



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1L9U
Title : THERMUS AQUATICUS RNA POLYMERASE HOLOENZYME AT 4 Å
RESOLUTION
Authors : Murakami, K.S.; Masuda, S.; Darst, S.A.
Deposited on : 2002-03-26
Resolution : 4.00 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

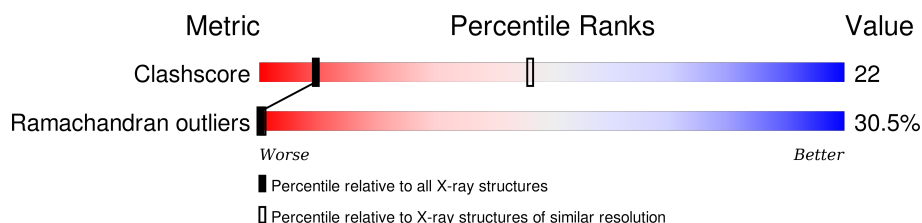
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.





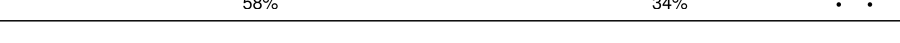
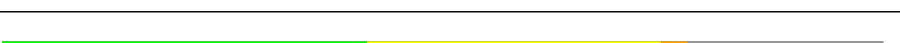
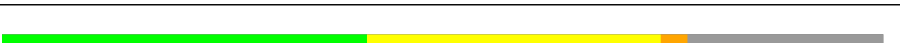


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 1052 (4.40-3.60) |
| Ramachandran outliers | 100387 | 1005 (4.40-3.60) |




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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 314 |  46% 24% • 29% |
| 1 | B | 314 |  49% 21% • 30% |
| 1 | J | 314 |  46% 24% • 29% |
| 1 | K | 314 |  49% 21% • 30% |
| 2 | C | 1118 |  58% 34% • • |
| 2 | L | 1118 |  58% 35% • • |
| 3 | D | 1524 |  41% 33% • 22% |
| 3 | M | 1524 |  41% 33% • 22% |
| 4 | E | 99 |  49% 42% • 7% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | N | 99 |  47% 44% • 7% |
| 5 | H | 332 |  75% 21% • • |
| 5 | Q | 332 |  75% 21% • • |

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18756 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 RNA POLYMERASE, ALPHA SUBUNIT.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|---------|-------|
| 1 | A | 224 | Total | C | N | 0 | 0 | 0 |
| | | | 672 | 448 | 224 | | | |
| 1 | B | 220 | Total | C | N | 0 | 0 | 0 |
| | | | 660 | 440 | 220 | | | |
| 1 | J | 224 | Total | C | N | 0 | 0 | 0 |
| | | | 672 | 448 | 224 | | | |
| 1 | K | 220 | Total | C | N | 0 | 0 | 0 |
| | | | 660 | 440 | 220 | | | |

- Molecule 2 is a protein called RNA POLYMERASE, BETA SUBUNIT.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|---------|---------|-------|
| 2 | C | 1084 | Total | C | N | 0 | 0 | 0 |
| | | | 3252 | 2168 | 1084 | | | |
| 2 | L | 1084 | Total | C | N | 0 | 0 | 0 |
| | | | 3252 | 2168 | 1084 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C | ? | - | GLU | DELETION | UNP Q9KWU7 |
| L | ? | - | GLU | DELETION | UNP Q9KWU7 |

- Molecule 3 is a protein called RNA POLYMERASE, BETA-PRIME SUBUNIT.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|---------|---------|-------|
| 3 | D | 1183 | Total | C | N | 0 | 0 | 0 |
| | | | 3549 | 2366 | 1183 | | | |
| 3 | M | 1183 | Total | C | N | 0 | 0 | 0 |
| | | | 3549 | 2366 | 1183 | | | |

- Molecule 4 is a protein called RNA POLYMERASE, OMEGA SUBUNIT.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|---------|---------|-------|
| 4 | E | 92 | Total | C | N | 0 | 0 | 0 |
| | | | 276 | 184 | 92 | | | |
| 4 | N | 92 | Total | C | N | 0 | 0 | 0 |
| | | | 276 | 184 | 92 | | | |

- Molecule 5 is a protein called SIGMA FACTOR SIGA.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|---------|---------|-------|
| 5 | H | 322 | Total | C | N | 0 | 0 | 0 |
| | | | 966 | 644 | 322 | | | |
| 5 | Q | 322 | Total | C | N | 0 | 0 | 0 |
| | | | 966 | 644 | 322 | | | |

There are 30 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| H | ? | - | ILE | DELETION | UNP Q9EZJ8 |
| H | ? | - | GLN | DELETION | UNP Q9EZJ8 |
| H | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| H | ? | - | ILE | DELETION | UNP Q9EZJ8 |
| H | ? | - | PRO | DELETION | UNP Q9EZJ8 |
| H | ? | - | GLY | DELETION | UNP Q9EZJ8 |
| H | ? | - | LEU | DELETION | UNP Q9EZJ8 |
| H | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| H | ? | - | GLU | DELETION | UNP Q9EZJ8 |
| H | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| H | ? | - | PRO | DELETION | UNP Q9EZJ8 |
| H | ? | - | ASP | DELETION | UNP Q9EZJ8 |
| H | ? | - | PRO | DELETION | UNP Q9EZJ8 |
| H | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| H | ? | - | THR | DELETION | UNP Q9EZJ8 |
| Q | ? | - | ILE | DELETION | UNP Q9EZJ8 |
| Q | ? | - | GLN | DELETION | UNP Q9EZJ8 |
| Q | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| Q | ? | - | ILE | DELETION | UNP Q9EZJ8 |
| Q | ? | - | PRO | DELETION | UNP Q9EZJ8 |
| Q | ? | - | GLY | DELETION | UNP Q9EZJ8 |
| Q | ? | - | LEU | DELETION | UNP Q9EZJ8 |
| Q | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| Q | ? | - | GLU | DELETION | UNP Q9EZJ8 |
| Q | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| Q | ? | - | PRO | DELETION | UNP Q9EZJ8 |
| Q | ? | - | ASP | DELETION | UNP Q9EZJ8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Q | ? | - | PRO | DELETION | UNP Q9EZJ8 |
| Q | ? | - | LYS | DELETION | UNP Q9EZJ8 |
| Q | ? | - | THR | DELETION | UNP Q9EZJ8 |

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6 | D | 1 | Total Mg 1 1 | 0 | 0 |
| 6 | M | 1 | Total Mg 1 1 | 0 | 0 |

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

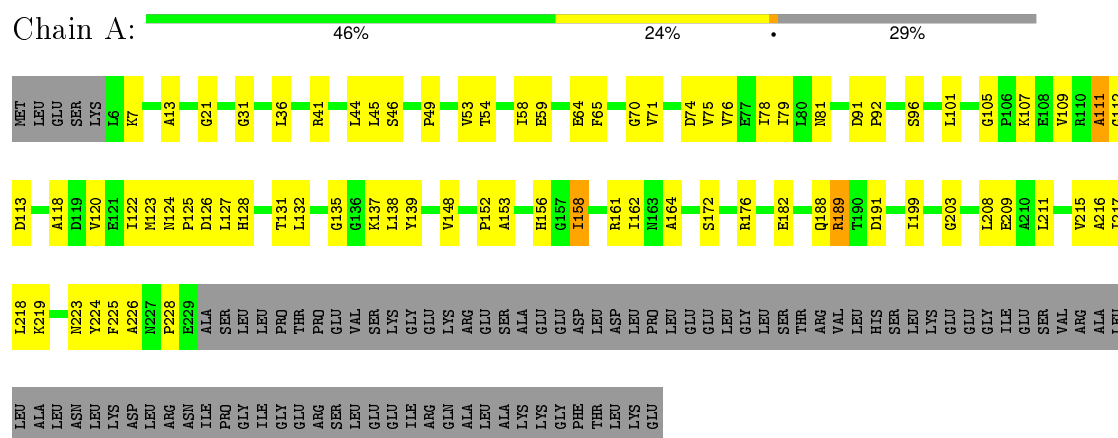
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7 | D | 2 | Total Zn 2 2 | 0 | 0 |
| 7 | M | 2 | Total Zn 2 2 | 0 | 0 |

3 Residue-property plots

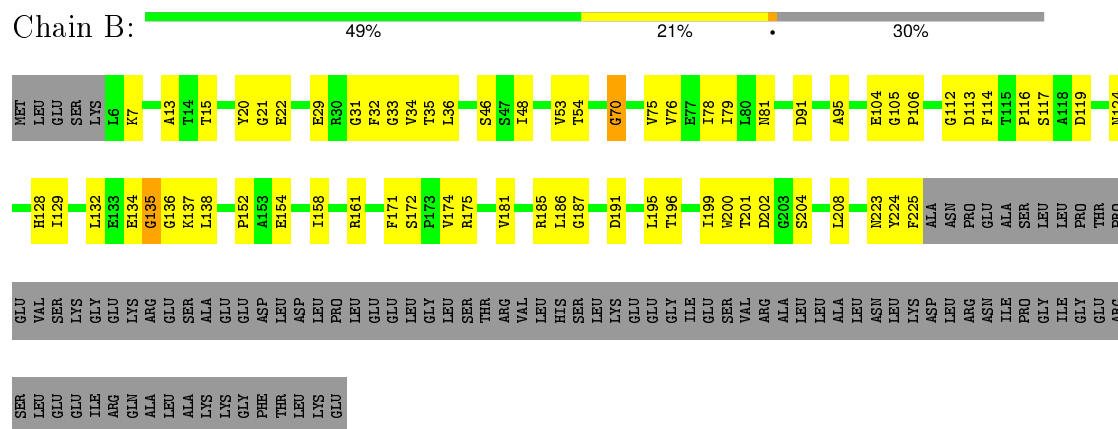
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

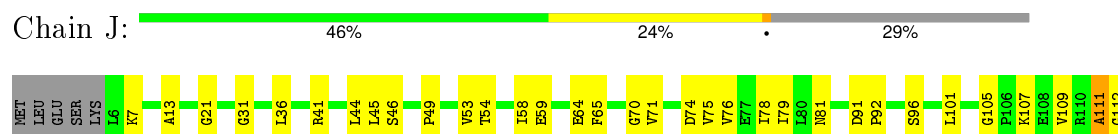
• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT

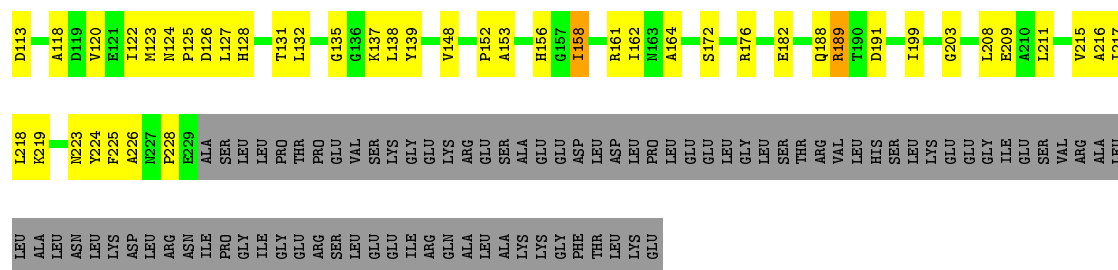


• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT

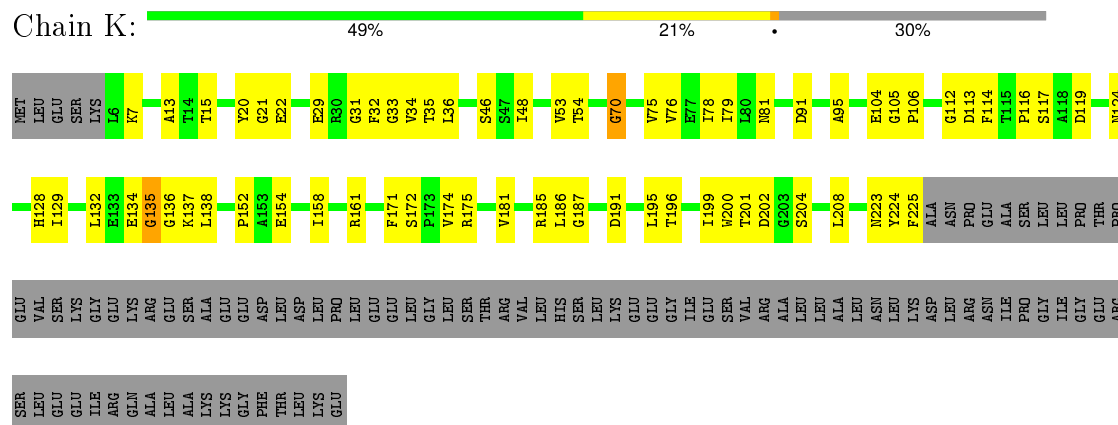


• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT

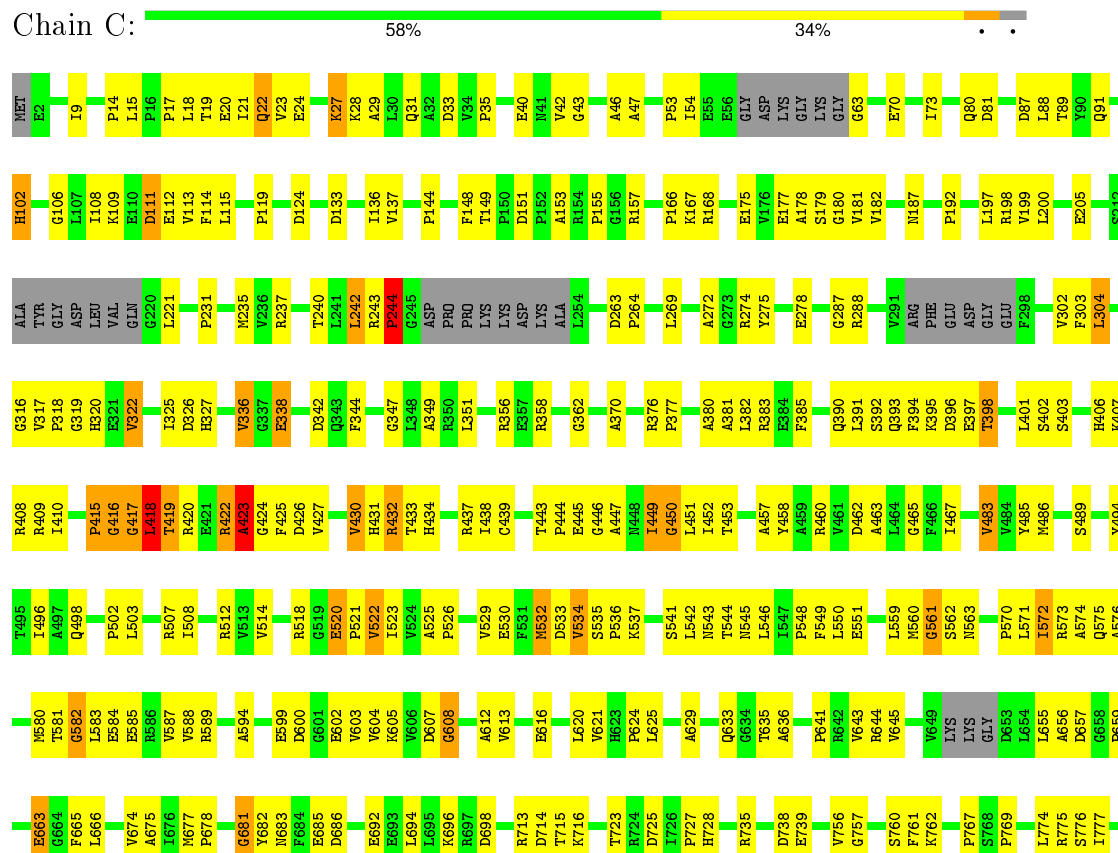


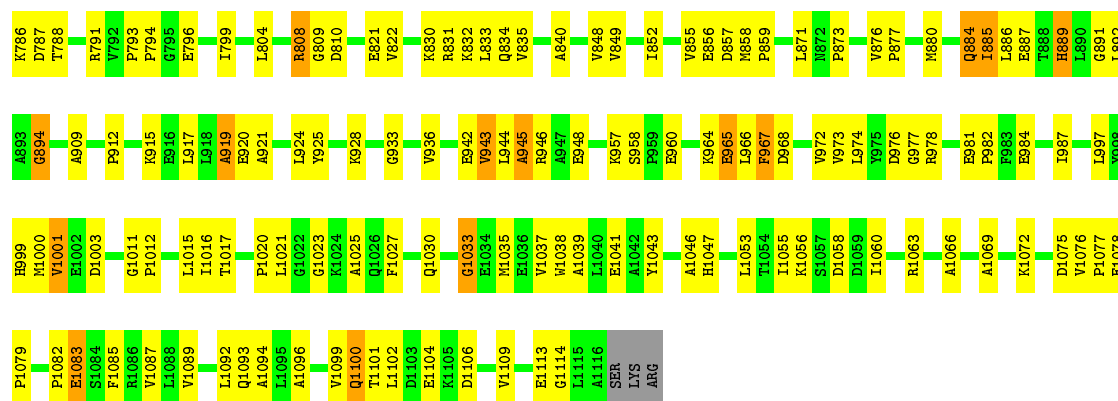


• Molecule 1: RNA POLYMERASE, ALPHA SUBUNIT



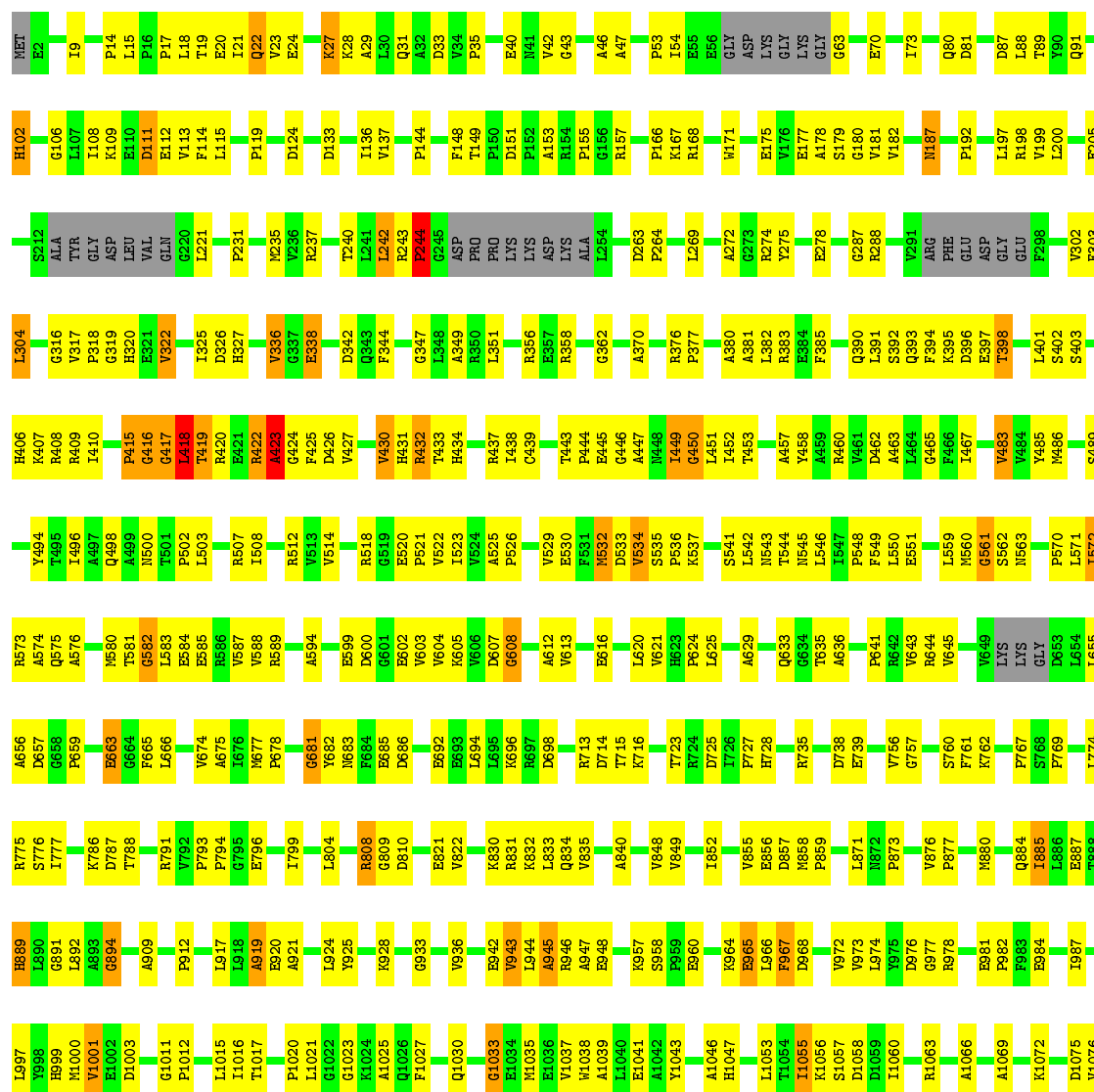
• Molecule 2: RNA POLYMERASE, BETA SUBUNIT

