



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 03:04 PM JST

PDB ID : 7D6E
EMDB ID : EMD-30593
Title : Structural insights into membrane remodeling by SNX1
Authors : Zhang, Y.; Pang, X.; Sun, F.
Deposited on : 2020-09-30
Resolution : 10.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

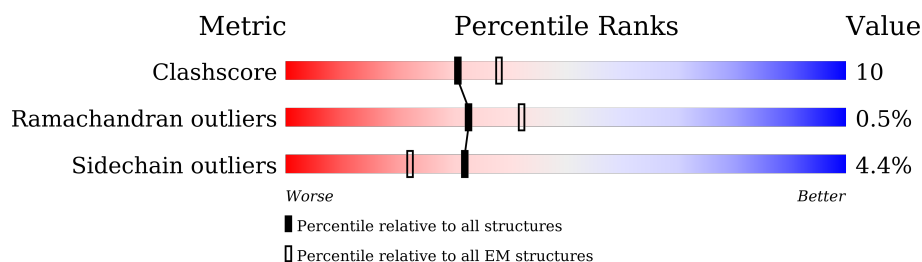
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 529 | |
| 1 | B | 529 | |
| 1 | C | 529 | |
| 1 | D | 529 | |
| 1 | E | 529 | |
| 1 | F | 529 | |
| 1 | G | 529 | |
| 1 | H | 529 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | I | 529 | |
| 1 | J | 529 | |
| 1 | K | 529 | |
| 1 | L | 529 | |
| 1 | M | 529 | |
| 1 | N | 529 | |
| 1 | O | 529 | |
| 1 | P | 529 | |
| 1 | Q | 529 | |
| 1 | R | 529 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 55872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sorting nexin-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | B | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | C | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | D | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | E | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | F | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | G | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | H | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | I | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | J | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | K | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | L | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | M | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | N | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | O | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | P | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |
| 1 | Q | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | R | 380 | Total | C | N | O | S | 0 | 0 |
| | | | 3104 | 1963 | 544 | 586 | 11 | | |

There are 144 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -7 | GLY | - | expression tag | UNP Q6NZD2 |
| A | -6 | PRO | - | expression tag | UNP Q6NZD2 |
| A | -5 | LEU | - | expression tag | UNP Q6NZD2 |
| A | -4 | GLY | - | expression tag | UNP Q6NZD2 |
| A | -3 | SER | - | expression tag | UNP Q6NZD2 |
| A | -2 | PRO | - | expression tag | UNP Q6NZD2 |
| A | -1 | GLU | - | expression tag | UNP Q6NZD2 |
| A | 0 | PHE | - | expression tag | UNP Q6NZD2 |
| B | -7 | GLY | - | expression tag | UNP Q6NZD2 |
| B | -6 | PRO | - | expression tag | UNP Q6NZD2 |
| B | -5 | LEU | - | expression tag | UNP Q6NZD2 |
| B | -4 | GLY | - | expression tag | UNP Q6NZD2 |
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| B | -1 | GLU | - | expression tag | UNP Q6NZD2 |
| B | 0 | PHE | - | expression tag | UNP Q6NZD2 |
| C | -7 | GLY | - | expression tag | UNP Q6NZD2 |
| C | -6 | PRO | - | expression tag | UNP Q6NZD2 |
| C | -5 | LEU | - | expression tag | UNP Q6NZD2 |
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| C | -3 | SER | - | expression tag | UNP Q6NZD2 |
| C | -2 | PRO | - | expression tag | UNP Q6NZD2 |
| C | -1 | GLU | - | expression tag | UNP Q6NZD2 |
| C | 0 | PHE | - | expression tag | UNP Q6NZD2 |
| D | -7 | GLY | - | expression tag | UNP Q6NZD2 |
| D | -6 | PRO | - | expression tag | UNP Q6NZD2 |
| D | -5 | LEU | - | expression tag | UNP Q6NZD2 |
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| E | -5 | LEU | - | expression tag | UNP Q6NZD2 |
| E | -4 | GLY | - | expression tag | UNP Q6NZD2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| E | -3 | SER | - | expression tag | UNP Q6NZD2 |
| E | -2 | PRO | - | expression tag | UNP Q6NZD2 |
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| F | -6 | PRO | - | expression tag | UNP Q6NZD2 |
| F | -5 | LEU | - | expression tag | UNP Q6NZD2 |
| F | -4 | GLY | - | expression tag | UNP Q6NZD2 |
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| I | -6 | PRO | - | expression tag | UNP Q6NZD2 |
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| J | -6 | PRO | - | expression tag | UNP Q6NZD2 |
| J | -5 | LEU | - | expression tag | UNP Q6NZD2 |
| J | -4 | GLY | - | expression tag | UNP Q6NZD2 |
| J | -3 | SER | - | expression tag | UNP Q6NZD2 |
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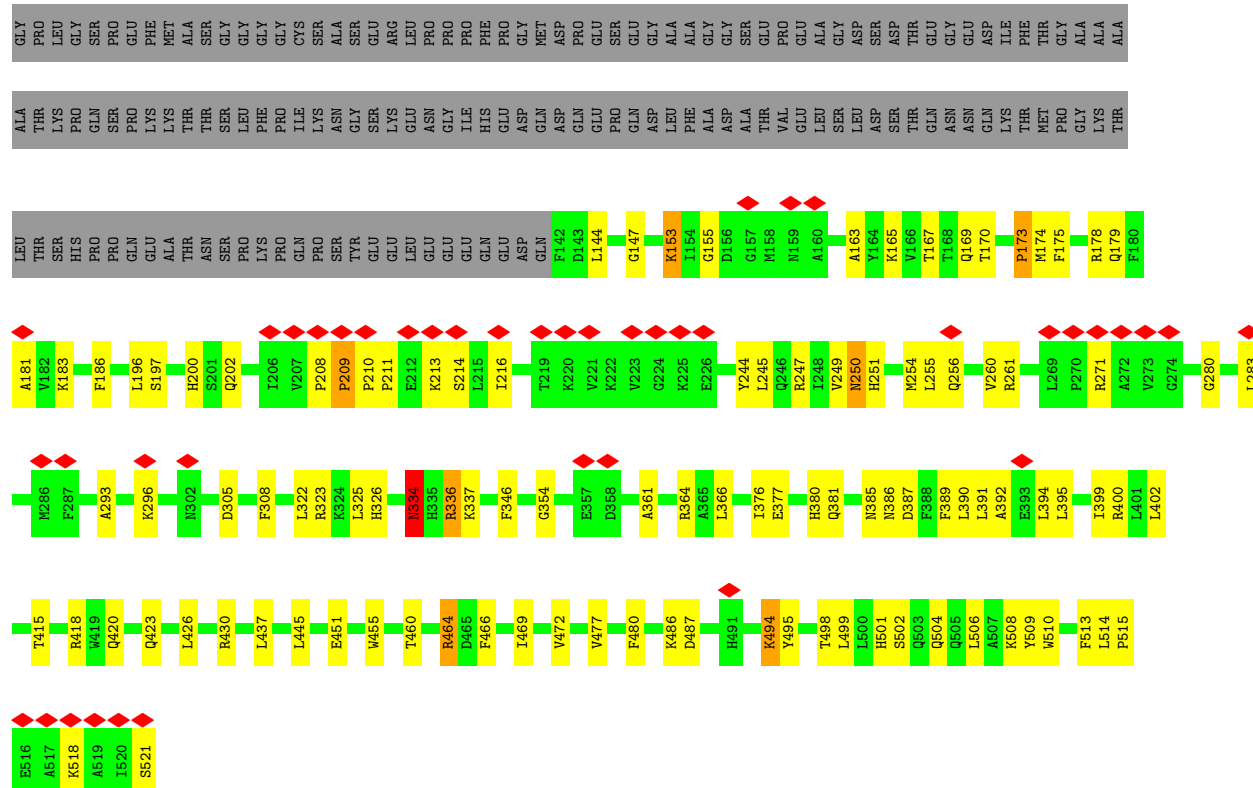
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| K | -6 | PRO | - | expression tag | UNP Q6NZD2 |
| K | -5 | LEU | - | expression tag | UNP Q6NZD2 |
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| L | -5 | LEU | - | expression tag | UNP Q6NZD2 |
| L | -4 | GLY | - | expression tag | UNP Q6NZD2 |
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| L | -1 | GLU | - | expression tag | UNP Q6NZD2 |
| L | 0 | PHE | - | expression tag | UNP Q6NZD2 |
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| M | -6 | PRO | - | expression tag | UNP Q6NZD2 |
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| M | -2 | PRO | - | expression tag | UNP Q6NZD2 |
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| O | -4 | GLY | - | expression tag | UNP Q6NZD2 |
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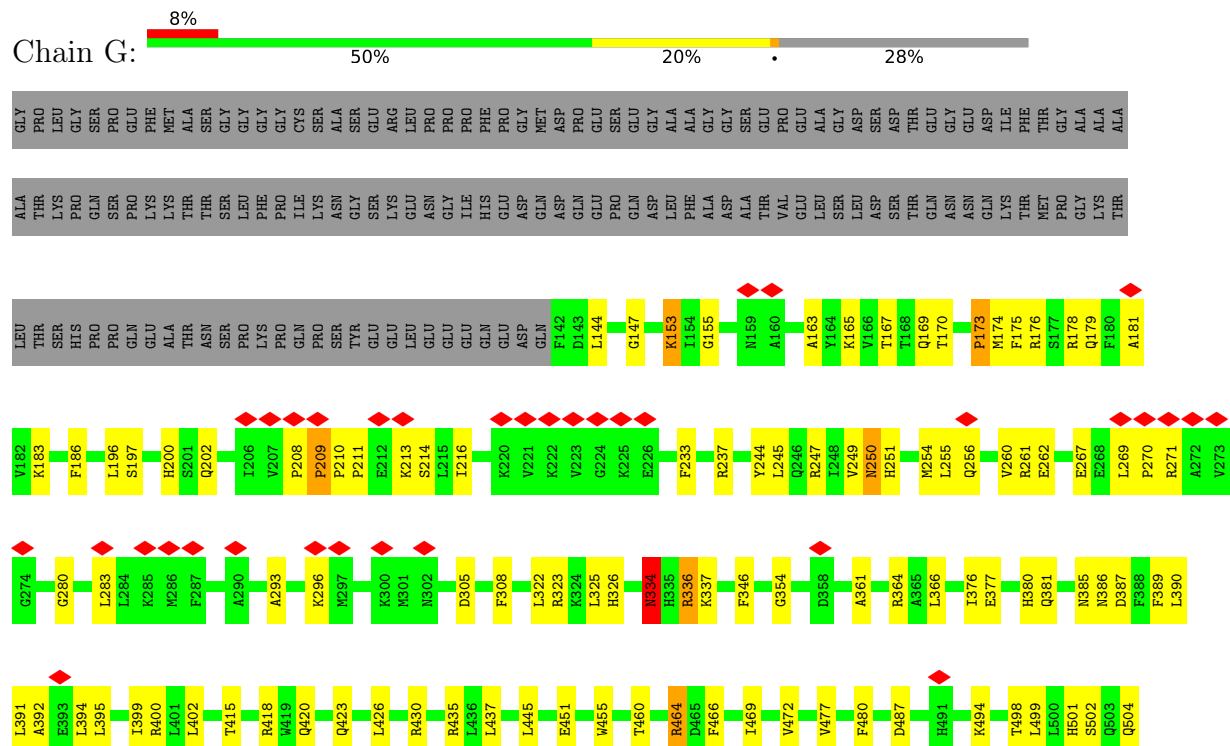
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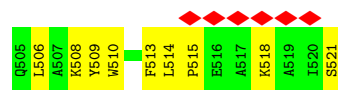




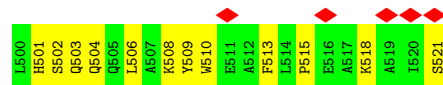
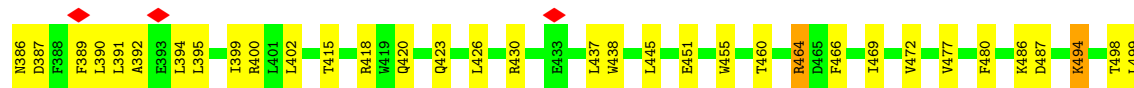
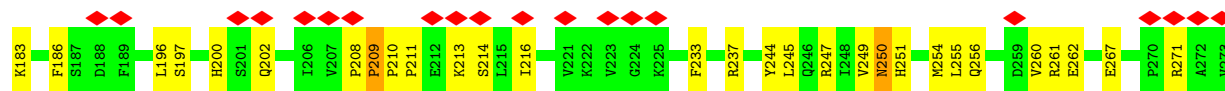
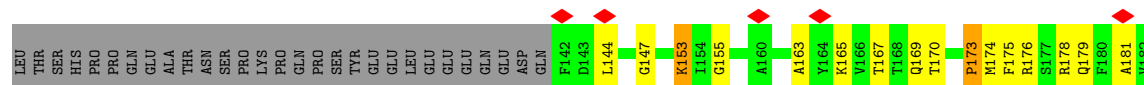
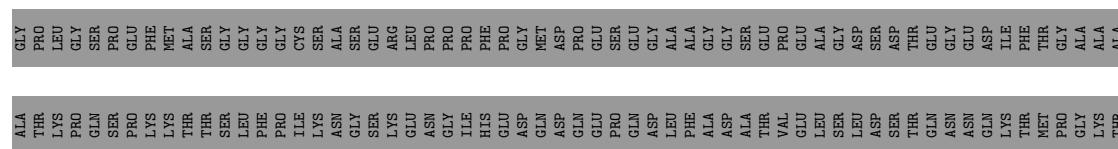
Chain F:

Chain G:

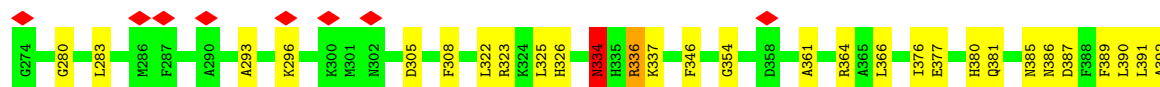
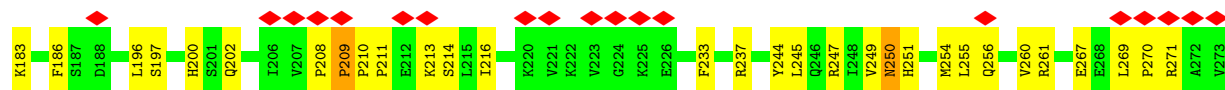
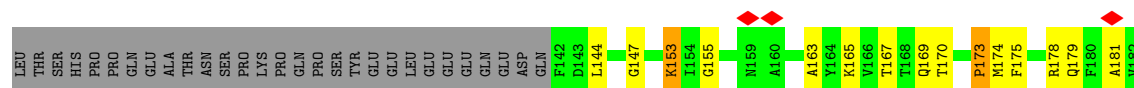
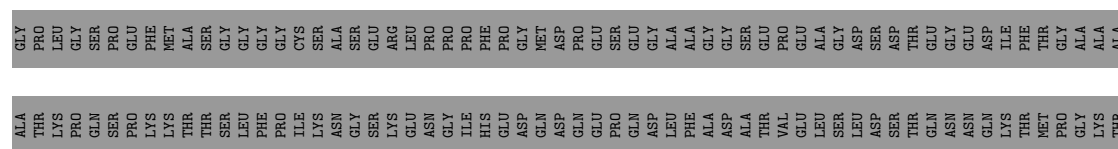


