD1 | 2.55 | 0.45 |
| 1:O:195:ASN:HD21 | 1:P:175:ALA:HB2 | 1.81 | 0.45 |
| 1:P:183:LYS:O | 1:P:187:PHE:HB3 | 2.16 | 0.45 |
| 1:R:105:ARG:HA | 1:R:111:THR:HG22 | 1.98 | 0.45 |
| 1:V:116:VAL:HG23 | 1:V:117:ALA:N | 2.32 | 0.45 |
| 1:W:134:GLU:HB2 | 2:W:201:HOH:O | 2.16 | 0.45 |
| 1:6:157:ILE:HG23 | 1:7:154:TYR:HB3 | 1.97 | 0.45 |
| 1:6:161:GLY:C | 1:6:163:PRO:HD3 | 2.37 | 0.45 |
| 1:D:145:LEU:O | 1:D:148:ALA:HB3 | 2.17 | 0.45 |
| 1:F:117:ALA:HB1 | 1:F:122:ILE:O | 2.17 | 0.45 |
| 1:G:122:ILE:HD11 | 1:G:127:VAL:HG22 | 1.99 | 0.45 |
| 1:I:129:ARG:HB3 | 1:I:134:GLU:CG | 2.46 | 0.45 |
| 1:2:120:ALA:HB1 | 1:2:145:LEU:HD22 | 1.98 | 0.45 |
| 1:3:182:ASN:HA | 1:3:185:THR:HB | 1.99 | 0.45 |
| 1:G:92:VAL:N | 2:G:204:HOH:O | 2.49 | 0.44 |
| 1:L:168:TYR:O | 1:L:168:TYR:CD1 | 2.70 | 0.44 |
| 1:O:169:ASP:HB3 | 1:O:172:MET:HA | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X:164:GLY:O | 1:Y:168:TYR:HE1 | 2.01 | 0.44 |
| 1:A:102:ALA:HA | 1:A:105:ARG:HD3 | 1.99 | 0.44 |
| 1:C:104:MET:CE | 1:C:131:MET:SD | 3.05 | 0.44 |
| 1:E:185:THR:HA | 1:E:188:ILE:HD12 | 1.99 | 0.44 |
| 1:I:103:TRP:CH2 | 1:I:156:MET:SD | 3.10 | 0.44 |
| 1:X:143:SER:HA | 1:X:153:ALA:HB2 | 1.99 | 0.44 |
| 1:Y:187:PHE:O | 1:Y:190:PHE:CD1 | 2.70 | 0.44 |
| 1:Z:151:HIS:NE2 | 1:Z:170:HIS:O | 2.49 | 0.44 |
| 1:6:132:LYS:O | 1:6:133:ALA:CB | 2.64 | 0.44 |
| 1:B:112:SER:HB2 | 1:B:115:LYS:HB2 | 1.98 | 0.44 |
| 1:E:138:THR:HG22 | 1:E:141:VAL:H | 1.82 | 0.44 |
| 1:J:102:ALA:HA | 1:J:105:ARG:NH2 | 2.32 | 0.44 |
| 1:M:96:ALA:HB2 | 1:M:157:ILE:HG22 | 1.98 | 0.44 |
| 1:P:103:TRP:HB3 | 1:P:149:PHE:CD1 | 2.52 | 0.44 |
| 1:Q:92:VAL:HG13 | 1:Q:157:ILE:HG23 | 1.98 | 0.44 |
| 1:Q:146:ALA:HB2 | 1:Q:156:MET:HE2 | 2.00 | 0.44 |
| 1:U:191:VAL:C | 1:U:193:GLU:HA | 2.37 | 0.44 |
| 1:W:192:PHE:O | 1:W:196:LYS:N | 2.46 | 0.44 |
| 1:2:168:TYR:CZ | 1:2:170:HIS:CE1 | 3.06 | 0.44 |
| 1:4:141:VAL:HG12 | 1:4:145:LEU:HD23 | 1.98 | 0.44 |
| 1:K:104:MET:HG2 | 1:K:149:PHE:CZ | 2.52 | 0.44 |
| 1:Z:157:ILE:HG13 | 1:1:154:TYR:CZ | 2.52 | 0.44 |
| 1:2:104:MET:SD | 1:2:131:MET:HG2 | 2.58 | 0.44 |
| 1:2:151:HIS:CE1 | 1:2:171:ARG:HB2 | 2.53 | 0.44 |
| 1:4:113:GLU:O | 1:4:114:LYS:HD2 | 2.18 | 0.44 |
| 1:G:157:ILE:HD12 | 1:H:157:ILE:HD11 | 2.00 | 0.44 |
| 1:O:178:GLN:O | 1:O:179:GLU:C | 2.55 | 0.44 |
| 1:V:110:MET:HG2 | 1:V:116:VAL:CG1 | 2.46 | 0.44 |
| 1:V:143:SER:HA | 1:V:153:ALA:HB2 | 2.00 | 0.44 |
| 1:Z:113:GLU:O | 1:Z:116:VAL:HG12 | 2.18 | 0.44 |
| 1:B:173:TYR:CZ | 1:B:181:LYS:CD | 3.00 | 0.44 |
| 1:E:93:GLU:HG3 | 1:F:139:ILE:HD11 | 1.99 | 0.44 |
| 1:I:157:ILE:HD11 | 1:J:153:ALA:C | 2.37 | 0.44 |
| 1:Q:162:ALA:HB3 | 1:Q:165:ILE:HD12 | 1.98 | 0.44 |
| 1:4:168:TYR:OH | 1:4:170:HIS:NE2 | 2.45 | 0.44 |
| 1:4:181:LYS:O | 1:4:185:THR:OG1 | 2.28 | 0.44 |
| 1:C:189:ASN:ND2 | 1:C:193:GLU:OE2 | 2.51 | 0.44 |
| 1:4:154:TYR:CD1 | 1:5:159:PRO:HD2 | 2.53 | 0.44 |
| 1:7:184:ILE:HB | 2:7:206:HOH:O | 2.17 | 0.44 |
| 1:A:161:GLY:O | 1:A:162:ALA:C | 2.55 | 0.44 |
| 1:P:142:LEU:HD11 | 1:P:156:MET:HE2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:176:LEU:CG | 1:Z:177:PRO:HD2 | 2.39 | 0.44 |
| 1:3:93:GLU:OE1 | 1:3:93:GLU:N | 2.47 | 0.44 |
| 1:A:166:ILE:HG12 | 1:B:173:TYR:CE1 | 2.53 | 0.44 |
| 1:X:120:ALA:HB3 | 1:X:122:ILE:HG12 | 1.99 | 0.44 |
| 1:G:111:THR:OG1 | 1:G:112:SER:N | 2.50 | 0.43 |
| 1:I:122:ILE:HG21 | 1:I:145:LEU:HD11 | 1.99 | 0.43 |
| 1:P:117:ALA:HB1 | 1:P:122:ILE:O | 2.18 | 0.43 |
| 1:Q:143:SER:HA | 1:Q:153:ALA:HB2 | 1.99 | 0.43 |
| 1:W:105:ARG:CG | 1:W:105:ARG:NH1 | 2.80 | 0.43 |
| 1:6:173:TYR:HB2 | 1:6:176:LEU:HD13 | 2.00 | 0.43 |
| 1:B:169:ASP:C | 1:B:169:ASP:OD1 | 2.55 | 0.43 |
| 1:C:104:MET:HB2 | 1:C:104:MET:HE2 | 1.64 | 0.43 |
| 1:N:143:SER:CA | 1:N:153:ALA:HB2 | 2.43 | 0.43 |
| 1:N:178:GLN:OE1 | 1:N:181:LYS:CD | 2.66 | 0.43 |
| 1:P:126:THR:HG22 | 1:P:128:ASN:N | 2.33 | 0.43 |
| 1:Q:173:TYR:CZ | 1:R:166:ILE:HG12 | 2.53 | 0.43 |
| 1:V:110:MET:SD | 1:V:115:LYS:CG | 3.06 | 0.43 |
| 1:3:113:GLU:HG2 | 1:3:114:LYS:CD | 2.48 | 0.43 |
| 1:4:168:TYR:HD2 | 1:4:172:MET:HE1 | 1.83 | 0.43 |
| 1:4:168:TYR:CZ | 1:5:165:ILE:HG13 | 2.53 | 0.43 |
| 1:A:99:THR:HA | 1:A:102:ALA:HB3 | 2.00 | 0.43 |
| 1:E:101:ASN:OD1 | 1:E:131:MET:SD | 2.76 | 0.43 |