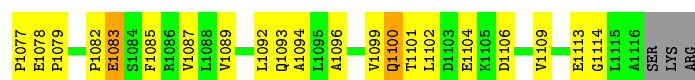




• Molecule 2: RNA POLYMERASE, BETA SUBUNIT

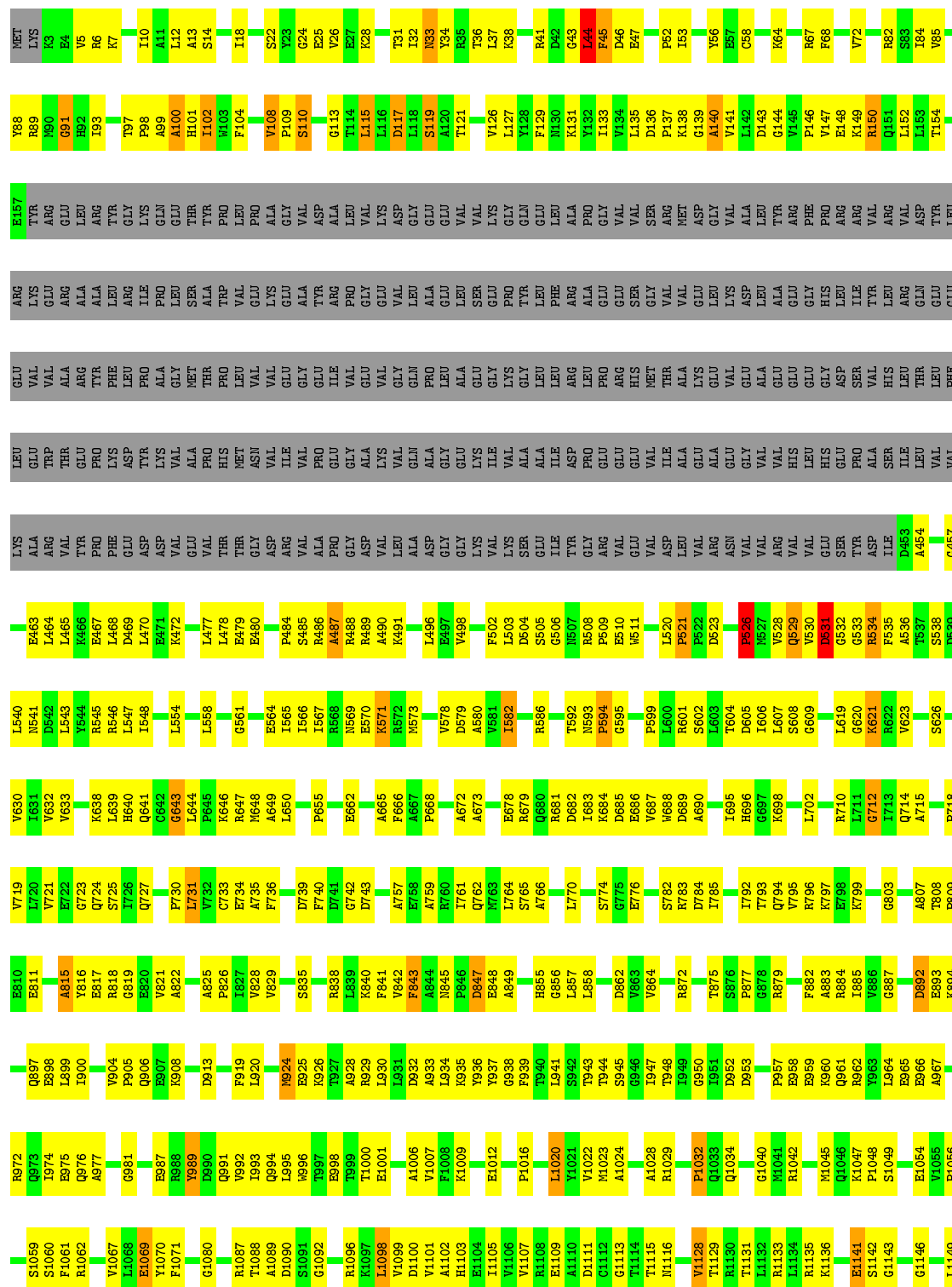
Chain L: 58% 35%



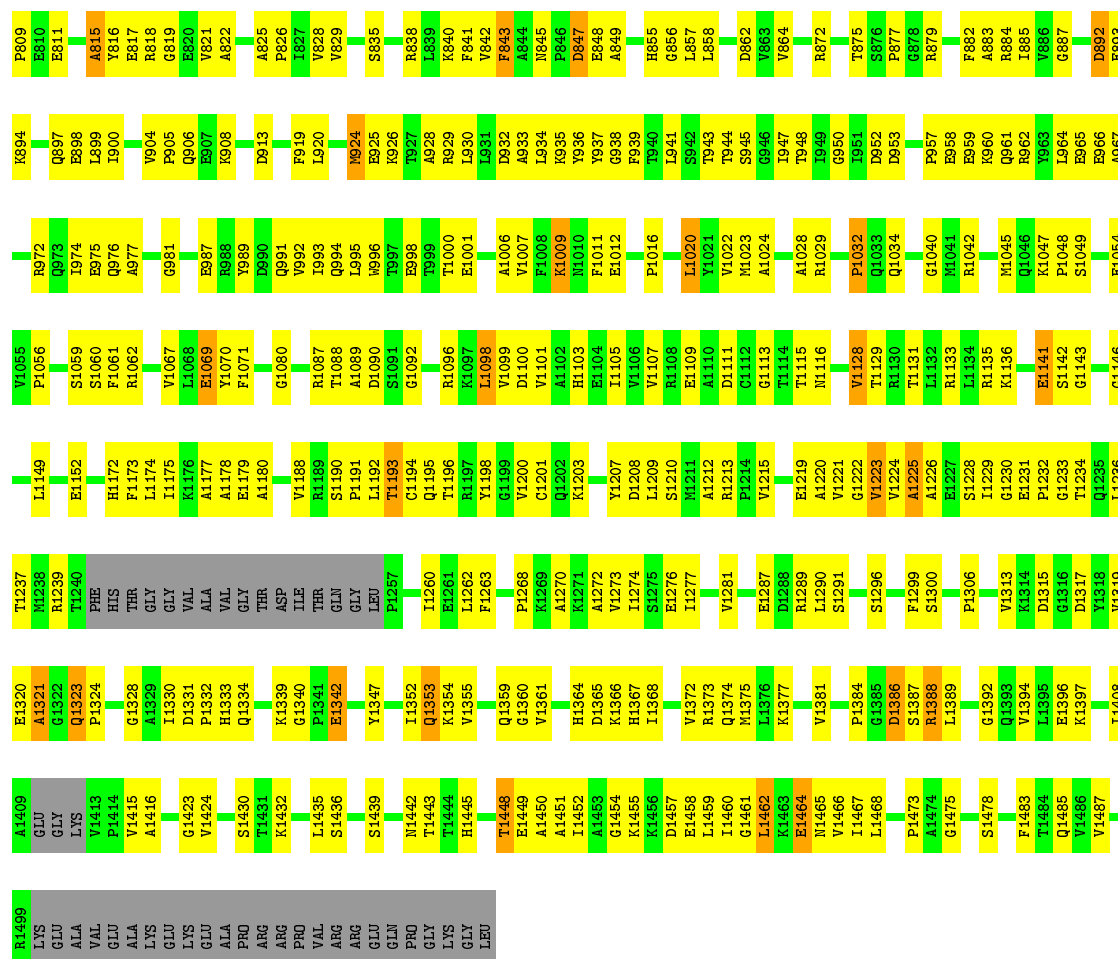


• Molecule 3: RNA POLYMERASE, BETA-PRIME SUBUNIT

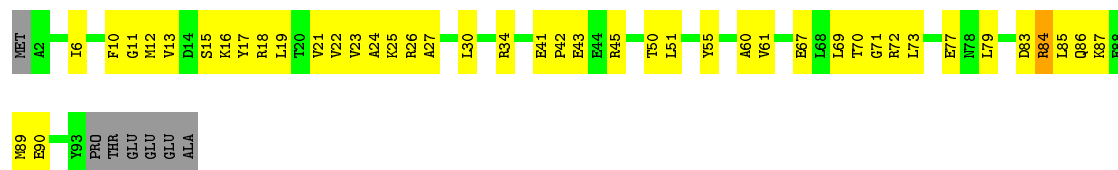
Chain D: 41% 33% 22%



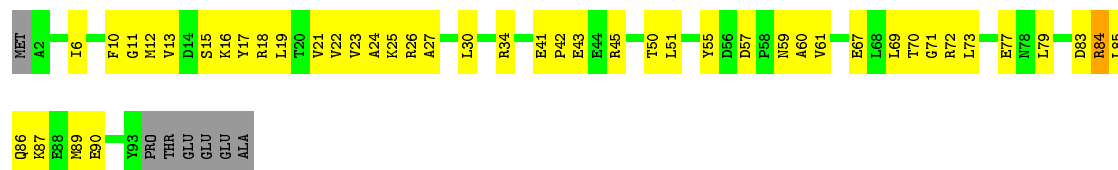




- Molecule 4: RNA POLYMERASE, OMEGA SUBUNIT

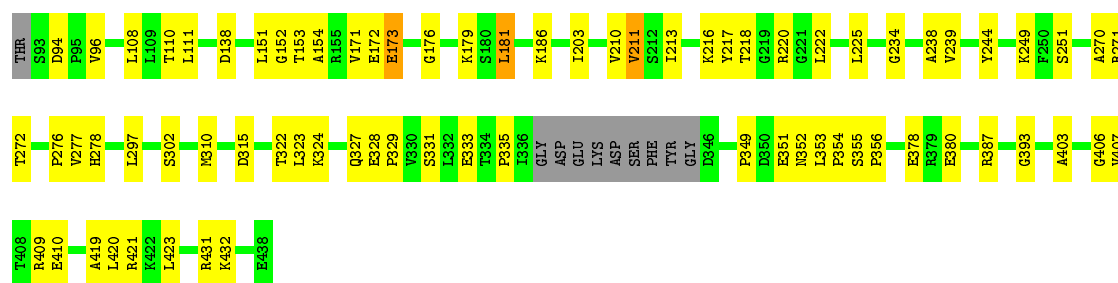


- Molecule 4: RNA POLYMERASE, OMEGA SUBUNIT

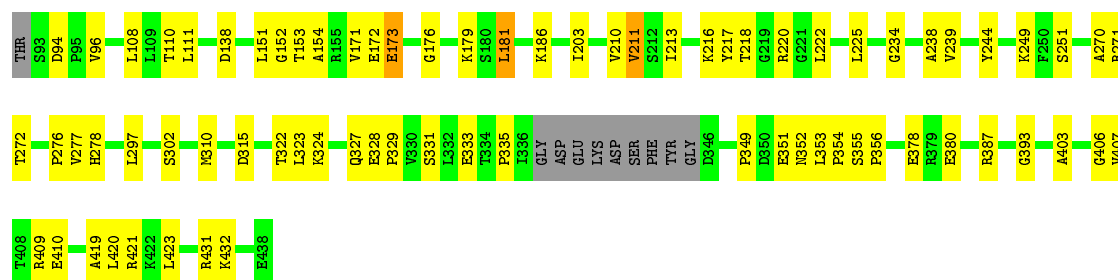


- Molecule 5: SIGMA FACTOR SIGA





- Molecule 5: SIGMA FACTOR SIGA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 155.00Å 271.20Å 155.30Å 90.00° 91.40° 90.00° | Depositor |
| Resolution (Å) | (Not available) – 4.00 | Depositor |
| % Data completeness (in resolution range) | (Not available) ((Not available)-4.00) | Depositor |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | ? | Depositor |
| R, R_{free} | (Not available) , (Not available) | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 18756 | wwPDB-VP |
| Average B, all atoms (Å ²) | 25.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.37 | 0/671 | 1.02 | 0/670 |
| 1 | B | 0.36 | 0/659 | 1.11 | 0/658 |
| 1 | J | 0.37 | 0/671 | 1.02 | 0/670 |
| 1 | K | 0.36 | 0/659 | 1.11 | 0/658 |
| 2 | C | 0.85 | 9/3246 (0.3%) | 1.37 | 15/3240 (0.5%) |
| 2 | L | 0.85 | 9/3246 (0.3%) | 1.37 | 15/3240 (0.5%) |
| 3 | D | 0.94 | 21/3545 (0.6%) | 1.34 | 21/3541 (0.6%) |
| 3 | M | 0.94 | 21/3545 (0.6%) | 1.34 | 21/3541 (0.6%) |
| 4 | E | 0.34 | 0/275 | 0.87 | 0/274 |
| 4 | N | 0.34 | 0/275 | 0.87 | 0/274 |
| 5 | H | 0.59 | 3/964 (0.3%) | 0.85 | 4/962 (0.4%) |
| 5 | Q | 0.59 | 3/964 (0.3%) | 0.85 | 4/962 (0.4%) |
| All | All | 0.80 | 66/18720 (0.4%) | 1.26 | 80/18690 (0.4%) |

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 |
|-----|-------|---------------------|---------------------|
| 2 | C | 0 | 8 |
| 2 | L | 0 | 8 |
| 3 | D | 0 | 7 |
| 3 | M | 0 | 7 |
| All | All | 0 | 30 |

All (66) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2 | C | 244 | PRO | C-N | -22.34 | 0.92 | 1.33 |
| 2 | L | 244 | PRO | C-N | -22.31 | 0.92 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 3 | D | 91 | GLY | C-N | -18.07 | 0.92 | 1.34 |
| 3 | M | 91 | GLY | C-N | -18.07 | 0.92 | 1.34 |
| 3 | D | 531 | ASP | C-N | -17.95 | 1.00 | 1.33 |
| 3 | M | 531 | ASP | C-N | -17.92 | 1.00 | 1.33 |
| 2 | C | 417 | GLY | C-N | -16.64 | 0.95 | 1.34 |
| 2 | L | 417 | GLY | C-N | -16.61 | 0.95 | 1.34 |
| 3 | M | 532 | GLY | C-N | 15.96 | 1.61 | 1.33 |
| 3 | D | 532 | GLY | C-N | 15.93 | 1.61 | 1.33 |
| 3 | D | 44 | LEU | C-N | 15.76 | 1.70 | 1.34 |
| 3 | M | 44 | LEU | C-N | 15.73 | 1.70 | 1.34 |
| 2 | L | 240 | THR | C-N | -15.27 | 0.98 | 1.34 |
| 2 | C | 240 | THR | C-N | -15.23 | 0.99 | 1.34 |
| 2 | L | 422 | ARG | C-N | -14.27 | 1.01 | 1.34 |
| 2 | C | 419 | THR | C-N | -14.27 | 1.01 | 1.34 |
| 2 | L | 418 | LEU | C-N | -14.26 | 1.01 | 1.34 |
| 2 | C | 422 | ARG | C-N | -14.24 | 1.01 | 1.34 |
| 2 | L | 419 | THR | C-N | -14.24 | 1.01 | 1.34 |
| 2 | C | 418 | LEU | C-N | -14.24 | 1.01 | 1.34 |
| 3 | D | 521 | PRO | C-N | -13.31 | 1.08 | 1.34 |
| 3 | M | 521 | PRO | C-N | -13.28 | 1.09 | 1.34 |
| 5 | H | 239 | VAL | C-N | -12.30 | 1.05 | 1.34 |
| 5 | Q | 239 | VAL | C-N | -12.27 | 1.05 | 1.34 |
| 3 | D | 529 | GLN | C-N | -11.91 | 1.06 | 1.34 |
| 3 | M | 529 | GLN | C-N | -11.90 | 1.06 | 1.34 |
| 2 | L | 423 | ALA | C-N | -10.79 | 1.13 | 1.33 |
| 2 | C | 423 | ALA | C-N | -10.75 | 1.13 | 1.33 |
| 3 | M | 526 | PRO | C-N | -10.69 | 1.09 | 1.34 |
| 3 | D | 526 | PRO | C-N | -10.66 | 1.09 | 1.34 |
| 3 | D | 533 | GLY | C-N | 10.19 | 1.57 | 1.34 |
| 3 | M | 533 | GLY | C-N | 10.19 | 1.57 | 1.34 |
| 3 | D | 1080 | GLY | C-N | 9.76 | 1.50 | 1.33 |
| 3 | M | 1080 | GLY | C-N | 9.74 | 1.50 | 1.33 |
| 3 | D | 1087 | ARG | C-N | -9.68 | 1.11 | 1.34 |
| 3 | M | 1087 | ARG | C-N | -9.65 | 1.11 | 1.34 |
| 3 | D | 113 | GLY | C-N | -9.33 | 1.12 | 1.34 |
| 3 | M | 113 | GLY | C-N | -9.30 | 1.12 | 1.34 |
| 3 | D | 115 | LEU | C-N | -7.80 | 1.16 | 1.34 |
| 3 | M | 115 | LEU | C-N | -7.79 | 1.16 | 1.34 |
| 3 | M | 113 | GLY | N-CA | -7.71 | 1.34 | 1.46 |
| 3 | D | 113 | GLY | N-CA | -7.70 | 1.34 | 1.46 |
| 3 | D | 538 | SER | C-N | 7.54 | 1.51 | 1.34 |
| 3 | M | 538 | SER | C-N | 7.53 | 1.51 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2 | C | 416 | GLY | C-N | -7.38 | 1.19 | 1.33 |
| 2 | L | 416 | GLY | C-N | -7.34 | 1.19 | 1.33 |
| 3 | M | 528 | VAL | C-N | 7.15 | 1.50 | 1.34 |
| 3 | D | 528 | VAL | C-N | 7.14 | 1.50 | 1.34 |
| 3 | D | 93 | ILE | C-N | -7.03 | 1.17 | 1.34 |
| 3 | M | 93 | ILE | C-N | -7.03 | 1.17 | 1.34 |
| 5 | H | 238 | ALA | N-CA | 6.76 | 1.59 | 1.46 |
| 5 | Q | 238 | ALA | N-CA | 6.75 | 1.59 | 1.46 |
| 2 | L | 415 | PRO | C-N | 6.10 | 1.44 | 1.33 |
| 2 | C | 415 | PRO | C-N | 6.07 | 1.44 | 1.33 |
| 3 | D | 523 | ASP | C-N | -5.78 | 1.20 | 1.34 |
| 3 | M | 523 | ASP | C-N | -5.76 | 1.20 | 1.34 |
| 3 | D | 534 | ARG | C-N | -5.72 | 1.20 | 1.34 |
| 3 | M | 534 | ARG | C-N | -5.68 | 1.21 | 1.34 |
| 3 | M | 1089 | ALA | C-N | -5.39 | 1.21 | 1.34 |
| 5 | Q | 234 | GLY | CA-C | -5.39 | 1.43 | 1.51 |
| 3 | D | 1089 | ALA | C-N | -5.39 | 1.21 | 1.34 |
| 5 | H | 234 | GLY | CA-C | -5.36 | 1.43 | 1.51 |
| 3 | M | 88 | TYR | C-N | 5.30 | 1.46 | 1.34 |
| 3 | D | 88 | TYR | C-N | 5.29 | 1.46 | 1.34 |
| 3 | D | 1096 | ARG | C-N | -5.11 | 1.22 | 1.34 |
| 3 | M | 1096 | ARG | C-N | -5.09 | 1.22 | 1.34 |

All (80) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | L | 244 | PRO | CA-C-N | 24.93 | 166.06 | 116.20 |
| 2 | C | 244 | PRO | CA-C-N | 24.90 | 166.00 | 116.20 |
| 2 | L | 417 | GLY | C-N-CA | 20.66 | 173.35 | 121.70 |
| 2 | C | 417 | GLY | C-N-CA | 20.66 | 173.34 | 121.70 |
| 3 | D | 531 | ASP | CA-C-N | 19.67 | 155.53 | 116.20 |
| 3 | M | 531 | ASP | CA-C-N | 19.63 | 155.46 | 116.20 |
| 2 | C | 419 | THR | C-N-CA | 19.39 | 170.16 | 121.70 |
| 2 | L | 419 | THR | C-N-CA | 19.38 | 170.14 | 121.70 |
| 3 | M | 534 | ARG | C-N-CA | 18.67 | 168.37 | 121.70 |
| 3 | D | 534 | ARG | C-N-CA | 18.66 | 168.35 | 121.70 |
| 2 | C | 244 | PRO | C-N-CA | 17.86 | 159.81 | 122.30 |
| 2 | L | 244 | PRO | C-N-CA | 17.85 | 159.78 | 122.30 |
| 3 | D | 529 | GLN | C-N-CA | 15.36 | 160.09 | 121.70 |
| 3 | M | 529 | GLN | C-N-CA | 15.34 | 160.05 | 121.70 |
| 2 | C | 242 | LEU | C-N-CA | 14.61 | 158.21 | 121.70 |
| 2 | L | 242 | LEU | C-N-CA | 14.61 | 158.22 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 2 | C | 422 | ARG | C-N-CA | 14.25 | 157.32 | 121.70 |
| 2 | L | 422 | ARG | C-N-CA | 14.25 | 157.32 | 121.70 |
| 2 | C | 422 | ARG | CA-C-N | 14.14 | 148.30 | 117.20 |
| 2 | L | 422 | ARG | CA-C-N | 14.11 | 148.25 | 117.20 |
| 3 | D | 531 | ASP | C-N-CA | 13.62 | 150.90 | 122.30 |
| 3 | M | 531 | ASP | C-N-CA | 13.62 | 150.90 | 122.30 |
| 2 | L | 417 | GLY | CA-C-N | 13.47 | 146.84 | 117.20 |
| 2 | C | 417 | GLY | CA-C-N | 13.47 | 146.84 | 117.20 |
| 3 | D | 91 | GLY | CA-C-N | 13.04 | 145.89 | 117.20 |
| 3 | M | 91 | GLY | CA-C-N | 13.04 | 145.89 | 117.20 |
| 3 | M | 526 | PRO | C-N-CA | 11.58 | 150.64 | 121.70 |
| 3 | D | 526 | PRO | C-N-CA | 11.57 | 150.64 | 121.70 |
| 2 | L | 418 | LEU | C-N-CA | 10.82 | 148.75 | 121.70 |
| 2 | C | 418 | LEU | C-N-CA | 10.80 | 148.71 | 121.70 |
| 3 | D | 534 | ARG | CA-C-N | 10.79 | 140.93 | 117.20 |
| 3 | M | 534 | ARG | CA-C-N | 10.78 | 140.91 | 117.20 |
| 3 | D | 91 | GLY | C-N-CA | 10.65 | 148.32 | 121.70 |
| 3 | M | 91 | GLY | C-N-CA | 10.65 | 148.32 | 121.70 |
| 3 | D | 88 | TYR | C-N-CA | -10.27 | 96.02 | 121.70 |
| 3 | M | 88 | TYR | C-N-CA | -10.26 | 96.06 | 121.70 |
| 3 | D | 526 | PRO | CA-C-N | 10.03 | 139.26 | 117.20 |
| 3 | M | 526 | PRO | CA-C-N | 10.03 | 139.26 | 117.20 |
| 3 | D | 88 | TYR | CA-C-N | -9.85 | 95.53 | 117.20 |
| 3 | M | 88 | TYR | CA-C-N | -9.85 | 95.54 | 117.20 |
| 3 | M | 532 | GLY | CA-C-N | 9.51 | 135.22 | 116.20 |
| 3 | D | 532 | GLY | CA-C-N | 9.50 | 135.20 | 116.20 |
| 2 | L | 418 | LEU | CA-C-N | 8.52 | 135.95 | 117.20 |
| 2 | C | 418 | LEU | CA-C-N | 8.49 | 135.89 | 117.20 |
| 2 | C | 242 | LEU | CA-C-N | 7.84 | 134.45 | 117.20 |
| 2 | L | 242 | LEU | CA-C-N | 7.84 | 134.45 | 117.20 |
| 3 | D | 1088 | THR | C-N-CA | 7.80 | 141.20 | 121.70 |
| 3 | M | 1088 | THR | C-N-CA | 7.79 | 141.17 | 121.70 |
| 5 | H | 225 | LEU | CA-C-N | 6.65 | 131.84 | 117.20 |
| 5 | Q | 225 | LEU | CA-C-N | 6.65 | 131.83 | 117.20 |
| 2 | L | 423 | ALA | CA-C-N | 6.59 | 129.39 | 116.20 |
| 2 | C | 423 | ALA | CA-C-N | 6.59 | 129.38 | 116.20 |
| 3 | M | 1128 | VAL | N-CA-C | -6.48 | 93.50 | 111.00 |
| 3 | D | 1128 | VAL | N-CA-C | -6.47 | 93.52 | 111.00 |
| 3 | D | 113 | GLY | CA-C-N | 6.34 | 131.14 | 117.20 |
| 3 | M | 113 | GLY | CA-C-N | 6.32 | 131.11 | 117.20 |
| 5 | H | 173 | GLU | N-CA-C | 6.20 | 127.74 | 111.00 |
| 5 | Q | 173 | GLU | N-CA-C | 6.19 | 127.72 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3 | D | 1080 | GLY | CA-C-N | -6.11 | 103.98 | 116.20 |
| 3 | M | 1080 | GLY | CA-C-N | -6.11 | 103.98 | 116.20 |
| 2 | C | 416 | GLY | CA-C-N | 6.09 | 128.38 | 116.20 |
| 2 | L | 416 | GLY | CA-C-N | 6.07 | 128.34 | 116.20 |
| 3 | D | 93 | ILE | C-N-CA | 6.06 | 136.85 | 121.70 |
| 3 | M | 93 | ILE | C-N-CA | 6.05 | 136.83 | 121.70 |
| 3 | D | 44 | LEU | C-N-CA | -6.01 | 106.66 | 121.70 |
| 2 | C | 416 | GLY | C-N-CA | 6.01 | 134.92 | 122.30 |
| 3 | M | 44 | LEU | C-N-CA | -6.01 | 106.68 | 121.70 |
| 2 | L | 416 | GLY | C-N-CA | 6.00 | 134.89 | 122.30 |
| 2 | C | 419 | THR | CA-C-N | 5.63 | 129.58 | 117.20 |
| 2 | L | 419 | THR | CA-C-N | 5.62 | 129.57 | 117.20 |
| 3 | D | 536 | ALA | N-CA-C | 5.50 | 125.84 | 111.00 |
| 3 | M | 536 | ALA | N-CA-C | 5.49 | 125.83 | 111.00 |
| 5 | H | 225 | LEU | C-N-CA | 5.46 | 135.36 | 121.70 |
| 5 | Q | 225 | LEU | C-N-CA | 5.46 | 135.36 | 121.70 |
| 3 | M | 89 | ARG | C-N-CA | -5.24 | 108.61 | 121.70 |
| 5 | Q | 239 | VAL | CA-C-N | -5.24 | 105.68 | 117.20 |
| 3 | D | 89 | ARG | C-N-CA | -5.23 | 108.63 | 121.70 |
| 5 | H | 239 | VAL | CA-C-N | -5.23 | 105.70 | 117.20 |
| 3 | D | 521 | PRO | CA-C-N | 5.14 | 131.49 | 117.10 |
| 3 | M | 521 | PRO | CA-C-N | 5.13 | 131.48 | 117.10 |

There are no chirality outliers.