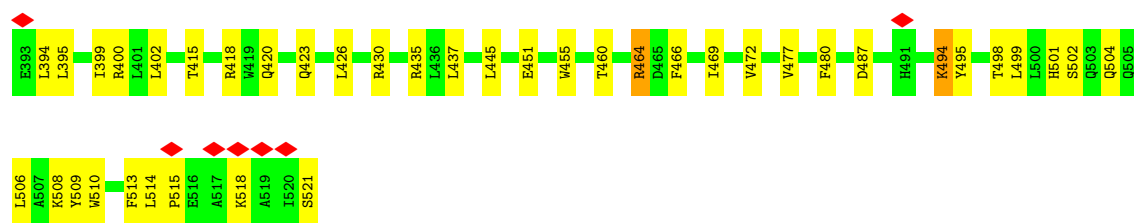


• Molecule 1: Sorting nexin-1

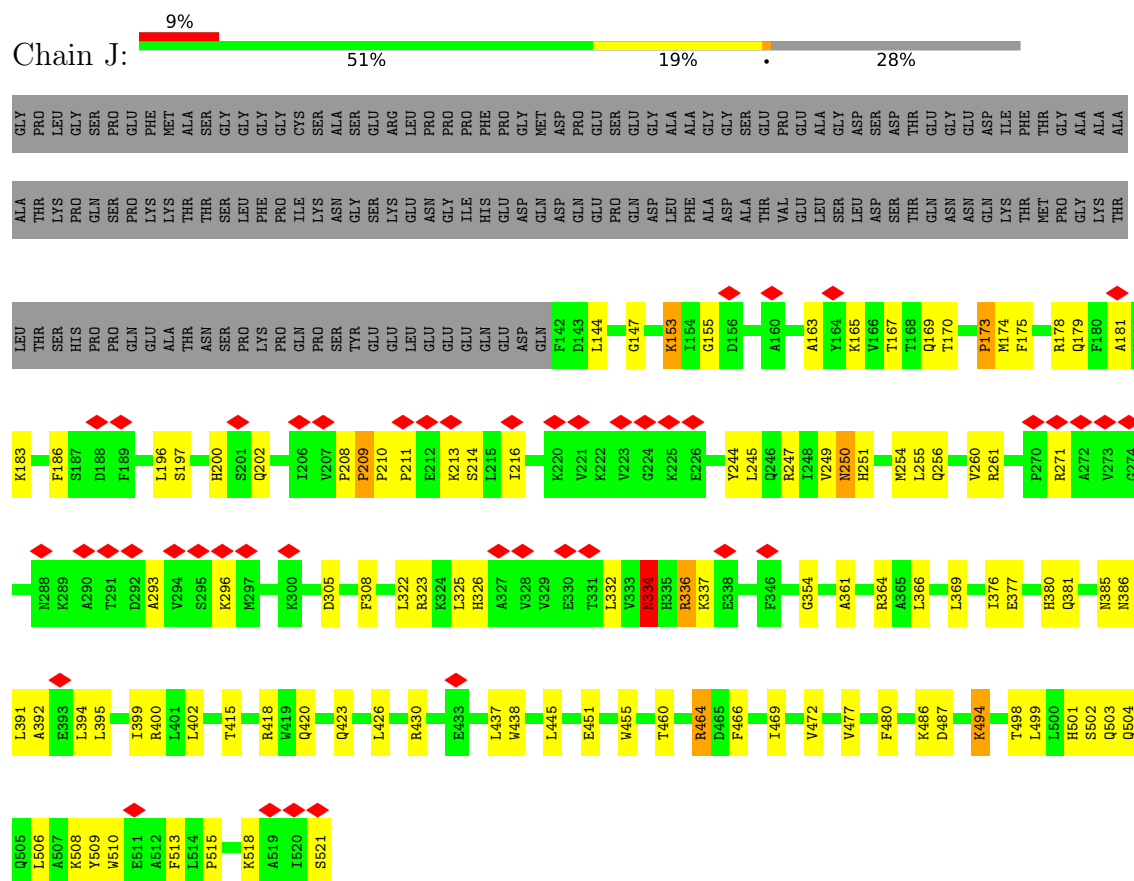


• Molecule 1: Sorting nexin-1

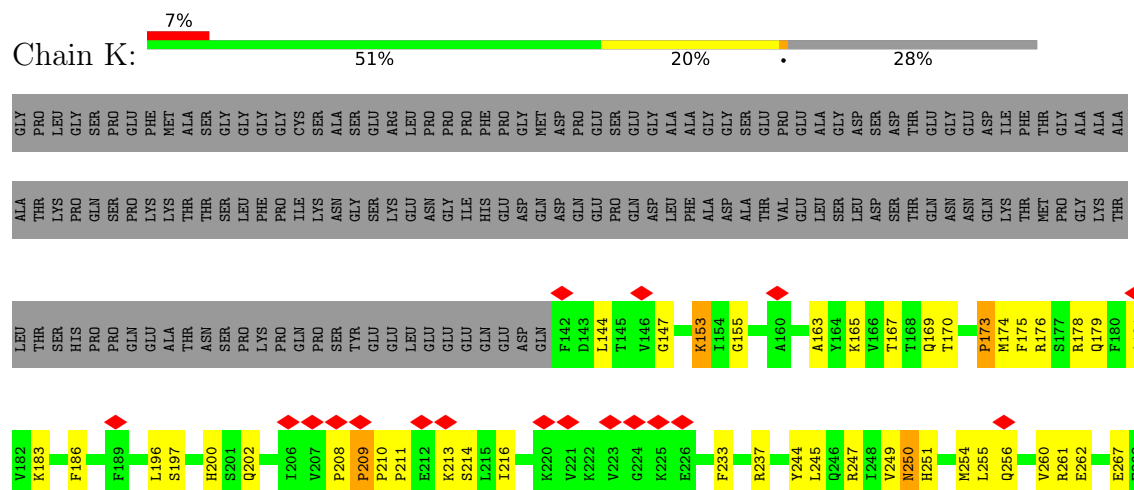


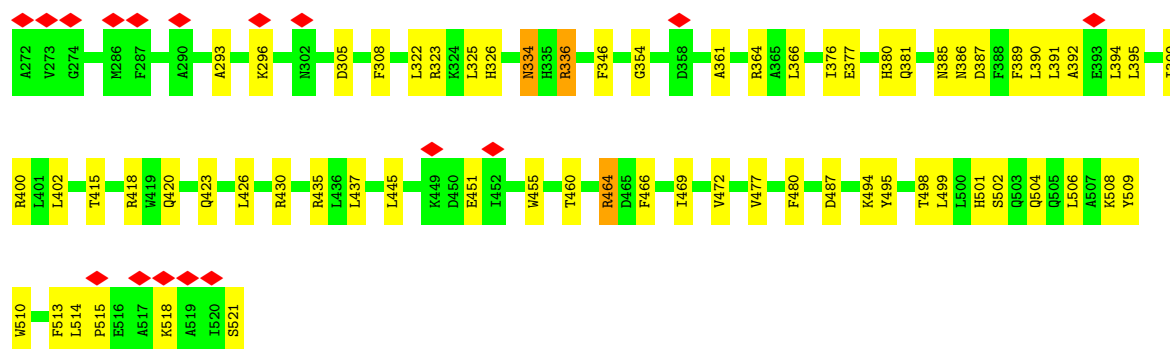


• Molecule 1: Sorting nexin-1

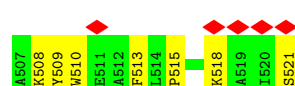
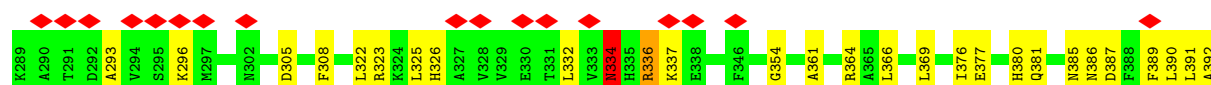
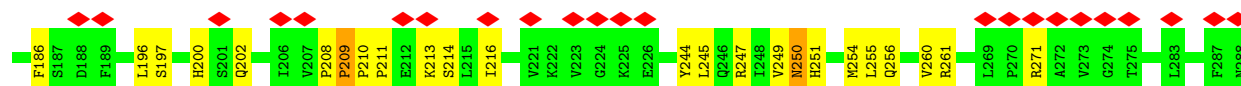
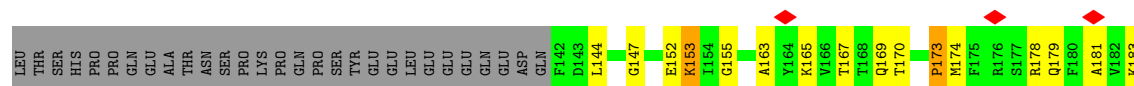
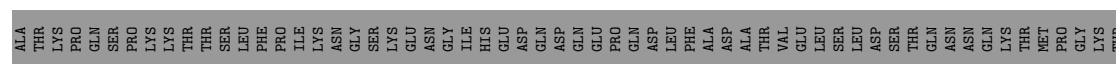
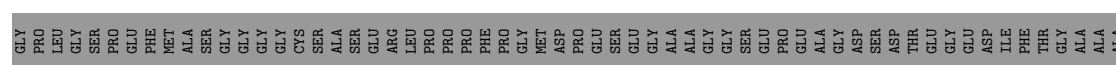


• Molecule 1: Sorting nexin-1

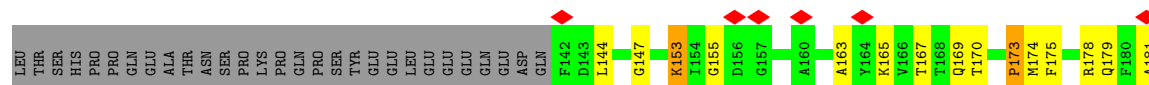
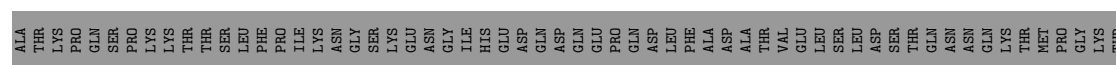
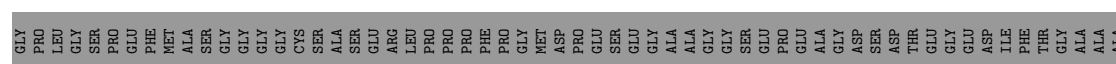


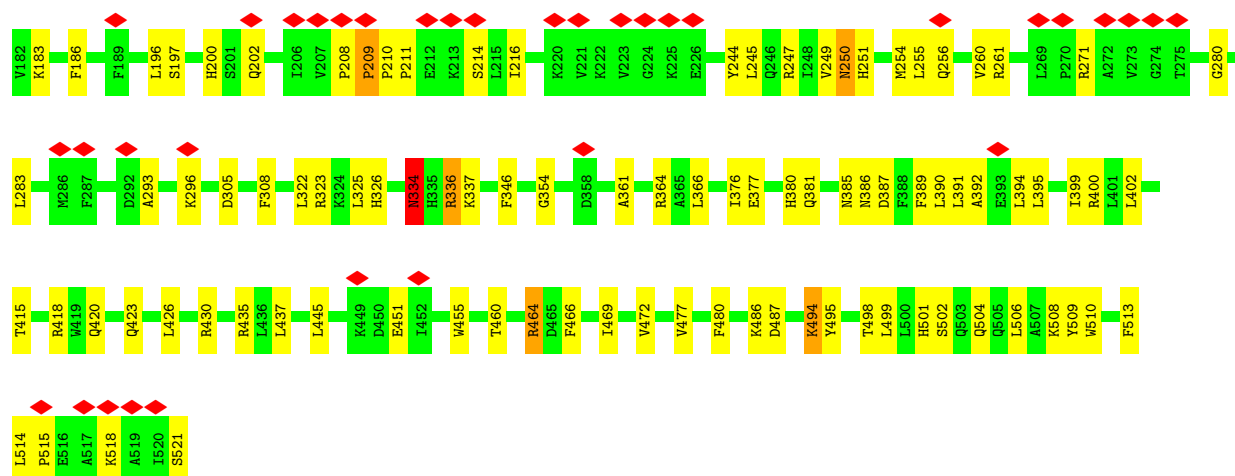


• Molecule 1: Sorting nexin-1



• Molecule 1: Sorting nexin-1





• Molecule 1: Sorting nexin-1



GLY PRO LEU LYS GLN SER PRO GLU PHE MET ALA SER GLY GLY GLY CYS SER ALA SER ASP MET GLN PRO GLU ARG LEU LEU PRO GLY PHE PRO GLY MET GLN ASP GLY ALA GLY GLY SER GLU VAL PRO GLU ALA GLY SER ASP THR GLN GLY ASP THR ILE ASP PHE THR GLY ALA ALA

ALA THR LYS PRO GLN SER PRO GLU PHE THR SER LEU PHE THR SER ASN ILE LYS GLY SER THR LEU HIS ASP GLN ASP THR VAL GLU LEU SER LEU ASP THR GLN ASN GLN LYS MET THR PRO GLY LYS THR

LEU THR HIS PRO PRO GLU ALA THR ASN PRO SER TYR GLU GLU GLU GLN GLU ASP F142 F143 L144 G147 E152 K153 I154 G155 A163 Y164 K165 V166 T167 Q169 T170 P173 M174 F175 R176 S177 R178 Q179 F180 A181 V182 K183

F186 S187 D188 F189 L196 S197 H200 S201 Q202 I206 V207 P208 P209 P210 P211 E212 K213 S214 I215 I216 V221 K222 V223 G224 K225 E226 F233 R237 Y244 L245 Q246 R247 V249 N250 H251 M254 L255 Q256 V260 R261 E262 L269 P270 R271 A272 G274

L283 F287 N288 K289 A290 A292 D292 A293 V294 S295 K296 M297 K300 D305 F308 L322 R323 K324 H326 A327 V328 V329 E330 T331 L332 V333 R334 R335 R336 K337 E338 F346 G354 D358 A361 R364 A365 L366 L369 I376 E377 Q381 N385 N386

D387 F388 F389 L390 L391 A392 E393 L394 L395 I399 R400 L401 L402 T415 R418 W419 Q420 Q423 L426 R430 E433 L437 W438 L445 E451 W455 T460 R464 D465 F466 I469 V472 V477 F480 D487 K494 T498 L499 L500 H501

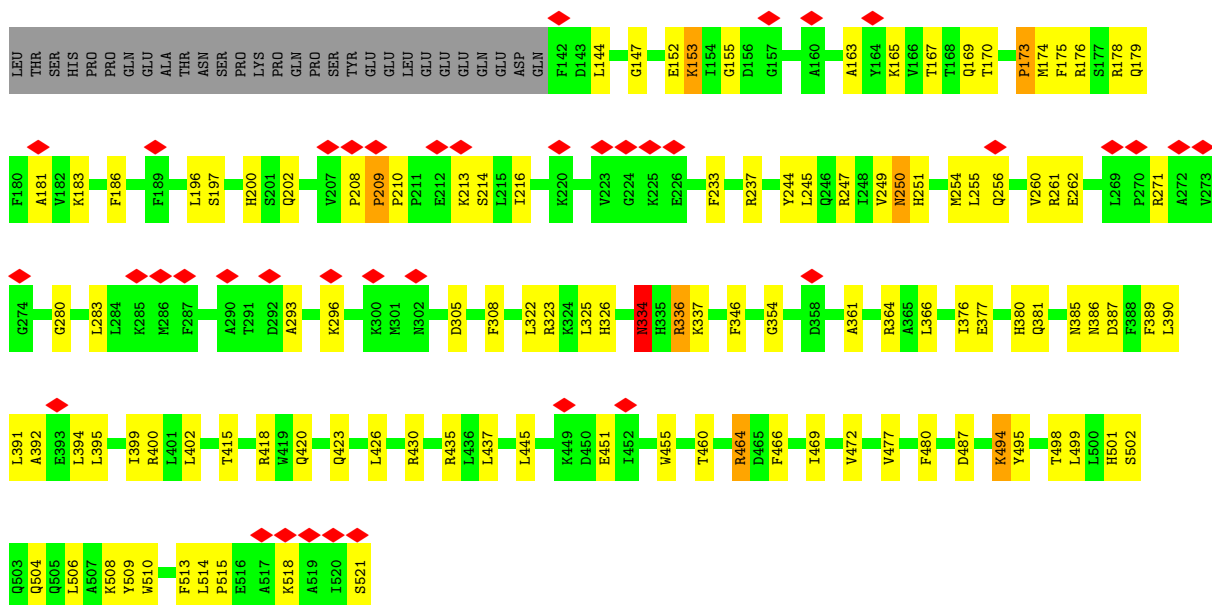
S502 Q503 Q504 Q505 L506 A507 K508 Y509 W510 E511 A512 F513 L514 P515 K518 A519 I520 S521