| 1:F:177:PRO:HA | 1:G:105:ARG:CZ | 2.49 | 0.43 |
| 1:G:162:ALA:N | 2:G:203:HOH:O | 2.47 | 0.43 |
| 1:O:173:TYR:CZ | 1:P:191:VAL:HG23 | 2.54 | 0.43 |
| 1:V:97:ALA:CB | 1:V:133:ALA:HB2 | 2.47 | 0.43 |
| 1:6:162:ALA:N | 1:6:163:PRO:CD | 2.80 | 0.43 |
| 1:7:170:HIS:CD2 | 1:7:171:ARG:N | 2.87 | 0.43 |
| 1:M:170:HIS:O | 1:M:170:HIS:CD2 | 2.71 | 0.43 |
| 1:O:152:GLU:O | 1:O:155:GLU:HG3 | 2.19 | 0.43 |
| 1:V:116:VAL:HG23 | 1:V:127:VAL:HG21 | 2.01 | 0.43 |
| 1:X:125:ALA:O | 1:X:129:ARG:HG2 | 2.19 | 0.43 |
| 1:2:110:MET:HE1 | 1:2:148:ALA:HB1 | 2.00 | 0.43 |
| 1:C:143:SER:O | 1:C:147:ARG:HG3 | 2.17 | 0.43 |
| 1:K:108:THR:OG1 | 1:K:109:GLU:N | 2.50 | 0.43 |
| 1:K:111:THR:OG1 | 1:K:112:SER:N | 2.48 | 0.43 |
| 1:T:173:TYR:CD1 | 1:T:173:TYR:C | 2.92 | 0.43 |
| 1:F:110:MET:SD | 1:F:116:VAL:HA | 2.58 | 0.43 |
| 1:H:180:GLU:HA | 1:H:180:GLU:OE1 | 2.19 | 0.43 |
| 1:K:114:LYS:HA | 1:K:127:VAL:HG23 | 2.00 | 0.43 |
| 1:V:98:ALA:HB2 | 1:X:163:PRO:HB3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:92:VAL:CG2 | 1:G:157:ILE:HG23 | 2.49 | 0.43 |
| 1:G:187:PHE:CD2 | 1:H:187:PHE:CD2 | 3.07 | 0.43 |
| 1:H:130:ILE:HG12 | 1:H:137:THR:OG1 | 2.19 | 0.43 |
| 1:I:96:ALA:HB2 | 1:I:157:ILE:HG22 | 2.01 | 0.43 |
| 1:Z:100:LEU:CD1 | 1:Z:156:MET:HE3 | 2.48 | 0.43 |
| 1:Z:128:ASN:OD1 | 1:Z:131:MET:CE | 2.67 | 0.43 |
| 1:H:106:LYS:O | 1:H:107:ASP:CB | 2.66 | 0.43 |
| 1:I:120:ALA:HB3 | 1:I:122:ILE:HG13 | 2.01 | 0.43 |
| 1:J:172:MET:HG3 | 1:J:175:ALA:CB | 2.47 | 0.43 |
| 1:K:183:LYS:CG | 1:K:184:ILE:N | 2.81 | 0.43 |
| 1:R:113:GLU:HG3 | 1:R:114:LYS:N | 2.33 | 0.43 |
| 1:3:95:GLN:N | 2:3:202:HOH:O | 2.52 | 0.43 |
| 1:B:125:ALA:N | 2:B:205:HOH:O | 2.47 | 0.43 |
| 1:M:127:VAL:HA | 1:M:130:ILE:HG22 | 2.00 | 0.43 |
| 1:M:182:ASN:O | 1:M:183:LYS:C | 2.56 | 0.43 |
| 1:V:122:ILE:HD12 | 1:V:141:VAL:HG22 | 2.00 | 0.43 |
| 1:V:134:GLU:CG | 1:Y:171:ARG:NH2 | 2.82 | 0.43 |
| 1:3:171:ARG:C | 1:3:173:TYR:N | 2.72 | 0.43 |
| 1:6:99:THR:HG22 | 1:6:103:TRP:CE2 | 2.54 | 0.43 |
| 1:6:162:ALA:N | 1:6:163:PRO:HD3 | 2.34 | 0.43 |
| 1:C:103:TRP:HB3 | 1:C:149:PHE:CZ | 2.54 | 0.43 |
| 1:E:176:LEU:HD21 | 1:F:192:PHE:HD1 | 1.82 | 0.43 |
| 1:N:128:ASN:ND2 | 2:N:205:HOH:O | 2.45 | 0.43 |
| 1:W:189:ASN:O | 1:W:192:PHE:HB2 | 2.19 | 0.43 |
| 1:X:164:GLY:H | 1:Y:170:HIS:CE1 | 2.37 | 0.43 |
| 1:4:136:SER:HG | 1:5:140:GLY:H | 1.63 | 0.43 |
| 1:F:130:ILE:HD13 | 1:F:145:LEU:HD11 | 2.00 | 0.42 |
| 1:O:152:GLU:HG3 | 1:P:163:PRO:HG3 | 2.01 | 0.42 |
| 1:Y:104:MET:HG3 | 2:Y:202:HOH:O | 2.19 | 0.42 |
| 1:Z:122:ILE:HG22 | 1:Z:123:GLY:H | 1.83 | 0.42 |
| 1:1:189:ASN:HA | 1:1:192:PHE:CE2 | 2.54 | 0.42 |
| 1:2:158:ILE:HD13 | 1:3:154:TYR:CG | 2.54 | 0.42 |
| 1:E:173:TYR:CZ | 1:E:181:LYS:HD2 | 2.54 | 0.42 |
| 1:M:97:ALA:CA | 1:M:131:MET:HB3 | 2.48 | 0.42 |
| 1:M:192:PHE:CZ | 1:W:186:SER:HB2 | 2.54 | 0.42 |
| 1:N:107:ASP:O | 1:N:110:MET:HG3 | 2.19 | 0.42 |
| 1:N:147:ARG:NH2 | 1:N:152:GLU:OE1 | 2.51 | 0.42 |
| 1:N:178:GLN:O | 1:N:181:LYS:HD3 | 2.19 | 0.42 |
| 1:R:97:ALA:O | 1:R:101:ASN:ND2 | 2.52 | 0.42 |
| 1:R:171:ARG:NE | 2:R:204:HOH:O | 2.51 | 0.42 |
| 1:V:183:LYS:NZ | 2:V:204:HOH:O | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2:184:ILE:HG12 | 1:3:187:PHE:HE2 | 1.84 | 0.42 |
| 1:D:101:ASN:ND2 | 1:F:160:VAL:HA | 2.33 | 0.42 |
| 1:G:111:THR:HG23 | 1:G:116:VAL:CG1 | 2.49 | 0.42 |
| 1:I:187:PHE:CE2 | 1:I:190:PHE:CG | 3.08 | 0.42 |
| 1:M:128:ASN:OD1 | 1:M:129:ARG:HG3 | 2.18 | 0.42 |
| 1:V:132:LYS:O | 1:V:133:ALA:HB3 | 2.19 | 0.42 |
| 1:6:157:ILE:HG23 | 1:7:154:TYR:HB2 | 2.00 | 0.42 |
| 1:B:108:THR:C | 1:B:110:MET:H | 2.22 | 0.42 |
| 1:D:111:THR:OG1 | 1:F:167:ASP:OD2 | 2.34 | 0.42 |
| 1:H:186:SER:HA | 1:H:189:ASN:HB2 | 2.01 | 0.42 |
| 1:Q:153:ALA:HA | 1:Q:156:MET:HE2 | 2.01 | 0.42 |
| 1:2:97:ALA:O | 1:2:101:ASN:ND2 | 2.52 | 0.42 |
| 1:3:158:ILE:HG13 | 1:3:158:ILE:O | 2.19 | 0.42 |
| 1:G:95:GLN:HG3 | 1:G:156:MET:O | 2.19 | 0.42 |
| 1:M:192:PHE:HZ | 1:W:186:SER:HB2 | 1.83 | 0.42 |
| 1:N:152:GLU:HB3 | 1:N:155:GLU:HG3 | 2.02 | 0.42 |
| 1:Z:93:GLU:OE1 | 1:Z:93:GLU:N | 2.39 | 0.42 |
| 1:Z:126:THR:N | 1:Z:127:VAL:HG22 | 2.35 | 0.42 |
| 1:2:173:TYR:OH | 1:3:166:ILE:HG23 | 2.19 | 0.42 |
| 1:6:136:SER:OG | 1:7:140:GLY:N | 2.51 | 0.42 |
| 1:A:142:LEU:HA | 2:A:208:HOH:O | 2.19 | 0.42 |