All (30) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | C | 242 | LEU | Peptide |
| 2 | C | 244 | PRO | Peptide |
| 2 | C | 416 | GLY | Peptide |
| 2 | C | 417 | GLY | Peptide |
| 2 | C | 418 | LEU | Peptide |
| 2 | C | 419 | THR | Peptide |
| 2 | C | 422 | ARG | Peptide |
| 2 | C | 423 | ALA | Peptide |
| 3 | D | 115 | LEU | Peptide |
| 3 | D | 521 | PRO | Peptide |
| 3 | D | 526 | PRO | Peptide |
| 3 | D | 529 | GLN | Peptide |
| 3 | D | 531 | ASP | Peptide |
| 3 | D | 534 | ARG | Peptide |
| 3 | D | 91 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | L | 242 | LEU | Peptide |
| 2 | L | 244 | PRO | Peptide |
| 2 | L | 416 | GLY | Peptide |
| 2 | L | 417 | GLY | Peptide |
| 2 | L | 418 | LEU | Peptide |
| 2 | L | 419 | THR | Peptide |
| 2 | L | 422 | ARG | Peptide |
| 2 | L | 423 | ALA | Peptide |
| 3 | M | 115 | LEU | Peptide |
| 3 | M | 521 | PRO | Peptide |
| 3 | M | 526 | PRO | Peptide |
| 3 | M | 529 | GLN | Peptide |
| 3 | M | 531 | ASP | Peptide |
| 3 | M | 534 | ARG | Peptide |
| 3 | M | 91 | GLY | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 672 | 0 | 241 | 13 | 0 |
| 1 | B | 660 | 0 | 238 | 10 | 0 |
| 1 | J | 672 | 0 | 241 | 13 | 0 |
| 1 | K | 660 | 0 | 238 | 9 | 0 |
| 2 | C | 3252 | 0 | 1190 | 105 | 0 |
| 2 | L | 3252 | 0 | 1190 | 107 | 0 |
| 3 | D | 3549 | 0 | 1280 | 135 | 0 |
| 3 | M | 3549 | 0 | 1280 | 134 | 0 |
| 4 | E | 276 | 0 | 96 | 14 | 0 |
| 4 | N | 276 | 0 | 96 | 15 | 0 |
| 5 | H | 966 | 0 | 342 | 14 | 0 |
| 5 | Q | 966 | 0 | 342 | 14 | 0 |
| 6 | D | 1 | 0 | 0 | 0 | 0 |
| 6 | M | 1 | 0 | 0 | 0 | 0 |
| 7 | D | 2 | 0 | 0 | 0 | 0 |
| 7 | M | 2 | 0 | 0 | 0 | 0 |
| All | All | 18756 | 0 | 6774 | 571 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (571) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 3:D:44:LEU:C | 3:D:45:PHE:N | 1.70 | 1.42 |
| 3:M:44:LEU:C | 3:M:45:PHE:N | 1.70 | 1.41 |
| 3:M:933:ALA:C | 3:M:935:LYS:H | 1.80 | 0.83 |
| 2:L:1033:GLY:HA2 | 3:M:620:GLY:HA2 | 1.60 | 0.82 |
| 2:L:542:LEU:C | 2:L:544:THR:H | 1.83 | 0.82 |
| 2:C:1033:GLY:HA2 | 3:D:620:GLY:HA2 | 1.60 | 0.82 |
| 3:D:933:ALA:C | 3:D:935:LYS:H | 1.81 | 0.81 |
| 2:C:1033:GLY:CA | 3:D:620:GLY:HA2 | 2.10 | 0.81 |
| 2:L:1033:GLY:CA | 3:M:620:GLY:HA2 | 2.10 | 0.81 |
| 2:C:542:LEU:C | 2:C:544:THR:H | 1.83 | 0.80 |
| 3:D:152:LEU:C | 3:D:154:THR:H | 1.85 | 0.80 |
| 3:D:44:LEU:C | 3:D:46:ASP:H | 1.85 | 0.80 |
| 3:M:44:LEU:C | 3:M:46:ASP:H | 1.85 | 0.79 |
| 2:L:533:ASP:C | 2:L:535:SER:H | 1.86 | 0.78 |
| 2:C:533:ASP:C | 2:C:535:SER:H | 1.86 | 0.78 |
| 3:D:578:VAL:C | 3:D:580:ALA:H | 1.87 | 0.78 |
| 2:C:681:GLY:C | 2:C:683:ASN:H | 1.88 | 0.77 |
| 3:M:578:VAL:C | 3:M:580:ALA:H | 1.87 | 0.77 |
| 3:M:152:LEU:C | 3:M:154:THR:H | 1.85 | 0.77 |
| 3:D:1069:GLU:C | 3:D:1071:PHE:H | 1.89 | 0.76 |
| 2:L:559:LEU:C | 2:L:561:GLY:H | 1.89 | 0.76 |
| 2:C:349:ALA:C | 2:C:351:LEU:H | 1.89 | 0.76 |
| 3:D:44:LEU:C | 3:D:45:PHE:CA | 2.54 | 0.76 |
| 2:C:559:LEU:C | 2:C:561:GLY:H | 1.89 | 0.76 |
| 3:M:1069:GLU:C | 3:M:1071:PHE:H | 1.89 | 0.76 |
| 3:M:44:LEU:C | 3:M:45:PHE:CA | 2.53 | 0.76 |
| 2:L:349:ALA:C | 2:L:351:LEU:H | 1.89 | 0.75 |
| 2:L:681:GLY:C | 2:L:683:ASN:H | 1.88 | 0.75 |
| 5:H:151:LEU:C | 5:H:153:THR:H | 1.93 | 0.72 |
| 2:L:383:ARG:C | 2:L:385:PHE:H | 1.93 | 0.71 |
| 3:M:604:THR:C | 3:M:606:ILE:H | 1.94 | 0.71 |
| 2:C:383:ARG:C | 2:C:385:PHE:H | 1.93 | 0.71 |
| 3:D:604:THR:C | 3:D:606:ILE:H | 1.94 | 0.70 |
| 5:Q:151:LEU:C | 5:Q:153:THR:H | 1.93 | 0.70 |
| 3:D:1022:VAL:C | 3:D:1024:ALA:H | 1.96 | 0.69 |
| 2:L:1100:GLN:C | 2:L:1102:LEU:H | 1.97 | 0.69 |
| 3:M:975:GLU:C | 3:M:977:ALA:H | 1.96 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 2:L:544:THR:C | 2:L:546:LEU:H | 1.97 | 0.68 |
| 2:C:1100:GLN:C | 2:C:1102:LEU:H | 1.97 | 0.68 |
| 3:D:975:GLU:C | 3:D:977:ALA:H | 1.96 | 0.67 |
| 3:M:1022:VAL:C | 3:M:1024:ALA:H | 1.96 | 0.67 |
| 2:C:544:THR:C | 2:C:546:LEU:H | 1.97 | 0.67 |
| 5:H:276:PRO:C | 5:H:278:HIS:H | 1.98 | 0.67 |
| 2:C:1092:LEU:C | 2:C:1094:ALA:H | 1.97 | 0.67 |
| 2:C:1092:LEU:C | 2:C:1094:ALA:N | 2.48 | 0.67 |
| 2:L:1092:LEU:C | 2:L:1094:ALA:N | 2.48 | 0.67 |
| 4:E:25:LYS:C | 4:E:27:ALA:H | 1.98 | 0.67 |
| 3:D:1060:SER:C | 3:D:1062:ARG:H | 1.98 | 0.66 |
| 2:C:347:GLY:C | 2:C:349:ALA:H | 1.99 | 0.66 |
| 4:N:25:LYS:C | 4:N:27:ALA:H | 1.98 | 0.66 |
| 3:M:1060:SER:C | 3:M:1062:ARG:H | 1.98 | 0.65 |
| 2:L:347:GLY:C | 2:L:349:ALA:H | 1.99 | 0.65 |
| 2:L:1092:LEU:C | 2:L:1094:ALA:H | 1.97 | 0.65 |
| 3:M:1448:THR:C | 3:M:1450:ALA:H | 2.01 | 0.65 |
| 2:L:406:HIS:C | 2:L:408:ARG:H | 2.01 | 0.65 |
| 3:M:933:ALA:C | 3:M:935:LYS:N | 2.50 | 0.64 |
| 5:Q:276:PRO:C | 5:Q:278:HIS:H | 1.98 | 0.64 |
| 3:D:1448:THR:C | 3:D:1450:ALA:H | 2.01 | 0.64 |
| 3:D:734:GLU:C | 3:D:736:PHE:H | 2.01 | 0.64 |
| 2:C:542:LEU:C | 2:C:544:THR:N | 2.51 | 0.63 |
| 2:L:542:LEU:C | 2:L:544:THR:N | 2.51 | 0.63 |
| 3:M:734:GLU:C | 3:M:736:PHE:H | 2.01 | 0.63 |
| 2:L:437:ARG:C | 2:L:439:CYS:H | 2.02 | 0.63 |
| 2:C:406:HIS:C | 2:C:408:ARG:H | 2.01 | 0.63 |
| 3:M:1191:PRO:C | 3:M:1193:THR:H | 2.01 | 0.63 |
| 2:C:430:VAL:C | 2:C:432:ARG:H | 2.02 | 0.63 |
| 2:C:437:ARG:C | 2:C:439:CYS:H | 2.02 | 0.63 |
| 2:L:430:VAL:C | 2:L:432:ARG:H | 2.02 | 0.62 |
| 3:D:1191:PRO:C | 3:D:1193:THR:H | 2.01 | 0.62 |
| 2:L:1100:GLN:C | 2:L:1102:LEU:N | 2.53 | 0.62 |
| 3:M:957:PRO:C | 3:M:959:GLU:H | 2.03 | 0.62 |
| 4:E:70:THR:C | 4:E:72:ARG:H | 2.02 | 0.62 |
| 5:H:270:ALA:C | 5:H:272:THR:H | 2.02 | 0.62 |
| 3:D:44:LEU:CA | 3:D:45:PHE:N | 2.62 | 0.62 |
| 3:D:957:PRO:C | 3:D:959:GLU:H | 2.03 | 0.62 |
| 2:L:549:PHE:C | 2:L:551:GLU:H | 2.03 | 0.61 |
| 3:M:643:GLY:HA3 | 3:M:727:GLN:H | 1.65 | 0.61 |
| 2:L:523:ILE:C | 2:L:525:ALA:N | 2.51 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 4:N:70:THR:C | 4:N:72:ARG:H | 2.02 | 0.61 |
| 3:D:643:GLY:HA3 | 3:D:727:GLN:H | 1.65 | 0.61 |
| 3:M:44:LEU:CA | 3:M:45:PHE:N | 2.62 | 0.61 |
| 2:C:561:GLY:C | 2:C:563:ASN:H | 2.04 | 0.61 |
| 5:Q:270:ALA:C | 5:Q:272:THR:H | 2.02 | 0.61 |
| 3:M:855:HIS:C | 3:M:857:LEU:H | 2.04 | 0.61 |
| 3:M:152:LEU:C | 3:M:154:THR:N | 2.54 | 0.61 |
| 2:L:450:GLY:C | 2:L:452:ILE:H | 2.04 | 0.61 |
| 3:D:855:HIS:C | 3:D:857:LEU:H | 2.04 | 0.61 |
| 2:L:561:GLY:C | 2:L:563:ASN:H | 2.04 | 0.61 |
| 2:C:1100:GLN:C | 2:C:1102:LEU:N | 2.53 | 0.60 |
| 4:E:11:GLY:C | 4:E:13:VAL:H | 2.05 | 0.60 |
| 3:M:757:ALA:C | 3:M:759:ALA:H | 2.04 | 0.60 |
| 4:N:11:GLY:C | 4:N:13:VAL:H | 2.05 | 0.60 |
| 2:L:681:GLY:C | 2:L:683:ASN:N | 2.55 | 0.60 |
| 2:C:549:PHE:C | 2:C:551:GLU:H | 2.03 | 0.60 |
| 3:M:688:TRP:C | 3:M:690:ALA:H | 2.05 | 0.60 |
| 2:C:450:GLY:C | 2:C:452:ILE:H | 2.04 | 0.60 |
| 3:M:639:LEU:C | 3:M:641:GLN:H | 2.05 | 0.59 |
| 2:C:178:ALA:C | 2:C:180:GLY:H | 2.05 | 0.59 |
| 3:D:688:TRP:C | 3:D:690:ALA:H | 2.05 | 0.59 |
| 3:M:119:SER:C | 3:M:121:THR:H | 2.05 | 0.59 |
| 2:C:559:LEU:C | 2:C:561:GLY:N | 2.55 | 0.59 |
| 2:L:178:ALA:C | 2:L:180:GLY:H | 2.05 | 0.59 |
| 2:C:406:HIS:C | 2:C:408:ARG:N | 2.55 | 0.59 |
| 3:D:757:ALA:C | 3:D:759:ALA:H | 2.04 | 0.59 |
| 3:M:845:ASN:C | 3:M:847:ASP:H | 2.06 | 0.59 |
| 3:M:503:LEU:C | 3:M:505:SER:H | 2.06 | 0.59 |
| 3:M:1141:GLU:C | 3:M:1143:GLY:H | 2.06 | 0.59 |
| 3:D:639:LEU:C | 3:D:641:GLN:H | 2.05 | 0.59 |
| 2:L:325:ILE:C | 2:L:327:HIS:H | 2.06 | 0.59 |
| 3:D:44:LEU:C | 3:D:46:ASP:N | 2.56 | 0.59 |
| 3:M:578:VAL:C | 3:M:580:ALA:N | 2.56 | 0.59 |
| 2:L:559:LEU:C | 2:L:561:GLY:N | 2.55 | 0.59 |
| 3:M:1340:GLY:C | 3:M:1342:GLU:H | 2.06 | 0.59 |
| 2:C:581:THR:C | 2:C:583:LEU:H | 2.06 | 0.59 |
| 3:D:119:SER:C | 3:D:121:THR:H | 2.05 | 0.59 |
| 3:D:1226:ALA:C | 3:D:1228:SER:H | 2.06 | 0.59 |
| 2:L:581:THR:C | 2:L:583:LEU:H | 2.06 | 0.59 |
| 3:D:503:LEU:C | 3:D:505:SER:H | 2.06 | 0.58 |
| 3:D:1340:GLY:C | 3:D:1342:GLU:H | 2.07 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:C:483:VAL:C | 2:C:485:TYR:H | 2.07 | 0.58 |
| 2:L:349:ALA:C | 2:L:351:LEU:N | 2.56 | 0.58 |
| 2:C:111:ASP:C | 2:C:113:VAL:H | 2.07 | 0.58 |
| 2:L:406:HIS:C | 2:L:408:ARG:N | 2.55 | 0.58 |
| 2:C:808:ARG:C | 2:C:810:ASP:H | 2.07 | 0.58 |
| 2:C:325:ILE:C | 2:C:327:HIS:H | 2.06 | 0.58 |
| 2:C:424:GLY:C | 2:C:426:ASP:H | 2.06 | 0.58 |
| 1:A:217:ILE:C | 1:A:219:LYS:H | 2.06 | 0.58 |
| 2:L:424:GLY:C | 2:L:426:ASP:H | 2.06 | 0.58 |
| 2:C:523:ILE:C | 2:C:525:ALA:N | 2.51 | 0.58 |
| 2:L:808:ARG:C | 2:L:810:ASP:H | 2.07 | 0.58 |
| 3:D:1032:PRO:C | 3:D:1034:GLN:H | 2.08 | 0.58 |
| 2:L:885:ILE:C | 2:L:887:GLU:N | 2.56 | 0.58 |
| 3:M:1032:PRO:C | 3:M:1034:GLN:H | 2.07 | 0.58 |
| 3:M:44:LEU:C | 3:M:46:ASP:N | 2.55 | 0.58 |
| 3:D:933:ALA:C | 3:D:935:LYS:N | 2.50 | 0.58 |
| 3:D:119:SER:C | 3:D:121:THR:N | 2.58 | 0.58 |
| 3:D:467:GLU:C | 3:D:469:ASP:H | 2.08 | 0.57 |
| 3:D:578:VAL:C | 3:D:580:ALA:N | 2.56 | 0.57 |
| 2:L:533:ASP:C | 2:L:535:SER:N | 2.57 | 0.57 |
| 3:M:108:VAL:C | 3:M:110:SER:N | 2.57 | 0.57 |
| 3:D:845:ASN:C | 3:D:847:ASP:N | 2.58 | 0.57 |
| 2:L:111:ASP:C | 2:L:113:VAL:H | 2.07 | 0.57 |
| 3:D:845:ASN:C | 3:D:847:ASP:H | 2.05 | 0.57 |
| 3:D:877:PRO:C | 3:D:879:ARG:H | 2.08 | 0.57 |
| 2:L:1015:LEU:C | 2:L:1017:THR:H | 2.08 | 0.57 |
| 3:M:1226:ALA:C | 3:M:1228:SER:H | 2.06 | 0.57 |
| 3:M:509:PRO:C | 3:M:511:TRP:H | 2.08 | 0.57 |
| 2:C:533:ASP:C | 2:C:535:SER:N | 2.57 | 0.57 |
| 2:C:943:VAL:C | 2:C:945:ALA:N | 2.58 | 0.57 |
| 1:J:217:ILE:C | 1:J:219:LYS:H | 2.06 | 0.57 |
| 2:C:885:ILE:C | 2:C:887:GLU:N | 2.56 | 0.57 |
| 3:M:845:ASN:C | 3:M:847:ASP:N | 2.58 | 0.57 |
| 3:M:467:GLU:C | 3:M:469:ASP:H | 2.08 | 0.57 |
| 2:L:1033:GLY:HA3 | 3:M:620:GLY:HA2 | 1.86 | 0.56 |
| 2:C:349:ALA:C | 2:C:351:LEU:N | 2.56 | 0.56 |
| 3:M:117:ASP:C | 3:M:119:SER:H | 2.07 | 0.56 |
| 3:D:1069:GLU:C | 3:D:1071:PHE:N | 2.58 | 0.56 |
| 3:M:924:MET:C | 3:M:926:LYS:H | 2.09 | 0.56 |
| 3:D:1141:GLU:C | 3:D:1143:GLY:H | 2.06 | 0.56 |
| 3:D:117:ASP:C | 3:D:119:SER:H | 2.07 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:C:1015:LEU:C | 2:C:1017:THR:H | 2.08 | 0.56 |
| 3:D:924:MET:C | 3:D:926:LYS:H | 2.09 | 0.56 |
| 3:M:119:SER:C | 3:M:121:THR:N | 2.58 | 0.56 |
| 2:C:681:GLY:C | 2:C:683:ASN:N | 2.55 | 0.56 |
| 2:C:383:ARG:C | 2:C:385:PHE:N | 2.59 | 0.56 |
| 2:L:383:ARG:C | 2:L:385:PHE:N | 2.59 | 0.56 |
| 3:M:1069:GLU:C | 3:M:1071:PHE:N | 2.58 | 0.56 |
| 2:C:1023:GLY:C | 2:C:1025:ALA:H | 2.09 | 0.56 |
| 2:L:483:VAL:C | 2:L:485:TYR:H | 2.07 | 0.56 |
| 2:L:943:VAL:C | 2:L:945:ALA:N | 2.58 | 0.56 |
| 2:L:889:HIS:C | 2:L:891:GLY:N | 2.58 | 0.56 |
| 5:H:151:LEU:C | 5:H:153:THR:N | 2.59 | 0.56 |
| 2:C:889:HIS:C | 2:C:891:GLY:N | 2.58 | 0.56 |
| 2:C:1033:GLY:HA3 | 3:D:620:GLY:HA2 | 1.86 | 0.56 |