• Molecule 1: Sorting nexin-1

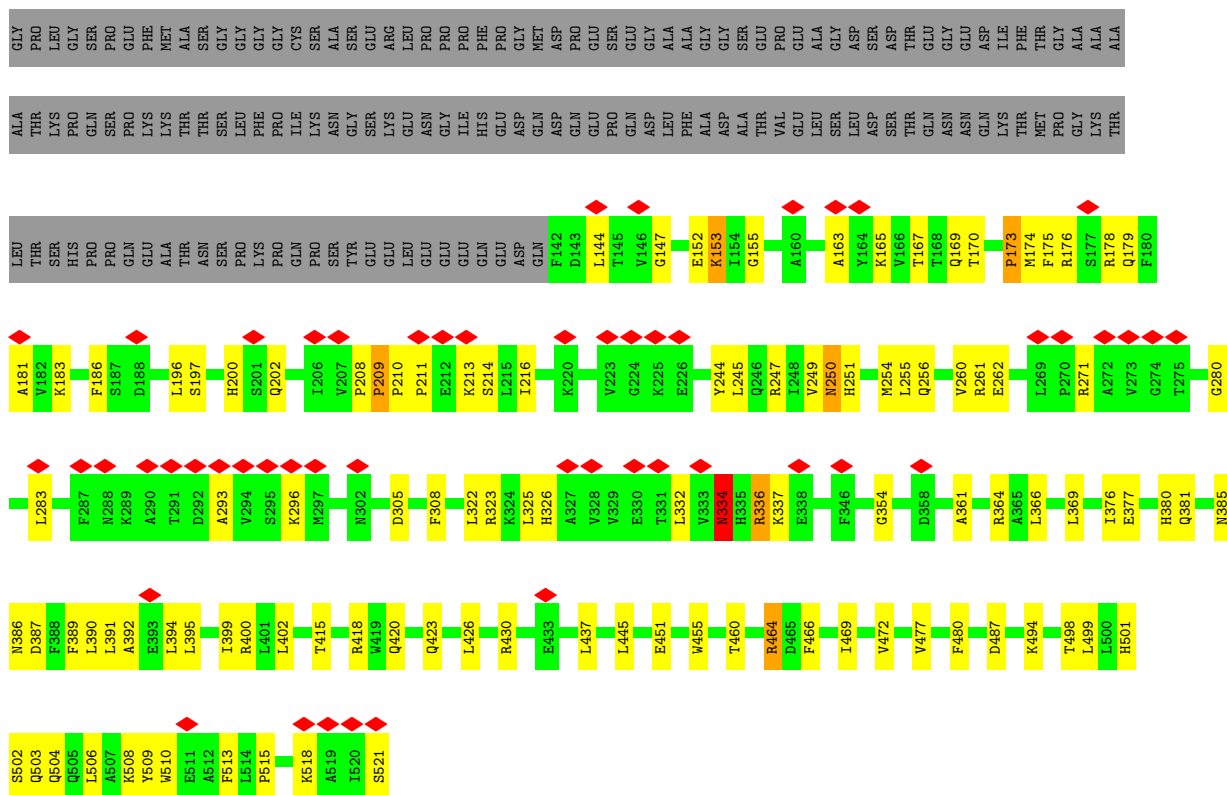


GLY PRO LEU LYS GLN SER PRO GLU PHE MET ALA SER GLY GLY GLY CYS SER ALA SER ASP MET GLN PRO GLU ARG LEU LEU PRO GLY PHE PRO GLY MET GLN ASP GLY ALA GLY GLY SER GLU VAL PRO GLU ALA GLY SER ASP THR GLN GLY ASP THR ILE ASP PHE THR GLY ALA ALA

ALA THR LYS PRO GLN SER PRO GLU PHE THR SER ASN ILE LYS GLY SER THR LEU HIS ASP GLN ASP THR VAL GLU LEU SER LEU ASP THR GLN ASN GLN LYS MET THR PRO GLY LYS THR

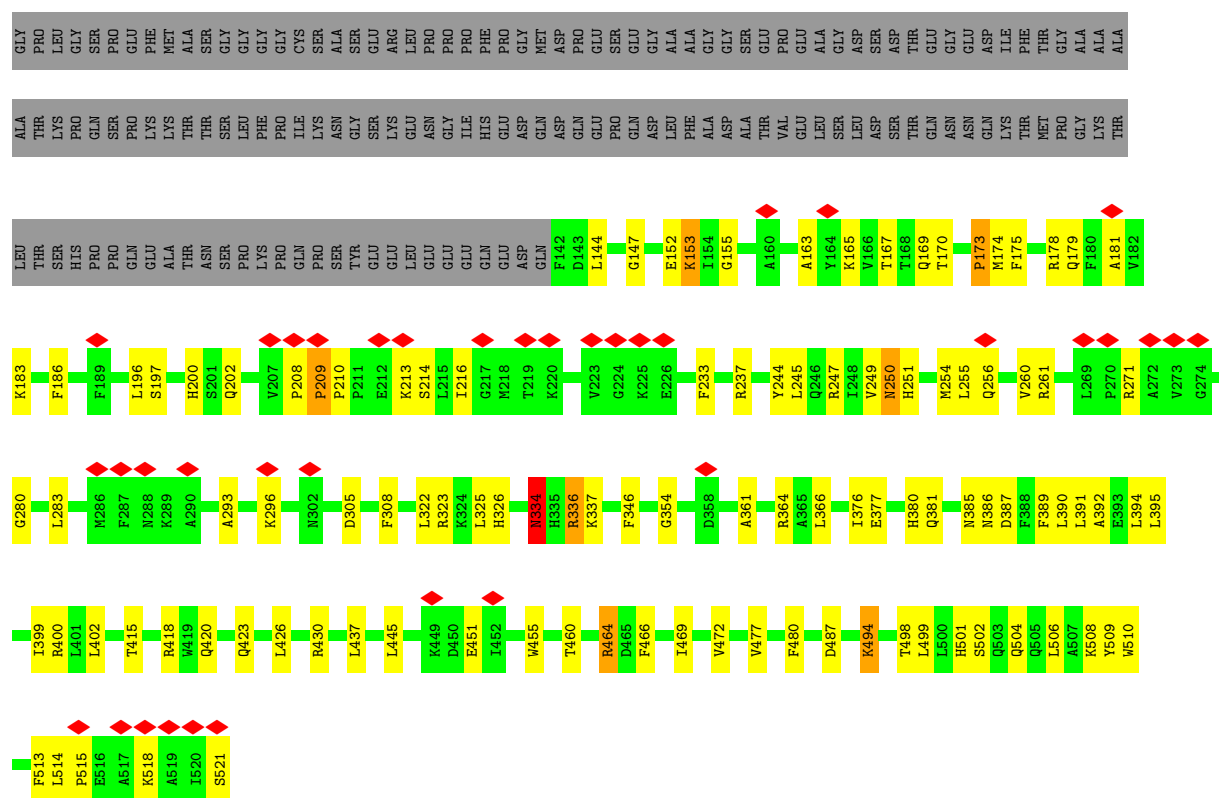


- Molecule 1: Sorting nexin-1

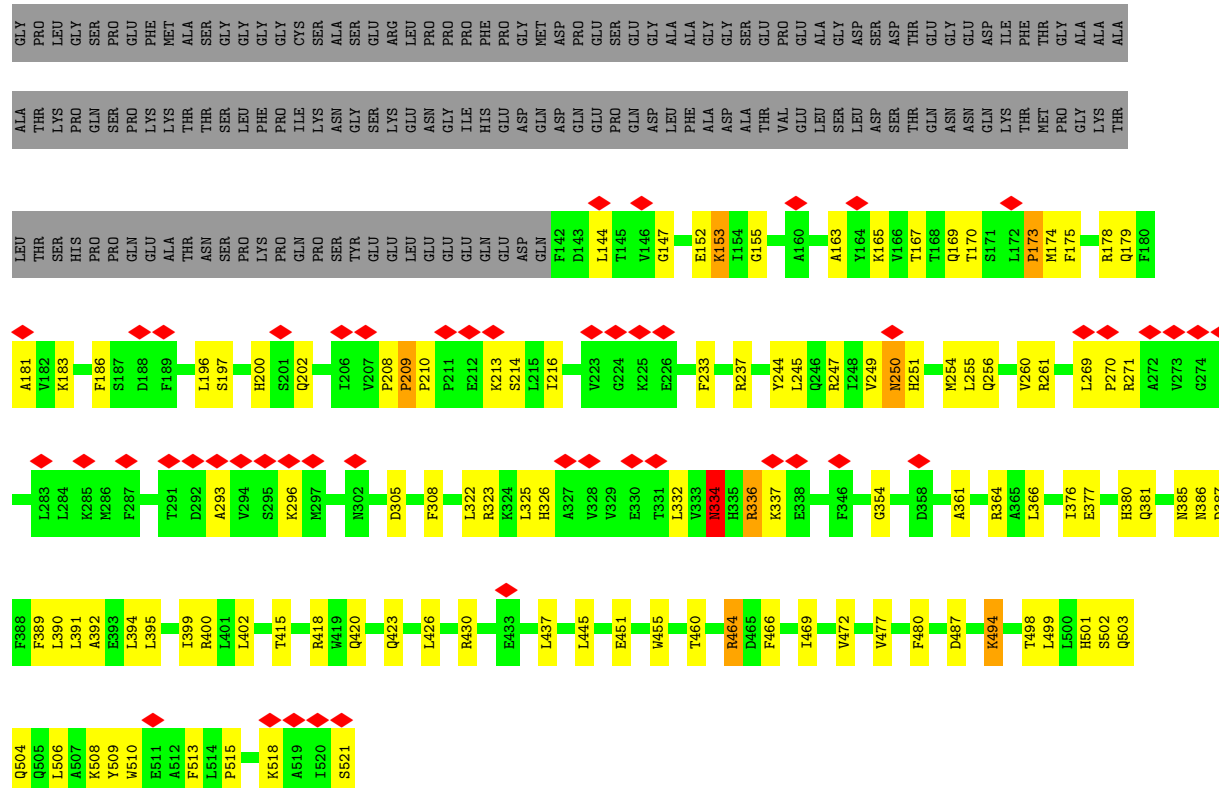


- Molecule 1: Sorting nexin-1





• Molecule 1: Sorting nexin-1



4 Experimental information

| Property | Value | Source |
|------------------------------------|--|-----------|
| EM reconstruction method | HELICAL | Depositor |
| Imposed symmetry | HELICAL, twist=51.51°, rise=7.51 Å, axial sym=C1 | Depositor |
| Number of segments used | 11677 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF was multiplied to each micrographs before tubes selection, and finally CTF amplitude correction was performed following 3D reconstruction | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{Å}^2$) | 25 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 59000 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 7.946 | Depositor |
| Minimum map value | -4.401 | Depositor |
| Average map value | 0.044 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 2.1 | Depositor |
| Map size (Å) | 511.19998, 511.19998, 170.4 | wwPDB |
| Map dimensions | 360, 360, 120 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.42, 1.42, 1.42 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | B | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | C | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | D | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | E | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | F | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | G | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | H | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | I | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | J | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | K | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | L | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | M | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | N | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | O | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | P | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | Q | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| 1 | R | 0.37 | 2/3159 (0.1%) | 0.69 | 0/4248 |
| All | All | 0.37 | 36/56862 (0.1%) | 0.69 | 0/76464 |

All (36) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | I | 334 | ASN | C-N | 7.07 | 1.50 | 1.34 |
| 1 | P | 334 | ASN | C-N | 7.07 | 1.50 | 1.34 |
| 1 | H | 334 | ASN | C-N | 7.07 | 1.50 | 1.34 |
| 1 | M | 334 | ASN | C-N | 7.06 | 1.50 | 1.34 |
| 1 | N | 334 | ASN | C-N | 7.06 | 1.50 | 1.34 |
| 1 | B | 334 | ASN | C-N | 7.06 | 1.50 | 1.34 |
| 1 | C | 334 | ASN | C-N | 7.06 | 1.50 | 1.34 |
| 1 | D | 334 | ASN | C-N | 7.06 | 1.50 | 1.34 |
| 1 | E | 334 | ASN | C-N | 7.06 | 1.50 | 1.34 |
| 1 | J | 334 | ASN | C-N | 7.05 | 1.50 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | K | 334 | ASN | C-N | 7.05 | 1.50 | 1.34 |
| 1 | G | 334 | ASN | C-N | 7.05 | 1.50 | 1.34 |
| 1 | O | 334 | ASN | C-N | 7.05 | 1.50 | 1.34 |
| 1 | L | 334 | ASN | C-N | 7.04 | 1.50 | 1.34 |
| 1 | F | 334 | ASN | C-N | 7.03 | 1.50 | 1.34 |
| 1 | A | 334 | ASN | C-N | 7.02 | 1.50 | 1.34 |
| 1 | R | 334 | ASN | C-N | 7.02 | 1.50 | 1.34 |
| 1 | Q | 334 | ASN | C-N | 7.01 | 1.50 | 1.34 |
| 1 | D | 325 | LEU | C-N | 6.53 | 1.49 | 1.34 |
| 1 | N | 325 | LEU | C-N | 6.53 | 1.49 | 1.34 |
| 1 | J | 325 | LEU | C-N | 6.52 | 1.49 | 1.34 |
| 1 | C | 325 | LEU | C-N | 6.51 | 1.49 | 1.34 |
| 1 | O | 325 | LEU | C-N | 6.51 | 1.49 | 1.34 |
| 1 | Q | 325 | LEU | C-N | 6.51 | 1.49 | 1.34 |
| 1 | L | 325 | LEU | C-N | 6.51 | 1.49 | 1.34 |
| 1 | R | 325 | LEU | C-N | 6.50 | 1.49 | 1.34 |
| 1 | H | 325 | LEU | C-N | 6.50 | 1.49 | 1.34 |
| 1 | P | 325 | LEU | C-N | 6.50 | 1.49 | 1.34 |
| 1 | A | 325 | LEU | C-N | 6.50 | 1.49 | 1.34 |
| 1 | M | 325 | LEU | C-N | 6.49 | 1.49 | 1.34 |
| 1 | F | 325 | LEU | C-N | 6.49 | 1.49 | 1.34 |
| 1 | I | 325 | LEU | C-N | 6.49 | 1.49 | 1.34 |
| 1 | K | 325 | LEU | C-N | 6.49 | 1.49 | 1.34 |
| 1 | G | 325 | LEU | C-N | 6.48 | 1.49 | 1.34 |
| 1 | E | 325 | LEU | C-N | 6.48 | 1.49 | 1.34 |
| 1 | B | 325 | LEU | C-N | 6.45 | 1.48 | 1.34 |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3104 | 0 | 3127 | 65 | 0 |
| 1 | B | 3104 | 0 | 3127 | 65 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | C | 3104 | 0 | 3127 | 63 | 0 |
| 1 | D | 3104 | 0 | 3127 | 63 | 0 |
| 1 | E | 3104 | 0 | 3127 | 63 | 0 |
| 1 | F | 3104 | 0 | 3127 | 63 | 0 |
| 1 | G | 3104 | 0 | 3127 | 66 | 0 |
| 1 | H | 3104 | 0 | 3127 | 66 | 0 |
| 1 | I | 3104 | 0 | 3127 | 66 | 0 |
| 1 | J | 3104 | 0 | 3127 | 64 | 0 |
| 1 | K | 3104 | 0 | 3127 | 63 | 0 |
| 1 | L | 3104 | 0 | 3127 | 63 | 0 |
| 1 | M | 3104 | 0 | 3127 | 64 | 0 |
| 1 | N | 3104 | 0 | 3127 | 66 | 0 |
| 1 | O | 3104 | 0 | 3127 | 66 | 0 |
| 1 | P | 3104 | 0 | 3127 | 63 | 0 |
| 1 | Q | 3104 | 0 | 3127 | 62 | 0 |
| 1 | R | 3104 | 0 | 3127 | 62 | 0 |
| All | All | 55872 | 0 | 56286 | 1097 | 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 10.