| 1:K:105:ARG:HA | 1:K:107:ASP:HB2 | 2.01 | 0.42 |
| 1:K:145:LEU:C | 1:K:145:LEU:HD23 | 2.39 | 0.42 |
| 1:M:97:ALA:CB | 1:M:131:MET:HB3 | 2.50 | 0.42 |
| 1:W:122:ILE:HD11 | 1:W:126:THR:HB | 2.02 | 0.42 |
| 1:Z:100:LEU:HD11 | 1:Z:156:MET:HE3 | 2.01 | 0.42 |
| 1:2:139:ILE:HD11 | 1:3:142:LEU:HD22 | 2.02 | 0.42 |
| 1:3:160:VAL:HG13 | 1:5:131:MET:O | 2.19 | 0.42 |
| 1:6:168:TYR:OH | 1:7:166:ILE:HD11 | 2.20 | 0.42 |
| 1:A:195:ASN:ND2 | 1:B:180:GLU:OE2 | 2.50 | 0.42 |
| 1:I:158:ILE:HG22 | 1:J:154:TYR:CG | 2.54 | 0.42 |
| 1:N:94:LYS:HD2 | 1:N:94:LYS:N | 2.34 | 0.42 |
| 1:T:173:TYR:HB2 | 1:U:192:PHE:HZ | 1.84 | 0.42 |
| 1:F:130:ILE:HG12 | 1:F:137:THR:HG21 | 2.00 | 0.42 |
| 1:I:154:TYR:HB3 | 1:J:158:ILE:HA | 2.02 | 0.42 |
| 1:I:157:ILE:CD1 | 1:J:153:ALA:HB3 | 2.50 | 0.42 |
| 1:I:187:PHE:CE2 | 1:I:190:PHE:CD1 | 3.08 | 0.42 |
| 1:L:188:ILE:O | 1:L:191:VAL:HG22 | 2.19 | 0.42 |
| 1:O:137:THR:HG22 | 1:O:138:THR:N | 2.35 | 0.42 |
| 1:X:187:PHE:O | 1:X:191:VAL:HG23 | 2.19 | 0.42 |
| 1:Z:97:ALA:HB2 | 1:Z:133:ALA:CB | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z:171:ARG:HG3 | 1:1:164:GLY:CA | 2.37 | 0.42 |
| 1:6:171:ARG:O | 1:6:172:MET:C | 2.57 | 0.42 |
| 1:7:112:SER:O | 1:7:115:LYS:HG3 | 2.19 | 0.42 |
| 1:H:176:LEU:O | 1:H:181:LYS:NZ | 2.49 | 0.42 |
| 1:O:103:TRP:HB3 | 1:O:149:PHE:CE2 | 2.55 | 0.42 |
| 1:1:160:VAL:HG11 | 1:7:97:ALA:CB | 2.49 | 0.42 |
| 1:2:96:ALA:CB | 1:2:100:LEU:HD23 | 2.44 | 0.42 |
| 1:7:162:ALA:HB1 | 1:7:163:PRO:CA | 2.42 | 0.42 |
| 1:G:122:ILE:CD1 | 1:G:145:LEU:HD21 | 2.49 | 0.42 |
| 1:H:110:MET:HB3 | 1:H:115:LYS:HG3 | 2.00 | 0.42 |
| 1:K:162:ALA:HB1 | 1:K:163:PRO:HD2 | 2.02 | 0.42 |
| 1:M:97:ALA:HB2 | 1:M:131:MET:C | 2.41 | 0.42 |
| 1:P:116:VAL:HG12 | 1:P:145:LEU:HD11 | 2.01 | 0.42 |
| 1:2:104:MET:CG | 1:2:105:ARG:N | 2.83 | 0.42 |
| 1:3:100:LEU:HD13 | 1:3:145:LEU:HD23 | 2.02 | 0.42 |
| 1:5:115:LYS:HA | 1:5:118:VAL:HG22 | 2.01 | 0.42 |
| 1:F:92:VAL:N | 2:F:206:HOH:O | 2.52 | 0.41 |
| 1:O:174:ALA:O | 1:O:181:LYS:CE | 2.67 | 0.41 |
| 1:1:184:ILE:O | 1:1:188:ILE:HG12 | 2.20 | 0.41 |
| 1:3:157:ILE:HG22 | 1:3:157:ILE:O | 2.20 | 0.41 |
| 1:6:103:TRP:CZ2 | 1:6:151:HIS:ND1 | 2.86 | 0.41 |
| 1:B:112:SER:N | 2:B:206:HOH:O | 2.54 | 0.41 |
| 1:G:111:THR:CG2 | 1:G:116:VAL:HG12 | 2.50 | 0.41 |
| 1:G:136:SER:HB2 | 1:H:138:THR:CG2 | 2.50 | 0.41 |
| 1:G:148:ALA:N | 2:G:207:HOH:O | 2.53 | 0.41 |
| 1:R:194:GLN:NE2 | 1:Z:183:LYS:HD3 | 2.35 | 0.41 |
| 1:2:122:ILE:HD11 | 1:2:145:LEU:HD21 | 2.03 | 0.41 |
| 1:C:164:GLY:HA3 | 1:D:170:HIS:HB3 | 2.02 | 0.41 |
| 1:I:157:ILE:HG12 | 1:J:157:ILE:HD11 | 2.02 | 0.41 |
| 1:I:168:TYR:CE1 | 1:J:166:ILE:HD12 | 2.55 | 0.41 |
| 1:K:174:ALA:HB2 | 1:L:163:PRO:CB | 2.50 | 0.41 |
| 1:M:103:TRP:CZ3 | 1:M:156:MET:HG2 | 2.55 | 0.41 |
| 1:N:182:ASN:HB3 | 1:N:186:SER:CA | 2.51 | 0.41 |
| 1:Z:94:LYS:O | 1:Z:97:ALA:N | 2.52 | 0.41 |
| 1:Z:169:ASP:OD1 | 1:Z:170:HIS:N | 2.53 | 0.41 |
| 1:1:105:ARG:NH1 | 2:1:204:HOH:O | 2.53 | 0.41 |
| 1:4:142:LEU:HD23 | 1:4:153:ALA:HB1 | 2.01 | 0.41 |
| 1:J:162:ALA:O | 1:J:165:ILE:HG12 | 2.19 | 0.41 |
| 1:K:159:PRO:O | 1:K:165:ILE:CD1 | 2.69 | 0.41 |
| 1:P:97:ALA:HB2 | 1:P:131:MET:O | 2.20 | 0.41 |
| 1:U:155:GLU:HA | 1:U:158:ILE:CD1 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:113:GLU:HG2 | 1:D:131:MET:HE1 | 2.01 | 0.41 |
| 1:X:164:GLY:C | 1:Y:170:HIS:CD2 | 2.93 | 0.41 |
| 1:4:173:TYR:CD2 | 1:4:176:LEU:HB2 | 2.55 | 0.41 |
| 1:C:92:VAL:N | 2:C:205:HOH:O | 2.52 | 0.41 |
| 1:1:117:ALA:O | 1:1:121:GLY:N | 2.54 | 0.41 |
| 1:4:138:THR:HA | 1:5:138:THR:HA | 2.03 | 0.41 |
| 1:4:173:TYR:OH | 1:4:180:GLU:CD | 2.59 | 0.41 |
| 1:4:191:VAL:HG23 | 1:4:191:VAL:O | 2.20 | 0.41 |
| 1:B:167:ASP:O | 1:B:168:TYR:HB3 | 2.20 | 0.41 |
| 1:N:103:TRP:CZ3 | 1:N:156:MET:HG2 | 2.55 | 0.41 |
| 1:O:152:GLU:O | 1:O:154:TYR:N | 2.54 | 0.41 |
| 1:X:117:ALA:HB1 | 2:X:202:HOH:O | 2.19 | 0.41 |
| 1:Z:138:THR:HG21 | 2:1:201:HOH:O | 2.20 | 0.41 |
| 1:5:117:ALA:CB | 1:5:127:VAL:HG21 | 2.49 | 0.41 |
| 1:E:143:SER:HA | 1:E:153:ALA:HB2 | 2.03 | 0.41 |
| 1:G:136:SER:HB2 | 1:H:138:THR:HG23 | 2.01 | 0.41 |
| 1:J:124:PRO:C | 1:J:126:THR:H | 2.23 | 0.41 |
| 1:P:158:ILE:O | 1:P:158:ILE:HG13 | 2.21 | 0.41 |
| 1:Q:187:PHE:HA | 1:Q:190:PHE:HD2 | 1.74 | 0.41 |