| 2:C:424:GLY:C | 2:C:426:ASP:N | 2.58 | 0.56 |
| 2:L:424:GLY:C | 2:L:426:ASP:N | 2.58 | 0.56 |
| 2:C:885:ILE:C | 2:C:887:GLU:H | 2.09 | 0.55 |
| 3:D:108:VAL:C | 3:D:110:SER:N | 2.58 | 0.55 |
| 3:M:487:ALA:C | 3:M:489:ARG:H | 2.10 | 0.55 |
| 3:M:877:PRO:C | 3:M:879:ARG:H | 2.08 | 0.55 |
| 2:L:1023:GLY:C | 2:L:1025:ALA:H | 2.09 | 0.55 |
| 3:D:509:PRO:C | 3:D:511:TRP:H | 2.08 | 0.55 |
| 1:A:71:VAL:H | 2:C:608:GLY:CA | 2.20 | 0.55 |
| 2:C:380:ALA:C | 2:C:382:LEU:H | 2.10 | 0.55 |
| 2:C:570:PRO:C | 2:C:572:ILE:H | 2.09 | 0.55 |
| 2:L:447:ALA:C | 2:L:449:ILE:H | 2.10 | 0.55 |
| 1:J:71:VAL:H | 2:L:608:GLY:CA | 2.20 | 0.55 |
| 3:M:1289:ARG:C | 3:M:1291:SER:H | 2.10 | 0.54 |
| 2:L:885:ILE:C | 2:L:887:GLU:H | 2.09 | 0.54 |
| 2:L:380:ALA:C | 2:L:382:LEU:H | 2.10 | 0.54 |
| 3:D:1332:PRO:C | 3:D:1334:GLN:H | 2.10 | 0.54 |
| 3:M:1022:VAL:C | 3:M:1024:ALA:N | 2.61 | 0.54 |
| 3:D:993:ILE:C | 3:D:995:LEU:H | 2.11 | 0.54 |
| 2:L:570:PRO:C | 2:L:572:ILE:H | 2.09 | 0.54 |
| 3:D:1289:ARG:C | 3:D:1291:SER:H | 2.10 | 0.54 |
| 2:L:356:ARG:C | 2:L:358:ARG:H | 2.11 | 0.54 |
| 3:D:1022:VAL:C | 3:D:1024:ALA:N | 2.61 | 0.54 |
| 1:J:217:ILE:C | 1:J:219:LYS:N | 2.61 | 0.54 |
| 3:D:152:LEU:C | 3:D:154:THR:N | 2.54 | 0.54 |
| 1:A:217:ILE:C | 1:A:219:LYS:N | 2.61 | 0.54 |
| 3:D:487:ALA:C | 3:D:489:ARG:H | 2.10 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:34:VAL:C | 1:B:36:LEU:N | 2.61 | 0.53 |
| 2:L:892:LEU:C | 2:L:894:GLY:H | 2.12 | 0.53 |
| 2:L:532:MET:C | 2:L:534:VAL:H | 2.12 | 0.53 |
| 2:L:336:VAL:C | 2:L:338:GLU:H | 2.11 | 0.53 |
| 2:C:571:LEU:C | 2:C:573:ARG:H | 2.11 | 0.53 |
| 2:C:447:ALA:C | 2:C:449:ILE:H | 2.10 | 0.53 |
| 2:C:892:LEU:C | 2:C:894:GLY:H | 2.12 | 0.53 |
| 1:K:34:VAL:C | 1:K:36:LEU:N | 2.61 | 0.53 |
| 3:M:1340:GLY:C | 3:M:1342:GLU:N | 2.62 | 0.53 |
| 2:L:571:LEU:C | 2:L:573:ARG:H | 2.11 | 0.53 |
| 3:M:993:ILE:C | 3:M:995:LEU:H | 2.11 | 0.53 |
| 3:D:465:LEU:C | 3:D:467:GLU:H | 2.12 | 0.52 |
| 3:M:470:LEU:C | 3:M:472:LYS:H | 2.13 | 0.52 |
| 3:M:1332:PRO:C | 3:M:1334:GLN:H | 2.11 | 0.52 |
| 1:K:105:GLY:HA2 | 1:K:136:GLY:HA3 | 1.91 | 0.52 |
| 2:C:336:VAL:C | 2:C:338:GLU:H | 2.11 | 0.52 |
| 2:L:544:THR:C | 2:L:546:LEU:N | 2.63 | 0.52 |
| 2:C:356:ARG:C | 2:C:358:ARG:H | 2.11 | 0.52 |
| 3:D:685:ASP:C | 3:D:687:VAL:H | 2.13 | 0.52 |
| 3:M:604:THR:C | 3:M:606:ILE:N | 2.62 | 0.52 |
| 2:C:532:MET:C | 2:C:534:VAL:H | 2.12 | 0.52 |
| 5:Q:151:LEU:C | 5:Q:153:THR:N | 2.59 | 0.52 |
| 3:M:685:ASP:C | 3:M:687:VAL:H | 2.13 | 0.52 |
| 1:J:79:ILE:C | 1:J:81:ASN:H | 2.13 | 0.52 |
| 3:D:924:MET:C | 3:D:926:LYS:N | 2.64 | 0.52 |
| 1:A:79:ILE:C | 1:A:81:ASN:H | 2.13 | 0.52 |
| 1:B:105:GLY:HA2 | 1:B:136:GLY:HA3 | 1.91 | 0.51 |
| 3:D:541:ASN:C | 3:D:543:LEU:N | 2.61 | 0.51 |
| 5:Q:322:THR:C | 5:Q:324:LYS:H | 2.14 | 0.51 |
| 3:D:1196:THR:C | 3:D:1198:TYR:H | 2.12 | 0.51 |
| 3:D:1020:LEU:C | 3:D:1022:VAL:H | 2.14 | 0.51 |
| 3:D:604:THR:C | 3:D:606:ILE:N | 2.62 | 0.51 |
| 3:D:1340:GLY:C | 3:D:1342:GLU:N | 2.62 | 0.51 |
| 3:M:924:MET:C | 3:M:926:LYS:N | 2.64 | 0.51 |
| 3:M:465:LEU:C | 3:M:467:GLU:H | 2.12 | 0.51 |
| 3:M:102:ILE:C | 3:M:104:PHE:N | 2.64 | 0.51 |
| 5:H:322:THR:C | 5:H:324:LYS:H | 2.14 | 0.51 |
| 3:M:1196:THR:C | 3:M:1198:TYR:H | 2.12 | 0.51 |
| 2:C:544:THR:C | 2:C:546:LEU:N | 2.63 | 0.51 |
| 3:M:1332:PRO:C | 3:M:1334:GLN:N | 2.64 | 0.51 |
| 3:M:1020:LEU:C | 3:M:1022:VAL:H | 2.14 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 3:D:108:VAL:C | 3:D:110:SER:H | 2.14 | 0.51 |
| 2:L:919:ALA:C | 2:L:921:ALA:N | 2.64 | 0.51 |
| 3:D:960:LYS:C | 3:D:962:ARG:H | 2.15 | 0.50 |
| 2:L:1041:GLU:C | 2:L:1043:TYR:N | 2.64 | 0.50 |
| 3:M:957:PRO:C | 3:M:959:GLU:N | 2.65 | 0.50 |
| 3:M:950:GLY:C | 3:M:952:ASP:N | 2.63 | 0.50 |
| 2:C:723:THR:C | 2:C:725:ASP:H | 2.14 | 0.50 |
| 3:M:960:LYS:C | 3:M:962:ARG:H | 2.15 | 0.50 |
| 2:C:396:ASP:C | 2:C:398:THR:H | 2.15 | 0.50 |
| 3:D:1332:PRO:C | 3:D:1334:GLN:N | 2.64 | 0.50 |
| 3:D:960:LYS:C | 3:D:962:ARG:N | 2.65 | 0.50 |
| 2:L:723:THR:C | 2:L:725:ASP:H | 2.15 | 0.50 |
| 1:J:223:ASN:C | 1:J:225:PHE:N | 2.65 | 0.50 |
| 3:D:957:PRO:C | 3:D:959:GLU:N | 2.65 | 0.50 |
| 2:C:581:THR:C | 2:C:583:LEU:N | 2.65 | 0.50 |
| 3:D:470:LEU:C | 3:D:472:LYS:H | 2.13 | 0.50 |
| 2:L:302:VAL:C | 2:L:304:LEU:H | 2.15 | 0.50 |
| 3:M:108:VAL:C | 3:M:110:SER:H | 2.14 | 0.50 |
| 3:M:960:LYS:C | 3:M:962:ARG:N | 2.65 | 0.50 |
| 2:L:396:ASP:C | 2:L:398:THR:H | 2.15 | 0.50 |
| 2:L:523:ILE:C | 2:L:525:ALA:H | 2.15 | 0.50 |
| 2:C:111:ASP:C | 2:C:113:VAL:N | 2.65 | 0.50 |
| 2:C:198:ARG:C | 2:C:200:LEU:H | 2.15 | 0.50 |
| 3:M:541:ASN:C | 3:M:543:LEU:N | 2.61 | 0.50 |
| 3:D:1331:ASP:C | 3:D:1333:HIS:N | 2.65 | 0.50 |
| 5:Q:276:PRO:C | 5:Q:278:HIS:N | 2.65 | 0.49 |
| 2:C:523:ILE:C | 2:C:525:ALA:H | 2.15 | 0.49 |
| 1:J:70:GLY:HA3 | 1:J:135:GLY:HA3 | 1.93 | 0.49 |
| 3:D:950:GLY:C | 3:D:952:ASP:N | 2.63 | 0.49 |
| 2:L:892:LEU:C | 2:L:894:GLY:N | 2.66 | 0.49 |
| 2:C:302:VAL:C | 2:C:304:LEU:H | 2.15 | 0.49 |
| 1:A:223:ASN:C | 1:A:225:PHE:N | 2.65 | 0.49 |
| 3:D:1223:VAL:C | 3:D:1225:ALA:N | 2.65 | 0.49 |
| 1:B:31:GLY:C | 1:B:33:GLY:H | 2.15 | 0.49 |
| 2:L:111:ASP:C | 2:L:113:VAL:N | 2.65 | 0.49 |
| 3:M:975:GLU:C | 3:M:977:ALA:N | 2.65 | 0.49 |
| 2:L:581:THR:C | 2:L:583:LEU:N | 2.65 | 0.49 |
| 2:C:1041:GLU:C | 2:C:1043:TYR:N | 2.64 | 0.49 |
| 1:A:70:GLY:HA3 | 1:A:135:GLY:HA3 | 1.93 | 0.49 |
| 3:M:593:ASN:CA | 3:M:594:PRO:C | 2.81 | 0.49 |
| 2:L:774:LEU:C | 2:L:776:SER:N | 2.66 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------|--------------------------|-------------------|
| 2:C:919:ALA:C | 2:C:921:ALA:N | 2.64 | 0.49 |
| 2:L:198:ARG:C | 2:L:200:LEU:H | 2.15 | 0.49 |
| 3:M:1331:ASP:C | 3:M:1333:HIS:N | 2.65 | 0.49 |
| 2:C:89:THR:C | 2:C:91:GLN:H | 2.17 | 0.49 |
| 3:D:34:TYR:C | 3:D:36:THR:N | 2.66 | 0.49 |
| 4:N:25:LYS:C | 4:N:27:ALA:N | 2.66 | 0.48 |
| 2:C:774:LEU:C | 2:C:776:SER:N | 2.66 | 0.48 |
| 2:C:892:LEU:C | 2:C:894:GLY:N | 2.66 | 0.48 |
| 3:M:989:TYR:C | 3:M:991:GLN:N | 2.66 | 0.48 |
| 3:D:593:ASN:CA | 3:D:594:PRO:C | 2.81 | 0.48 |
| 3:D:1228:SER:C | 3:D:1230:GLY:H | 2.16 | 0.48 |
| 2:L:532:MET:C | 2:L:534:VAL:N | 2.67 | 0.48 |
| 2:C:532:MET:C | 2:C:534:VAL:N | 2.67 | 0.48 |
| 1:K:31:GLY:C | 1:K:33:GLY:H | 2.15 | 0.48 |
| 2:L:1033:GLY:HA2 | 3:M:620:GLY:CA | 2.37 | 0.48 |
| 3:D:975:GLU:C | 3:D:977:ALA:N | 2.65 | 0.48 |
| 3:M:1228:SER:C | 3:M:1230:GLY:H | 2.16 | 0.48 |
| 1:B:172:SER:C | 1:B:174:VAL:H | 2.17 | 0.48 |
| 2:L:89:THR:C | 2:L:91:GLN:H | 2.16 | 0.48 |
| 3:M:34:TYR:C | 3:M:36:THR:N | 2.66 | 0.48 |
| 2:C:27:LYS:C | 2:C:29:ALA:N | 2.67 | 0.48 |
| 1:K:223:ASN:C | 1:K:225:PHE:H | 2.17 | 0.48 |
| 2:C:1085:PHE:C | 2:C:1087:VAL:N | 2.66 | 0.48 |
| 3:M:1223:VAL:C | 3:M:1225:ALA:N | 2.65 | 0.48 |
| 2:L:1085:PHE:C | 2:L:1087:VAL:N | 2.66 | 0.48 |
| 3:M:1226:ALA:C | 3:M:1228:SER:N | 2.68 | 0.47 |
| 3:M:100:ALA:C | 3:M:102:ILE:H | 2.18 | 0.47 |
| 3:M:710:ARG:C | 3:M:712:GLY:N | 2.65 | 0.47 |
| 4:E:25:LYS:C | 4:E:27:ALA:N | 2.66 | 0.47 |
| 3:D:1141:GLU:C | 3:D:1143:GLY:N | 2.68 | 0.47 |
| 1:A:122:ILE:C | 1:A:124:ASN:H | 2.18 | 0.47 |
| 3:D:1191:PRO:C | 3:D:1193:THR:N | 2.67 | 0.47 |
| 3:M:877:PRO:C | 3:M:879:ARG:N | 2.68 | 0.47 |
| 1:B:223:ASN:C | 1:B:225:PHE:H | 2.17 | 0.47 |
| 3:M:1060:SER:C | 3:M:1062:ARG:N | 2.67 | 0.47 |
| 3:M:1448:THR:C | 3:M:1450:ALA:N | 2.67 | 0.47 |
| 4:E:43:GLU:C | 4:E:45:ARG:H | 2.18 | 0.47 |
| 4:E:43:GLU:C | 4:E:45:ARG:N | 2.67 | 0.47 |
| 1:K:172:SER:C | 1:K:174:VAL:H | 2.17 | 0.47 |
| 2:L:583:LEU:C | 2:L:585:GLU:N | 2.68 | 0.47 |
| 3:D:1321:ALA:C | 3:D:1323:GLN:H | 2.16 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 2:L:342:ASP:C | 2:L:344:PHE:H | 2.18 | 0.47 |
| 2:C:582:GLY:C | 2:C:584:GLU:N | 2.68 | 0.47 |
| 3:D:102:ILE:C | 3:D:104:PHE:N | 2.64 | 0.47 |
| 3:D:100:ALA:C | 3:D:102:ILE:H | 2.18 | 0.47 |
| 1:J:122:ILE:C | 1:J:124:ASN:H | 2.18 | 0.47 |
| 3:M:734:GLU:C | 3:M:736:PHE:N | 2.68 | 0.47 |
| 2:C:272:ALA:C | 2:C:274:ARG:N | 2.67 | 0.47 |
| 3:D:877:PRO:C | 3:D:879:ARG:N | 2.68 | 0.46 |
| 3:D:989:TYR:C | 3:D:991:GLN:N | 2.66 | 0.46 |
| 4:N:43:GLU:C | 4:N:45:ARG:N | 2.68 | 0.46 |
| 3:D:734:GLU:C | 3:D:736:PHE:N | 2.68 | 0.46 |
| 5:H:270:ALA:C | 5:H:272:THR:N | 2.69 | 0.46 |
| 1:K:223:ASN:C | 1:K:225:PHE:N | 2.68 | 0.46 |
| 2:L:1083:GLU:C | 2:L:1085:PHE:N | 2.66 | 0.46 |
| 2:L:27:LYS:C | 2:L:29:ALA:N | 2.67 | 0.46 |
| 2:C:342:ASP:C | 2:C:344:PHE:H | 2.18 | 0.46 |
| 3:M:1220:ALA:C | 3:M:1222:GLY:N | 2.68 | 0.46 |
| 1:B:223:ASN:C | 1:B:225:PHE:N | 2.68 | 0.46 |
| 2:L:1001:VAL:C | 2:L:1003:ASP:N | 2.68 | 0.46 |
| 5:H:378:GLU:C | 5:H:380:GLU:H | 2.19 | 0.46 |
| 2:C:1001:VAL:C | 2:C:1003:ASP:N | 2.68 | 0.46 |
| 3:M:1321:ALA:C | 3:M:1323:GLN:H | 2.16 | 0.46 |
| 3:M:841:PHE:C | 3:M:843:PHE:H | 2.19 | 0.46 |
| 3:D:150:ARG:C | 3:D:152:LEU:H | 2.19 | 0.46 |
| 5:Q:270:ALA:C | 5:Q:272:THR:N | 2.69 | 0.46 |
| 5:Q:179:LYS:C | 5:Q:181:LEU:H | 2.19 | 0.46 |
| 3:M:148:GLU:C | 3:M:150:ARG:H | 2.18 | 0.46 |
| 5:Q:216:LYS:C | 5:Q:218:THR:H | 2.19 | 0.46 |
| 3:D:148:GLU:C | 3:D:150:ARG:H | 2.18 | 0.46 |
| 3:M:580:ALA:C | 3:M:582:ILE:N | 2.69 | 0.46 |
| 2:C:583:LEU:C | 2:C:585:GLU:N | 2.68 | 0.46 |
| 3:D:1226:ALA:C | 3:D:1228:SER:N | 2.68 | 0.46 |
| 2:C:342:ASP:C | 2:C:344:PHE:N | 2.70 | 0.46 |
| 5:Q:421:ARG:C | 5:Q:423:LEU:H | 2.19 | 0.46 |
| 5:H:216:LYS:C | 5:H:218:THR:H | 2.19 | 0.46 |
| 3:D:117:ASP:C | 3:D:119:SER:N | 2.70 | 0.46 |
| 2:C:1083:GLU:C | 2:C:1085:PHE:N | 2.66 | 0.46 |
| 3:M:150:ARG:C | 3:M:152:LEU:H | 2.19 | 0.46 |
| 3:M:688:TRP:C | 3:M:690:ALA:N | 2.69 | 0.46 |
| 3:M:487:ALA:C | 3:M:489:ARG:N | 2.70 | 0.46 |
| 2:L:272:ALA:C | 2:L:274:ARG:N | 2.67 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------|--------------------------|-------------------|
| 1:J:118:ALA:C | 1:J:120:VAL:H | 2.20 | 0.46 |
| 3:M:508:ARG:C | 3:M:510:GLU:H | 2.19 | 0.46 |
| 3:D:580:ALA:C | 3:D:582:ILE:N | 2.69 | 0.45 |
| 4:N:43:GLU:C | 4:N:45:ARG:H | 2.18 | 0.45 |
| 5:Q:378:GLU:C | 5:Q:380:GLU:H | 2.19 | 0.45 |
| 3:D:1090:ASP:C | 3:D:1092:GLY:N | 2.69 | 0.45 |
| 3:D:508:ARG:C | 3:D:510:GLU:H | 2.19 | 0.45 |
| 2:L:437:ARG:C | 2:L:439:CYS:N | 2.69 | 0.45 |
| 3:D:841:PHE:C | 3:D:843:PHE:H | 2.19 | 0.45 |
| 2:L:976:ASP:C | 2:L:978:ARG:H | 2.19 | 0.45 |
| 3:D:1060:SER:C | 3:D:1062:ARG:N | 2.67 | 0.45 |
| 3:D:740:PHE:C | 3:D:742:GLY:H | 2.20 | 0.45 |
| 3:D:688:TRP:C | 3:D:690:ALA:N | 2.69 | 0.45 |
| 2:L:774:LEU:C | 2:L:776:SER:H | 2.20 | 0.45 |
| 3:M:892:ASP:C | 3:M:894:LYS:N | 2.70 | 0.45 |
| 3:D:930:LEU:C | 3:D:932:ASP:N | 2.69 | 0.45 |
| 1:J:111:ALA:C | 1:J:113:ASP:H | 2.20 | 0.45 |