All (1097) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:D:426:LEU:O | 1:D:430:ARG:HB2 | 1.81 | 0.81 |
| 1:L:426:LEU:O | 1:L:430:ARG:HB2 | 1.81 | 0.81 |
| 1:R:426:LEU:O | 1:R:430:ARG:HB2 | 1.81 | 0.81 |
| 1:N:426:LEU:O | 1:N:430:ARG:HB2 | 1.81 | 0.81 |
| 1:J:426:LEU:O | 1:J:430:ARG:HB2 | 1.81 | 0.81 |
| 1:C:426:LEU:O | 1:C:430:ARG:HB2 | 1.81 | 0.80 |
| 1:E:426:LEU:O | 1:E:430:ARG:HB2 | 1.81 | 0.80 |
| 1:Q:426:LEU:O | 1:Q:430:ARG:HB2 | 1.81 | 0.80 |
| 1:H:426:LEU:O | 1:H:430:ARG:HB2 | 1.81 | 0.80 |
| 1:I:426:LEU:O | 1:I:430:ARG:HB2 | 1.81 | 0.80 |
| 1:K:426:LEU:O | 1:K:430:ARG:HB2 | 1.81 | 0.80 |
| 1:O:426:LEU:O | 1:O:430:ARG:HB2 | 1.81 | 0.80 |
| 1:A:426:LEU:O | 1:A:430:ARG:HB2 | 1.81 | 0.80 |
| 1:B:426:LEU:O | 1:B:430:ARG:HB2 | 1.81 | 0.80 |
| 1:P:426:LEU:O | 1:P:430:ARG:HB2 | 1.81 | 0.80 |
| 1:F:426:LEU:O | 1:F:430:ARG:HB2 | 1.81 | 0.80 |
| 1:G:426:LEU:O | 1:G:430:ARG:HB2 | 1.81 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:M:426:LEU:O | 1:M:430:ARG:HB2 | 1.81 | 0.79 |
| 1:F:451:GLU:O | 1:F:455:TRP:HB2 | 1.83 | 0.79 |
| 1:Q:451:GLU:O | 1:Q:455:TRP:HB2 | 1.84 | 0.78 |
| 1:C:451:GLU:O | 1:C:455:TRP:HB2 | 1.84 | 0.78 |
| 1:D:451:GLU:O | 1:D:455:TRP:HB2 | 1.84 | 0.78 |
| 1:R:451:GLU:O | 1:R:455:TRP:HB2 | 1.83 | 0.78 |
| 1:A:451:GLU:O | 1:A:455:TRP:HB2 | 1.83 | 0.78 |
| 1:B:451:GLU:O | 1:B:455:TRP:HB2 | 1.83 | 0.78 |
| 1:P:451:GLU:O | 1:P:455:TRP:HB2 | 1.83 | 0.78 |
| 1:O:451:GLU:O | 1:O:455:TRP:HB2 | 1.84 | 0.78 |
| 1:E:451:GLU:O | 1:E:455:TRP:HB2 | 1.83 | 0.78 |
| 1:H:451:GLU:O | 1:H:455:TRP:HB2 | 1.83 | 0.77 |
| 1:I:451:GLU:O | 1:I:455:TRP:HB2 | 1.83 | 0.77 |
| 1:N:451:GLU:O | 1:N:455:TRP:HB2 | 1.83 | 0.77 |
| 1:G:451:GLU:O | 1:G:455:TRP:HB2 | 1.83 | 0.77 |
| 1:K:451:GLU:O | 1:K:455:TRP:HB2 | 1.83 | 0.76 |
| 1:J:451:GLU:O | 1:J:455:TRP:HB2 | 1.83 | 0.76 |
| 1:L:451:GLU:O | 1:L:455:TRP:HB2 | 1.84 | 0.76 |
| 1:M:451:GLU:O | 1:M:455:TRP:HB2 | 1.84 | 0.75 |
| 1:D:504:GLN:O | 1:D:508:LYS:HB2 | 1.92 | 0.70 |
| 1:C:504:GLN:O | 1:C:508:LYS:HB2 | 1.92 | 0.69 |
| 1:G:504:GLN:O | 1:G:508:LYS:HB2 | 1.92 | 0.69 |
| 1:R:504:GLN:O | 1:R:508:LYS:HB2 | 1.92 | 0.69 |
| 1:N:504:GLN:O | 1:N:508:LYS:HB2 | 1.92 | 0.69 |
| 1:Q:504:GLN:O | 1:Q:508:LYS:HB2 | 1.92 | 0.69 |
| 1:M:504:GLN:O | 1:M:508:LYS:HB2 | 1.92 | 0.69 |
| 1:K:504:GLN:O | 1:K:508:LYS:HB2 | 1.92 | 0.69 |
| 1:H:504:GLN:O | 1:H:508:LYS:HB2 | 1.92 | 0.69 |
| 1:J:504:GLN:O | 1:J:508:LYS:HB2 | 1.92 | 0.69 |
| 1:A:504:GLN:O | 1:A:508:LYS:HB2 | 1.92 | 0.69 |
| 1:E:504:GLN:O | 1:E:508:LYS:HB2 | 1.92 | 0.69 |
| 1:I:504:GLN:O | 1:I:508:LYS:HB2 | 1.92 | 0.68 |
| 1:O:504:GLN:O | 1:O:508:LYS:HB2 | 1.92 | 0.68 |
| 1:P:504:GLN:O | 1:P:508:LYS:HB2 | 1.92 | 0.68 |
| 1:B:504:GLN:O | 1:B:508:LYS:HB2 | 1.92 | 0.68 |
| 1:L:504:GLN:O | 1:L:508:LYS:HB2 | 1.92 | 0.68 |
| 1:F:504:GLN:O | 1:F:508:LYS:HB2 | 1.92 | 0.68 |
| 1:L:210:PRO:HB3 | 1:L:400:ARG:HH12 | 1.60 | 0.67 |
| 1:O:210:PRO:HB3 | 1:O:400:ARG:HH12 | 1.60 | 0.67 |
| 1:A:210:PRO:HB3 | 1:A:400:ARG:HH12 | 1.60 | 0.67 |
| 1:D:210:PRO:HB3 | 1:D:400:ARG:HH12 | 1.58 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:210:PRO:HB3 | 1:K:400:ARG:HH12 | 1.60 | 0.67 |
| 1:I:210:PRO:HB3 | 1:I:400:ARG:HH12 | 1.60 | 0.67 |
| 1:J:210:PRO:HB3 | 1:J:400:ARG:HH12 | 1.60 | 0.67 |
| 1:F:210:PRO:HB3 | 1:F:400:ARG:HH12 | 1.60 | 0.66 |
| 1:B:210:PRO:HB3 | 1:B:400:ARG:HH12 | 1.60 | 0.66 |
| 1:E:210:PRO:HB3 | 1:E:400:ARG:HH12 | 1.60 | 0.66 |
| 1:G:210:PRO:HB3 | 1:G:400:ARG:HH12 | 1.60 | 0.66 |
| 1:M:210:PRO:HB3 | 1:M:400:ARG:HH12 | 1.59 | 0.66 |
| 1:P:210:PRO:HB3 | 1:P:400:ARG:HH12 | 1.60 | 0.66 |
| 1:H:210:PRO:HB3 | 1:H:400:ARG:HH12 | 1.60 | 0.66 |
| 1:R:210:PRO:HB3 | 1:R:400:ARG:HH12 | 1.60 | 0.66 |
| 1:N:210:PRO:HB3 | 1:N:400:ARG:HH12 | 1.60 | 0.65 |
| 1:E:336:ARG:NH2 | 1:E:381:GLN:O | 2.30 | 0.65 |
| 1:N:336:ARG:NH2 | 1:N:381:GLN:O | 2.30 | 0.65 |
| 1:D:336:ARG:NH2 | 1:D:381:GLN:O | 2.30 | 0.65 |
| 1:I:336:ARG:NH2 | 1:I:381:GLN:O | 2.30 | 0.65 |
| 1:P:336:ARG:NH2 | 1:P:381:GLN:O | 2.30 | 0.65 |
| 1:B:336:ARG:NH2 | 1:B:381:GLN:O | 2.30 | 0.64 |
| 1:G:336:ARG:NH2 | 1:G:381:GLN:O | 2.30 | 0.64 |
| 1:Q:210:PRO:HB3 | 1:Q:400:ARG:HH12 | 1.59 | 0.64 |
| 1:R:336:ARG:NH2 | 1:R:381:GLN:O | 2.30 | 0.64 |
| 1:K:336:ARG:NH2 | 1:K:381:GLN:O | 2.30 | 0.64 |
| 1:L:336:ARG:NH2 | 1:L:381:GLN:O | 2.30 | 0.64 |
| 1:C:210:PRO:HB3 | 1:C:400:ARG:HH12 | 1.60 | 0.64 |
| 1:J:336:ARG:NH2 | 1:J:381:GLN:O | 2.30 | 0.64 |
| 1:M:336:ARG:NH2 | 1:M:381:GLN:O | 2.30 | 0.64 |
| 1:C:336:ARG:NH2 | 1:C:381:GLN:O | 2.30 | 0.64 |
| 1:K:163:ALA:HB1 | 1:K:183:LYS:HD2 | 1.80 | 0.64 |
| 1:Q:336:ARG:NH2 | 1:Q:381:GLN:O | 2.30 | 0.64 |
| 1:M:163:ALA:HB1 | 1:M:183:LYS:HD2 | 1.80 | 0.63 |
| 1:A:163:ALA:HB1 | 1:A:183:LYS:HD2 | 1.80 | 0.63 |
| 1:C:163:ALA:HB1 | 1:C:183:LYS:HD2 | 1.80 | 0.63 |
| 1:E:163:ALA:HB1 | 1:E:183:LYS:HD2 | 1.80 | 0.63 |
| 1:I:163:ALA:HB1 | 1:I:183:LYS:HD2 | 1.80 | 0.63 |
| 1:F:336:ARG:NH2 | 1:F:381:GLN:O | 2.30 | 0.63 |
| 1:G:163:ALA:HB1 | 1:G:183:LYS:HD2 | 1.80 | 0.63 |
| 1:O:163:ALA:HB1 | 1:O:183:LYS:HD2 | 1.80 | 0.63 |
| 1:Q:163:ALA:HB1 | 1:Q:183:LYS:HD2 | 1.80 | 0.63 |
| 1:A:336:ARG:NH2 | 1:A:381:GLN:O | 2.30 | 0.63 |
| 1:H:336:ARG:NH2 | 1:H:381:GLN:O | 2.30 | 0.63 |
| 1:O:336:ARG:NH2 | 1:O:381:GLN:O | 2.30 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:O:186:PHE:HE2 | 1:O:214:SER:HB3 | 1.64 | 0.63 |
| 1:D:163:ALA:HB1 | 1:D:183:LYS:HD2 | 1.80 | 0.63 |
| 1:H:186:PHE:HE2 | 1:H:214:SER:HB3 | 1.64 | 0.63 |
| 1:J:186:PHE:HE2 | 1:J:214:SER:HB3 | 1.64 | 0.63 |
| 1:C:186:PHE:HE2 | 1:C:214:SER:HB3 | 1.65 | 0.62 |
| 1:F:163:ALA:HB1 | 1:F:183:LYS:HD2 | 1.80 | 0.62 |
| 1:Q:186:PHE:HE2 | 1:Q:214:SER:HB3 | 1.65 | 0.62 |
| 1:J:163:ALA:HB1 | 1:J:183:LYS:HD2 | 1.80 | 0.62 |
| 1:L:163:ALA:HB1 | 1:L:183:LYS:HD2 | 1.80 | 0.62 |
| 1:A:186:PHE:HE2 | 1:A:214:SER:HB3 | 1.65 | 0.62 |
| 1:R:163:ALA:HB1 | 1:R:183:LYS:HD2 | 1.80 | 0.62 |
| 1:B:163:ALA:HB1 | 1:B:183:LYS:HD2 | 1.80 | 0.62 |
| 1:F:186:PHE:HE2 | 1:F:214:SER:HB3 | 1.64 | 0.62 |
| 1:M:186:PHE:HE2 | 1:M:214:SER:HB3 | 1.64 | 0.62 |
| 1:K:186:PHE:HE2 | 1:K:214:SER:HB3 | 1.64 | 0.62 |
| 1:N:163:ALA:HB1 | 1:N:183:LYS:HD2 | 1.80 | 0.62 |
| 1:L:186:PHE:HE2 | 1:L:214:SER:HB3 | 1.64 | 0.62 |
| 1:R:186:PHE:HE2 | 1:R:214:SER:HB3 | 1.64 | 0.62 |
| 1:E:186:PHE:HE2 | 1:E:214:SER:HB3 | 1.64 | 0.62 |
| 1:P:163:ALA:HB1 | 1:P:183:LYS:HD2 | 1.80 | 0.62 |
| 1:D:186:PHE:HE2 | 1:D:214:SER:HB3 | 1.65 | 0.62 |
| 1:H:163:ALA:HB1 | 1:H:183:LYS:HD2 | 1.80 | 0.62 |
| 1:N:186:PHE:HE2 | 1:N:214:SER:HB3 | 1.64 | 0.62 |
| 1:G:186:PHE:HE2 | 1:G:214:SER:HB3 | 1.64 | 0.61 |
| 1:P:186:PHE:HE2 | 1:P:214:SER:HB3 | 1.64 | 0.61 |
| 1:B:186:PHE:HE2 | 1:B:214:SER:HB3 | 1.64 | 0.61 |
| 1:I:186:PHE:HE2 | 1:I:214:SER:HB3 | 1.65 | 0.60 |
| 1:F:361:ALA:O | 1:F:521:SER:OG | 2.20 | 0.58 |
| 1:N:361:ALA:O | 1:N:521:SER:OG | 2.20 | 0.58 |
| 1:A:361:ALA:O | 1:A:521:SER:OG | 2.20 | 0.58 |
| 1:O:361:ALA:O | 1:O:521:SER:OG | 2.20 | 0.58 |
| 1:C:361:ALA:O | 1:C:521:SER:OG | 2.20 | 0.58 |
| 1:H:361:ALA:O | 1:H:521:SER:OG | 2.20 | 0.58 |
| 1:Q:361:ALA:O | 1:Q:521:SER:OG | 2.20 | 0.58 |
| 1:L:361:ALA:O | 1:L:521:SER:OG | 2.20 | 0.57 |
| 1:D:361:ALA:O | 1:D:521:SER:OG | 2.20 | 0.57 |
| 1:R:361:ALA:O | 1:R:521:SER:OG | 2.20 | 0.57 |
| 1:H:165:LYS:NZ | 1:H:167:THR:OG1 | 2.38 | 0.57 |
| 1:G:165:LYS:NZ | 1:G:167:THR:OG1 | 2.38 | 0.57 |
| 1:J:165:LYS:NZ | 1:J:167:THR:OG1 | 2.38 | 0.57 |
| 1:L:165:LYS:NZ | 1:L:167:THR:OG1 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:165:LYS:NZ | 1:P:167:THR:OG1 | 2.38 | 0.57 |
| 1:Q:165:LYS:NZ | 1:Q:167:THR:OG1 | 2.38 | 0.57 |
| 1:B:165:LYS:NZ | 1:B:167:THR:OG1 | 2.38 | 0.57 |
| 1:C:165:LYS:NZ | 1:C:167:THR:OG1 | 2.38 | 0.57 |
| 1:E:165:LYS:NZ | 1:E:167:THR:OG1 | 2.38 | 0.57 |
| 1:F:165:LYS:NZ | 1:F:167:THR:OG1 | 2.38 | 0.57 |
| 1:D:165:LYS:NZ | 1:D:167:THR:OG1 | 2.38 | 0.56 |
| 1:M:361:ALA:O | 1:M:521:SER:OG | 2.20 | 0.56 |
| 1:K:165:LYS:NZ | 1:K:167:THR:OG1 | 2.38 | 0.56 |
| 1:M:165:LYS:NZ | 1:M:167:THR:OG1 | 2.38 | 0.56 |
| 1:O:165:LYS:NZ | 1:O:167:THR:OG1 | 2.38 | 0.56 |
| 1:R:165:LYS:NZ | 1:R:167:THR:OG1 | 2.38 | 0.56 |
| 1:A:165:LYS:NZ | 1:A:167:THR:OG1 | 2.38 | 0.56 |
| 1:E:361:ALA:O | 1:E:521:SER:OG | 2.20 | 0.56 |
| 1:I:165:LYS:NZ | 1:I:167:THR:OG1 | 2.38 | 0.56 |
| 1:J:361:ALA:O | 1:J:521:SER:OG | 2.20 | 0.56 |
| 1:N:165:LYS:NZ | 1:N:167:THR:OG1 | 2.38 | 0.56 |