| 1:V:110:MET:HG2 | 1:V:116:VAL:HG13 | 2.02 | 0.41 |
| 1:7:183:LYS:O | 1:7:187:PHE:HB3 | 2.20 | 0.41 |
| 1:B:171:ARG:HG2 | 1:B:172:MET:N | 2.36 | 0.41 |
| 1:C:176:LEU:HB3 | 1:C:180:GLU:CD | 2.38 | 0.41 |
| 1:D:173:TYR:CE1 | 1:D:181:LYS:HG2 | 2.56 | 0.41 |
| 1:L:173:TYR:HA | 1:L:176:LEU:HG | 2.03 | 0.41 |
| 1:O:176:LEU:HD12 | 1:O:181:LYS:HZ3 | 1.85 | 0.41 |
| 1:P:170:HIS:O | 1:P:171:ARG:C | 2.58 | 0.41 |
| 1:R:173:TYR:CE1 | 1:R:181:LYS:HG3 | 2.56 | 0.41 |
| 1:U:110:MET:HG3 | 1:U:116:VAL:HG22 | 2.03 | 0.41 |
| 1:W:185:THR:O | 1:W:189:ASN:ND2 | 2.53 | 0.41 |
| 1:X:110:MET:HG3 | 1:X:111:THR:H | 1.84 | 0.41 |
| 1:X:142:LEU:HA | 1:X:145:LEU:HB2 | 2.02 | 0.41 |
| 1:Z:169:ASP:O | 1:Z:172:MET:N | 2.45 | 0.41 |
| 1:2:116:VAL:O | 1:2:121:GLY:N | 2.53 | 0.41 |
| 1:4:103:TRP:CH2 | 1:4:156:MET:CG | 3.04 | 0.41 |
| 1:C:122:ILE:HG21 | 1:C:126:THR:HG21 | 2.03 | 0.41 |
| 1:M:172:MET:O | 1:M:181:LYS:NZ | 2.51 | 0.41 |
| 1:Z:139:ILE:HG21 | 1:1:142:LEU:HD23 | 2.03 | 0.41 |
| 1:4:168:TYR:CE2 | 1:4:170:HIS:CD2 | 3.08 | 0.41 |
| 1:7:145:LEU:O | 1:7:149:PHE:N | 2.52 | 0.41 |
| 1:B:169:ASP:CG | 1:B:172:MET:HG2 | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:180:GLU:HA | 1:B:183:LYS:HE2 | 2.02 | 0.40 |
| 1:E:190:PHE:CZ | 1:5:190:PHE:HA | 2.56 | 0.40 |
| 1:F:187:PHE:CE1 | 1:F:191:VAL:HG11 | 2.56 | 0.40 |
| 1:U:142:LEU:HD23 | 1:U:153:ALA:HB1 | 2.03 | 0.40 |
| 1:V:113:GLU:OE2 | 1:V:125:ALA:HA | 2.21 | 0.40 |
| 1:Z:176:LEU:HD12 | 1:Z:177:PRO:HD3 | 2.03 | 0.40 |
| 1:4:93:GLU:HG3 | 1:5:139:ILE:HD11 | 2.03 | 0.40 |
| 1:B:122:ILE:HG22 | 1:B:123:GLY:N | 2.34 | 0.40 |
| 1:E:154:TYR:OH | 1:F:165:ILE:HD11 | 2.21 | 0.40 |
| 1:M:182:ASN:C | 1:M:184:ILE:N | 2.74 | 0.40 |
| 1:N:165:ILE:HG22 | 1:N:166:ILE:H | 1.84 | 0.40 |
| 1:N:192:PHE:O | 1:N:193:GLU:CB | 2.65 | 0.40 |
| 1:X:178:GLN:CD | 1:X:178:GLN:N | 2.74 | 0.40 |
| 1:Y:132:LYS:NZ | 2:Y:204:HOH:O | 2.53 | 0.40 |
| 1:Z:111:THR:HG22 | 1:Z:112:SER:H | 1.87 | 0.40 |
| 1:4:122:ILE:HG22 | 1:4:126:THR:OG1 | 2.20 | 0.40 |
| 1:6:176:LEU:HG | 1:6:180:GLU:HG3 | 2.04 | 0.40 |
| 1:B:184:ILE:O | 1:B:188:ILE:HG12 | 2.21 | 0.40 |
| 1:C:107:ASP:HA | 1:C:110:MET:HG2 | 2.02 | 0.40 |
| 1:H:189:ASN:CA | 1:H:191:VAL:HG23 | 2.49 | 0.40 |
| 1:V:110:MET:HE3 | 1:V:112:SER:N | 2.34 | 0.40 |
| 1:W:111:THR:HG21 | 2:W:208:HOH:O | 2.21 | 0.40 |
| 1:3:100:LEU:HD22 | 1:3:130:ILE:HG22 | 2.03 | 0.40 |
| 1:3:165:ILE:HG23 | 1:3:166:ILE:N | 2.36 | 0.40 |
| 1:3:188:ILE:O | 1:3:191:VAL:HG23 | 2.21 | 0.40 |
| 1:4:92:VAL:HG13 | 1:4:93:GLU:N | 2.37 | 0.40 |
| 1:5:171:ARG:CG | 1:5:172:MET:N | 2.77 | 0.40 |
| 1:6:181:LYS:HE2 | 1:7:166:ILE:HG21 | 2.04 | 0.40 |
| 1:O:183:LYS:HA | 1:O:186:SER:HB3 | 2.02 | 0.40 |
| 1:Q:146:ALA:HB2 | 1:Q:156:MET:CE | 2.51 | 0.40 |
| 1:U:179:GLU:O | 1:U:183:LYS:N | 2.52 | 0.40 |
| 1:1:95:GLN:OE1 | 1:1:159:PRO:HA | 2.21 | 0.40 |
| 1:1:130:ILE:CD1 | 1:1:141:VAL:HG11 | 2.51 | 0.40 |
| 1:6:142:LEU:HD13 | 1:6:155:GLU:HG3 | 2.02 | 0.40 |
| 1:F:162:ALA:N | 1:F:163:PRO:CD | 2.85 | 0.40 |
| 1:M:106:LYS:HG2 | 1:M:107:ASP:H | 1.87 | 0.40 |
| 1:M:107:ASP:OD1 | 1:M:107:ASP:N | 2.55 | 0.40 |
| 1:N:153:ALA:C | 1:N:155:GLU:H | 2.25 | 0.40 |
| 1:N:157:ILE:HG22 | 2:N:201:HOH:O | 2.21 | 0.40 |
| 1:Z:173:TYR:O | 1:Z:174:ALA:C | 2.59 | 0.40 |
| 1:1:92:VAL:HG13 | 1:1:93:GLU:H | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2:155:GLU:O | 1:2:158:ILE:HG22 | 2.22 | 0.40 |
| 1:4:145:LEU:HD12 | 1:4:146:ALA:N | 2.35 | 0.40 |
| 1:5:164:GLY:O | 1:5:165:ILE:CB | 2.70 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:167:ASP:OD1 | 1:Y:111:THR:O[1_465] | 2.04 | 0.16 |
| 1:I:133:ALA:O | 1:L:147:ARG:NH1[1_455] | 2.12 | 0.08 |

## 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 | 1 | 103/107 (96%) | 92 (89%) | 9 (9%) | 2 (2%) | 8 | 33 |
| 1 | 2 | 99/107 (92%) | 85 (86%) | 13 (13%) | 1 (1%) | 15 | 50 |
| 1 | 3 | 98/107 (92%) | 88 (90%) | 6 (6%) | 4 (4%) | 3 | 14 |
| 1 | 4 | 98/107 (92%) | 81 (83%) | 15 (15%) | 2 (2%) | 7 | 32 |
| 1 | 5 | 98/107 (92%) | 85 (87%) | 10 (10%) | 3 (3%) | 4 | 20 |
| 1 | 6 | 99/107 (92%) | 73 (74%) | 17 (17%) | 9 (9%) | 1 | 3 |
| 1 | 7 | 103/107 (96%) | 79 (77%) | 19 (18%) | 5 (5%) | 2 | 11 |
| 1 | A | 103/107 (96%) | 98 (95%) | 5 (5%) | 0 | 100 | 100 |