| 5:H:421:ARG:C | 5:H:423:LEU:H | 2.19 | 0.45 |
| 5:H:179:LYS:C | 5:H:181:LEU:H | 2.19 | 0.45 |
| 3:M:740:PHE:C | 3:M:742:GLY:H | 2.20 | 0.45 |
| 1:J:156:HIS:C | 1:J:158:ILE:H | 2.20 | 0.45 |
| 2:C:1033:GLY:HA2 | 3:D:620:GLY:CA | 2.37 | 0.45 |
| 3:M:1141:GLU:C | 3:M:1143:GLY:N | 2.68 | 0.45 |
| 2:L:342:ASP:C | 2:L:344:PHE:N | 2.70 | 0.45 |
| 4:E:84:ARG:C | 4:E:86:GLN:N | 2.70 | 0.45 |
| 3:D:619:LEU:C | 3:D:621:LYS:H | 2.20 | 0.45 |
| 3:D:1196:THR:C | 3:D:1198:TYR:N | 2.70 | 0.45 |
| 1:A:111:ALA:C | 1:A:113:ASP:H | 2.20 | 0.45 |
| 3:D:487:ALA:C | 3:D:489:ARG:N | 2.70 | 0.45 |
| 1:K:34:VAL:C | 1:K:36:LEU:H | 2.21 | 0.45 |
| 4:E:86:GLN:C | 4:E:89:MET:H | 2.20 | 0.45 |
| 2:C:63:GLY:HA3 | 2:C:102:HIS:CA | 2.47 | 0.45 |
| 4:N:86:GLN:C | 4:N:89:MET:H | 2.20 | 0.45 |
| 3:M:619:LEU:C | 3:M:621:LYS:H | 2.20 | 0.45 |
| 3:M:1260:ILE:C | 3:M:1262:LEU:N | 2.68 | 0.45 |
| 2:C:450:GLY:C | 2:C:452:ILE:N | 2.70 | 0.44 |
| 2:C:178:ALA:C | 2:C:180:GLY:N | 2.70 | 0.44 |
| 3:M:117:ASP:C | 3:M:119:SER:N | 2.69 | 0.44 |
| 3:D:470:LEU:C | 3:D:472:LYS:N | 2.71 | 0.44 |
| 2:C:976:ASP:C | 2:C:978:ARG:H | 2.19 | 0.44 |
| 3:M:1462:LEU:C | 3:M:1464:GLU:N | 2.69 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 2:L:63:GLY:HA3 | 2:L:102:HIS:CA | 2.47 | 0.44 |
| 3:D:892:ASP:C | 3:D:894:LYS:N | 2.70 | 0.44 |
| 1:B:79:ILE:C | 1:B:81:ASN:N | 2.70 | 0.44 |
| 3:M:470:LEU:C | 3:M:472:LYS:N | 2.71 | 0.44 |
| 3:D:1260:ILE:C | 3:D:1262:LEU:N | 2.68 | 0.44 |
| 2:L:450:GLY:C | 2:L:452:ILE:N | 2.70 | 0.44 |
| 2:C:774:LEU:C | 2:C:776:SER:H | 2.20 | 0.44 |
| 1:A:156:HIS:C | 1:A:158:ILE:H | 2.20 | 0.44 |
| 3:M:1090:ASP:C | 3:M:1092:GLY:N | 2.69 | 0.44 |
| 5:Q:211:VAL:C | 5:Q:213:ILE:H | 2.20 | 0.44 |
| 3:M:937:TYR:C | 3:M:939:PHE:N | 2.70 | 0.44 |
| 3:D:710:ARG:C | 3:D:712:GLY:N | 2.65 | 0.44 |
| 5:H:276:PRO:C | 5:H:278:HIS:N | 2.65 | 0.44 |
| 3:M:639:LEU:C | 3:M:641:GLN:N | 2.71 | 0.44 |
| 3:D:639:LEU:C | 3:D:641:GLN:N | 2.71 | 0.44 |
| 5:Q:179:LYS:C | 5:Q:181:LEU:N | 2.71 | 0.44 |
| 2:C:1041:GLU:C | 2:C:1043:TYR:H | 2.21 | 0.44 |
| 3:D:1220:ALA:C | 3:D:1222:GLY:N | 2.68 | 0.44 |
| 1:K:79:ILE:C | 1:K:81:ASN:N | 2.70 | 0.44 |
| 5:H:211:VAL:C | 5:H:213:ILE:H | 2.20 | 0.44 |
| 2:C:325:ILE:C | 2:C:327:HIS:N | 2.71 | 0.44 |
| 3:D:1448:THR:C | 3:D:1450:ALA:N | 2.67 | 0.44 |
| 3:M:1191:PRO:C | 3:M:1193:THR:N | 2.67 | 0.44 |
| 2:L:20:GLU:C | 2:L:22:GLN:N | 2.71 | 0.44 |
| 3:D:1172:HIS:C | 3:D:1174:LEU:N | 2.70 | 0.44 |
| 3:D:1321:ALA:C | 3:D:1323:GLN:N | 2.71 | 0.44 |
| 2:C:692:GLU:C | 2:C:694:LEU:N | 2.70 | 0.44 |
| 3:D:815:ALA:C | 3:D:817:GLU:H | 2.21 | 0.44 |
| 3:M:930:LEU:C | 3:M:932:ASP:N | 2.69 | 0.44 |
| 1:B:34:VAL:C | 1:B:36:LEU:H | 2.21 | 0.43 |
| 3:M:1196:THR:C | 3:M:1198:TYR:N | 2.70 | 0.43 |
| 5:H:179:LYS:C | 5:H:181:LEU:N | 2.71 | 0.43 |
| 3:M:996:TRP:C | 3:M:998:GLU:N | 2.69 | 0.43 |
| 1:K:70:GLY:HA3 | 1:K:135:GLY:HA3 | 2.00 | 0.43 |
| 2:L:919:ALA:C | 2:L:921:ALA:H | 2.21 | 0.43 |
| 4:N:84:ARG:C | 4:N:86:GLN:N | 2.70 | 0.43 |
| 2:L:430:VAL:C | 2:L:432:ARG:N | 2.72 | 0.43 |
| 3:D:757:ALA:C | 3:D:759:ALA:N | 2.70 | 0.43 |
| 3:D:993:ILE:C | 3:D:995:LEU:N | 2.71 | 0.43 |
| 2:L:1041:GLU:C | 2:L:1043:TYR:H | 2.21 | 0.43 |
| 2:C:965:GLU:C | 2:C:967:PHE:N | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:D:855:HIS:C | 3:D:857:LEU:N | 2.70 | 0.43 |
| 3:M:22:SER:C | 3:M:24:GLY:H | 2.22 | 0.43 |
| 3:M:815:ALA:C | 3:M:817:GLU:H | 2.21 | 0.43 |
| 2:L:946:ARG:C | 2:L:948:GLU:N | 2.71 | 0.43 |
| 1:A:118:ALA:C | 1:A:120:VAL:H | 2.20 | 0.43 |
| 4:N:11:GLY:C | 4:N:13:VAL:N | 2.71 | 0.43 |
| 2:L:582:GLY:C | 2:L:584:GLU:N | 2.68 | 0.43 |
| 2:C:561:GLY:C | 2:C:563:ASN:N | 2.71 | 0.43 |
| 3:M:1386:ASP:C | 3:M:1388:ARG:H | 2.22 | 0.43 |
| 3:M:602:SER:C | 3:M:604:THR:H | 2.22 | 0.43 |
| 3:D:22:SER:C | 3:D:24:GLY:H | 2.22 | 0.43 |
| 3:M:1172:HIS:C | 3:M:1174:LEU:N | 2.70 | 0.43 |
| 2:C:20:GLU:C | 2:C:22:GLN:N | 2.71 | 0.43 |
| 4:N:70:THR:C | 4:N:72:ARG:N | 2.69 | 0.43 |
| 2:C:583:LEU:C | 2:C:585:GLU:H | 2.21 | 0.43 |
| 2:C:919:ALA:C | 2:C:921:ALA:H | 2.21 | 0.43 |
| 3:D:1386:ASP:C | 3:D:1388:ARG:H | 2.22 | 0.43 |
| 4:E:70:THR:C | 4:E:72:ARG:N | 2.69 | 0.43 |
| 3:D:937:TYR:C | 3:D:939:PHE:N | 2.70 | 0.43 |
| 4:E:83:ASP:C | 4:E:85:LEU:H | 2.22 | 0.43 |
| 1:B:70:GLY:HA3 | 1:B:135:GLY:HA3 | 2.00 | 0.43 |
| 3:D:1462:LEU:C | 3:D:1464:GLU:N | 2.69 | 0.43 |
| 1:J:71:VAL:C | 2:L:608:GLY:HA2 | 2.40 | 0.42 |
| 3:M:1321:ALA:C | 3:M:1323:GLN:N | 2.71 | 0.42 |
| 2:C:946:ARG:C | 2:C:948:GLU:N | 2.71 | 0.42 |
| 3:M:731:LEU:C | 3:M:733:CYS:N | 2.70 | 0.42 |
| 2:L:692:GLU:C | 2:L:694:LEU:N | 2.70 | 0.42 |
| 3:M:643:GLY:HA3 | 3:M:727:GLN:N | 2.33 | 0.42 |
| 2:L:178:ALA:C | 2:L:180:GLY:N | 2.70 | 0.42 |
| 2:L:917:LEU:C | 2:L:919:ALA:N | 2.73 | 0.42 |
| 3:M:937:TYR:C | 3:M:939:PHE:H | 2.23 | 0.42 |
| 3:M:764:LEU:C | 3:M:766:ALA:N | 2.73 | 0.42 |
| 3:D:731:LEU:C | 3:D:733:CYS:N | 2.70 | 0.42 |
| 3:M:467:GLU:C | 3:M:469:ASP:N | 2.73 | 0.42 |
| 2:L:570:PRO:C | 2:L:572:ILE:N | 2.72 | 0.42 |
| 2:C:302:VAL:C | 2:C:304:LEU:N | 2.73 | 0.42 |
| 3:M:1098:LEU:C | 3:M:1100:ASP:N | 2.72 | 0.42 |
| 1:A:189:ARG:C | 1:A:191:ASP:H | 2.22 | 0.42 |
| 1:J:79:ILE:C | 1:J:81:ASN:N | 2.72 | 0.42 |
| 3:M:1009:LYS:C | 3:M:1011:PHE:N | 2.70 | 0.42 |
| 3:D:996:TRP:C | 3:D:998:GLU:N | 2.69 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 2:L:549:PHE:C | 2:L:551:GLU:N | 2.72 | 0.42 |
| 3:M:855:HIS:C | 3:M:857:LEU:N | 2.70 | 0.42 |
| 3:D:937:TYR:C | 3:D:939:PHE:H | 2.23 | 0.42 |
| 2:L:583:LEU:C | 2:L:585:GLU:H | 2.21 | 0.42 |
| 1:A:71:VAL:C | 2:C:608:GLY:HA2 | 2.40 | 0.42 |
| 2:C:917:LEU:C | 2:C:919:ALA:N | 2.73 | 0.42 |
| 2:C:320:HIS:C | 2:C:322:VAL:H | 2.23 | 0.42 |
| 4:E:17:TYR:C | 4:E:19:LEU:N | 2.72 | 0.42 |
| 3:M:885:ILE:C | 3:M:887:GLY:N | 2.73 | 0.42 |
| 2:L:1015:LEU:C | 2:L:1017:THR:N | 2.73 | 0.42 |
| 3:D:1098:LEU:C | 3:D:1100:ASP:N | 2.72 | 0.42 |
| 4:N:17:TYR:C | 4:N:19:LEU:N | 2.72 | 0.42 |
| 4:N:67:GLU:C | 4:N:69:LEU:H | 2.24 | 0.42 |
| 4:E:67:GLU:C | 4:E:69:LEU:H | 2.24 | 0.42 |
| 2:L:965:GLU:C | 2:L:967:PHE:N | 2.71 | 0.42 |
| 2:C:437:ARG:C | 2:C:439:CYS:N | 2.69 | 0.42 |
| 3:M:993:ILE:C | 3:M:995:LEU:N | 2.71 | 0.42 |
| 1:J:189:ARG:C | 1:J:191:ASP:H | 2.22 | 0.42 |
| 4:N:83:ASP:C | 4:N:85:LEU:H | 2.22 | 0.42 |
| 4:E:11:GLY:C | 4:E:13:VAL:N | 2.71 | 0.41 |
| 1:A:79:ILE:C | 1:A:81:ASN:N | 2.72 | 0.41 |
| 2:C:1001:VAL:C | 2:C:1003:ASP:H | 2.23 | 0.41 |
| 3:D:602:SER:C | 3:D:604:THR:H | 2.22 | 0.41 |
| 2:L:1001:VAL:C | 2:L:1003:ASP:H | 2.23 | 0.41 |
| 4:N:84:ARG:C | 4:N:87:LYS:H | 2.24 | 0.41 |
| 3:D:941:LEU:C | 3:D:943:THR:N | 2.71 | 0.41 |
| 3:D:764:LEU:C | 3:D:766:ALA:N | 2.72 | 0.41 |
| 3:D:764:LEU:C | 3:D:766:ALA:H | 2.24 | 0.41 |
| 3:D:885:ILE:C | 3:D:887:GLY:N | 2.73 | 0.41 |
| 3:M:491:LYS:C | 3:M:493:ARG:N | 2.73 | 0.41 |
| 2:L:320:HIS:C | 2:L:322:VAL:H | 2.23 | 0.41 |
| 2:L:171:TRP:H | 2:L:187:ASN:CA | 2.33 | 0.41 |
| 3:D:82:ARG:C | 3:D:84:ILE:H | 2.23 | 0.41 |
| 2:C:663:GLU:C | 2:C:665:PHE:H | 2.24 | 0.41 |
| 2:C:549:PHE:C | 2:C:551:GLU:N | 2.72 | 0.41 |
| 3:M:1090:ASP:C | 3:M:1092:GLY:H | 2.23 | 0.41 |
| 3:M:1353:GLN:C | 3:M:1355:VAL:N | 2.74 | 0.41 |
| 2:L:463:ALA:C | 2:L:465:GLY:N | 2.72 | 0.41 |
| 2:L:347:GLY:C | 2:L:349:ALA:N | 2.70 | 0.41 |
| 2:L:808:ARG:C | 2:L:810:ASP:N | 2.73 | 0.41 |
| 2:C:1015:LEU:C | 2:C:1017:THR:N | 2.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 3:M:56:TYR:C | 3:M:58:CYS:H | 2.24 | 0.41 |
| 2:C:430:VAL:C | 2:C:432:ARG:N | 2.72 | 0.41 |
| 2:L:325:ILE:C | 2:L:327:HIS:N | 2.71 | 0.41 |
| 3:D:465:LEU:C | 3:D:467:GLU:N | 2.72 | 0.41 |
| 3:M:21:TRP:C | 3:M:23:TYR:N | 2.73 | 0.41 |
| 3:D:1129:THR:C | 3:D:1131:THR:H | 2.24 | 0.41 |
| 3:D:1270:ALA:C | 3:D:1272:ALA:H | 2.23 | 0.41 |
| 3:M:541:ASN:C | 3:M:543:LEU:H | 2.24 | 0.41 |
| 3:D:1331:ASP:C | 3:D:1333:HIS:H | 2.24 | 0.41 |
| 2:C:463:ALA:C | 2:C:465:GLY:N | 2.72 | 0.41 |
| 3:M:1270:ALA:C | 3:M:1272:ALA:H | 2.23 | 0.41 |
| 3:D:1020:LEU:C | 3:D:1022:VAL:N | 2.74 | 0.41 |
| 3:D:1090:ASP:C | 3:D:1092:GLY:H | 2.23 | 0.41 |
| 3:D:56:TYR:C | 3:D:58:CYS:H | 2.24 | 0.41 |
| 3:M:1129:THR:C | 3:M:1131:THR:H | 2.24 | 0.41 |
| 2:L:943:VAL:C | 2:L:945:ALA:H | 2.24 | 0.41 |
| 3:D:541:ASN:C | 3:D:543:LEU:H | 2.24 | 0.41 |
| 2:L:302:VAL:C | 2:L:304:LEU:N | 2.73 | 0.41 |
| 3:M:82:ARG:C | 3:M:84:ILE:H | 2.23 | 0.41 |
| 3:M:941:LEU:C | 3:M:943:THR:N | 2.71 | 0.41 |
| 2:L:561:GLY:C | 2:L:563:ASN:N | 2.71 | 0.41 |
| 3:D:643:GLY:HA3 | 3:D:727:GLN:N | 2.33 | 0.41 |
| 3:M:1032:PRO:C | 3:M:1034:GLN:N | 2.74 | 0.41 |
| 2:C:884:GLN:C | 2:C:886:LEU:N | 2.75 | 0.41 |
| 5:Q:94:ASP:C | 5:Q:96:VAL:H | 2.25 | 0.41 |
| 2:C:570:PRO:C | 2:C:572:ILE:N | 2.72 | 0.40 |
| 2:C:520:GLU:C | 2:C:522:VAL:N | 2.75 | 0.40 |
| 4:N:57:ASP:C | 4:N:59:ASN:H | 2.25 | 0.40 |
| 1:B:172:SER:C | 1:B:174:VAL:N | 2.75 | 0.40 |
| 4:E:84:ARG:C | 4:E:87:LYS:H | 2.24 | 0.40 |
| 3:D:1100:ASP:C | 3:D:1102:ALA:N | 2.75 | 0.40 |
| 2:L:1055:ILE:C | 2:L:1057:SER:H | 2.25 | 0.40 |
| 3:D:31:THR:C | 3:D:33:ASN:H | 2.25 | 0.40 |
| 3:M:31:THR:C | 3:M:33:ASN:H | 2.25 | 0.40 |
| 2:C:915:LYS:C | 2:C:917:LEU:N | 2.73 | 0.40 |
| 3:D:571:LYS:C | 3:D:573:MET:N | 2.74 | 0.40 |
| 3:D:138:LYS:C | 3:D:140:ALA:H | 2.25 | 0.40 |
| 2:L:663:GLU:C | 2:L:665:PHE:H | 2.24 | 0.40 |
| 3:M:571:LYS:C | 3:M:573:MET:N | 2.74 | 0.40 |
| 3:D:1353:GLN:C | 3:D:1355:VAL:N | 2.74 | 0.40 |
| 3:M:1331:ASP:C | 3:M:1333:HIS:H | 2.24 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|--------------|--------------------------|-------------------|
| 5:H:94:ASP:C | 5:H:96:VAL:H | 2.25 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|------------|-------------|---|
| 1 | A | 222/314 (71%) | 95 (43%) | 65 (29%) | 62 (28%) | 0 | 0 |
| 1 | B | 218/314 (69%) | 110 (50%) | 53 (24%) | 55 (25%) | 0 | 1 |
| 1 | J | 222/314 (71%) | 95 (43%) | 65 (29%) | 62 (28%) | 0 | 0 |
| 1 | K | 218/314 (69%) | 110 (50%) | 53 (24%) | 55 (25%) | 0 | 1 |
| 2 | C | 1072/1118 (96%) | 439 (41%) | 296 (28%) | 337 (31%) | 0 | 0 |
| 2 | L | 1072/1118 (96%) | 439 (41%) | 294 (27%) | 339 (32%) | 0 | 0 |
| 3 | D | 1175/1524 (77%) | 456 (39%) | 307 (26%) | 412 (35%) | 0 | 0 |
| 3 | M | 1175/1524 (77%) | 456 (39%) | 309 (26%) | 410 (35%) | 0 | 0 |
| 4 | E | 90/99 (91%) | 40 (44%) | 24 (27%) | 26 (29%) | 0 | 0 |
| 4 | N | 90/99 (91%) | 40 (44%) | 24 (27%) | 26 (29%) | 0 | 0 |
| 5 | H | 318/332 (96%) | 209 (66%) | 57 (18%) | 52 (16%) | 0 | 5 |
| 5 | Q | 318/332 (96%) | 209 (66%) | 57 (18%) | 52 (16%) | 0 | 5 |
| All | All | 6190/7402 (84%) | 2698 (44%) | 1604 (26%) | 1888 (30%) | 0 | 0 |