| 1:F:173:PRO:HA | 1:F:178:ARG:HH22 | 1.71 | 0.56 |
| 1:Q:173:PRO:HA | 1:Q:178:ARG:HH22 | 1.71 | 0.56 |
| 1:C:173:PRO:HA | 1:C:178:ARG:HH22 | 1.71 | 0.56 |
| 1:E:173:PRO:HA | 1:E:178:ARG:HH22 | 1.71 | 0.55 |
| 1:A:173:PRO:HA | 1:A:178:ARG:HH22 | 1.71 | 0.55 |
| 1:O:173:PRO:HA | 1:O:178:ARG:HH22 | 1.71 | 0.55 |
| 1:M:293:ALA:HA | 1:M:296:LYS:HE3 | 1.89 | 0.55 |
| 1:O:293:ALA:HA | 1:O:296:LYS:HE3 | 1.89 | 0.55 |
| 1:A:293:ALA:HA | 1:A:296:LYS:HE3 | 1.89 | 0.55 |
| 1:H:173:PRO:HA | 1:H:178:ARG:HH22 | 1.71 | 0.55 |
| 1:K:293:ALA:HA | 1:K:296:LYS:HE3 | 1.89 | 0.55 |
| 1:B:361:ALA:O | 1:B:521:SER:OG | 2.20 | 0.55 |
| 1:P:173:PRO:HA | 1:P:178:ARG:HH22 | 1.71 | 0.55 |
| 1:K:173:PRO:HA | 1:K:178:ARG:HH22 | 1.71 | 0.55 |
| 1:B:173:PRO:HA | 1:B:178:ARG:HH22 | 1.71 | 0.55 |
| 1:C:293:ALA:HA | 1:C:296:LYS:HE3 | 1.89 | 0.55 |
| 1:L:173:PRO:HA | 1:L:178:ARG:HH22 | 1.71 | 0.55 |
| 1:P:361:ALA:O | 1:P:521:SER:OG | 2.20 | 0.55 |
| 1:Q:293:ALA:HA | 1:Q:296:LYS:HE3 | 1.89 | 0.55 |
| 1:R:173:PRO:HA | 1:R:178:ARG:HH22 | 1.71 | 0.55 |
| 1:L:293:ALA:HA | 1:L:296:LYS:HE3 | 1.89 | 0.55 |
| 1:N:293:ALA:HA | 1:N:296:LYS:HE3 | 1.89 | 0.55 |
| 1:B:399:ILE:HD13 | 1:B:402:LEU:HD12 | 1.90 | 0.54 |
| 1:J:293:ALA:HA | 1:J:296:LYS:HE3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:399:ILE:HD13 | 1:J:402:LEU:HD12 | 1.90 | 0.54 |
| 1:D:173:PRO:HA | 1:D:178:ARG:HH22 | 1.71 | 0.54 |
| 1:I:173:PRO:HA | 1:I:178:ARG:HH22 | 1.71 | 0.54 |
| 1:I:399:ILE:HD13 | 1:I:402:LEU:HD12 | 1.90 | 0.54 |
| 1:N:399:ILE:HD13 | 1:N:402:LEU:HD12 | 1.90 | 0.54 |
| 1:P:399:ILE:HD13 | 1:P:402:LEU:HD12 | 1.90 | 0.54 |
| 1:H:293:ALA:HA | 1:H:296:LYS:HE3 | 1.89 | 0.54 |
| 1:I:293:ALA:HA | 1:I:296:LYS:HE3 | 1.89 | 0.54 |
| 1:K:399:ILE:HD13 | 1:K:402:LEU:HD12 | 1.90 | 0.54 |
| 1:E:399:ILE:HD13 | 1:E:402:LEU:HD12 | 1.90 | 0.54 |
| 1:G:173:PRO:HA | 1:G:178:ARG:HH22 | 1.71 | 0.54 |
| 1:G:399:ILE:HD13 | 1:G:402:LEU:HD12 | 1.89 | 0.54 |
| 1:H:399:ILE:HD13 | 1:H:402:LEU:HD12 | 1.90 | 0.54 |
| 1:J:173:PRO:HA | 1:J:178:ARG:HH22 | 1.71 | 0.54 |
| 1:L:399:ILE:HD13 | 1:L:402:LEU:HD12 | 1.89 | 0.54 |
| 1:K:361:ALA:O | 1:K:521:SER:OG | 2.20 | 0.54 |
| 1:M:399:ILE:HD13 | 1:M:402:LEU:HD12 | 1.89 | 0.54 |
| 1:O:399:ILE:HD13 | 1:O:402:LEU:HD12 | 1.90 | 0.54 |
| 1:P:293:ALA:HA | 1:P:296:LYS:HE3 | 1.89 | 0.54 |
| 1:B:293:ALA:HA | 1:B:296:LYS:HE3 | 1.89 | 0.54 |
| 1:C:399:ILE:HD13 | 1:C:402:LEU:HD12 | 1.90 | 0.54 |
| 1:D:399:ILE:HD13 | 1:D:402:LEU:HD12 | 1.90 | 0.54 |
| 1:E:293:ALA:HA | 1:E:296:LYS:HE3 | 1.89 | 0.54 |
| 1:Q:399:ILE:HD13 | 1:Q:402:LEU:HD12 | 1.90 | 0.54 |
| 1:R:399:ILE:HD13 | 1:R:402:LEU:HD12 | 1.89 | 0.54 |
| 1:A:399:ILE:HD13 | 1:A:402:LEU:HD12 | 1.90 | 0.54 |
| 1:F:293:ALA:HA | 1:F:296:LYS:HE3 | 1.89 | 0.54 |
| 1:G:361:ALA:O | 1:G:521:SER:OG | 2.20 | 0.54 |
| 1:D:293:ALA:HA | 1:D:296:LYS:HE3 | 1.89 | 0.53 |
| 1:D:502:SER:O | 1:D:506:LEU:HB3 | 2.09 | 0.53 |
| 1:F:399:ILE:HD13 | 1:F:402:LEU:HD12 | 1.90 | 0.53 |
| 1:H:420:GLN:OE1 | 1:H:423:GLN:NE2 | 2.42 | 0.53 |
| 1:N:420:GLN:OE1 | 1:N:423:GLN:NE2 | 2.42 | 0.53 |
| 1:A:420:GLN:OE1 | 1:A:423:GLN:NE2 | 2.42 | 0.53 |
| 1:J:420:GLN:OE1 | 1:J:423:GLN:NE2 | 2.42 | 0.53 |
| 1:N:173:PRO:HA | 1:N:178:ARG:HH22 | 1.71 | 0.53 |
| 1:O:420:GLN:OE1 | 1:O:423:GLN:NE2 | 2.42 | 0.53 |
| 1:G:420:GLN:OE1 | 1:G:423:GLN:NE2 | 2.42 | 0.53 |
| 1:I:420:GLN:OE1 | 1:I:423:GLN:NE2 | 2.42 | 0.53 |
| 1:K:506:LEU:HD21 | 1:L:506:LEU:HD21 | 1.90 | 0.53 |
| 1:M:420:GLN:OE1 | 1:M:423:GLN:NE2 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:293:ALA:HA | 1:R:296:LYS:HE3 | 1.89 | 0.53 |
| 1:C:506:LEU:HD21 | 1:D:506:LEU:HD21 | 1.90 | 0.53 |
| 1:K:420:GLN:OE1 | 1:K:423:GLN:NE2 | 2.42 | 0.53 |
| 1:L:420:GLN:OE1 | 1:L:423:GLN:NE2 | 2.42 | 0.53 |
| 1:M:173:PRO:HA | 1:M:178:ARG:HH22 | 1.71 | 0.53 |
| 1:R:502:SER:O | 1:R:506:LEU:HB3 | 2.09 | 0.53 |
| 1:P:420:GLN:OE1 | 1:P:423:GLN:NE2 | 2.42 | 0.53 |
| 1:Q:506:LEU:HD21 | 1:R:506:LEU:HD21 | 1.90 | 0.53 |
| 1:C:502:SER:O | 1:C:506:LEU:HB3 | 2.09 | 0.53 |
| 1:E:502:SER:O | 1:E:506:LEU:HB3 | 2.09 | 0.53 |
| 1:F:420:GLN:OE1 | 1:F:423:GLN:NE2 | 2.42 | 0.53 |
| 1:M:506:LEU:HD21 | 1:N:506:LEU:HD21 | 1.90 | 0.53 |
| 1:K:510:TRP:HZ3 | 1:L:499:LEU:HG | 1.73 | 0.53 |
| 1:B:420:GLN:OE1 | 1:B:423:GLN:NE2 | 2.42 | 0.53 |
| 1:I:361:ALA:O | 1:I:521:SER:OG | 2.20 | 0.53 |
| 1:M:466:PHE:HA | 1:M:469:ILE:HG12 | 1.91 | 0.53 |
| 1:Q:502:SER:O | 1:Q:506:LEU:HB3 | 2.09 | 0.53 |
| 1:Q:510:TRP:HZ3 | 1:R:499:LEU:HG | 1.73 | 0.53 |
| 1:G:293:ALA:HA | 1:G:296:LYS:HE3 | 1.89 | 0.53 |
| 1:I:466:PHE:HA | 1:I:469:ILE:HG12 | 1.91 | 0.53 |
| 1:I:510:TRP:HZ3 | 1:J:499:LEU:HG | 1.73 | 0.53 |
| 1:K:466:PHE:HA | 1:K:469:ILE:HG12 | 1.91 | 0.53 |
| 1:Q:420:GLN:OE1 | 1:Q:423:GLN:NE2 | 2.42 | 0.53 |
| 1:A:506:LEU:HD21 | 1:B:506:LEU:HD21 | 1.90 | 0.52 |
| 1:E:510:TRP:HZ3 | 1:F:499:LEU:HG | 1.73 | 0.52 |
| 1:H:502:SER:O | 1:H:506:LEU:HB3 | 2.09 | 0.52 |
| 1:A:466:PHE:HA | 1:A:469:ILE:HG12 | 1.91 | 0.52 |
| 1:A:502:SER:O | 1:A:506:LEU:HB3 | 2.09 | 0.52 |
| 1:C:510:TRP:HZ3 | 1:D:499:LEU:HG | 1.73 | 0.52 |
| 1:G:502:SER:O | 1:G:506:LEU:HB3 | 2.09 | 0.52 |
| 1:I:506:LEU:HD21 | 1:J:506:LEU:HD21 | 1.90 | 0.52 |
| 1:M:510:TRP:HZ3 | 1:N:499:LEU:HG | 1.73 | 0.52 |
| 1:O:502:SER:O | 1:O:506:LEU:HB3 | 2.09 | 0.52 |
| 1:O:506:LEU:HD21 | 1:P:506:LEU:HD21 | 1.90 | 0.52 |
| 1:C:420:GLN:OE1 | 1:C:423:GLN:NE2 | 2.42 | 0.52 |
| 1:M:251:HIS:HB2 | 1:M:254:MET:HB2 | 1.92 | 0.52 |
| 1:O:466:PHE:HA | 1:O:469:ILE:HG12 | 1.91 | 0.52 |
| 1:G:506:LEU:HD21 | 1:H:506:LEU:HD21 | 1.90 | 0.52 |
| 1:K:251:HIS:HB2 | 1:K:254:MET:HB2 | 1.92 | 0.52 |
| 1:E:420:GLN:OE1 | 1:E:423:GLN:NE2 | 2.42 | 0.52 |
| 1:E:469:ILE:HA | 1:E:472:VAL:HG22 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:506:LEU:HD21 | 1:F:506:LEU:HD21 | 1.90 | 0.52 |
| 1:L:502:SER:O | 1:L:506:LEU:HB3 | 2.09 | 0.52 |
| 1:M:502:SER:O | 1:M:506:LEU:HB3 | 2.09 | 0.52 |
| 1:P:502:SER:O | 1:P:506:LEU:HB3 | 2.09 | 0.52 |
| 1:A:251:HIS:HB2 | 1:A:254:MET:HB2 | 1.92 | 0.52 |
| 1:F:502:SER:O | 1:F:506:LEU:HB3 | 2.09 | 0.52 |
| 1:G:469:ILE:HA | 1:G:472:VAL:HG22 | 1.92 | 0.52 |
| 1:I:251:HIS:HB2 | 1:I:254:MET:HB2 | 1.91 | 0.52 |
| 1:K:502:SER:O | 1:K:506:LEU:HB3 | 2.09 | 0.52 |
| 1:N:466:PHE:HA | 1:N:469:ILE:HG12 | 1.91 | 0.52 |
| 1:N:502:SER:O | 1:N:506:LEU:HB3 | 2.09 | 0.52 |
| 1:O:251:HIS:HB2 | 1:O:254:MET:HB2 | 1.92 | 0.52 |
| 1:B:469:ILE:HA | 1:B:472:VAL:HG22 | 1.92 | 0.52 |
| 1:D:420:GLN:OE1 | 1:D:423:GLN:NE2 | 2.42 | 0.52 |
| 1:D:469:ILE:HA | 1:D:472:VAL:HG22 | 1.92 | 0.52 |
| 1:L:466:PHE:HA | 1:L:469:ILE:HG12 | 1.91 | 0.52 |
| 1:O:510:TRP:HZ3 | 1:P:499:LEU:HG | 1.73 | 0.52 |
| 1:R:469:ILE:HA | 1:R:472:VAL:HG22 | 1.92 | 0.52 |
| 1:A:510:TRP:HZ3 | 1:B:499:LEU:HG | 1.73 | 0.52 |
| 1:F:469:ILE:HA | 1:F:472:VAL:HG22 | 1.92 | 0.52 |
| 1:G:466:PHE:HA | 1:G:469:ILE:HG12 | 1.92 | 0.52 |
| 1:H:438:TRP:HD1 | 1:I:435:ARG:HH21 | 1.57 | 0.52 |
| 1:J:502:SER:O | 1:J:506:LEU:HB3 | 2.09 | 0.52 |
| 1:B:502:SER:O | 1:B:506:LEU:HB3 | 2.09 | 0.52 |
| 1:C:466:PHE:HA | 1:C:469:ILE:HG12 | 1.91 | 0.52 |
| 1:G:510:TRP:HZ3 | 1:H:499:LEU:HG | 1.73 | 0.52 |
| 1:Q:466:PHE:HA | 1:Q:469:ILE:HG12 | 1.91 | 0.52 |
| 1:Q:469:ILE:HA | 1:Q:472:VAL:HG22 | 1.92 | 0.52 |
| 1:R:420:GLN:OE1 | 1:R:423:GLN:NE2 | 2.42 | 0.52 |
| 1:P:469:ILE:HA | 1:P:472:VAL:HG22 | 1.92 | 0.52 |
| 1:J:466:PHE:HA | 1:J:469:ILE:HG12 | 1.92 | 0.51 |
| 1:N:469:ILE:HA | 1:N:472:VAL:HG22 | 1.92 | 0.51 |
| 1:C:469:ILE:HA | 1:C:472:VAL:HG22 | 1.92 | 0.51 |
| 1:H:466:PHE:HA | 1:H:469:ILE:HG12 | 1.91 | 0.51 |
| 1:I:502:SER:O | 1:I:506:LEU:HB3 | 2.09 | 0.51 |
| 1:K:499:LEU:HG | 1:L:510:TRP:HZ3 | 1.75 | 0.51 |
| 1:B:354:GLY:HA3 | 1:B:366:LEU:HD21 | 1.93 | 0.51 |
| 1:C:499:LEU:HG | 1:D:510:TRP:HZ3 | 1.75 | 0.51 |
| 1:E:466:PHE:HA | 1:E:469:ILE:HG12 | 1.92 | 0.51 |
| 1:E:499:LEU:HG | 1:F:510:TRP:HZ3 | 1.75 | 0.51 |
| 1:J:354:GLY:HA3 | 1:J:366:LEU:HD21 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:504:GLN:O | 1:C:508:LYS:CB | 2.59 | 0.51 |
| 1:F:504:GLN:O | 1:F:508:LYS:CB | 2.59 | 0.51 |
| 1:I:469:ILE:HA | 1:I:472:VAL:HG22 | 1.92 | 0.51 |
| 1:P:354:GLY:HA3 | 1:P:366:LEU:HD21 | 1.93 | 0.51 |
| 1:P:466:PHE:HA | 1:P:469:ILE:HG12 | 1.91 | 0.51 |
| 1:Q:499:LEU:HG | 1:R:510:TRP:HZ3 | 1.75 | 0.51 |
| 1:Q:504:GLN:O | 1:Q:508:LYS:CB | 2.59 | 0.51 |
| 1:F:251:HIS:HB2 | 1:F:254:MET:HB2 | 1.92 | 0.51 |
| 1:H:354:GLY:HA3 | 1:H:366:LEU:HD21 | 1.93 | 0.51 |