| 1 | B | 103/107 (96%) | 95 (92%) | 7 (7%) | 1 (1%) | 15 | 50 |
| 1 | C | 103/107 (96%) | 95 (92%) | 7 (7%) | 1 (1%) | 15 | 50 |
| 1 | D | 99/107 (92%) | 93 (94%) | 6 (6%) | 0 | 100 | 100 |
| 1 | E | 103/107 (96%) | 98 (95%) | 5 (5%) | 0 | 100 | 100 |
| 1 | F | 103/107 (96%) | 101 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | G | 103/107 (96%) | 96 (93%) | 7 (7%) | 0 | 100 | 100 |
| 1 | H | 100/107 (94%) | 94 (94%) | 4 (4%) | 2 (2%) | 7 | 32 |
| 1 | I | 103/107 (96%) | 87 (84%) | 11 (11%) | 5 (5%) | 2 | 11 |
| 1 | J | 101/107 (94%) | 89 (88%) | 11 (11%) | 1 (1%) | 15 | 50 |
| 1 | K | 103/107 (96%) | 84 (82%) | 13 (13%) | 6 (6%) | 1 | 8 |
| 1 | L | 103/107 (96%) | 90 (87%) | 11 (11%) | 2 (2%) | 8 | 33 |
| 1 | M | 103/107 (96%) | 80 (78%) | 21 (20%) | 2 (2%) | 8 | 33 |
| 1 | N | 100/107 (94%) | 85 (85%) | 11 (11%) | 4 (4%) | 3 | 15 |
| 1 | O | 103/107 (96%) | 86 (84%) | 13 (13%) | 4 (4%) | 3 | 15 |
| 1 | P | 98/107 (92%) | 82 (84%) | 10 (10%) | 6 (6%) | 1 | 7 |
| 1 | Q | 103/107 (96%) | 98 (95%) | 5 (5%) | 0 | 100 | 100 |
| 1 | R | 103/107 (96%) | 99 (96%) | 3 (3%) | 1 (1%) | 15 | 50 |
| 1 | T | 103/107 (96%) | 97 (94%) | 5 (5%) | 1 (1%) | 15 | 50 |
| 1 | U | 101/107 (94%) | 98 (97%) | 3 (3%) | 0 | 100 | 100 |
| 1 | V | 103/107 (96%) | 97 (94%) | 6 (6%) | 0 | 100 | 100 |
| 1 | W | 103/107 (96%) | 100 (97%) | 3 (3%) | 0 | 100 | 100 |
| 1 | X | 103/107 (96%) | 96 (93%) | 6 (6%) | 1 (1%) | 15 | 50 |
| 1 | Y | 103/107 (96%) | 90 (87%) | 12 (12%) | 1 (1%) | 15 | 50 |
| 1 | Z | 98/107 (92%) | 82 (84%) | 13 (13%) | 3 (3%) | 4 | 20 |
| All | All | 3249/3424 (95%) | 2893 (89%) | 289 (9%) | 67 (2%) | 7 | 30 |

All (67) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 115 | LYS |
| 1 | I | 190 | PHE |
| 1 | N | 110 | MET |
| 1 | N | 165 | ILE |
| 1 | P | 112 | SER |
| 1 | 5 | 165 | ILE |
| 1 | B | 107 | ASP |
| 1 | H | 191 | VAL |
| 1 | I | 116 | VAL |
| 1 | I | 135 | VAL |
| 1 | I | 188 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 153 | ALA |
| 1 | K | 160 | VAL |
| 1 | N | 172 | MET |
| 1 | O | 108 | THR |
| 1 | O | 109 | GLU |
| 1 | O | 153 | ALA |
| 1 | O | 155 | GLU |
| 1 | P | 111 | THR |
| 1 | X | 111 | THR |
| 1 | Z | 170 | HIS |
| 1 | 3 | 172 | MET |
| 1 | 4 | 160 | VAL |
| 1 | 5 | 174 | ALA |
| 1 | 6 | 133 | ALA |
| 1 | 7 | 110 | MET |
| 1 | 7 | 173 | TYR |
| 1 | H | 109 | GLU |
| 1 | K | 114 | LYS |
| 1 | M | 171 | ARG |
| 1 | P | 110 | MET |
| 1 | P | 190 | PHE |
| 1 | R | 111 | THR |
| 1 | Z | 190 | PHE |
| 1 | 1 | 160 | VAL |
| 1 | 3 | 162 | ALA |
| 1 | 6 | 96 | ALA |
| 1 | 6 | 98 | ALA |
| 1 | 6 | 108 | THR |
| 1 | 6 | 152 | GLU |
| 1 | 6 | 170 | HIS |
| 1 | 7 | 168 | TYR |
| 1 | L | 166 | ILE |
| 1 | M | 114 | LYS |
| 1 | P | 153 | ALA |
| 1 | T | 124 | PRO |
| 1 | Z | 127 | VAL |
| 1 | 3 | 123 | GLY |
| 1 | 3 | 173 | TYR |
| 1 | 5 | 172 | MET |
| 1 | 7 | 128 | ASN |
| 1 | C | 177 | PRO |
| 1 | K | 113 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 133 | ALA |
| 1 | L | 107 | ASP |
| 1 | N | 143 | SER |
| 1 | 2 | 110 | MET |
| 1 | 6 | 163 | PRO |
| 1 | 6 | 177 | PRO |
| 1 | 6 | 191 | VAL |
| 1 | Y | 160 | VAL |
| 1 | 1 | 177 | PRO |
| 1 | J | 124 | PRO |
| 1 | P | 160 | VAL |
| 1 | K | 184 | ILE |
| 1 | 4 | 177 | PRO |
| 1 | 7 | 163 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 1 | 84/86 (98%) | 82 (98%) | 2 (2%) | 49 | 78 |
| 1 | 2 | 80/86 (93%) | 75 (94%) | 5 (6%) | 18 | 49 |
| 1 | 3 | 79/86 (92%) | 76 (96%) | 3 (4%) | 33 | 67 |
| 1 | 4 | 79/86 (92%) | 75 (95%) | 4 (5%) | 24 | 57 |
| 1 | 5 | 79/86 (92%) | 75 (95%) | 4 (5%) | 24 | 57 |
| 1 | 6 | 80/86 (93%) | 73 (91%) | 7 (9%) | 10 | 34 |
| 1 | 7 | 84/86 (98%) | 80 (95%) | 4 (5%) | 25 | 60 |
| 1 | A | 84/86 (98%) | 81 (96%) | 3 (4%) | 35 | 68 |
| 1 | B | 84/86 (98%) | 80 (95%) | 4 (5%) | 25 | 60 |
| 1 | C | 84/86 (98%) | 77 (92%) | 7 (8%) | 11 | 37 |
| 1 | D | 80/86 (93%) | 78 (98%) | 2 (2%) | 47 | 77 |
| 1 | E | 84/86 (98%) | 82 (98%) | 2 (2%) | 49 | 78 |
| 1 | F | 84/86 (98%) | 84 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | G | 84/86 (98%) | 79 (94%) | 5 (6%) | 19 | 51 |
| 1 | H | 81/86 (94%) | 79 (98%) | 2 (2%) | 47 | 77 |
| 1 | I | 84/86 (98%) | 80 (95%) | 4 (5%) | 25 | 60 |