All (1888) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 59 | GLU |
| 1 | A | 64 | GLU |
| 1 | A | 76 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 125 | PRO |
| 1 | A | 137 | LYS |
| 1 | A | 148 | VAL |
| 1 | A | 153 | ALA |
| 1 | A | 158 | ILE |
| 1 | A | 162 | ILE |
| 1 | A | 172 | SER |
| 1 | A | 176 | ARG |
| 1 | A | 182 | GLU |
| 1 | A | 188 | GLN |
| 1 | A | 199 | ILE |
| 1 | A | 208 | LEU |
| 1 | A | 216 | ALA |
| 1 | A | 226 | ALA |
| 1 | B | 7 | LYS |
| 1 | B | 15 | THR |
| 1 | B | 29 | GLU |
| 1 | B | 54 | THR |
| 1 | B | 75 | VAL |
| 1 | B | 91 | ASP |
| 1 | B | 104 | GLU |
| 1 | B | 106 | PRO |
| 1 | B | 114 | PHE |
| 1 | B | 128 | HIS |
| 1 | B | 135 | GLY |
| 1 | B | 158 | ILE |
| 1 | B | 171 | PHE |
| 1 | B | 181 | VAL |
| 1 | B | 185 | ARG |
| 1 | B | 186 | LEU |
| 1 | B | 191 | ASP |
| 1 | B | 195 | LEU |
| 1 | B | 200 | TRP |
| 1 | B | 224 | TYR |
| 2 | C | 17 | PRO |
| 2 | C | 22 | GLN |
| 2 | C | 27 | LYS |
| 2 | C | 31 | GLN |
| 2 | C | 33 | ASP |
| 2 | C | 40 | GLU |
| 2 | C | 42 | VAL |
| 2 | C | 46 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 47 | ALA |
| 2 | C | 54 | ILE |
| 2 | C | 70 | GLU |
| 2 | C | 80 | GLN |
| 2 | C | 88 | LEU |
| 2 | C | 102 | HIS |
| 2 | C | 109 | LYS |
| 2 | C | 111 | ASP |
| 2 | C | 114 | PHE |
| 2 | C | 115 | LEU |
| 2 | C | 136 | ILE |
| 2 | C | 137 | VAL |
| 2 | C | 153 | ALA |
| 2 | C | 155 | PRO |
| 2 | C | 168 | ARG |
| 2 | C | 182 | VAL |
| 2 | C | 187 | ASN |
| 2 | C | 199 | VAL |
| 2 | C | 221 | LEU |
| 2 | C | 244 | PRO |
| 2 | C | 263 | ASP |
| 2 | C | 264 | PRO |
| 2 | C | 269 | LEU |
| 2 | C | 275 | TYR |
| 2 | C | 278 | GLU |
| 2 | C | 288 | ARG |
| 2 | C | 322 | VAL |
| 2 | C | 336 | VAL |
| 2 | C | 370 | ALA |
| 2 | C | 392 | SER |
| 2 | C | 395 | LYS |
| 2 | C | 397 | GLU |
| 2 | C | 398 | THR |
| 2 | C | 402 | SER |
| 2 | C | 409 | ARG |
| 2 | C | 418 | LEU |
| 2 | C | 420 | ARG |
| 2 | C | 425 | PHE |
| 2 | C | 430 | VAL |
| 2 | C | 431 | HIS |
| 2 | C | 432 | ARG |
| 2 | C | 434 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 444 | PRO |
| 2 | C | 449 | ILE |
| 2 | C | 451 | LEU |
| 2 | C | 457 | ALA |
| 2 | C | 483 | VAL |
| 2 | C | 496 | ILE |
| 2 | C | 498 | GLN |
| 2 | C | 503 | LEU |
| 2 | C | 518 | ARG |
| 2 | C | 522 | VAL |
| 2 | C | 526 | PRO |
| 2 | C | 530 | GLU |
| 2 | C | 532 | MET |
| 2 | C | 537 | LYS |
| 2 | C | 541 | SER |
| 2 | C | 543 | ASN |
| 2 | C | 545 | ASN |
| 2 | C | 548 | PRO |
| 2 | C | 574 | ALA |
| 2 | C | 580 | MET |
| 2 | C | 587 | VAL |
| 2 | C | 588 | VAL |
| 2 | C | 599 | GLU |
| 2 | C | 603 | VAL |
| 2 | C | 604 | VAL |
| 2 | C | 612 | ALA |
| 2 | C | 616 | GLU |
| 2 | C | 629 | ALA |
| 2 | C | 633 | GLN |
| 2 | C | 641 | PRO |
| 2 | C | 643 | VAL |
| 2 | C | 644 | ARG |
| 2 | C | 656 | ALA |
| 2 | C | 657 | ASP |
| 2 | C | 663 | GLU |
| 2 | C | 677 | MET |
| 2 | C | 713 | ARG |
| 2 | C | 714 | ASP |
| 2 | C | 715 | THR |
| 2 | C | 728 | HIS |
| 2 | C | 735 | ARG |
| 2 | C | 738 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 760 | SER |
| 2 | C | 762 | LYS |
| 2 | C | 767 | PRO |
| 2 | C | 788 | THR |
| 2 | C | 804 | LEU |
| 2 | C | 831 | ARG |
| 2 | C | 832 | LYS |
| 2 | C | 840 | ALA |
| 2 | C | 848 | VAL |
| 2 | C | 849 | VAL |
| 2 | C | 871 | LEU |
| 2 | C | 880 | MET |
| 2 | C | 884 | GLN |
| 2 | C | 885 | ILE |
| 2 | C | 919 | ALA |
| 2 | C | 920 | GLU |
| 2 | C | 944 | LEU |
| 2 | C | 957 | LYS |
| 2 | C | 964 | LYS |
| 2 | C | 965 | GLU |
| 2 | C | 967 | PHE |
| 2 | C | 973 | VAL |
| 2 | C | 974 | LEU |
| 2 | C | 984 | GLU |
| 2 | C | 999 | HIS |
| 2 | C | 1000 | MET |
| 2 | C | 1011 | GLY |
| 2 | C | 1012 | PRO |
| 2 | C | 1021 | LEU |
| 2 | C | 1027 | PHE |
| 2 | C | 1035 | MET |
| 2 | C | 1038 | TRP |
| 2 | C | 1053 | LEU |
| 2 | C | 1075 | ASP |
| 2 | C | 1078 | GLU |
| 2 | C | 1104 | GLU |
| 3 | D | 5 | VAL |
| 3 | D | 10 | ILE |
| 3 | D | 12 | LEU |
| 3 | D | 13 | ALA |
| 3 | D | 26 | VAL |
| 3 | D | 28 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 33 | ASN |
| 3 | D | 41 | ARG |
| 3 | D | 52 | PRO |
| 3 | D | 64 | LYS |
| 3 | D | 97 | THR |
| 3 | D | 98 | PRO |
| 3 | D | 100 | ALA |
| 3 | D | 109 | PRO |
| 3 | D | 110 | SER |
| 3 | D | 117 | ASP |
| 3 | D | 119 | SER |
| 3 | D | 126 | VAL |
| 3 | D | 131 | LYS |
| 3 | D | 140 | ALA |
| 3 | D | 141 | VAL |
| 3 | D | 143 | ASP |
| 3 | D | 146 | PRO |
| 3 | D | 147 | VAL |
| 3 | D | 454 | ALA |
| 3 | D | 477 | LEU |
| 3 | D | 478 | LEU |
| 3 | D | 479 | GLU |
| 3 | D | 484 | PRO |
| 3 | D | 486 | ARG |
| 3 | D | 487 | ALA |
| 3 | D | 488 | ARG |
| 3 | D | 491 | LYS |
| 3 | D | 526 | PRO |
| 3 | D | 530 | VAL |
| 3 | D | 531 | ASP |
| 3 | D | 535 | PHE |
| 3 | D | 547 | LEU |
| 3 | D | 548 | ILE |
| 3 | D | 564 | GLU |
| 3 | D | 565 | ILE |
| 3 | D | 571 | LYS |
| 3 | D | 582 | ILE |
| 3 | D | 607 | LEU |
| 3 | D | 626 | SER |
| 3 | D | 630 | VAL |
| 3 | D | 633 | VAL |
| 3 | D | 638 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 646 | LYS |
| 3 | D | 647 | ARG |
| 3 | D | 648 | MET |
| 3 | D | 649 | ALA |
| 3 | D | 650 | LEU |
| 3 | D | 655 | PRO |
| 3 | D | 662 | GLU |
| 3 | D | 665 | ALA |
| 3 | D | 668 | PRO |
| 3 | D | 672 | ALA |
| 3 | D | 678 | GLU |
| 3 | D | 679 | ARG |
| 3 | D | 682 | ASP |
| 3 | D | 684 | LYS |
| 3 | D | 696 | HIS |
| 3 | D | 702 | LEU |
| 3 | D | 718 | PRO |
| 3 | D | 725 | SER |
| 3 | D | 730 | PRO |
| 3 | D | 731 | LEU |
| 3 | D | 739 | ASP |
| 3 | D | 762 | GLN |
| 3 | D | 770 | LEU |
| 3 | D | 782 | SER |
| 3 | D | 793 | THR |
| 3 | D | 795 | VAL |
| 3 | D | 797 | LYS |
| 3 | D | 799 | LYS |
| 3 | D | 807 | ALA |
| 3 | D | 808 | THR |
| 3 | D | 811 | GLU |
| 3 | D | 815 | ALA |
| 3 | D | 821 | VAL |
| 3 | D | 825 | ALA |
| 3 | D | 826 | PRO |
| 3 | D | 828 | VAL |
| 3 | D | 829 | VAL |
| 3 | D | 835 | SER |
| 3 | D | 838 | ARG |
| 3 | D | 840 | LYS |
| 3 | D | 842 | VAL |
| 3 | D | 848 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 849 | ALA |
| 3 | D | 862 | ASP |
| 3 | D | 875 | THR |
| 3 | D | 898 | GLU |
| 3 | D | 899 | LEU |
| 3 | D | 900 | ILE |
| 3 | D | 905 | PRO |
| 3 | D | 908 | LYS |
| 3 | D | 919 | PHE |
| 3 | D | 924 | MET |
| 3 | D | 925 | GLU |
| 3 | D | 947 | ILE |
| 3 | D | 948 | THR |
| 3 | D | 953 | ASP |
| 3 | D | 961 | GLN |
| 3 | D | 966 | GLU |
| 3 | D | 1000 | THR |
| 3 | D | 1006 | ALA |
| 3 | D | 1016 | PRO |
| 3 | D | 1023 | MET |
| 3 | D | 1028 | ALA |
| 3 | D | 1029 | ARG |
| 3 | D | 1040 | GLY |
| 3 | D | 1045 | MET |
| 3 | D | 1054 | GLU |
| 3 | D | 1059 | SER |
| 3 | D | 1061 | PHE |
| 3 | D | 1067 | VAL |
| 3 | D | 1109 | GLU |
| 3 | D | 1111 | ASP |
| 3 | D | 1113 | GLY |
| 3 | D | 1116 | ASN |
| 3 | D | 1141 | GLU |
| 3 | D | 1149 | LEU |
| 3 | D | 1152 | GLU |
| 3 | D | 1178 | ALA |
| 3 | D | 1190 | SER |
| 3 | D | 1194 | CYS |
| 3 | D | 1195 | GLN |
| 3 | D | 1201 | CYS |
| 3 | D | 1203 | LYS |
| 3 | D | 1208 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 1209 | LEU |
| 3 | D | 1210 | SER |
| 3 | D | 1219 | GLU |
| 3 | D | 1223 | VAL |
| 3 | D | 1224 | VAL |
| 3 | D | 1225 | ALA |
| 3 | D | 1231 | GLU |
| 3 | D | 1232 | PRO |
| 3 | D | 1234 | THR |
| 3 | D | 1236 | LEU |
| 3 | D | 1239 | ARG |
| 3 | D | 1268 | PRO |
| 3 | D | 1276 | GLU |
| 3 | D | 1281 | VAL |
| 3 | D | 1296 | SER |
| 3 | D | 1300 | SER |
| 3 | D | 1306 | PRO |
| 3 | D | 1313 | VAL |
| 3 | D | 1320 | GLU |
| 3 | D | 1321 | ALA |
| 3 | D | 1323 | GLN |
| 3 | D | 1330 | ILE |
| 3 | D | 1347 | TYR |
| 3 | D | 1364 | HIS |
| 3 | D | 1366 | LYS |
| 3 | D | 1367 | HIS |
| 3 | D | 1373 | ARG |
| 3 | D | 1374 | GLN |
| 3 | D | 1375 | MET |
| 3 | D | 1384 | PRO |
| 3 | D | 1388 | ARG |
| 3 | D | 1394 | VAL |
| 3 | D | 1396 | GLU |
| 3 | D | 1408 | ILE |
| 3 | D | 1424 | VAL |
| 3 | D | 1436 | SER |
| 3 | D | 1439 | SER |
| 3 | D | 1442 | ASN |
| 3 | D | 1445 | HIS |
| 3 | D | 1448 | THR |
| 3 | D | 1451 | ALA |
| 3 | D | 1452 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 1455 | LYS |
| 3 | D | 1457 | ASP |
| 3 | D | 1458 | GLU |
| 3 | D | 1462 | LEU |
| 3 | D | 1464 | GLU |
| 3 | D | 1483 | PHE |
| 3 | D | 1487 | VAL |
| 4 | E | 16 | LYS |
| 4 | E | 21 | VAL |
| 4 | E | 30 | LEU |
| 4 | E | 34 | ARG |
| 4 | E | 42 | PRO |
| 4 | E | 50 | THR |
| 4 | E | 51 | LEU |
| 4 | E | 60 | ALA |
| 4 | E | 61 | VAL |
| 4 | E | 77 | GLU |
| 4 | E | 90 | GLU |
| 5 | H | 171 | VAL |
| 5 | H | 203 | ILE |
| 5 | H | 211 | VAL |
| 5 | H | 220 | ARG |
| 5 | H | 249 | LYS |
| 5 | H | 251 | SER |
| 5 | H | 328 | GLU |
| 5 | H | 329 | PRO |
| 5 | H | 333 | GLU |
| 5 | H | 335 | PRO |
| 5 | H | 352 | ASN |
| 5 | H | 407 | VAL |
| 5 | H | 409 | ARG |
| 5 | H | 420 | LEU |
| 5 | H | 432 | LYS |
| 1 | J | 59 | GLU |
| 1 | J | 64 | GLU |
| 1 | J | 76 | VAL |
| 1 | J | 125 | PRO |
| 1 | J | 137 | LYS |
| 1 | J | 148 | VAL |
| 1 | J | 153 | ALA |
| 1 | J | 158 | ILE |
| 1 | J | 162 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 172 | SER |
| 1 | J | 176 | ARG |
| 1 | J | 182 | GLU |
| 1 | J | 188 | GLN |
| 1 | J | 199 | ILE |
| 1 | J | 208 | LEU |
| 1 | J | 216 | ALA |
| 1 | J | 226 | ALA |
| 1 | K | 7 | LYS |
| 1 | K | 15 | THR |
| 1 | K | 29 | GLU |
| 1 | K | 54 | THR |
| 1 | K | 75 | VAL |
| 1 | K | 91 | ASP |
| 1 | K | 104 | GLU |
| 1 | K | 106 | PRO |
| 1 | K | 114 | PHE |
| 1 | K | 128 | HIS |
| 1 | K | 135 | GLY |
| 1 | K | 158 | ILE |
| 1 | K | 171 | PHE |
| 1 | K | 181 | VAL |
| 1 | K | 185 | ARG |
| 1 | K | 186 | LEU |
| 1 | K | 191 | ASP |
| 1 | K | 195 | LEU |
| 1 | K | 200 | TRP |
| 1 | K | 224 | TYR |
| 2 | L | 17 | PRO |
| 2 | L | 22 | GLN |
| 2 | L | 27 | LYS |
| 2 | L | 31 | GLN |
| 2 | L | 33 | ASP |
| 2 | L | 40 | GLU |
| 2 | L | 42 | VAL |
| 2 | L | 46 | ALA |
| 2 | L | 47 | ALA |
| 2 | L | 54 | ILE |
| 2 | L | 70 | GLU |
| 2 | L | 80 | GLN |
| 2 | L | 88 | LEU |
| 2 | L | 102 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | L | 109 | LYS |
| 2 | L | 111 | ASP |
| 2 | L | 114 | PHE |
| 2 | L | 115 | LEU |
| 2 | L | 136 | ILE |
| 2 | L | 137 | VAL |
| 2 | L | 153 | ALA |
| 2 | L | 155 | PRO |
| 2 | L | 168 | ARG |
| 2 | L | 182 | VAL |
| 2 | L | 187 | ASN |
| 2 | L | 199 | VAL |
| 2 | L | 221 | LEU |
| 2 | L | 244 | PRO |
| 2 | L | 263 | ASP |
| 2 | L | 264 | PRO |
| 2 | L | 269 | LEU |
| 2 | L | 275 | TYR |
| 2 | L | 278 | GLU |
| 2 | L | 288 | ARG |
| 2 | L | 322 | VAL |
| 2 | L | 336 | VAL |
| 2 | L | 370 | ALA |
| 2 | L | 392 | SER |
| 2 | L | 395 | LYS |
| 2 | L | 397 | GLU |
| 2 | L | 398 | THR |
| 2 | L | 402 | SER |
| 2 | L | 409 | ARG |
| 2 | L | 418 | LEU |
| 2 | L | 420 | ARG |
| 2 | L | 425 | PHE |
| 2 | L | 430 | VAL |
| 2 | L | 431 | HIS |
| 2 | L | 432 | ARG |
| 2 | L | 434 | HIS |
| 2 | L | 444 | PRO |
| 2 | L | 449 | ILE |
| 2 | L | 451 | LEU |
| 2 | L | 457 | ALA |
| 2 | L | 483 | VAL |
| 2 | L | 496 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | L | 498 | GLN |
| 2 | L | 503 | LEU |
| 2 | L | 518 | ARG |
| 2 | L | 522 | VAL |
| 2 | L | 526 | PRO |
| 2 | L | 530 | GLU |
| 2 | L | 532 | MET |
| 2 | L | 537 | LYS |
| 2 | L | 541 | SER |
| 2 | L | 543 | ASN |
| 2 | L | 545 | ASN |
| 2 | L | 548 | PRO |
| 2 | L | 574 | ALA |
| 2 | L | 580 | MET |
| 2 | L | 587 | VAL |
| 2 | L | 588 | VAL |
| 2 | L | 599 | GLU |
| 2 | L | 603 | VAL |
| 2 | L | 604 | VAL |
| 2 | L | 612 | ALA |
| 2 | L | 616 | GLU |
| 2 | L | 629 | ALA |
| 2 | L | 633 | GLN |
| 2 | L | 641 | PRO |
| 2 | L | 643 | VAL |
| 2 | L | 644 | ARG |
| 2 | L | 656 | ALA |
| 2 | L | 657 | ASP |
| 2 | L | 663 | GLU |
| 2 | L | 677 | MET |
| 2 | L | 713 | ARG |
| 2 | L | 714 | ASP |
| 2 | L | 715 | THR |
| 2 | L | 728 | HIS |
| 2 | L | 735 | ARG |
| 2 | L | 738 | ASP |
| 2 | L | 760 | SER |
| 2 | L | 762 | LYS |
| 2 | L | 767 | PRO |
| 2 | L | 788 | THR |
| 2 | L | 804 | LEU |
| 2 | L | 831 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | L | 832 | LYS |
| 2 | L | 840 | ALA |
| 2 | L | 848 | VAL |
| 2 | L | 849 | VAL |
| 2 | L | 871 | LEU |
| 2 | L | 880 | MET |
| 2 | L | 884 | GLN |
| 2 | L | 885 | ILE |
| 2 | L | 919 | ALA |
| 2 | L | 920 | GLU |
| 2 | L | 944 | LEU |
| 2 | L | 957 | LYS |
| 2 | L | 964 | LYS |
| 2 | L | 965 | GLU |
| 2 | L | 967 | PHE |
| 2 | L | 973 | VAL |
| 2 | L | 974 | LEU |
| 2 | L | 984 | GLU |
| 2 | L | 999 | HIS |
| 2 | L | 1000 | MET |
| 2 | L | 1011 | GLY |
| 2 | L | 1012 | PRO |
| 2 | L | 1021 | LEU |
| 2 | L | 1027 | PHE |
| 2 | L | 1035 | MET |
| 2 | L | 1038 | TRP |
| 2 | L | 1053 | LEU |
| 2 | L | 1075 | ASP |
| 2 | L | 1078 | GLU |
| 2 | L | 1104 | GLU |
| 3 | M | 5 | VAL |
| 3 | M | 10 | ILE |
| 3 | M | 12 | LEU |
| 3 | M | 13 | ALA |
| 3 | M | 26 | VAL |
| 3 | M | 28 | LYS |
| 3 | M | 33 | ASN |
| 3 | M | 41 | ARG |
| 3 | M | 52 | PRO |
| 3 | M | 64 | LYS |
| 3 | M | 97 | THR |
| 3 | M | 98 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | M | 100 | ALA |
| 3 | M | 109 | PRO |
| 3 | M | 110 | SER |
| 3 | M | 117 | ASP |
| 3 | M | 119 | SER |
| 3 | M | 126 | VAL |
| 3 | M | 131 | LYS |
| 3 | M | 140 | ALA |
| 3 | M | 141 | VAL |
| 3 | M | 143 | ASP |
| 3 | M | 146 | PRO |
| 3 | M | 147 | VAL |
| 3 | M | 454 | ALA |
| 3 | M | 477 | LEU |
| 3 | M | 478 | LEU |
| 3 | M | 479 | GLU |
| 3 | M | 484 | PRO |
| 3 | M | 486 | ARG |
| 3 | M | 487 | ALA |
| 3 | M | 488 | ARG |
| 3 | M | 491 | LYS |
| 3 | M | 526 | PRO |
| 3 | M | 530 | VAL |
| 3 | M | 531 | ASP |
| 3 | M | 535 | PHE |
| 3 | M | 547 | LEU |
| 3 | M | 548 | ILE |
| 3 | M | 564 | GLU |
| 3 | M | 565 | ILE |
| 3 | M | 571 | LYS |
| 3 | M | 582 | ILE |
| 3 | M | 607 | LEU |
| 3 | M | 626 | SER |
| 3 | M | 630 | VAL |
| 3 | M | 633 | VAL |
| 3 | M | 638 | LYS |
| 3 | M | 646 | LYS |
| 3 | M | 647 | ARG |
| 3 | M | 648 | MET |
| 3 | M | 649 | ALA |
| 3 | M | 650 | LEU |
| 3 | M | 655 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | M | 662 | GLU |
| 3 | M | 665 | ALA |
| 3 | M | 668 | PRO |
| 3 | M | 672 | ALA |
| 3 | M | 678 | GLU |
| 3 | M | 679 | ARG |
| 3 | M | 682 | ASP |
| 3 | M | 684 | LYS |
| 3 | M | 696 | HIS |
| 3 | M | 702 | LEU |
| 3 | M | 718 | PRO |
| 3 | M | 725 | SER |
| 3 | M | 730 | PRO |
| 3 | M | 731 | LEU |
| 3 | M | 739 | ASP |
| 3 | M | 762 | GLN |
| 3 | M | 770 | LEU |
| 3 | M | 782 | SER |
| 3 | M | 793 | THR |
| 3 | M | 795 | VAL |
| 3 | M | 797 | LYS |
| 3 | M | 799 | LYS |
| 3 | M | 807 | ALA |
| 3 | M | 808 | THR |
| 3 | M | 811 | GLU |
| 3 | M | 815 | ALA |
| 3 | M | 821 | VAL |
| 3 | M | 825 | ALA |
| 3 | M | 826 | PRO |
| 3 | M | 828 | VAL |
| 3 | M | 829 | VAL |
| 3 | M | 835 | SER |
| 3 | M | 838 | ARG |
| 3 | M | 840 | LYS |
| 3 | M | 842 | VAL |
| 3 | M | 848 | GLU |
| 3 | M | 849 | ALA |
| 3 | M | 862 | ASP |
| 3 | M | 875 | THR |
| 3 | M | 898 | GLU |