| 1:L:354:GLY:HA3 | 1:L:366:LEU:HD21 | 1.93 | 0.51 |
| 1:N:354:GLY:HA3 | 1:N:366:LEU:HD21 | 1.93 | 0.51 |
| 1:B:466:PHE:HA | 1:B:469:ILE:HG12 | 1.91 | 0.51 |
| 1:B:504:GLN:O | 1:B:508:LYS:CB | 2.59 | 0.51 |
| 1:C:251:HIS:HB2 | 1:C:254:MET:HB2 | 1.92 | 0.51 |
| 1:D:251:HIS:HB2 | 1:D:254:MET:HB2 | 1.92 | 0.51 |
| 1:G:354:GLY:HA3 | 1:G:366:LEU:HD21 | 1.93 | 0.51 |
| 1:I:504:GLN:O | 1:I:508:LYS:CB | 2.59 | 0.51 |
| 1:Q:251:HIS:HB2 | 1:Q:254:MET:HB2 | 1.92 | 0.51 |
| 1:A:469:ILE:HA | 1:A:472:VAL:HG22 | 1.92 | 0.51 |
| 1:E:354:GLY:HA3 | 1:E:366:LEU:HD21 | 1.93 | 0.51 |
| 1:H:251:HIS:HB2 | 1:H:254:MET:HB2 | 1.92 | 0.51 |
| 1:I:247:ARG:HA | 1:I:250:ASN:HB2 | 1.93 | 0.51 |
| 1:I:354:GLY:HA3 | 1:I:366:LEU:HD21 | 1.93 | 0.51 |
| 1:M:354:GLY:HA3 | 1:M:366:LEU:HD21 | 1.93 | 0.51 |
| 1:N:251:HIS:HB2 | 1:N:254:MET:HB2 | 1.92 | 0.51 |
| 1:N:504:GLN:O | 1:N:508:LYS:CB | 2.59 | 0.51 |
| 1:P:504:GLN:O | 1:P:508:LYS:CB | 2.59 | 0.51 |
| 1:C:249:VAL:HA | 1:C:255:LEU:HD22 | 1.93 | 0.51 |
| 1:E:249:VAL:HA | 1:E:255:LEU:HD22 | 1.93 | 0.51 |
| 1:K:354:GLY:HA3 | 1:K:366:LEU:HD21 | 1.93 | 0.51 |
| 1:M:153:LYS:HD2 | 1:M:155:GLY:H | 1.76 | 0.51 |
| 1:O:469:ILE:HA | 1:O:472:VAL:HG22 | 1.92 | 0.51 |
| 1:P:251:HIS:HB2 | 1:P:254:MET:HB2 | 1.92 | 0.51 |
| 1:R:466:PHE:HA | 1:R:469:ILE:HG12 | 1.91 | 0.51 |
| 1:B:251:HIS:HB2 | 1:B:254:MET:HB2 | 1.92 | 0.51 |
| 1:C:354:GLY:HA3 | 1:C:366:LEU:HD21 | 1.93 | 0.51 |
| 1:D:208:PRO:HB2 | 1:D:244:TYR:HA | 1.93 | 0.51 |
| 1:E:251:HIS:HB2 | 1:E:254:MET:HB2 | 1.92 | 0.51 |
| 1:F:249:VAL:HA | 1:F:255:LEU:HD22 | 1.93 | 0.51 |
| 1:F:466:PHE:HA | 1:F:469:ILE:HG12 | 1.91 | 0.51 |
| 1:G:251:HIS:HB2 | 1:G:254:MET:HB2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:153:LYS:HD2 | 1:H:155:GLY:H | 1.76 | 0.51 |
| 1:J:153:LYS:HD2 | 1:J:155:GLY:H | 1.76 | 0.51 |
| 1:J:251:HIS:HB2 | 1:J:254:MET:HB2 | 1.92 | 0.51 |
| 1:L:251:HIS:HB2 | 1:L:254:MET:HB2 | 1.92 | 0.51 |
| 1:O:153:LYS:HD2 | 1:O:155:GLY:H | 1.76 | 0.51 |
| 1:O:354:GLY:HA3 | 1:O:366:LEU:HD21 | 1.93 | 0.51 |
| 1:A:153:LYS:HD2 | 1:A:155:GLY:H | 1.76 | 0.51 |
| 1:A:354:GLY:HA3 | 1:A:366:LEU:HD21 | 1.93 | 0.51 |
| 1:D:354:GLY:HA3 | 1:D:366:LEU:HD21 | 1.93 | 0.51 |
| 1:H:469:ILE:HA | 1:H:472:VAL:HG22 | 1.92 | 0.51 |
| 1:L:153:LYS:HD2 | 1:L:155:GLY:H | 1.76 | 0.51 |
| 1:M:504:GLN:O | 1:M:508:LYS:CB | 2.59 | 0.51 |
| 1:Q:354:GLY:HA3 | 1:Q:366:LEU:HD21 | 1.93 | 0.51 |
| 1:R:251:HIS:HB2 | 1:R:254:MET:HB2 | 1.92 | 0.51 |
| 1:R:354:GLY:HA3 | 1:R:366:LEU:HD21 | 1.93 | 0.51 |
| 1:D:249:VAL:HA | 1:D:255:LEU:HD22 | 1.93 | 0.50 |
| 1:G:499:LEU:HG | 1:H:510:TRP:HZ3 | 1.75 | 0.50 |
| 1:H:504:GLN:O | 1:H:508:LYS:CB | 2.59 | 0.50 |
| 1:L:469:ILE:HA | 1:L:472:VAL:HG22 | 1.92 | 0.50 |
| 1:P:249:VAL:HA | 1:P:255:LEU:HD22 | 1.93 | 0.50 |
| 1:Q:249:VAL:HA | 1:Q:255:LEU:HD22 | 1.93 | 0.50 |
| 1:R:249:VAL:HA | 1:R:255:LEU:HD22 | 1.93 | 0.50 |
| 1:A:499:LEU:HG | 1:B:510:TRP:HZ3 | 1.75 | 0.50 |
| 1:D:466:PHE:HA | 1:D:469:ILE:HG12 | 1.91 | 0.50 |
| 1:F:354:GLY:HA3 | 1:F:366:LEU:HD21 | 1.93 | 0.50 |
| 1:I:153:LYS:HD2 | 1:I:155:GLY:H | 1.76 | 0.50 |
| 1:M:469:ILE:HA | 1:M:472:VAL:HG22 | 1.92 | 0.50 |
| 1:N:144:LEU:HA | 1:N:170:THR:HG23 | 1.94 | 0.50 |
| 1:O:499:LEU:HG | 1:P:510:TRP:HZ3 | 1.75 | 0.50 |
| 1:J:504:GLN:O | 1:J:508:LYS:CB | 2.59 | 0.50 |
| 1:K:469:ILE:HA | 1:K:472:VAL:HG22 | 1.92 | 0.50 |
| 1:L:144:LEU:HA | 1:L:170:THR:HG23 | 1.94 | 0.50 |
| 1:B:249:VAL:HA | 1:B:255:LEU:HD22 | 1.93 | 0.50 |
| 1:G:504:GLN:O | 1:G:508:LYS:CB | 2.59 | 0.50 |
| 1:J:144:LEU:HA | 1:J:170:THR:HG23 | 1.94 | 0.50 |
| 1:L:247:ARG:HA | 1:L:250:ASN:HB2 | 1.93 | 0.50 |
| 1:B:144:LEU:HA | 1:B:170:THR:HG23 | 1.94 | 0.50 |
| 1:C:153:LYS:HD2 | 1:C:155:GLY:H | 1.76 | 0.50 |
| 1:C:247:ARG:HA | 1:C:250:ASN:HB2 | 1.93 | 0.50 |
| 1:K:247:ARG:HA | 1:K:250:ASN:HB2 | 1.93 | 0.50 |
| 1:N:247:ARG:HA | 1:N:250:ASN:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:249:VAL:HA | 1:G:255:LEU:HD22 | 1.93 | 0.50 |
| 1:H:144:LEU:HA | 1:H:170:THR:HG23 | 1.94 | 0.50 |
| 1:K:249:VAL:HA | 1:K:255:LEU:HD22 | 1.93 | 0.50 |
| 1:L:438:TRP:HD1 | 1:M:435:ARG:HH21 | 1.60 | 0.50 |
| 1:M:499:LEU:HG | 1:N:510:TRP:HZ3 | 1.75 | 0.50 |
| 1:O:144:LEU:HA | 1:O:170:THR:HG23 | 1.94 | 0.50 |
| 1:O:504:GLN:O | 1:O:508:LYS:CB | 2.59 | 0.50 |
| 1:P:144:LEU:HA | 1:P:170:THR:HG23 | 1.94 | 0.50 |
| 1:Q:247:ARG:HA | 1:Q:250:ASN:HB2 | 1.93 | 0.50 |
| 1:A:249:VAL:HA | 1:A:255:LEU:HD22 | 1.93 | 0.50 |
| 1:L:504:GLN:O | 1:L:508:LYS:CB | 2.59 | 0.50 |
| 1:N:153:LYS:HD2 | 1:N:155:GLY:H | 1.76 | 0.50 |
| 1:Q:153:LYS:HD2 | 1:Q:155:GLY:H | 1.76 | 0.50 |
| 1:A:247:ARG:HA | 1:A:250:ASN:HB2 | 1.93 | 0.50 |
| 1:A:504:GLN:O | 1:A:508:LYS:CB | 2.59 | 0.50 |
| 1:G:247:ARG:HA | 1:G:250:ASN:HB2 | 1.93 | 0.50 |
| 1:M:144:LEU:HA | 1:M:170:THR:HG23 | 1.94 | 0.50 |
| 1:M:249:VAL:HA | 1:M:255:LEU:HD22 | 1.93 | 0.50 |
| 1:O:249:VAL:HA | 1:O:255:LEU:HD22 | 1.93 | 0.50 |
| 1:A:144:LEU:HA | 1:A:170:THR:HG23 | 1.94 | 0.50 |
| 1:C:144:LEU:HA | 1:C:170:THR:HG23 | 1.94 | 0.50 |
| 1:C:514:LEU:HD22 | 1:D:503:GLN:HE22 | 1.77 | 0.50 |
| 1:D:504:GLN:O | 1:D:508:LYS:CB | 2.59 | 0.50 |
| 1:E:247:ARG:HA | 1:E:250:ASN:HB2 | 1.93 | 0.50 |
| 1:F:153:LYS:HD2 | 1:F:155:GLY:H | 1.76 | 0.50 |
| 1:J:469:ILE:HA | 1:J:472:VAL:HG22 | 1.92 | 0.50 |
| 1:O:247:ARG:HA | 1:O:250:ASN:HB2 | 1.93 | 0.50 |
| 1:Q:514:LEU:HD22 | 1:R:503:GLN:HE22 | 1.77 | 0.50 |
| 1:R:153:LYS:HD2 | 1:R:155:GLY:H | 1.76 | 0.50 |
| 1:I:249:VAL:HA | 1:I:255:LEU:HD22 | 1.93 | 0.49 |
| 1:Q:144:LEU:HA | 1:Q:170:THR:HG23 | 1.94 | 0.49 |
| 1:D:153:LYS:HD2 | 1:D:155:GLY:H | 1.76 | 0.49 |
| 1:H:249:VAL:HA | 1:H:255:LEU:HD22 | 1.93 | 0.49 |
| 1:B:247:ARG:HA | 1:B:250:ASN:HB2 | 1.93 | 0.49 |
| 1:E:514:LEU:HD22 | 1:F:503:GLN:HE22 | 1.77 | 0.49 |
| 1:I:144:LEU:HA | 1:I:170:THR:HG23 | 1.94 | 0.49 |
| 1:K:144:LEU:HA | 1:K:170:THR:HG23 | 1.94 | 0.49 |
| 1:R:504:GLN:O | 1:R:508:LYS:CB | 2.59 | 0.49 |
| 1:I:499:LEU:HG | 1:J:510:TRP:HZ3 | 1.75 | 0.49 |
| 1:K:153:LYS:HD2 | 1:K:155:GLY:H | 1.76 | 0.49 |
| 1:K:504:GLN:O | 1:K:508:LYS:CB | 2.59 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:247:ARG:HA | 1:P:250:ASN:HB2 | 1.93 | 0.49 |
| 1:B:153:LYS:HD2 | 1:B:155:GLY:H | 1.76 | 0.49 |
| 1:E:144:LEU:HA | 1:E:170:THR:HG23 | 1.94 | 0.49 |
| 1:E:153:LYS:HD2 | 1:E:155:GLY:H | 1.76 | 0.49 |
| 1:G:305:ASP:HA | 1:G:308:PHE:HB2 | 1.94 | 0.49 |
| 1:G:514:LEU:HD22 | 1:H:503:GLN:HE22 | 1.77 | 0.49 |
| 1:I:305:ASP:HA | 1:I:308:PHE:HB2 | 1.94 | 0.49 |
| 1:D:144:LEU:HA | 1:D:170:THR:HG23 | 1.94 | 0.49 |
| 1:E:305:ASP:HA | 1:E:308:PHE:HB2 | 1.94 | 0.49 |
| 1:F:305:ASP:HA | 1:F:308:PHE:HB2 | 1.94 | 0.49 |
| 1:H:247:ARG:HA | 1:H:250:ASN:HB2 | 1.93 | 0.49 |
| 1:J:247:ARG:HA | 1:J:250:ASN:HB2 | 1.93 | 0.49 |
| 1:N:249:VAL:HA | 1:N:255:LEU:HD22 | 1.93 | 0.49 |
| 1:P:153:LYS:HD2 | 1:P:155:GLY:H | 1.76 | 0.49 |
| 1:R:247:ARG:HA | 1:R:250:ASN:HB2 | 1.93 | 0.49 |
| 1:F:247:ARG:HA | 1:F:250:ASN:HB2 | 1.93 | 0.49 |
| 1:G:153:LYS:HD2 | 1:G:155:GLY:H | 1.76 | 0.49 |
| 1:H:305:ASP:HA | 1:H:308:PHE:HB2 | 1.94 | 0.49 |
| 1:C:305:ASP:HA | 1:C:308:PHE:HB2 | 1.94 | 0.49 |
| 1:D:169:GLN:NE2 | 1:D:179:GLN:OE1 | 2.46 | 0.49 |
| 1:L:249:VAL:HA | 1:L:255:LEU:HD22 | 1.93 | 0.49 |
| 1:A:305:ASP:HA | 1:A:308:PHE:HB2 | 1.94 | 0.49 |
| 1:J:169:GLN:NE2 | 1:J:179:GLN:OE1 | 2.46 | 0.49 |
| 1:L:169:GLN:NE2 | 1:L:179:GLN:OE1 | 2.46 | 0.49 |
| 1:M:247:ARG:HA | 1:M:250:ASN:HB2 | 1.93 | 0.49 |
| 1:R:144:LEU:HA | 1:R:170:THR:HG23 | 1.94 | 0.49 |
| 1:D:247:ARG:HA | 1:D:250:ASN:HB2 | 1.93 | 0.49 |
| 1:D:305:ASP:HA | 1:D:308:PHE:HB2 | 1.94 | 0.49 |
| 1:F:144:LEU:HA | 1:F:170:THR:HG23 | 1.94 | 0.49 |
| 1:J:249:VAL:HA | 1:J:255:LEU:HD22 | 1.93 | 0.49 |
| 1:O:514:LEU:HD22 | 1:P:503:GLN:HE22 | 1.77 | 0.49 |
| 1:Q:305:ASP:HA | 1:Q:308:PHE:HB2 | 1.94 | 0.49 |
| 1:R:169:GLN:NE2 | 1:R:179:GLN:OE1 | 2.46 | 0.49 |
| 1:A:514:LEU:HD22 | 1:B:503:GLN:HE22 | 1.77 | 0.48 |
| 1:B:305:ASP:HA | 1:B:308:PHE:HB2 | 1.94 | 0.48 |
| 1:G:144:LEU:HA | 1:G:170:THR:HG23 | 1.94 | 0.48 |
| 1:K:169:GLN:NE2 | 1:K:179:GLN:OE1 | 2.46 | 0.48 |
| 1:Q:169:GLN:NE2 | 1:Q:179:GLN:OE1 | 2.46 | 0.48 |
| 1:R:305:ASP:HA | 1:R:308:PHE:HB2 | 1.94 | 0.48 |
| 1:C:169:GLN:NE2 | 1:C:179:GLN:OE1 | 2.46 | 0.48 |
| 1:K:305:ASP:HA | 1:K:308:PHE:HB2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:305:ASP:HA | 1:O:308:PHE:HB2 | 1.94 | 0.48 |