| 1 | J | 82/86 (95%) | 77 (94%) | 5 (6%) | 18 | 51 |
| 1 | K | 84/86 (98%) | 79 (94%) | 5 (6%) | 19 | 51 |
| 1 | L | 84/86 (98%) | 78 (93%) | 6 (7%) | 14 | 44 |
| 1 | M | 84/86 (98%) | 75 (89%) | 9 (11%) | 6 | 24 |
| 1 | N | 81/86 (94%) | 76 (94%) | 5 (6%) | 18 | 50 |
| 1 | O | 84/86 (98%) | 76 (90%) | 8 (10%) | 8 | 30 |
| 1 | P | 79/86 (92%) | 75 (95%) | 4 (5%) | 24 | 57 |
| 1 | Q | 84/86 (98%) | 80 (95%) | 4 (5%) | 25 | 60 |
| 1 | R | 84/86 (98%) | 82 (98%) | 2 (2%) | 49 | 78 |
| 1 | T | 84/86 (98%) | 81 (96%) | 3 (4%) | 35 | 68 |
| 1 | U | 82/86 (95%) | 80 (98%) | 2 (2%) | 49 | 78 |
| 1 | V | 84/86 (98%) | 83 (99%) | 1 (1%) | 71 | 89 |
| 1 | W | 84/86 (98%) | 82 (98%) | 2 (2%) | 49 | 78 |
| 1 | X | 84/86 (98%) | 78 (93%) | 6 (7%) | 14 | 44 |
| 1 | Y | 84/86 (98%) | 82 (98%) | 2 (2%) | 49 | 78 |
| 1 | Z | 79/86 (92%) | 71 (90%) | 8 (10%) | 7 | 27 |
| All | All | 2641/2752 (96%) | 2511 (95%) | 130 (5%) | 25 | 59 |

All (130) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 113 | GLU |
| 1 | A | 136 | SER |
| 1 | A | 193 | GLU |
| 1 | B | 105 | ARG |
| 1 | B | 171 | ARG |
| 1 | B | 182 | ASN |
| 1 | B | 185 | THR |
| 1 | C | 99 | THR |
| 1 | C | 114 | LYS |
| 1 | C | 115 | LYS |
| 1 | C | 122 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 176 | LEU |
| 1 | C | 180 | GLU |
| 1 | C | 195 | ASN |
| 1 | D | 170 | HIS |
| 1 | D | 185 | THR |
| 1 | E | 138 | THR |
| 1 | E | 167 | ASP |
| 1 | G | 110 | MET |
| 1 | G | 111 | THR |
| 1 | G | 127 | VAL |
| 1 | G | 147 | ARG |
| 1 | G | 149 | PHE |
| 1 | H | 171 | ARG |
| 1 | H | 178 | GLN |
| 1 | I | 114 | LYS |
| 1 | I | 115 | LYS |
| 1 | I | 127 | VAL |
| 1 | I | 178 | GLN |
| 1 | J | 95 | GLN |
| 1 | J | 110 | MET |
| 1 | J | 142 | LEU |
| 1 | J | 154 | TYR |
| 1 | J | 176 | LEU |
| 1 | K | 105 | ARG |
| 1 | K | 114 | LYS |
| 1 | K | 130 | ILE |
| 1 | K | 132 | LYS |
| 1 | K | 189 | ASN |
| 1 | L | 93 | GLU |
| 1 | L | 138 | THR |
| 1 | L | 145 | LEU |
| 1 | L | 152 | GLU |
| 1 | L | 179 | GLU |
| 1 | L | 193 | GLU |
| 1 | M | 94 | LYS |
| 1 | M | 107 | ASP |
| 1 | M | 110 | MET |
| 1 | M | 118 | VAL |
| 1 | M | 128 | ASN |
| 1 | M | 173 | TYR |
| 1 | M | 176 | LEU |
| 1 | M | 182 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 192 | PHE |
| 1 | N | 113 | GLU |
| 1 | N | 151 | HIS |
| 1 | N | 171 | ARG |
| 1 | N | 176 | LEU |
| 1 | N | 178 | GLN |
| 1 | O | 94 | LYS |
| 1 | O | 109 | GLU |
| 1 | O | 151 | HIS |
| 1 | O | 152 | GLU |
| 1 | O | 170 | HIS |
| 1 | O | 171 | ARG |
| 1 | O | 190 | PHE |
| 1 | O | 194 | GLN |
| 1 | P | 93 | GLU |
| 1 | P | 110 | MET |
| 1 | P | 111 | THR |
| 1 | P | 115 | LYS |
| 1 | Q | 92 | VAL |
| 1 | Q | 157 | ILE |
| 1 | Q | 176 | LEU |
| 1 | Q | 180 | GLU |
| 1 | R | 136 | SER |
| 1 | R | 167 | ASP |
| 1 | T | 101 | ASN |
| 1 | T | 111 | THR |
| 1 | T | 136 | SER |
| 1 | U | 107 | ASP |
| 1 | U | 178 | GLN |
| 1 | V | 115 | LYS |
| 1 | W | 178 | GLN |
| 1 | W | 185 | THR |
| 1 | X | 110 | MET |
| 1 | X | 111 | THR |
| 1 | X | 115 | LYS |
| 1 | X | 166 | ILE |
| 1 | X | 172 | MET |
| 1 | X | 196 | LYS |
| 1 | Y | 94 | LYS |
| 1 | Y | 176 | LEU |
| 1 | Z | 111 | THR |
| 1 | Z | 129 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Z | 134 | GLU |
| 1 | Z | 156 | MET |
| 1 | Z | 158 | ILE |
| 1 | Z | 167 | ASP |
| 1 | Z | 184 | ILE |
| 1 | Z | 191 | VAL |
| 1 | 1 | 107 | ASP |
| 1 | 1 | 179 | GLU |
| 1 | 2 | 100 | LEU |
| 1 | 2 | 105 | ARG |
| 1 | 2 | 110 | MET |
| 1 | 2 | 122 | ILE |
| 1 | 2 | 135 | VAL |
| 1 | 3 | 122 | ILE |
| 1 | 3 | 141 | VAL |
| 1 | 3 | 172 | MET |
| 1 | 4 | 104 | MET |
| 1 | 4 | 129 | ARG |
| 1 | 4 | 170 | HIS |
| 1 | 4 | 190 | PHE |
| 1 | 5 | 130 | ILE |
| 1 | 5 | 171 | ARG |
| 1 | 5 | 172 | MET |
| 1 | 5 | 173 | TYR |
| 1 | 6 | 92 | VAL |
| 1 | 6 | 132 | LYS |
| 1 | 6 | 136 | SER |
| 1 | 6 | 147 | ARG |
| 1 | 6 | 156 | MET |
| 1 | 6 | 169 | ASP |
| 1 | 6 | 170 | HIS |
| 1 | 7 | 101 | ASN |
| 1 | 7 | 106 | LYS |
| 1 | 7 | 122 | ILE |
| 1 | 7 | 170 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 101 | ASN |
| 1 | G | 128 | ASN |
| 1 | G | 151 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 194 | GLN |
| 1 | I | 178 | GLN |