| 3 | M | 899 | LEU |
| 3 | M | 900 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | M | 905 | PRO |
| 3 | M | 908 | LYS |
| 3 | M | 919 | PHE |
| 3 | M | 924 | MET |
| 3 | M | 925 | GLU |
| 3 | M | 947 | ILE |
| 3 | M | 948 | THR |
| 3 | M | 953 | ASP |
| 3 | M | 961 | GLN |
| 3 | M | 966 | GLU |
| 3 | M | 1000 | THR |
| 3 | M | 1006 | ALA |
| 3 | M | 1016 | PRO |
| 3 | M | 1023 | MET |
| 3 | M | 1028 | ALA |
| 3 | M | 1029 | ARG |
| 3 | M | 1040 | GLY |
| 3 | M | 1045 | MET |
| 3 | M | 1054 | GLU |
| 3 | M | 1059 | SER |
| 3 | M | 1061 | PHE |
| 3 | M | 1067 | VAL |
| 3 | M | 1109 | GLU |
| 3 | M | 1111 | ASP |
| 3 | M | 1113 | GLY |
| 3 | M | 1116 | ASN |
| 3 | M | 1141 | GLU |
| 3 | M | 1149 | LEU |
| 3 | M | 1152 | GLU |
| 3 | M | 1178 | ALA |
| 3 | M | 1190 | SER |
| 3 | M | 1194 | CYS |
| 3 | M | 1195 | GLN |
| 3 | M | 1201 | CYS |
| 3 | M | 1203 | LYS |
| 3 | M | 1208 | ASP |
| 3 | M | 1209 | LEU |
| 3 | M | 1210 | SER |
| 3 | M | 1219 | GLU |
| 3 | M | 1223 | VAL |
| 3 | M | 1224 | VAL |
| 3 | M | 1225 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | M | 1231 | GLU |
| 3 | M | 1232 | PRO |
| 3 | M | 1234 | THR |
| 3 | M | 1236 | LEU |
| 3 | M | 1239 | ARG |
| 3 | M | 1268 | PRO |
| 3 | M | 1276 | GLU |
| 3 | M | 1281 | VAL |
| 3 | M | 1296 | SER |
| 3 | M | 1300 | SER |
| 3 | M | 1306 | PRO |
| 3 | M | 1313 | VAL |
| 3 | M | 1320 | GLU |
| 3 | M | 1321 | ALA |
| 3 | M | 1323 | GLN |
| 3 | M | 1330 | ILE |
| 3 | M | 1347 | TYR |
| 3 | M | 1364 | HIS |
| 3 | M | 1366 | LYS |
| 3 | M | 1367 | HIS |
| 3 | M | 1373 | ARG |
| 3 | M | 1374 | GLN |
| 3 | M | 1375 | MET |
| 3 | M | 1384 | PRO |
| 3 | M | 1388 | ARG |
| 3 | M | 1394 | VAL |
| 3 | M | 1396 | GLU |
| 3 | M | 1408 | ILE |
| 3 | M | 1424 | VAL |
| 3 | M | 1436 | SER |
| 3 | M | 1439 | SER |
| 3 | M | 1442 | ASN |
| 3 | M | 1445 | HIS |
| 3 | M | 1448 | THR |
| 3 | M | 1451 | ALA |
| 3 | M | 1452 | ILE |
| 3 | M | 1455 | LYS |
| 3 | M | 1457 | ASP |
| 3 | M | 1458 | GLU |
| 3 | M | 1462 | LEU |
| 3 | M | 1464 | GLU |
| 3 | M | 1483 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | M | 1487 | VAL |
| 4 | N | 16 | LYS |
| 4 | N | 21 | VAL |
| 4 | N | 30 | LEU |
| 4 | N | 34 | ARG |
| 4 | N | 42 | PRO |
| 4 | N | 50 | THR |
| 4 | N | 51 | LEU |
| 4 | N | 60 | ALA |
| 4 | N | 61 | VAL |
| 4 | N | 77 | GLU |
| 4 | N | 90 | GLU |
| 5 | Q | 171 | VAL |
| 5 | Q | 203 | ILE |
| 5 | Q | 211 | VAL |
| 5 | Q | 220 | ARG |
| 5 | Q | 249 | LYS |
| 5 | Q | 251 | SER |
| 5 | Q | 328 | GLU |
| 5 | Q | 329 | PRO |
| 5 | Q | 333 | GLU |
| 5 | Q | 335 | PRO |
| 5 | Q | 352 | ASN |
| 5 | Q | 407 | VAL |
| 5 | Q | 409 | ARG |
| 5 | Q | 420 | LEU |
| 5 | Q | 432 | LYS |
| 1 | A | 13 | ALA |
| 1 | A | 36 | LEU |
| 1 | A | 44 | LEU |
| 1 | A | 46 | SER |
| 1 | A | 54 | THR |
| 1 | A | 65 | PHE |
| 1 | A | 107 | LYS |
| 1 | A | 112 | GLY |
| 1 | A | 123 | MET |
| 1 | A | 126 | ASP |
| 1 | A | 132 | LEU |
| 1 | A | 138 | LEU |
| 1 | A | 164 | ALA |
| 1 | A | 189 | ARG |
| 1 | A | 209 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 211 | LEU |
| 1 | A | 215 | VAL |
| 1 | A | 224 | TYR |
| 1 | A | 228 | PRO |
| 1 | B | 35 | THR |
| 1 | B | 53 | VAL |
| 1 | B | 70 | GLY |
| 1 | B | 78 | ILE |
| 1 | B | 112 | GLY |
| 1 | B | 117 | SER |
| 1 | B | 137 | LYS |
| 1 | B | 138 | LEU |
| 1 | B | 152 | PRO |
| 1 | B | 196 | THR |
| 1 | B | 201 | THR |
| 1 | B | 202 | ASP |
| 1 | B | 204 | SER |
| 1 | B | 208 | LEU |
| 2 | C | 24 | GLU |
| 2 | C | 28 | LYS |
| 2 | C | 43 | GLY |
| 2 | C | 81 | ASP |
| 2 | C | 108 | ILE |
| 2 | C | 112 | GLU |
| 2 | C | 133 | ASP |
| 2 | C | 144 | PRO |
| 2 | C | 157 | ARG |
| 2 | C | 177 | GLU |
| 2 | C | 179 | SER |
| 2 | C | 237 | ARG |
| 2 | C | 316 | GLY |
| 2 | C | 326 | ASP |
| 2 | C | 338 | GLU |
| 2 | C | 381 | ALA |
| 2 | C | 391 | LEU |
| 2 | C | 393 | GLN |
| 2 | C | 423 | ALA |
| 2 | C | 427 | VAL |
| 2 | C | 438 | ILE |
| 2 | C | 445 | GLU |
| 2 | C | 450 | GLY |
| 2 | C | 458 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 460 | ARG |
| 2 | C | 489 | SER |
| 2 | C | 494 | TYR |
| 2 | C | 502 | PRO |
| 2 | C | 508 | ILE |
| 2 | C | 514 | VAL |
| 2 | C | 529 | VAL |
| 2 | C | 534 | VAL |
| 2 | C | 536 | PRO |
| 2 | C | 550 | LEU |
| 2 | C | 560 | MET |
| 2 | C | 582 | GLY |
| 2 | C | 589 | ARG |
| 2 | C | 600 | ASP |
| 2 | C | 605 | LYS |
| 2 | C | 608 | GLY |
| 2 | C | 620 | LEU |
| 2 | C | 635 | THR |
| 2 | C | 655 | LEU |
| 2 | C | 666 | LEU |
| 2 | C | 685 | GLU |
| 2 | C | 698 | ASP |
| 2 | C | 761 | PHE |
| 2 | C | 769 | PRO |
| 2 | C | 775 | ARG |
| 2 | C | 787 | ASP |
| 2 | C | 791 | ARG |
| 2 | C | 793 | PRO |
| 2 | C | 808 | ARG |
| 2 | C | 809 | GLY |
| 2 | C | 855 | VAL |
| 2 | C | 857 | ASP |
| 2 | C | 876 | VAL |
| 2 | C | 877 | PRO |
| 2 | C | 894 | GLY |
| 2 | C | 928 | LYS |
| 2 | C | 933 | GLY |
| 2 | C | 945 | ALA |
| 2 | C | 960 | GLU |
| 2 | C | 968 | ASP |
| 2 | C | 972 | VAL |
| 2 | C | 981 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 987 | ILE |
| 2 | C | 1001 | VAL |
| 2 | C | 1037 | VAL |
| 2 | C | 1046 | ALA |
| 2 | C | 1056 | LYS |
| 2 | C | 1060 | ILE |
| 2 | C | 1066 | ALA |
| 2 | C | 1079 | PRO |
| 2 | C | 1082 | PRO |
| 2 | C | 1083 | GLU |
| 2 | C | 1093 | GLN |
| 2 | C | 1096 | ALA |
| 2 | C | 1106 | ASP |
| 2 | C | 1113 | GLU |
| 2 | C | 1114 | GLY |
| 3 | D | 7 | LYS |
| 3 | D | 14 | SER |
| 3 | D | 18 | ILE |
| 3 | D | 32 | ILE |
| 3 | D | 37 | LEU |
| 3 | D | 43 | GLY |
| 3 | D | 45 | PHE |
| 3 | D | 47 | GLU |
| 3 | D | 67 | ARG |
| 3 | D | 72 | VAL |
| 3 | D | 85 | VAL |
| 3 | D | 99 | ALA |
| 3 | D | 102 | ILE |
| 3 | D | 127 | LEU |
| 3 | D | 129 | PHE |
| 3 | D | 139 | GLY |
| 3 | D | 464 | LEU |
| 3 | D | 480 | GLU |
| 3 | D | 485 | SER |
| 3 | D | 498 | VAL |
| 3 | D | 502 | PHE |
| 3 | D | 506 | GLY |
| 3 | D | 540 | LEU |
| 3 | D | 545 | ARG |
| 3 | D | 558 | LEU |
| 3 | D | 567 | ILE |
| 3 | D | 586 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 595 | GLY |
| 3 | D | 601 | ARG |
| 3 | D | 605 | ASP |
| 3 | D | 609 | GLY |
| 3 | D | 621 | LYS |
| 3 | D | 640 | HIS |
| 3 | D | 643 | GLY |
| 3 | D | 681 | ARG |
| 3 | D | 686 | GLU |
| 3 | D | 689 | ASP |
| 3 | D | 695 | ILE |
| 3 | D | 712 | GLY |
| 3 | D | 715 | ALA |
| 3 | D | 723 | GLY |
| 3 | D | 724 | GLN |
| 3 | D | 735 | ALA |
| 3 | D | 776 | GLU |
| 3 | D | 783 | ARG |
| 3 | D | 784 | ASP |
| 3 | D | 794 | GLN |
| 3 | D | 796 | ARG |
| 3 | D | 803 | GLY |
| 3 | D | 819 | GLY |
| 3 | D | 822 | ALA |
| 3 | D | 864 | VAL |
| 3 | D | 872 | ARG |
| 3 | D | 892 | ASP |
| 3 | D | 893 | GLU |
| 3 | D | 897 | GLN |
| 3 | D | 913 | ASP |
| 3 | D | 920 | LEU |
| 3 | D | 928 | ALA |
| 3 | D | 936 | TYR |
| 3 | D | 958 | GLU |
| 3 | D | 964 | LEU |
| 3 | D | 994 | GLN |
| 3 | D | 1001 | GLU |
| 3 | D | 1020 | LEU |
| 3 | D | 1042 | ARG |
| 3 | D | 1056 | PRO |
| 3 | D | 1070 | TYR |
| 3 | D | 1099 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 1142 | SER |
| 3 | D | 1146 | GLY |
| 3 | D | 1173 | PHE |
| 3 | D | 1175 | ILE |
| 3 | D | 1179 | GLU |
| 3 | D | 1180 | ALA |
| 3 | D | 1188 | VAL |
| 3 | D | 1200 | VAL |
| 3 | D | 1212 | ALA |
| 3 | D | 1215 | VAL |
| 3 | D | 1233 | GLY |
| 3 | D | 1237 | THR |
| 3 | D | 1263 | PHE |
| 3 | D | 1273 | VAL |
| 3 | D | 1287 | GLU |
| 3 | D | 1328 | GLY |
| 3 | D | 1339 | LYS |
| 3 | D | 1353 | GLN |
| 3 | D | 1360 | GLY |
| 3 | D | 1361 | VAL |
| 3 | D | 1365 | ASP |
| 3 | D | 1381 | VAL |
| 3 | D | 1386 | ASP |
| 3 | D | 1397 | LYS |
| 3 | D | 1430 | SER |
| 3 | D | 1449 | GLU |
| 3 | D | 1454 | GLY |
| 3 | D | 1466 | VAL |
| 3 | D | 1473 | PRO |
| 3 | D | 1475 | GLY |
| 4 | E | 6 | ILE |
| 4 | E | 10 | PHE |
| 4 | E | 12 | MET |
| 4 | E | 15 | SER |
| 4 | E | 22 | VAL |
| 4 | E | 23 | VAL |
| 4 | E | 24 | ALA |
| 4 | E | 41 | GLU |
| 5 | H | 108 | LEU |
| 5 | H | 111 | LEU |
| 5 | H | 152 | GLY |
| 5 | H | 172 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | H | 173 | GLU |
| 5 | H | 176 | GLY |
| 5 | H | 186 | LYS |
| 5 | H | 277 | VAL |
| 5 | H | 315 | ASP |
| 5 | H | 331 | SER |
| 5 | H | 349 | PRO |
| 5 | H | 351 | GLU |
| 5 | H | 387 | ARG |
| 5 | H | 406 | GLY |
| 5 | H | 410 | GLU |
| 5 | H | 419 | ALA |
| 5 | H | 431 | ARG |
| 1 | J | 13 | ALA |
| 1 | J | 36 | LEU |
| 1 | J | 44 | LEU |
| 1 | J | 46 | SER |
| 1 | J | 54 | THR |
| 1 | J | 65 | PHE |
| 1 | J | 107 | LYS |
| 1 | J | 112 | GLY |
| 1 | J | 123 | MET |
| 1 | J | 126 | ASP |
| 1 | J | 132 | LEU |
| 1 | J | 138 | LEU |
| 1 | J | 164 | ALA |
| 1 | J | 189 | ARG |
| 1 | J | 209 | GLU |
| 1 | J | 211 | LEU |
| 1 | J | 215 | VAL |
| 1 | J | 224 | TYR |
| 1 | J | 228 | PRO |
| 1 | K | 35 | THR |
| 1 | K | 53 | VAL |
| 1 | K | 70 | GLY |
| 1 | K | 78 | ILE |
| 1 | K | 112 | GLY |
| 1 | K | 117 | SER |
| 1 | K | 137 | LYS |
| 1 | K | 138 | LEU |
| 1 | K | 152 | PRO |
| 1 | K | 196 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 201 | THR |
| 1 | K | 202 | ASP |
| 1 | K | 204 | SER |
| 1 | K | 208 | LEU |
| 2 | L | 24 | GLU |
| 2 | L | 28 | LYS |
| 2 | L | 43 | GLY |
| 2 | L | 81 | ASP |
| 2 | L | 108 | ILE |
| 2 | L | 112 | GLU |
| 2 | L | 133 | ASP |
| 2 | L | 144 | PRO |
| 2 | L | 157 | ARG |
| 2 | L | 177 | GLU |
| 2 | L | 179 | SER |
| 2 | L | 237 | ARG |
| 2 | L | 316 | GLY |
| 2 | L | 326 | ASP |
| 2 | L | 338 | GLU |
| 2 | L | 381 | ALA |
| 2 | L | 391 | LEU |
| 2 | L | 393 | GLN |
| 2 | L | 423 | ALA |
| 2 | L | 427 | VAL |
| 2 | L | 438 | ILE |
| 2 | L | 445 | GLU |
| 2 | L | 450 | GLY |
| 2 | L | 458 | TYR |
| 2 | L | 460 | ARG |
| 2 | L | 489 | SER |
| 2 | L | 494 | TYR |
| 2 | L | 502 | PRO |
| 2 | L | 508 | ILE |
| 2 | L | 514 | VAL |
| 2 | L | 529 | VAL |
| 2 | L | 534 | VAL |
| 2 | L | 536 | PRO |
| 2 | L | 550 | LEU |
| 2 | L | 560 | MET |
| 2 | L | 582 | GLY |
| 2 | L | 589 | ARG |
| 2 | L | 600 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | L | 605 | LYS |
| 2 | L | 608 | GLY |
| 2 | L | 620 | LEU |
| 2 | L | 635 | THR |
| 2 | L | 655 | LEU |
| 2 | L | 666 | LEU |
| 2 | L | 685 | GLU |
| 2 | L | 698 | ASP |
| 2 | L | 761 | PHE |
| 2 | L | 769 | PRO |
| 2 | L | 775 | ARG |
| 2 | L | 787 | ASP |
| 2 | L | 791 | ARG |
| 2 | L | 793 | PRO |
| 2 | L | 808 | ARG |
| 2 | L | 809 | GLY |
| 2 | L | 855 | VAL |
| 2 | L | 857 | ASP |
| 2 | L | 876 | VAL |
| 2 | L | 877 | PRO |
| 2 | L | 894 | GLY |
| 2 | L | 928 | LYS |
| 2 | L | 933 | GLY |
| 2 | L | 945 | ALA |
| 2 | L | 960 | GLU |
| 2 | L | 968 | ASP |
| 2 | L | 972 | VAL |
| 2 | L | 981 | GLU |
| 2 | L | 987 | ILE |
| 2 | L | 1001 | VAL |
| 2 | L | 1037 | VAL |
| 2 | L | 1046 | ALA |
| 2 | L | 1056 | LYS |
| 2 | L | 1060 | ILE |
| 2 | L | 1066 | ALA |
| 2 | L | 1079 | PRO |
| 2 | L | 1082 | PRO |
| 2 | L | 1083 | GLU |
| 2 | L | 1093 | GLN |
| 2 | L | 1096 | ALA |
| 2 | L | 1106 | ASP |
| 2 | L | 1113 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | L | 1114 | GLY |
| 3 | M | 7 | LYS |
| 3 | M | 14 | SER |
| 3 | M | 18 | ILE |
| 3 | M | 32 | ILE |
| 3 | M | 37 | LEU |
| 3 | M | 43 | GLY |
| 3 | M | 45 | PHE |
| 3 | M | 47 | GLU |
| 3 | M | 67 | ARG |
| 3 | M | 72 | VAL |
| 3 | M | 85 | VAL |
| 3 | M | 99 | ALA |
| 3 | M | 102 | ILE |
| 3 | M | 127 | LEU |
| 3 | M | 129 | PHE |
| 3 | M | 139 | GLY |
| 3 | M | 464 | LEU |
| 3 | M | 480 | GLU |
| 3 | M | 485 | SER |
| 3 | M | 498 | VAL |
| 3 | M | 502 | PHE |
| 3 | M | 506 | GLY |
| 3 | M | 540 | LEU |
| 3 | M | 545 | ARG |
| 3 | M | 558 | LEU |
| 3 | M | 567 | ILE |
| 3 | M | 586 | ARG |
| 3 | M | 595 | GLY |
| 3 | M | 601 | ARG |
| 3 | M | 605 | ASP |
| 3 | M | 609 | GLY |
| 3 | M | 621 | LYS |
| 3 | M | 640 | HIS |
| 3 | M | 643 | GLY |
| 3 | M | 681 | ARG |
| 3 | M | 686 | GLU |
| 3 | M | 689 | ASP |
| 3 | M | 695 | ILE |
| 3 | M | 712 | GLY |
| 3 | M | 715 | ALA |
| 3 | M | 723 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | M | 724 | GLN |
| 3 | M | 735 | ALA |
| 3 | M | 776 | GLU |
| 3 | M | 783 | ARG |
| 3 | M | 784 | ASP |
| 3 | M | 794 | GLN |
| 3 | M | 796 | ARG |
| 3 | M | 803 | GLY |
| 3 | M | 819 | GLY |
| 3 | M | 822 | ALA |
| 3 | M | 864 | VAL |
| 3 | M | 872 | ARG |
| 3 | M | 892 | ASP |
| 3 | M | 893 | GLU |
| 3 | M | 897 | GLN |
| 3 | M | 913 | ASP |
| 3 | M | 920 | LEU |
| 3 | M | 928 | ALA |
| 3 | M | 936 | TYR |
| 3 | M | 958 | GLU |
| 3 | M | 964 | LEU |
| 3 | M | 994 | GLN |
| 3 | M | 1001 | GLU |
| 3 | M | 1020 | LEU |
| 3 | M | 1042 | ARG |
| 3 | M | 1056 | PRO |
| 3 | M | 1070 | TYR |
| 3 | M | 1099 | VAL |
| 3 | M | 1142 | SER |
| 3 | M | 1146 | GLY |
| 3 | M | 1173 | PHE |
| 3 | M | 1175 | ILE |
| 3 | M | 1179 | GLU |
| 3 | M | 1180 | ALA |
| 3 | M | 1188 | VAL |
| 3 | M | 1200 | VAL |
| 3 | M | 1212 | ALA |
| 3 | M | 1215 | VAL |
| 3 | M | 1233 | GLY |
| 3 | M | 1237 | THR |
| 3 | M | 1263 | PHE |
| 3 | M | 1273 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | M | 1287 | GLU |
| 3 | M | 1328 | GLY |
| 3 | M | 1339 | LYS |
| 3 | M | 1353 | GLN |
| 3 | M | 1360 | GLY |
| 3 | M | 1361 | VAL |
| 3 | M | 1365 | ASP |
| 3 | M | 1381 | VAL |
| 3 | M | 1386 | ASP |
| 3 | M | 1397 | LYS |
| 3 | M | 1430 | SER |
| 3 | M | 1449 | GLU |
| 3 | M | 1454 | GLY |
| 3 | M | 1466 | VAL |
| 3 | M | 1473 | PRO |
| 3 | M | 1475 | GLY |
| 4 | N | 6 | ILE |
| 4 | N | 10 | PHE |
| 4 | N | 12 | MET |
| 4 | N | 15 | SER |
| 4 | N | 22 | VAL |
| 4 | N | 23 | VAL |
| 4 | N | 24 | ALA |
| 4 | N | 41 | GLU |
| 5 | Q | 108 | LEU |
| 5 | Q | 111 | LEU |
| 5 | Q | 152 | GLY |
| 5 | Q | 172 | GLU |
| 5 | Q | 173 | GLU |
| 5 | Q | 176 | GLY |
| 5 | Q | 186 | LYS |
| 5 | Q | 277 | VAL |
| 5 | Q | 315 | ASP |
| 5 | Q | 331 | SER |
| 5 | Q | 349 | PRO |
| 5 | Q | 351 | GLU |
| 5 | Q | 387 | ARG |
| 5 | Q | 406 | GLY |
| 5 | Q | 410 | GLU |
| 5 | Q | 419 | ALA |
| 5 | Q | 431 | ARG |
| 1 | A | 7 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 31 | GLY |
| 1 | A | 49 | PRO |
| 1 | A | 74 | ASP |
| 1 | A | 96 | SER |
| 1 | A | 101 | LEU |
| 1 | A | 105 | GLY |
| 1 | A | 109 | VAL |
| 1 | A | 111 | ALA |
| 1 | A | 131 | THR |
| 1 | A | 161 | ARG |
| 1 | B | 32 | PHE |
| 1 | B | 95 | ALA |
| 1 | B | 116 | PRO |
| 1 | B | 132 | LEU |
| 1 | B | 134 | GLU |
| 1 | B | 161 | ARG |
| 2 | C | 14 | PRO |
| 2 | C | 18 | LEU |
| 2 | C | 19 | THR |
| 2 | C | 53 | PRO |
| 2 | C | 166 | PRO |
| 2 | C | 362 | GLY |
| 2 | C | 401 | LEU |
| 2 | C | 410 | ILE |
| 2 | C | 433 | THR |
| 2 | C | 453 | THR |
| 2 | C | 462 | ASP |
| 2 | C | 467 | ILE |
| 2 | C | 486 | MET |
| 2 | C | 507 | ARG |
| 2 | C | 512 | ARG |
| 2 | C | 561 | GLY |
| 2 | C | 575 | GLN |
| 2 | C | 594 | ALA |
| 2 | C | 613 | VAL |
| 2 | C | 625 | LEU |
| 2 | C | 645 | VAL |
| 2 | C | 686 | ASP |
| 2 | C | 696 | LYS |