| 1:C:147:GLY:N | 1:C:167:THR:O | 2.46 | 0.48 |
| 1:C:460:THR:O | 1:C:464:ARG:NE | 2.37 | 0.48 |
| 1:E:169:GLN:NE2 | 1:E:179:GLN:OE1 | 2.46 | 0.48 |
| 1:G:169:GLN:NE2 | 1:G:179:GLN:OE1 | 2.46 | 0.48 |
| 1:M:169:GLN:NE2 | 1:M:179:GLN:OE1 | 2.46 | 0.48 |
| 1:M:514:LEU:HD22 | 1:N:503:GLN:HE22 | 1.77 | 0.48 |
| 1:B:147:GLY:N | 1:B:167:THR:O | 2.46 | 0.48 |
| 1:J:305:ASP:HA | 1:J:308:PHE:HB2 | 1.94 | 0.48 |
| 1:J:438:TRP:HD1 | 1:K:435:ARG:HH21 | 1.60 | 0.48 |
| 1:M:305:ASP:HA | 1:M:308:PHE:HB2 | 1.94 | 0.48 |
| 1:H:169:GLN:NE2 | 1:H:179:GLN:OE1 | 2.46 | 0.48 |
| 1:P:305:ASP:HA | 1:P:308:PHE:HB2 | 1.94 | 0.48 |
| 1:Q:147:GLY:N | 1:Q:167:THR:O | 2.46 | 0.48 |
| 1:E:504:GLN:O | 1:E:508:LYS:CB | 2.59 | 0.48 |
| 1:I:214:SER:O | 1:I:216:ILE:HG23 | 2.14 | 0.48 |
| 1:K:514:LEU:HD22 | 1:L:503:GLN:HE22 | 1.77 | 0.48 |
| 1:M:385:ASN:OD1 | 1:M:386:ASN:N | 2.47 | 0.48 |
| 1:N:169:GLN:NE2 | 1:N:179:GLN:OE1 | 2.46 | 0.48 |
| 1:N:305:ASP:HA | 1:N:308:PHE:HB2 | 1.94 | 0.48 |
| 1:N:385:ASN:OD1 | 1:N:386:ASN:N | 2.47 | 0.48 |
| 1:R:460:THR:O | 1:R:464:ARG:NE | 2.37 | 0.48 |
| 1:A:169:GLN:NE2 | 1:A:179:GLN:OE1 | 2.46 | 0.48 |
| 1:I:169:GLN:NE2 | 1:I:179:GLN:OE1 | 2.46 | 0.48 |
| 1:J:385:ASN:OD1 | 1:J:386:ASN:N | 2.47 | 0.48 |
| 1:L:214:SER:O | 1:L:216:ILE:HG23 | 2.14 | 0.48 |
| 1:L:305:ASP:HA | 1:L:308:PHE:HB2 | 1.94 | 0.48 |
| 1:O:169:GLN:NE2 | 1:O:179:GLN:OE1 | 2.46 | 0.48 |
| 1:A:214:SER:O | 1:A:216:ILE:HG23 | 2.14 | 0.48 |
| 1:I:385:ASN:OD1 | 1:I:386:ASN:N | 2.47 | 0.48 |
| 1:M:498:THR:HA | 1:M:501:HIS:CE1 | 2.49 | 0.48 |
| 1:F:169:GLN:NE2 | 1:F:179:GLN:OE1 | 2.46 | 0.48 |
| 1:F:460:THR:O | 1:F:464:ARG:NE | 2.37 | 0.48 |
| 1:F:498:THR:HA | 1:F:501:HIS:CE1 | 2.49 | 0.48 |
| 1:I:514:LEU:HD22 | 1:J:503:GLN:HE22 | 1.77 | 0.48 |
| 1:L:498:THR:HA | 1:L:501:HIS:CE1 | 2.49 | 0.48 |
| 1:B:169:GLN:NE2 | 1:B:179:GLN:OE1 | 2.46 | 0.48 |
| 1:C:385:ASN:OD1 | 1:C:386:ASN:N | 2.47 | 0.48 |
| 1:D:498:THR:HA | 1:D:501:HIS:CE1 | 2.49 | 0.48 |
| 1:G:498:THR:HA | 1:G:501:HIS:CE1 | 2.49 | 0.48 |
| 1:H:498:THR:HA | 1:H:501:HIS:CE1 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:385:ASN:OD1 | 1:L:386:ASN:N | 2.47 | 0.48 |
| 1:P:169:GLN:NE2 | 1:P:179:GLN:OE1 | 2.46 | 0.48 |
| 1:R:498:THR:HA | 1:R:501:HIS:CE1 | 2.49 | 0.48 |
| 1:I:147:GLY:N | 1:I:167:THR:O | 2.46 | 0.47 |
| 1:K:498:THR:HA | 1:K:501:HIS:CE1 | 2.49 | 0.47 |
| 1:O:214:SER:O | 1:O:216:ILE:HG23 | 2.14 | 0.47 |
| 1:Q:385:ASN:OD1 | 1:Q:386:ASN:N | 2.47 | 0.47 |
| 1:Q:460:THR:O | 1:Q:464:ARG:NE | 2.37 | 0.47 |
| 1:R:147:GLY:N | 1:R:167:THR:O | 2.46 | 0.47 |
| 1:C:214:SER:O | 1:C:216:ILE:HG23 | 2.14 | 0.47 |
| 1:H:214:SER:O | 1:H:216:ILE:HG23 | 2.14 | 0.47 |
| 1:D:460:THR:O | 1:D:464:ARG:NE | 2.37 | 0.47 |
| 1:E:460:THR:O | 1:E:464:ARG:NE | 2.37 | 0.47 |
| 1:E:498:THR:HA | 1:E:501:HIS:CE1 | 2.49 | 0.47 |
| 1:J:214:SER:O | 1:J:216:ILE:HG23 | 2.14 | 0.47 |
| 1:K:385:ASN:OD1 | 1:K:386:ASN:N | 2.47 | 0.47 |
| 1:K:460:THR:O | 1:K:464:ARG:NE | 2.37 | 0.47 |
| 1:N:498:THR:HA | 1:N:501:HIS:CE1 | 2.49 | 0.47 |
| 1:P:214:SER:O | 1:P:216:ILE:HG23 | 2.14 | 0.47 |
| 1:R:214:SER:O | 1:R:216:ILE:HG23 | 2.14 | 0.47 |
| 1:A:460:THR:O | 1:A:464:ARG:NE | 2.37 | 0.47 |
| 1:A:498:THR:HA | 1:A:501:HIS:CE1 | 2.49 | 0.47 |
| 1:B:498:THR:HA | 1:B:501:HIS:CE1 | 2.49 | 0.47 |
| 1:D:147:GLY:N | 1:D:167:THR:O | 2.46 | 0.47 |
| 1:D:214:SER:O | 1:D:216:ILE:HG23 | 2.14 | 0.47 |
| 1:E:214:SER:O | 1:E:216:ILE:HG23 | 2.14 | 0.47 |
| 1:F:214:SER:O | 1:F:216:ILE:HG23 | 2.14 | 0.47 |
| 1:N:214:SER:O | 1:N:216:ILE:HG23 | 2.14 | 0.47 |
| 1:O:498:THR:HA | 1:O:501:HIS:CE1 | 2.49 | 0.47 |
| 1:P:498:THR:HA | 1:P:501:HIS:CE1 | 2.49 | 0.47 |
| 1:A:385:ASN:OD1 | 1:A:386:ASN:N | 2.47 | 0.47 |
| 1:B:385:ASN:OD1 | 1:B:386:ASN:N | 2.47 | 0.47 |
| 1:E:385:ASN:OD1 | 1:E:386:ASN:N | 2.47 | 0.47 |
| 1:G:214:SER:O | 1:G:216:ILE:HG23 | 2.14 | 0.47 |
| 1:J:498:THR:HA | 1:J:501:HIS:CE1 | 2.49 | 0.47 |
| 1:N:460:THR:O | 1:N:464:ARG:NE | 2.37 | 0.47 |
| 1:D:385:ASN:OD1 | 1:D:386:ASN:N | 2.47 | 0.47 |
| 1:F:385:ASN:OD1 | 1:F:386:ASN:N | 2.47 | 0.47 |
| 1:G:385:ASN:OD1 | 1:G:386:ASN:N | 2.47 | 0.47 |
| 1:H:385:ASN:OD1 | 1:H:386:ASN:N | 2.47 | 0.47 |
| 1:K:214:SER:O | 1:K:216:ILE:HG23 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:385:ASN:OD1 | 1:O:386:ASN:N | 2.47 | 0.47 |
| 1:P:385:ASN:OD1 | 1:P:386:ASN:N | 2.47 | 0.47 |
| 1:R:385:ASN:OD1 | 1:R:386:ASN:N | 2.47 | 0.47 |
| 1:B:214:SER:O | 1:B:216:ILE:HG23 | 2.14 | 0.47 |
| 1:I:498:THR:HA | 1:I:501:HIS:CE1 | 2.49 | 0.47 |
| 1:K:377:GLU:HA | 1:K:380:HIS:CE1 | 2.50 | 0.47 |
| 1:L:147:GLY:N | 1:L:167:THR:O | 2.46 | 0.47 |
| 1:L:460:THR:O | 1:L:464:ARG:NE | 2.37 | 0.47 |
| 1:P:460:THR:O | 1:P:464:ARG:NE | 2.37 | 0.47 |
| 1:Q:214:SER:O | 1:Q:216:ILE:HG23 | 2.15 | 0.47 |
| 1:Q:498:THR:HA | 1:Q:501:HIS:CE1 | 2.49 | 0.47 |
| 1:C:498:THR:HA | 1:C:501:HIS:CE1 | 2.49 | 0.47 |
| 1:M:147:GLY:N | 1:M:167:THR:O | 2.46 | 0.47 |
| 1:H:377:GLU:HA | 1:H:380:HIS:CE1 | 2.50 | 0.47 |
| 1:M:377:GLU:HA | 1:M:380:HIS:CE1 | 2.50 | 0.47 |
| 1:M:174:MET:SD | 1:M:174:MET:N | 2.88 | 0.47 |
| 1:N:147:GLY:N | 1:N:167:THR:O | 2.46 | 0.47 |
| 1:A:147:GLY:N | 1:A:167:THR:O | 2.46 | 0.46 |
| 1:B:460:THR:O | 1:B:464:ARG:NE | 2.37 | 0.46 |
| 1:E:174:MET:SD | 1:E:174:MET:N | 2.88 | 0.46 |
| 1:E:377:GLU:HA | 1:E:380:HIS:CE1 | 2.50 | 0.46 |
| 1:J:377:GLU:HA | 1:J:380:HIS:CE1 | 2.50 | 0.46 |
| 1:M:214:SER:O | 1:M:216:ILE:HG23 | 2.15 | 0.46 |
| 1:M:460:THR:O | 1:M:464:ARG:NE | 2.37 | 0.46 |
| 1:C:174:MET:SD | 1:C:174:MET:N | 2.88 | 0.46 |
| 1:I:174:MET:SD | 1:I:174:MET:N | 2.88 | 0.46 |
| 1:O:386:ASN:OD1 | 1:O:387:ASP:N | 2.49 | 0.46 |
| 1:O:460:THR:O | 1:O:464:ARG:NE | 2.37 | 0.46 |
| 1:A:386:ASN:OD1 | 1:A:387:ASP:N | 2.49 | 0.46 |
| 1:K:386:ASN:OD1 | 1:K:387:ASP:N | 2.49 | 0.46 |
| 1:L:174:MET:SD | 1:L:174:MET:N | 2.88 | 0.46 |
| 1:N:377:GLU:HA | 1:N:380:HIS:CE1 | 2.50 | 0.46 |
| 1:P:377:GLU:HA | 1:P:380:HIS:CE1 | 2.50 | 0.46 |
| 1:Q:174:MET:SD | 1:Q:174:MET:N | 2.88 | 0.46 |
| 1:B:377:GLU:HA | 1:B:380:HIS:CE1 | 2.50 | 0.46 |
| 1:D:386:ASN:OD1 | 1:D:387:ASP:N | 2.49 | 0.46 |
| 1:G:322:LEU:HD13 | 1:G:395:LEU:HB2 | 1.98 | 0.46 |
| 1:G:386:ASN:OD1 | 1:G:387:ASP:N | 2.49 | 0.46 |
| 1:G:460:THR:O | 1:G:464:ARG:NE | 2.37 | 0.46 |
| 1:J:147:GLY:N | 1:J:167:THR:O | 2.46 | 0.46 |
| 1:L:377:GLU:HA | 1:L:380:HIS:CE1 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:147:GLY:N | 1:O:167:THR:O | 2.46 | 0.46 |
| 1:Q:377:GLU:HA | 1:Q:380:HIS:CE1 | 2.50 | 0.46 |
| 1:R:377:GLU:HA | 1:R:380:HIS:CE1 | 2.50 | 0.46 |
| 1:R:386:ASN:OD1 | 1:R:387:ASP:N | 2.49 | 0.46 |
| 1:C:377:GLU:HA | 1:C:380:HIS:CE1 | 2.50 | 0.46 |
| 1:D:377:GLU:HA | 1:D:380:HIS:CE1 | 2.50 | 0.46 |
| 1:I:377:GLU:HA | 1:I:380:HIS:CE1 | 2.50 | 0.46 |
| 1:I:386:ASN:OD1 | 1:I:387:ASP:N | 2.49 | 0.46 |
| 1:L:386:ASN:OD1 | 1:L:387:ASP:N | 2.49 | 0.46 |
| 1:N:386:ASN:OD1 | 1:N:387:ASP:N | 2.49 | 0.46 |
| 1:A:415:THR:HA | 1:A:418:ARG:HD2 | 1.98 | 0.46 |
| 1:I:322:LEU:HD13 | 1:I:395:LEU:HB2 | 1.98 | 0.46 |
| 1:J:415:THR:HA | 1:J:418:ARG:HD2 | 1.98 | 0.46 |
| 1:Q:322:LEU:HD13 | 1:Q:395:LEU:HB2 | 1.98 | 0.46 |
| 1:C:322:LEU:HD13 | 1:C:395:LEU:HB2 | 1.98 | 0.46 |
| 1:E:386:ASN:OD1 | 1:E:387:ASP:N | 2.49 | 0.46 |
| 1:F:386:ASN:OD1 | 1:F:387:ASP:N | 2.49 | 0.46 |
| 1:G:377:GLU:HA | 1:G:380:HIS:CE1 | 2.50 | 0.46 |
| 1:H:386:ASN:OD1 | 1:H:387:ASP:N | 2.49 | 0.46 |
| 1:H:460:THR:O | 1:H:464:ARG:NE | 2.37 | 0.46 |
| 1:K:415:THR:HA | 1:K:418:ARG:HD2 | 1.98 | 0.46 |
| 1:M:415:THR:HA | 1:M:418:ARG:HD2 | 1.98 | 0.46 |
| 1:P:386:ASN:OD1 | 1:P:387:ASP:N | 2.49 | 0.46 |
| 1:E:322:LEU:HD13 | 1:E:395:LEU:HB2 | 1.98 | 0.46 |
| 1:G:147:GLY:N | 1:G:167:THR:O | 2.46 | 0.46 |
| 1:H:415:THR:HA | 1:H:418:ARG:HD2 | 1.98 | 0.46 |
| 1:L:415:THR:HA | 1:L:418:ARG:HD2 | 1.98 | 0.46 |
| 1:N:174:MET:SD | 1:N:174:MET:N | 2.88 | 0.46 |
| 1:O:415:THR:HA | 1:O:418:ARG:HD2 | 1.98 | 0.46 |
| 1:B:386:ASN:OD1 | 1:B:387:ASP:N | 2.49 | 0.46 |
| 1:D:174:MET:SD | 1:D:174:MET:N | 2.88 | 0.46 |
| 1:F:174:MET:SD | 1:F:174:MET:N | 2.88 | 0.46 |
| 1:F:415:THR:HA | 1:F:418:ARG:HD2 | 1.98 | 0.46 |
| 1:K:174:MET:SD | 1:K:174:MET:N | 2.88 | 0.46 |
| 1:R:174:MET:SD | 1:R:174:MET:N | 2.88 | 0.46 |
| 1:F:377:GLU:HA | 1:F:380:HIS:CE1 | 2.50 | 0.46 |
| 1:I:346:PHE:HE2 | 1:J:332:LEU:HG | 1.81 | 0.46 |
| 1:J:460:THR:O | 1:J:464:ARG:NE | 2.37 | 0.46 |
| 1:K:322:LEU:HD13 | 1:K:395:LEU:HB2 | 1.98 | 0.46 |