| 1 | J | 182 | ASN |
| 1 | K | 189 | ASN |
| 1 | O | 95 | GLN |
| 1 | O | 128 | ASN |
| 1 | O | 151 | HIS |
| 1 | O | 170 | HIS |
| 1 | O | 195 | ASN |
| 1 | Q | 182 | ASN |
| 1 | R | 194 | GLN |
| 1 | T | 182 | ASN |
| 1 | T | 195 | ASN |
| 1 | U | 182 | ASN |
| 1 | W | 101 | ASN |
| 1 | X | 195 | ASN |
| 1 | Y | 195 | ASN |
| 1 | Z | 95 | GLN |
| 1 | Z | 178 | GLN |
| 1 | Z | 182 | ASN |
| 1 | 2 | 182 | ASN |
| 1 | 4 | 95 | GLN |
| 1 | 4 | 128 | ASN |
| 1 | 5 | 170 | HIS |
| 1 | 6 | 170 | HIS |
| 1 | 7 | 101 | ASN |
| 1 | 7 | 170 | 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

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

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 105/107 (98%) | 0.12 | 3 (2%) | 51 | 32 | 47, 87, 110, 116 | 0 |
| 1 | 2 | 101/107 (94%) | 0.47 | 9 (8%) | 9 | 5 | 61, 99, 133, 140 | 0 |
| 1 | 3 | 100/107 (93%) | 0.20 | 2 (2%) | 65 | 45 | 41, 83, 111, 139 | 0 |
| 1 | 4 | 100/107 (93%) | 0.66 | 18 (18%) | 1 | 1 | 64, 100, 138, 150 | 0 |
| 1 | 5 | 100/107 (93%) | 0.40 | 7 (7%) | 16 | 8 | 54, 94, 122, 139 | 0 |
| 1 | 6 | 101/107 (94%) | 0.92 | 18 (17%) | 1 | 1 | 55, 111, 136, 154 | 0 |
| 1 | 7 | 105/107 (98%) | 0.53 | 15 (14%) | 2 | 1 | 63, 99, 124, 129 | 0 |
| 1 | A | 105/107 (98%) | -0.07 | 2 (1%) | 66 | 46 | 33, 64, 96, 105 | 0 |
| 1 | B | 105/107 (98%) | -0.01 | 1 (0%) | 82 | 66 | 31, 54, 87, 99 | 0 |
| 1 | C | 105/107 (98%) | -0.08 | 2 (1%) | 66 | 46 | 34, 60, 92, 117 | 0 |
| 1 | D | 101/107 (94%) | -0.20 | 0 | 100 | 100 | 33, 49, 69, 79 | 0 |
| 1 | E | 105/107 (98%) | -0.16 | 0 | 100 | 100 | 37, 60, 84, 102 | 0 |
| 1 | F | 105/107 (98%) | -0.26 | 2 (1%) | 66 | 46 | 24, 46, 72, 83 | 0 |
| 1 | G | 105/107 (98%) | -0.17 | 1 (0%) | 82 | 66 | 35, 63, 116, 127 | 0 |
| 1 | H | 102/107 (95%) | -0.20 | 1 (0%) | 82 | 66 | 30, 52, 76, 85 | 0 |
| 1 | I | 105/107 (98%) | 0.52 | 7 (6%) | 17 | 9 | 60, 100, 126, 137 | 0 |
| 1 | J | 103/107 (96%) | 0.13 | 2 (1%) | 66 | 46 | 62, 89, 121, 134 | 0 |
| 1 | K | 105/107 (98%) | 0.48 | 11 (10%) | 6 | 3 | 69, 105, 132, 158 | 0 |
| 1 | L | 105/107 (98%) | 0.31 | 4 (3%) | 40 | 24 | 61, 85, 115, 118 | 0 |
| 1 | M | 105/107 (98%) | 0.53 | 9 (8%) | 10 | 5 | 75, 105, 142, 168 | 0 |
| 1 | N | 102/107 (95%) | 0.36 | 7 (6%) | 16 | 9 | 52, 92, 119, 125 | 0 |
| 1 | O | 105/107 (98%) | 0.62 | 14 (13%) | 3 | 1 | 66, 106, 123, 131 | 0 |
| 1 | P | 100/107 (93%) | 0.38 | 8 (8%) | 12 | 6 | 59, 91, 120, 133 | 0 |
| 1 | Q | 105/107 (98%) | 0.06 | 5 (4%) | 30 | 18 | 34, 64, 94, 104 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | R | 105/107 (98%) | -0.03 | 1 (0%) | 82 | 66 | 32, 53, 80, 106 | 0 |
| 1 | T | 105/107 (98%) | 0.01 | 2 (1%) | 66 | 46 | 41, 58, 100, 118 | 0 |
| 1 | U | 103/107 (96%) | -0.25 | 0 | 100 | 100 | 29, 42, 64, 74 | 0 |
| 1 | V | 105/107 (98%) | -0.08 | 1 (0%) | 82 | 66 | 40, 65, 89, 110 | 0 |
| 1 | W | 105/107 (98%) | -0.19 | 2 (1%) | 66 | 46 | 27, 45, 80, 97 | 0 |
| 1 | X | 105/107 (98%) | -0.10 | 2 (1%) | 66 | 46 | 38, 68, 111, 117 | 0 |
| 1 | Y | 105/107 (98%) | -0.05 | 3 (2%) | 51 | 32 | 32, 58, 95, 128 | 0 |
| 1 | Z | 100/107 (93%) | 0.56 | 14 (14%) | 2 | 1 | 64, 104, 132, 140 | 0 |
| All | All | 3313/3424 (96%) | 0.17 | 173 (5%) | 27 | 16 | 24, 77, 122, 168 | 0 |

All (173) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 4 | 102 | ALA | 7.7 |
| 1 | K | 117 | ALA | 7.1 |
| 1 | O | 92 | VAL | 6.4 |
| 1 | M | 195 | ASN | 5.9 |
| 1 | 6 | 160 | VAL | 5.5 |
| 1 | 6 | 161 | GLY | 5.4 |
| 1 | C | 111 | THR | 5.4 |
| 1 | P | 184 | ILE | 5.4 |
| 1 | P | 185 | THR | 5.2 |
| 1 | Z | 102 | ALA | 4.6 |
| 1 | O | 94 | LYS | 4.6 |
| 1 | 5 | 110 | MET | 4.5 |
| 1 | Z | 161 | GLY | 4.5 |
| 1 | 6 | 149 | PHE | 4.3 |
| 1 | 6 | 163 | PRO | 4.3 |
| 1 | 6 | 102 | ALA | 4.1 |
| 1 | O | 112 | SER | 4.0 |
| 1 | 4 | 159 | PRO | 4.0 |
| 1 | 6 | 128 | ASN | 4.0 |
| 1 | Z | 103 | TRP | 3.9 |
| 1 | 7 | 137 | THR | 3.9 |
| 1 | 2 | 128 | ASN | 3.8 |
| 1 | 7 | 177 | PRO | 3.8 |
| 1 | 4 | 96 | ALA | 3.8 |
| 1 | N | 130 | ILE | 3.7 |
| 1 | K | 102 | ALA | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 6 | 98 | ALA | 3.6 |
| 1 | K | 195 | ASN | 3.6 |
| 1 | 7 | 178 | GLN | 3.6 |
| 1 | R | 111 | THR | 3.6 |