| 2 | C | 821 | GLU |
| 2 | C | 856 | GLU |
| 2 | C | 873 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 909 | ALA |
| 2 | C | 924 | LEU |
| 2 | C | 936 | VAL |
| 2 | C | 997 | LEU |
| 2 | C | 1020 | PRO |
| 2 | C | 1030 | GLN |
| 2 | C | 1058 | ASP |
| 2 | C | 1069 | ALA |
| 2 | C | 1100 | GLN |
| 2 | C | 1109 | VAL |
| 3 | D | 25 | GLU |
| 3 | D | 44 | LEU |
| 3 | D | 53 | ILE |
| 3 | D | 68 | PHE |
| 3 | D | 133 | ILE |
| 3 | D | 149 | LYS |
| 3 | D | 463 | GLU |
| 3 | D | 561 | GLY |
| 3 | D | 566 | ILE |
| 3 | D | 569 | ASN |
| 3 | D | 579 | ASP |
| 3 | D | 698 | LYS |
| 3 | D | 714 | GLN |
| 3 | D | 818 | ARG |
| 3 | D | 847 | ASP |
| 3 | D | 858 | LEU |
| 3 | D | 904 | VAL |
| 3 | D | 938 | GLY |
| 3 | D | 945 | SER |
| 3 | D | 965 | GLU |
| 3 | D | 967 | ALA |
| 3 | D | 1009 | LYS |
| 3 | D | 1047 | LYS |
| 3 | D | 1048 | PRO |
| 3 | D | 1049 | SER |
| 3 | D | 1098 | LEU |
| 3 | D | 1103 | HIS |
| 3 | D | 1105 | ILE |
| 3 | D | 1128 | VAL |
| 3 | D | 1135 | ARG |
| 3 | D | 1192 | LEU |
| 3 | D | 1315 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 1359 | GLN |
| 3 | D | 1368 | ILE |
| 3 | D | 1387 | SER |
| 3 | D | 1389 | LEU |
| 3 | D | 1416 | ALA |
| 3 | D | 1435 | LEU |
| 3 | D | 1459 | LEU |
| 3 | D | 1465 | ASN |
| 3 | D | 1468 | LEU |
| 3 | D | 1485 | GLN |
| 4 | E | 18 | ARG |
| 4 | E | 71 | GLY |
| 4 | E | 84 | ARG |
| 5 | H | 181 | LEU |
| 5 | H | 297 | LEU |
| 5 | H | 327 | GLN |
| 5 | H | 353 | LEU |
| 1 | J | 7 | LYS |
| 1 | J | 31 | GLY |
| 1 | J | 49 | PRO |
| 1 | J | 74 | ASP |
| 1 | J | 96 | SER |
| 1 | J | 101 | LEU |
| 1 | J | 105 | GLY |
| 1 | J | 109 | VAL |
| 1 | J | 111 | ALA |
| 1 | J | 131 | THR |
| 1 | J | 161 | ARG |
| 1 | K | 32 | PHE |
| 1 | K | 95 | ALA |
| 1 | K | 116 | PRO |
| 1 | K | 132 | LEU |
| 1 | K | 134 | GLU |
| 1 | K | 161 | ARG |
| 2 | L | 14 | PRO |
| 2 | L | 18 | LEU |
| 2 | L | 19 | THR |
| 2 | L | 53 | PRO |
| 2 | L | 166 | PRO |
| 2 | L | 362 | GLY |
| 2 | L | 401 | LEU |
| 2 | L | 410 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | L | 433 | THR |
| 2 | L | 453 | THR |
| 2 | L | 462 | ASP |
| 2 | L | 467 | ILE |
| 2 | L | 486 | MET |
| 2 | L | 507 | ARG |
| 2 | L | 512 | ARG |
| 2 | L | 561 | GLY |
| 2 | L | 575 | GLN |
| 2 | L | 594 | ALA |
| 2 | L | 613 | VAL |
| 2 | L | 625 | LEU |
| 2 | L | 645 | VAL |
| 2 | L | 686 | ASP |
| 2 | L | 696 | LYS |
| 2 | L | 821 | GLU |
| 2 | L | 856 | GLU |
| 2 | L | 873 | PRO |
| 2 | L | 909 | ALA |
| 2 | L | 924 | LEU |
| 2 | L | 936 | VAL |
| 2 | L | 997 | LEU |
| 2 | L | 1020 | PRO |
| 2 | L | 1030 | GLN |
| 2 | L | 1058 | ASP |
| 2 | L | 1069 | ALA |
| 2 | L | 1100 | GLN |
| 2 | L | 1109 | VAL |
| 3 | M | 25 | GLU |
| 3 | M | 44 | LEU |
| 3 | M | 53 | ILE |
| 3 | M | 68 | PHE |
| 3 | M | 133 | ILE |
| 3 | M | 149 | LYS |
| 3 | M | 463 | GLU |
| 3 | M | 561 | GLY |
| 3 | M | 566 | ILE |
| 3 | M | 569 | ASN |
| 3 | M | 579 | ASP |
| 3 | M | 698 | LYS |
| 3 | M | 714 | GLN |
| 3 | M | 818 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | M | 847 | ASP |
| 3 | M | 858 | LEU |
| 3 | M | 883 | ALA |
| 3 | M | 904 | VAL |
| 3 | M | 938 | GLY |
| 3 | M | 945 | SER |
| 3 | M | 965 | GLU |
| 3 | M | 967 | ALA |
| 3 | M | 1009 | LYS |
| 3 | M | 1047 | LYS |
| 3 | M | 1048 | PRO |
| 3 | M | 1049 | SER |
| 3 | M | 1098 | LEU |
| 3 | M | 1103 | HIS |
| 3 | M | 1105 | ILE |
| 3 | M | 1128 | VAL |
| 3 | M | 1135 | ARG |
| 3 | M | 1192 | LEU |
| 3 | M | 1315 | ASP |
| 3 | M | 1359 | GLN |
| 3 | M | 1368 | ILE |
| 3 | M | 1387 | SER |
| 3 | M | 1389 | LEU |
| 3 | M | 1416 | ALA |
| 3 | M | 1435 | LEU |
| 3 | M | 1459 | LEU |
| 3 | M | 1465 | ASN |
| 3 | M | 1468 | LEU |
| 3 | M | 1485 | GLN |
| 4 | N | 18 | ARG |
| 4 | N | 71 | GLY |
| 4 | N | 84 | ARG |
| 5 | Q | 181 | LEU |
| 5 | Q | 297 | LEU |
| 5 | Q | 327 | GLN |
| 5 | Q | 353 | LEU |
| 1 | A | 78 | ILE |
| 1 | A | 91 | ASP |
| 1 | A | 128 | HIS |
| 1 | A | 152 | PRO |
| 1 | A | 218 | LEU |
| 1 | B | 13 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 20 | TYR |
| 1 | B | 21 | GLY |
| 1 | B | 22 | GLU |
| 1 | B | 46 | SER |
| 1 | B | 48 | ILE |
| 1 | B | 76 | VAL |
| 1 | B | 113 | ASP |
| 2 | C | 35 | PRO |
| 2 | C | 87 | ASP |
| 2 | C | 106 | GLY |
| 2 | C | 148 | PHE |
| 2 | C | 167 | LYS |
| 2 | C | 175 | GLU |
| 2 | C | 205 | GLU |
| 2 | C | 303 | PHE |
| 2 | C | 317 | VAL |
| 2 | C | 318 | PRO |
| 2 | C | 376 | ARG |
| 2 | C | 394 | PHE |
| 2 | C | 521 | PRO |
| 2 | C | 562 | SER |
| 2 | C | 572 | ILE |
| 2 | C | 607 | ASP |
| 2 | C | 636 | ALA |
| 2 | C | 659 | PRO |
| 2 | C | 675 | ALA |
| 2 | C | 682 | TYR |
| 2 | C | 716 | LYS |
| 2 | C | 739 | GLU |
| 2 | C | 756 | VAL |
| 2 | C | 777 | ILE |
| 2 | C | 786 | LYS |
| 2 | C | 796 | GLU |
| 2 | C | 822 | VAL |
| 2 | C | 830 | LYS |
| 2 | C | 833 | LEU |
| 2 | C | 834 | GLN |
| 2 | C | 942 | GLU |
| 2 | C | 943 | VAL |
| 2 | C | 1039 | ALA |
| 2 | C | 1072 | LYS |
| 2 | C | 1089 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 6 | ARG |
| 3 | D | 101 | HIS |
| 3 | D | 135 | LEU |
| 3 | D | 136 | ASP |
| 3 | D | 457 | GLY |
| 3 | D | 468 | LEU |
| 3 | D | 490 | ALA |
| 3 | D | 496 | LEU |
| 3 | D | 520 | LEU |
| 3 | D | 546 | ARG |
| 3 | D | 554 | LEU |
| 3 | D | 570 | GLU |
| 3 | D | 592 | THR |
| 3 | D | 594 | PRO |
| 3 | D | 608 | SER |
| 3 | D | 644 | LEU |
| 3 | D | 666 | PHE |
| 3 | D | 673 | ALA |
| 3 | D | 721 | VAL |
| 3 | D | 765 | SER |
| 3 | D | 785 | ILE |
| 3 | D | 843 | PHE |
| 3 | D | 883 | ALA |
| 3 | D | 934 | LEU |
| 3 | D | 944 | THR |
| 3 | D | 976 | GLN |
| 3 | D | 1069 | GLU |
| 3 | D | 1101 | VAL |
| 3 | D | 1115 | THR |
| 3 | D | 1177 | ALA |
| 3 | D | 1193 | THR |
| 3 | D | 1274 | ILE |
| 3 | D | 1277 | ILE |
| 3 | D | 1342 | GLU |
| 3 | D | 1352 | ILE |
| 3 | D | 1354 | LYS |
| 3 | D | 1377 | LYS |
| 3 | D | 1432 | LYS |
| 3 | D | 1460 | ILE |
| 4 | E | 26 | ARG |
| 4 | E | 73 | LEU |
| 4 | E | 79 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | H | 110 | THR |
| 5 | H | 217 | TYR |
| 5 | H | 222 | LEU |
| 5 | H | 271 | ARG |
| 5 | H | 310 | MET |
| 5 | H | 323 | LEU |
| 5 | H | 354 | PRO |
| 5 | H | 393 | GLY |
| 5 | H | 403 | ALA |
| 1 | J | 78 | ILE |
| 1 | J | 91 | ASP |
| 1 | J | 128 | HIS |
| 1 | J | 152 | PRO |
| 1 | J | 218 | LEU |
| 1 | K | 13 | ALA |
| 1 | K | 20 | TYR |
| 1 | K | 21 | GLY |
| 1 | K | 22 | GLU |
| 1 | K | 46 | SER |
| 1 | K | 48 | ILE |
| 1 | K | 76 | VAL |
| 1 | K | 113 | ASP |
| 2 | L | 35 | PRO |
| 2 | L | 87 | ASP |
| 2 | L | 106 | GLY |
| 2 | L | 148 | PHE |
| 2 | L | 167 | LYS |
| 2 | L | 175 | GLU |
| 2 | L | 205 | GLU |
| 2 | L | 303 | PHE |
| 2 | L | 317 | VAL |
| 2 | L | 318 | PRO |
| 2 | L | 376 | ARG |
| 2 | L | 394 | PHE |
| 2 | L | 521 | PRO |
| 2 | L | 562 | SER |
| 2 | L | 572 | ILE |
| 2 | L | 607 | ASP |
| 2 | L | 636 | ALA |
| 2 | L | 659 | PRO |
| 2 | L | 675 | ALA |
| 2 | L | 682 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | L | 716 | LYS |
| 2 | L | 739 | GLU |
| 2 | L | 756 | VAL |
| 2 | L | 777 | ILE |
| 2 | L | 786 | LYS |
| 2 | L | 796 | GLU |
| 2 | L | 822 | VAL |
| 2 | L | 830 | LYS |
| 2 | L | 833 | LEU |
| 2 | L | 834 | GLN |
| 2 | L | 942 | GLU |
| 2 | L | 943 | VAL |
| 2 | L | 1039 | ALA |
| 2 | L | 1072 | LYS |
| 2 | L | 1089 | VAL |
| 3 | M | 6 | ARG |
| 3 | M | 101 | HIS |
| 3 | M | 135 | LEU |
| 3 | M | 136 | ASP |
| 3 | M | 457 | GLY |
| 3 | M | 468 | LEU |
| 3 | M | 490 | ALA |
| 3 | M | 496 | LEU |
| 3 | M | 520 | LEU |
| 3 | M | 546 | ARG |
| 3 | M | 554 | LEU |
| 3 | M | 570 | GLU |
| 3 | M | 592 | THR |
| 3 | M | 594 | PRO |
| 3 | M | 608 | SER |
| 3 | M | 644 | LEU |
| 3 | M | 666 | PHE |
| 3 | M | 673 | ALA |
| 3 | M | 721 | VAL |
| 3 | M | 765 | SER |
| 3 | M | 785 | ILE |
| 3 | M | 843 | PHE |
| 3 | M | 934 | LEU |
| 3 | M | 944 | THR |
| 3 | M | 976 | GLN |
| 3 | M | 1069 | GLU |
| 3 | M | 1101 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | M | 1115 | THR |
| 3 | M | 1177 | ALA |
| 3 | M | 1193 | THR |
| 3 | M | 1274 | ILE |
| 3 | M | 1277 | ILE |
| 3 | M | 1342 | GLU |
| 3 | M | 1352 | ILE |
| 3 | M | 1354 | LYS |
| 3 | M | 1377 | LYS |
| 3 | M | 1432 | LYS |
| 3 | M | 1460 | ILE |
| 4 | N | 26 | ARG |
| 4 | N | 73 | LEU |
| 4 | N | 79 | LEU |
| 5 | Q | 110 | THR |
| 5 | Q | 217 | TYR |
| 5 | Q | 222 | LEU |
| 5 | Q | 271 | ARG |
| 5 | Q | 310 | MET |
| 5 | Q | 323 | LEU |
| 5 | Q | 354 | PRO |
| 5 | Q | 393 | GLY |
| 5 | Q | 403 | ALA |
| 1 | A | 41 | ARG |
| 1 | A | 45 | LEU |
| 1 | A | 53 | VAL |
| 1 | A | 127 | LEU |
| 1 | A | 139 | TYR |
| 1 | A | 203 | GLY |
| 1 | B | 119 | ASP |
| 1 | B | 154 | GLU |
| 1 | B | 175 | ARG |
| 1 | B | 187 | GLY |
| 2 | C | 15 | LEU |
| 2 | C | 21 | ILE |
| 2 | C | 73 | ILE |
| 2 | C | 124 | ASP |
| 2 | C | 149 | THR |
| 2 | C | 231 | PRO |
| 2 | C | 235 | MET |
| 2 | C | 243 | ARG |
| 2 | C | 377 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 407 | LYS |
| 2 | C | 576 | ALA |
| 2 | C | 624 | PRO |
| 2 | C | 681 | GLY |
| 2 | C | 889 | HIS |
| 2 | C | 925 | TYR |
| 2 | C | 958 | SER |
| 2 | C | 966 | LEU |
| 2 | C | 977 | GLY |
| 2 | C | 1047 | HIS |
| 2 | C | 1063 | ARG |
| 2 | C | 1101 | THR |
| 3 | D | 150 | ARG |
| 3 | D | 743 | ASP |
| 3 | D | 774 | SER |
| 3 | D | 816 | TYR |
| 3 | D | 906 | GLN |
| 3 | D | 929 | ARG |
| 3 | D | 972 | ARG |
| 3 | D | 1012 | GLU |
| 3 | D | 1107 | VAL |
| 3 | D | 1133 | ARG |
| 3 | D | 1136 | LYS |
| 3 | D | 1207 | TYR |
| 3 | D | 1229 | ILE |
| 3 | D | 1299 | PHE |
| 3 | D | 1317 | ASP |
| 3 | D | 1324 | PRO |
| 4 | E | 55 | TYR |
| 5 | H | 138 | ASP |
| 5 | H | 154 | ALA |
| 5 | H | 355 | SER |
| 1 | J | 41 | ARG |
| 1 | J | 45 | LEU |
| 1 | J | 53 | VAL |
| 1 | J | 127 | LEU |
| 1 | J | 139 | TYR |
| 1 | J | 203 | GLY |
| 1 | K | 119 | ASP |
| 1 | K | 154 | GLU |
| 1 | K | 175 | ARG |
| 1 | K | 187 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | L | 15 | LEU |
| 2 | L | 21 | ILE |
| 2 | L | 73 | ILE |
| 2 | L | 124 | ASP |
| 2 | L | 149 | THR |
| 2 | L | 231 | PRO |
| 2 | L | 235 | MET |
| 2 | L | 243 | ARG |
| 2 | L | 377 | PRO |
| 2 | L | 407 | LYS |
| 2 | L | 576 | ALA |
| 2 | L | 624 | PRO |
| 2 | L | 681 | GLY |
| 2 | L | 889 | HIS |
| 2 | L | 925 | TYR |
| 2 | L | 958 | SER |
| 2 | L | 966 | LEU |
| 2 | L | 977 | GLY |
| 2 | L | 1047 | HIS |
| 2 | L | 1063 | ARG |
| 2 | L | 1101 | THR |
| 3 | M | 150 | ARG |
| 3 | M | 743 | ASP |
| 3 | M | 774 | SER |
| 3 | M | 816 | TYR |
| 3 | M | 906 | GLN |
| 3 | M | 929 | ARG |
| 3 | M | 972 | ARG |
| 3 | M | 1012 | GLU |
| 3 | M | 1107 | VAL |
| 3 | M | 1133 | ARG |
| 3 | M | 1136 | LYS |
| 3 | M | 1207 | TYR |
| 3 | M | 1229 | ILE |
| 3 | M | 1299 | PHE |
| 3 | M | 1317 | ASP |
| 3 | M | 1324 | PRO |
| 4 | N | 55 | TYR |
| 5 | Q | 138 | ASP |
| 5 | Q | 154 | ALA |
| 5 | Q | 355 | SER |
| 1 | A | 58 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 75 | VAL |
| 2 | C | 9 | ILE |
| 2 | C | 23 | VAL |
| 2 | C | 197 | LEU |
| 2 | C | 390 | GLN |
| 2 | C | 403 | SER |
| 2 | C | 602 | GLU |
| 2 | C | 794 | PRO |
| 2 | C | 835 | VAL |
| 2 | C | 858 | MET |
| 2 | C | 859 | PRO |
| 3 | D | 504 | ASP |
| 3 | D | 623 | VAL |
| 3 | D | 882 | PHE |
| 3 | D | 884 | ARG |
| 3 | D | 981 | GLY |
| 3 | D | 987 | GLU |
| 3 | D | 989 | TYR |
| 3 | D | 1007 | VAL |
| 3 | D | 1213 | ARG |
| 3 | D | 1290 | LEU |
| 3 | D | 1319 | VAL |
| 3 | D | 1443 | THR |
| 3 | D | 1478 | SER |
| 5 | H | 244 | TYR |
| 5 | H | 302 | SER |
| 1 | J | 58 | ILE |
| 1 | J | 75 | VAL |
| 2 | L | 9 | ILE |
| 2 | L | 23 | VAL |
| 2 | L | 197 | LEU |
| 2 | L | 390 | GLN |
| 2 | L | 403 | SER |
| 2 | L | 500 | ASN |
| 2 | L | 602 | GLU |
| 2 | L | 794 | PRO |
| 2 | L | 835 | VAL |
| 2 | L | 858 | MET |
| 2 | L | 859 | PRO |
| 2 | L | 947 | ALA |
| 3 | M | 504 | ASP |
| 3 | M | 623 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | M | 882 | PHE |
| 3 | M | 884 | ARG |
| 3 | M | 981 | GLY |
| 3 | M | 987 | GLU |
| 3 | M | 1007 | VAL |
| 3 | M | 1213 | ARG |
| 3 | M | 1290 | LEU |
| 3 | M | 1319 | VAL |
| 3 | M | 1443 | THR |
| 3 | M | 1478 | SER |
| 5 | Q | 244 | TYR |
| 5 | Q | 302 | SER |
| 2 | C | 181 | VAL |
| 2 | C | 287 | GLY |
| 2 | C | 304 | LEU |
| 2 | C | 443 | THR |
| 2 | C | 520 | GLU |
| 2 | C | 912 | PRO |
| 2 | C | 1033 | GLY |
| 3 | D | 108 | VAL |
| 3 | D | 144 | GLY |
| 3 | D | 1032 | PRO |
| 3 | D | 1221 | VAL |
| 3 | D | 1392 | GLY |
| 2 | L | 181 | VAL |
| 2 | L | 287 | GLY |
| 2 | L | 304 | LEU |
| 2 | L | 443 | THR |
| 2 | L | 520 | GLU |
| 2 | L | 912 | PRO |
| 2 | L | 1033 | GLY |
| 3 | M | 108 | VAL |
| 3 | M | 144 | GLY |
| 3 | M | 1032 | PRO |
| 3 | M | 1221 | VAL |
| 3 | M | 1392 | GLY |
| 1 | A | 21 | GLY |
| 1 | A | 92 | PRO |
| 1 | B | 129 | ILE |
| 1 | B | 199 | ILE |
| 2 | C | 119 | PRO |
| 2 | C | 192 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 446 | GLY |
| 2 | C | 678 | PRO |
| 2 | C | 727 | PRO |
| 3 | D | 719 | VAL |
| 3 | D | 792 | ILE |
| 3 | D | 992 | VAL |
| 3 | D | 1372 | VAL |
| 3 | D | 1415 | VAL |
| 3 | D | 1461 | GLY |
| 5 | H | 210 | VAL |
| 5 | H | 356 | PRO |
| 1 | J | 21 | GLY |
| 1 | J | 92 | PRO |
| 1 | K | 129 | ILE |
| 1 | K | 199 | ILE |
| 2 | L | 119 | PRO |
| 2 | L | 192 | PRO |
| 2 | L | 446 | GLY |
| 2 | L | 678 | PRO |
| 2 | L | 727 | PRO |
| 3 | M | 719 | VAL |
| 3 | M | 761 | ILE |
| 3 | M | 792 | ILE |
| 3 | M | 992 | VAL |
| 3 | M | 1372 | VAL |
| 3 | M | 1415 | VAL |
| 3 | M | 1461 | GLY |
| 5 | Q | 210 | VAL |
| 5 | Q | 356 | PRO |
| 1 | B | 124 | ASN |
| 2 | C | 151 | ASP |
| 2 | C | 319 | GLY |
| 2 | C | 415 | PRO |
| 2 | C | 621 | VAL |
| 2 | C | 674 | VAL |
| 2 | C | 799 | ILE |
| 2 | C | 982 | PRO |
| 2 | C | 1077 | PRO |
| 2 | C | 1099 | VAL |
| 3 | D | 683 | ILE |
| 3 | D | 761 | ILE |
| 3 | D | 809 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 856 | GLY |
| 1 | K | 124 | ASN |
| 2 | L | 151 | ASP |
| 2 | L | 319 | GLY |
| 2 | L | 415 | PRO |
| 2 | L | 621 | VAL |
| 2 | L | 674 | VAL |
| 2 | L | 799 | ILE |
| 2 | L | 982 | PRO |
| 2 | L | 1077 | PRO |
| 2 | L | 1099 | VAL |
| 3 | M | 683 | ILE |
| 3 | M | 809 | PRO |
| 3 | M | 856 | GLY |
| 2 | C | 852 | ILE |
| 2 | C | 1055 | ILE |
| 3 | D | 38 | LYS |
| 2 | L | 852 | ILE |
| 2 | L | 1055 | ILE |
| 3 | M | 38 | LYS |
| 2 | C | 757 | GLY |
| 2 | C | 1016 | ILE |
| 2 | C | 1076 | VAL |
| 3 | D | 137 | PRO |
| 3 | D | 599 | PRO |
| 3 | D | 632 | VAL |
| 3 | D | 974 | ILE |
| 3 | D | 1423 | GLY |
| 3 | D | 1467 | ILE |
| 2 | L | 757 | GLY |
| 2 | L | 1016 | ILE |
| 2 | L | 1076 | VAL |
| 3 | M | 137 | PRO |
| 3 | M | 632 | VAL |
| 3 | M | 974 | ILE |
| 3 | M | 1423 | GLY |
| 3 | M | 1467 | ILE |

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.