| 1 | 7 | 150 | GLY | 3.5 |
| 1 | M | 159 | PRO | 3.5 |
| 1 | 2 | 185 | THR | 3.4 |
| 1 | 7 | 148 | ALA | 3.4 |
| 1 | K | 156 | MET | 3.4 |
| 1 | X | 118 | VAL | 3.4 |
| 1 | Z | 168 | TYR | 3.4 |
| 1 | C | 108 | THR | 3.4 |
| 1 | 1 | 164 | GLY | 3.3 |
| 1 | Z | 107 | ASP | 3.3 |
| 1 | Y | 193 | GLU | 3.3 |
| 1 | K | 132 | LYS | 3.3 |
| 1 | Z | 185 | THR | 3.3 |
| 1 | 7 | 119 | ALA | 3.3 |
| 1 | 7 | 111 | THR | 3.2 |
| 1 | 4 | 115 | LYS | 3.2 |
| 1 | 4 | 154 | TYR | 3.2 |
| 1 | I | 124 | PRO | 3.2 |
| 1 | 4 | 98 | ALA | 3.2 |
| 1 | 6 | 105 | ARG | 3.2 |
| 1 | 2 | 111 | THR | 3.2 |
| 1 | 4 | 131 | MET | 3.2 |
| 1 | 4 | 176 | LEU | 3.1 |
| 1 | B | 111 | THR | 3.1 |
| 1 | Z | 162 | ALA | 3.1 |
| 1 | 4 | 178 | GLN | 3.1 |
| 1 | Z | 125 | ALA | 3.1 |
| 1 | 4 | 114 | LYS | 3.0 |
| 1 | P | 112 | SER | 3.0 |
| 1 | M | 138 | THR | 3.0 |
| 1 | 6 | 190 | PHE | 2.9 |
| 1 | O | 146 | ALA | 2.9 |
| 1 | 2 | 108 | THR | 2.9 |
| 1 | Q | 111 | THR | 2.9 |
| 1 | 2 | 134 | GLU | 2.9 |
| 1 | N | 127 | VAL | 2.9 |
| 1 | 2 | 98 | ALA | 2.8 |
| 1 | O | 157 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | M | 128 | ASN | 2.8 |
| 1 | O | 175 | ALA | 2.8 |
| 1 | 4 | 105 | ARG | 2.8 |
| 1 | 4 | 94 | LYS | 2.8 |
| 1 | I | 104 | MET | 2.8 |
| 1 | O | 103 | TRP | 2.8 |
| 1 | 5 | 92 | VAL | 2.8 |
| 1 | M | 102 | ALA | 2.8 |
| 1 | I | 112 | SER | 2.7 |
| 1 | 6 | 107 | ASP | 2.7 |
| 1 | M | 174 | ALA | 2.7 |
| 1 | 2 | 168 | TYR | 2.7 |
| 1 | W | 190 | PHE | 2.7 |
| 1 | K | 96 | ALA | 2.7 |
| 1 | L | 175 | ALA | 2.7 |
| 1 | K | 126 | THR | 2.7 |
| 1 | 4 | 138 | THR | 2.7 |
| 1 | N | 171 | ARG | 2.7 |
| 1 | 6 | 133 | ALA | 2.7 |
| 1 | M | 118 | VAL | 2.7 |
| 1 | 4 | 95 | GLN | 2.7 |
| 1 | 7 | 92 | VAL | 2.7 |
| 1 | P | 125 | ALA | 2.7 |
| 1 | Q | 188 | ILE | 2.6 |
| 1 | L | 110 | MET | 2.6 |
| 1 | Z | 112 | SER | 2.6 |
| 1 | 5 | 108 | THR | 2.6 |
| 1 | M | 137 | THR | 2.6 |
| 1 | I | 194 | GLN | 2.6 |
| 1 | O | 187 | PHE | 2.6 |
| 1 | A | 111 | THR | 2.6 |
| 1 | V | 111 | THR | 2.6 |
| 1 | Q | 121 | GLY | 2.6 |
| 1 | 2 | 160 | VAL | 2.5 |
| 1 | Q | 120 | ALA | 2.5 |
| 1 | 6 | 162 | ALA | 2.5 |
| 1 | T | 124 | PRO | 2.5 |
| 1 | 5 | 146 | ALA | 2.5 |
| 1 | 6 | 148 | ALA | 2.5 |
| 1 | H | 111 | THR | 2.5 |
| 1 | K | 103 | TRP | 2.5 |
| 1 | 7 | 118 | VAL | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 3 | 110 | MET | 2.5 |
| 1 | I | 188 | ILE | 2.5 |
| 1 | Z | 117 | ALA | 2.5 |
| 1 | A | 194 | GLN | 2.5 |
| 1 | I | 151 | HIS | 2.5 |
| 1 | K | 129 | ARG | 2.4 |
| 1 | 7 | 113 | GLU | 2.4 |
| 1 | P | 186 | SER | 2.4 |
| 1 | N | 110 | MET | 2.4 |
| 1 | 5 | 168 | TYR | 2.4 |
| 1 | T | 110 | MET | 2.4 |
| 1 | Y | 176 | LEU | 2.4 |
| 1 | Q | 118 | VAL | 2.4 |
| 1 | F | 166 | ILE | 2.4 |
| 1 | O | 171 | ARG | 2.4 |
| 1 | 7 | 99 | THR | 2.3 |
| 1 | 2 | 110 | MET | 2.3 |
| 1 | I | 195 | ASN | 2.3 |
| 1 | O | 133 | ALA | 2.3 |
| 1 | 7 | 149 | PHE | 2.3 |
| 1 | J | 110 | MET | 2.3 |
| 1 | M | 103 | TRP | 2.3 |
| 1 | K | 157 | ILE | 2.3 |
| 1 | 1 | 128 | ASN | 2.3 |
| 1 | Y | 191 | VAL | 2.3 |
| 1 | 1 | 110 | MET | 2.3 |
| 1 | W | 194 | GLN | 2.3 |
| 1 | P | 180 | GLU | 2.3 |
| 1 | Z | 108 | THR | 2.3 |
| 1 | 6 | 108 | THR | 2.3 |
| 1 | O | 170 | HIS | 2.3 |
| 1 | N | 137 | THR | 2.2 |
| 1 | J | 170 | HIS | 2.2 |
| 1 | L | 136 | SER | 2.2 |
| 1 | 6 | 136 | SER | 2.2 |
| 1 | Z | 126 | THR | 2.2 |
| 1 | G | 193 | GLU | 2.2 |
| 1 | 4 | 99 | THR | 2.2 |
| 1 | 6 | 106 | LYS | 2.2 |
| 1 | O | 142 | LEU | 2.2 |
| 1 | N | 121 | GLY | 2.2 |
| 1 | 4 | 165 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | N | 151 | HIS | 2.2 |
| 1 | P | 144 | SER | 2.1 |
| 1 | 5 | 127 | VAL | 2.1 |
| 1 | 3 | 174 | ALA | 2.1 |
| 1 | O | 189 | ASN | 2.1 |
| 1 | 5 | 145 | LEU | 2.1 |
| 1 | L | 103 | TRP | 2.1 |
| 1 | Z | 156 | MET | 2.1 |
| 1 | 4 | 111 | THR | 2.1 |
| 1 | P | 168 | TYR | 2.1 |
| 1 | 4 | 101 | ASN | 2.1 |
| 1 | O | 93 | GLU | 2.1 |
| 1 | 7 | 141 | VAL | 2.1 |
| 1 | 6 | 103 | TRP | 2.1 |
| 1 | F | 187 | PHE | 2.1 |
| 1 | X | 185 | THR | 2.0 |
| 1 | Z | 111 | THR | 2.0 |
| 1 | 7 | 98 | ALA | 2.0 |
| 1 | 6 | 166 | ILE | 2.0 |
| 1 | 7 | 136 | SER | 2.0 |
| 1 | K | 131 | MET | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.