| 1:Q:386:ASN:OD1 | 1:Q:387:ASP:N | 2.49 | 0.46 |
| 1:A:377:GLU:HA | 1:A:380:HIS:CE1 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:502:SER:O | 1:D:506:LEU:CB | 2.64 | 0.45 |
| 1:E:502:SER:O | 1:E:506:LEU:CB | 2.65 | 0.45 |
| 1:F:147:GLY:N | 1:F:167:THR:O | 2.46 | 0.45 |
| 1:F:502:SER:O | 1:F:506:LEU:CB | 2.64 | 0.45 |
| 1:H:322:LEU:HD13 | 1:H:395:LEU:HB2 | 1.98 | 0.45 |
| 1:J:174:MET:SD | 1:J:174:MET:N | 2.88 | 0.45 |
| 1:J:386:ASN:OD1 | 1:J:387:ASP:N | 2.49 | 0.45 |
| 1:M:346:PHE:HE2 | 1:N:332:LEU:HG | 1.81 | 0.45 |
| 1:O:322:LEU:HD13 | 1:O:395:LEU:HB2 | 1.98 | 0.45 |
| 1:O:377:GLU:HA | 1:O:380:HIS:CE1 | 2.50 | 0.45 |
| 1:Q:346:PHE:HE2 | 1:R:332:LEU:HG | 1.82 | 0.45 |
| 1:R:502:SER:O | 1:R:506:LEU:CB | 2.65 | 0.45 |
| 1:A:322:LEU:HD13 | 1:A:395:LEU:HB2 | 1.98 | 0.45 |
| 1:C:346:PHE:HE2 | 1:D:332:LEU:HG | 1.82 | 0.45 |
| 1:C:415:THR:HA | 1:C:418:ARG:HD2 | 1.98 | 0.45 |
| 1:C:502:SER:O | 1:C:506:LEU:CB | 2.65 | 0.45 |
| 1:E:346:PHE:HE2 | 1:F:332:LEU:HG | 1.82 | 0.45 |
| 1:P:322:LEU:HD13 | 1:P:395:LEU:HB2 | 1.99 | 0.45 |
| 1:B:322:LEU:HD13 | 1:B:395:LEU:HB2 | 1.99 | 0.45 |
| 1:C:386:ASN:OD1 | 1:C:387:ASP:N | 2.49 | 0.45 |
| 1:H:502:SER:O | 1:H:506:LEU:CB | 2.65 | 0.45 |
| 1:Q:415:THR:HA | 1:Q:418:ARG:HD2 | 1.98 | 0.45 |
| 1:A:502:SER:O | 1:A:506:LEU:CB | 2.64 | 0.45 |
| 1:O:346:PHE:HE2 | 1:P:332:LEU:HG | 1.82 | 0.45 |
| 1:Q:502:SER:O | 1:Q:506:LEU:CB | 2.65 | 0.45 |
| 1:A:346:PHE:HE2 | 1:B:332:LEU:HG | 1.82 | 0.45 |
| 1:H:174:MET:SD | 1:H:174:MET:N | 2.88 | 0.45 |
| 1:M:322:LEU:HD13 | 1:M:395:LEU:HB2 | 1.98 | 0.45 |
| 1:M:386:ASN:OD1 | 1:M:387:ASP:N | 2.49 | 0.45 |
| 1:N:502:SER:O | 1:N:506:LEU:CB | 2.64 | 0.45 |
| 1:R:322:LEU:HD13 | 1:R:395:LEU:HB2 | 1.99 | 0.45 |
| 1:B:502:SER:O | 1:B:506:LEU:CB | 2.65 | 0.45 |
| 1:N:415:THR:HA | 1:N:418:ARG:HD2 | 1.98 | 0.45 |
| 1:P:147:GLY:N | 1:P:167:THR:O | 2.46 | 0.45 |
| 1:B:174:MET:SD | 1:B:174:MET:N | 2.88 | 0.45 |
| 1:G:346:PHE:HE2 | 1:H:332:LEU:HG | 1.81 | 0.45 |
| 1:I:415:THR:HA | 1:I:418:ARG:HD2 | 1.98 | 0.45 |
| 1:L:322:LEU:HD13 | 1:L:395:LEU:HB2 | 1.99 | 0.45 |
| 1:M:167:THR:HA | 1:M:181:ALA:HA | 1.99 | 0.45 |
| 1:P:502:SER:O | 1:P:506:LEU:CB | 2.65 | 0.45 |
| 1:R:415:THR:HA | 1:R:418:ARG:HD2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:322:LEU:HD13 | 1:D:395:LEU:HB2 | 1.99 | 0.45 |
| 1:H:167:THR:HA | 1:H:181:ALA:HA | 1.99 | 0.45 |
| 1:J:167:THR:HA | 1:J:181:ALA:HA | 1.99 | 0.45 |
| 1:K:147:GLY:N | 1:K:167:THR:O | 2.46 | 0.45 |
| 1:K:502:SER:O | 1:K:506:LEU:CB | 2.65 | 0.45 |
| 1:L:502:SER:O | 1:L:506:LEU:CB | 2.65 | 0.45 |
| 1:O:502:SER:O | 1:O:506:LEU:CB | 2.65 | 0.45 |
| 1:D:415:THR:HA | 1:D:418:ARG:HD2 | 1.98 | 0.45 |
| 1:H:210:PRO:HA | 1:H:211:PRO:HD3 | 1.89 | 0.45 |
| 1:I:502:SER:O | 1:I:506:LEU:CB | 2.65 | 0.45 |
| 1:P:174:MET:SD | 1:P:174:MET:N | 2.88 | 0.45 |
| 1:F:322:LEU:HD13 | 1:F:395:LEU:HB2 | 1.99 | 0.45 |
| 1:G:174:MET:SD | 1:G:174:MET:N | 2.88 | 0.45 |
| 1:O:167:THR:HA | 1:O:181:ALA:HA | 1.99 | 0.45 |
| 1:A:167:THR:HA | 1:A:181:ALA:HA | 1.99 | 0.44 |
| 1:E:377:GLU:O | 1:E:381:GLN:HB2 | 2.17 | 0.44 |
| 1:E:415:THR:HA | 1:E:418:ARG:HD2 | 1.98 | 0.44 |
| 1:G:502:SER:O | 1:G:506:LEU:CB | 2.65 | 0.44 |
| 1:K:167:THR:HA | 1:K:181:ALA:HA | 1.99 | 0.44 |
| 1:N:167:THR:HA | 1:N:181:ALA:HA | 1.99 | 0.44 |
| 1:B:210:PRO:HA | 1:B:211:PRO:HD3 | 1.90 | 0.44 |
| 1:K:376:ILE:O | 1:K:380:HIS:ND1 | 2.51 | 0.44 |
| 1:L:167:THR:HA | 1:L:181:ALA:HA | 1.99 | 0.44 |
| 1:P:377:GLU:O | 1:P:381:GLN:HB2 | 2.17 | 0.44 |
| 1:P:415:THR:HA | 1:P:418:ARG:HD2 | 1.98 | 0.44 |
| 1:B:377:GLU:O | 1:B:381:GLN:HB2 | 2.18 | 0.44 |
| 1:B:415:THR:HA | 1:B:418:ARG:HD2 | 1.98 | 0.44 |
| 1:C:377:GLU:O | 1:C:381:GLN:HB2 | 2.18 | 0.44 |
| 1:F:376:ILE:O | 1:F:380:HIS:ND1 | 2.51 | 0.44 |
| 1:I:167:THR:HA | 1:I:181:ALA:HA | 1.99 | 0.44 |
| 1:I:256:GLN:HA | 1:I:261:ARG:HH12 | 1.83 | 0.44 |
| 1:J:502:SER:O | 1:J:506:LEU:CB | 2.64 | 0.44 |
| 1:A:376:ILE:O | 1:A:380:HIS:ND1 | 2.51 | 0.44 |
| 1:G:377:GLU:O | 1:G:381:GLN:HB2 | 2.18 | 0.44 |
| 1:G:415:THR:HA | 1:G:418:ARG:HD2 | 1.98 | 0.44 |
| 1:J:322:LEU:HD13 | 1:J:395:LEU:HB2 | 1.99 | 0.44 |
| 1:M:376:ILE:O | 1:M:380:HIS:ND1 | 2.51 | 0.44 |
| 1:M:377:GLU:O | 1:M:381:GLN:HB2 | 2.18 | 0.44 |
| 1:M:502:SER:O | 1:M:506:LEU:CB | 2.65 | 0.44 |
| 1:O:376:ILE:O | 1:O:380:HIS:ND1 | 2.51 | 0.44 |
| 1:P:210:PRO:HA | 1:P:211:PRO:HD3 | 1.89 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:256:GLN:HA | 1:Q:261:ARG:HH12 | 1.83 | 0.44 |
| 1:Q:376:ILE:O | 1:Q:380:HIS:ND1 | 2.51 | 0.44 |
| 1:Q:377:GLU:O | 1:Q:381:GLN:HB2 | 2.18 | 0.44 |
| 1:C:256:GLN:HA | 1:C:261:ARG:HH12 | 1.83 | 0.44 |
| 1:C:376:ILE:O | 1:C:380:HIS:ND1 | 2.51 | 0.44 |
| 1:H:376:ILE:O | 1:H:380:HIS:ND1 | 2.51 | 0.44 |
| 1:J:377:GLU:O | 1:J:381:GLN:HB2 | 2.18 | 0.44 |
| 1:M:256:GLN:HA | 1:M:261:ARG:HH12 | 1.83 | 0.44 |
| 1:R:376:ILE:O | 1:R:380:HIS:ND1 | 2.51 | 0.44 |
| 1:R:377:GLU:O | 1:R:381:GLN:HB2 | 2.18 | 0.44 |
| 1:D:377:GLU:O | 1:D:381:GLN:HB2 | 2.17 | 0.44 |
| 1:H:147:GLY:N | 1:H:167:THR:O | 2.46 | 0.44 |
| 1:H:256:GLN:HA | 1:H:261:ARG:HH12 | 1.83 | 0.44 |
| 1:H:377:GLU:O | 1:H:381:GLN:HB2 | 2.18 | 0.44 |
| 1:I:377:GLU:O | 1:I:381:GLN:HB2 | 2.17 | 0.44 |
| 1:I:394:LEU:HD11 | 1:I:487:ASP:HB2 | 2.00 | 0.44 |
| 1:J:376:ILE:O | 1:J:380:HIS:ND1 | 2.51 | 0.44 |
| 1:L:256:GLN:HA | 1:L:261:ARG:HH12 | 1.83 | 0.44 |
| 1:L:376:ILE:O | 1:L:380:HIS:ND1 | 2.51 | 0.44 |
| 1:N:377:GLU:O | 1:N:381:GLN:HB2 | 2.18 | 0.44 |
| 1:O:174:MET:N | 1:O:174:MET:SD | 2.88 | 0.44 |
| 1:A:377:GLU:O | 1:A:381:GLN:HB2 | 2.18 | 0.44 |
| 1:B:256:GLN:HA | 1:B:261:ARG:HH12 | 1.83 | 0.44 |
| 1:D:256:GLN:HA | 1:D:261:ARG:HH12 | 1.83 | 0.44 |
| 1:E:147:GLY:N | 1:E:167:THR:O | 2.46 | 0.44 |
| 1:F:167:THR:HA | 1:F:181:ALA:HA | 1.99 | 0.44 |
| 1:F:256:GLN:HA | 1:F:261:ARG:HH12 | 1.83 | 0.44 |
| 1:K:346:PHE:HE2 | 1:L:332:LEU:HG | 1.82 | 0.44 |
| 1:K:394:LEU:HD11 | 1:K:487:ASP:HB2 | 2.00 | 0.44 |
| 1:R:256:GLN:HA | 1:R:261:ARG:HH12 | 1.83 | 0.44 |
| 1:E:256:GLN:HA | 1:E:261:ARG:HH12 | 1.83 | 0.44 |
| 1:G:167:THR:HA | 1:G:181:ALA:HA | 1.99 | 0.44 |
| 1:I:197:SER:HA | 1:I:200:HIS:CD2 | 2.53 | 0.44 |
| 1:N:394:LEU:HD11 | 1:N:487:ASP:HB2 | 2.00 | 0.44 |
| 1:O:377:GLU:O | 1:O:381:GLN:HB2 | 2.18 | 0.44 |
| 1:P:167:THR:HA | 1:P:181:ALA:HA | 1.99 | 0.44 |
| 1:P:256:GLN:HA | 1:P:261:ARG:HH12 | 1.83 | 0.44 |
| 1:A:174:MET:SD | 1:A:174:MET:N | 2.88 | 0.44 |
| 1:A:197:SER:HA | 1:A:200:HIS:CD2 | 2.53 | 0.44 |
| 1:C:167:THR:HA | 1:C:181:ALA:HA | 1.99 | 0.44 |
| 1:F:197:SER:HA | 1:F:200:HIS:CD2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:394:LEU:HD11 | 1:L:487:ASP:HB2 | 2.00 | 0.44 |
| 1:O:152:GLU:O | 1:O:163:ALA:N | 2.45 | 0.44 |
| 1:Q:167:THR:HA | 1:Q:181:ALA:HA | 1.99 | 0.44 |
| 1:G:256:GLN:HA | 1:G:261:ARG:HH12 | 1.83 | 0.43 |
| 1:M:210:PRO:HA | 1:M:211:PRO:HD3 | 1.89 | 0.43 |
| 1:Q:394:LEU:HD11 | 1:Q:487:ASP:HB2 | 2.00 | 0.43 |
| 1:B:167:THR:HA | 1:B:181:ALA:HA | 1.99 | 0.43 |
| 1:C:394:LEU:HD11 | 1:C:487:ASP:HB2 | 2.00 | 0.43 |
| 1:D:167:THR:HA | 1:D:181:ALA:HA | 1.99 | 0.43 |
| 1:K:377:GLU:O | 1:K:381:GLN:HB2 | 2.18 | 0.43 |
| 1:O:197:SER:HA | 1:O:200:HIS:CD2 | 2.53 | 0.43 |
| 1:R:167:THR:HA | 1:R:181:ALA:HA | 1.99 | 0.43 |
| 1:F:377:GLU:O | 1:F:381:GLN:HB2 | 2.17 | 0.43 |
| 1:G:394:LEU:HD11 | 1:G:487:ASP:HB2 | 2.00 | 0.43 |
| 1:H:197:SER:HA | 1:H:200:HIS:CD2 | 2.53 | 0.43 |
| 1:K:197:SER:HA | 1:K:200:HIS:CD2 | 2.53 | 0.43 |
| 1:N:197:SER:HA | 1:N:200:HIS:CD2 | 2.53 | 0.43 |
| 1:N:515:PRO:HA | 1:N:518:LYS:HE2 | 2.00 | 0.43 |
| 1:A:152:GLU:O | 1:A:163:ALA:N | 2.45 | 0.43 |
| 1:A:256:GLN:HA | 1:A:261:ARG:HH12 | 1.83 | 0.43 |
| 1:A:394:LEU:HD11 | 1:A:487:ASP:HB2 | 2.00 | 0.43 |
| 1:G:197:SER:HA | 1:G:200:HIS:CD2 | 2.53 | 0.43 |
| 1:H:515:PRO:HA | 1:H:518:LYS:HE2 | 2.00 | 0.43 |
| 1:J:197:SER:HA | 1:J:200:HIS:CD2 | 2.53 | 0.43 |
| 1:J:256:GLN:HA | 1:J:261:ARG:HH12 | 1.83 | 0.43 |
| 1:L:486:LYS:HE2 | 1:L:486:LYS:HB3 | 1.91 | 0.43 |
| 1:O:394:LEU:HD11 | 1:O:487:ASP:HB2 | 2.00 | 0.43 |
| 1:O:515:PRO:HA | 1:O:518:LYS:HE2 | 2.00 | 0.43 |
| 1:A:515:PRO:HA | 1:A:518:LYS:HE2 | 2.00 | 0.43 |
| 1:B:394:LEU:HD11 | 1:B:487:ASP:HB2 | 2.00 | 0.43 |
| 1:B:437:LEU:HB2 | 1:B:445:LEU:HD11 | 2.01 | 0.43 |
| 1:J:210:PRO:HA | 1:J:211:PRO:HD3 | 1.90 | 0.43 |
| 1:L:197:SER:HA | 1:L:200:HIS:CD2 | 2.53 | 0.43 |
| 1:L:377:GLU:O | 1:L:381:GLN:HB2 | 2.18 | 0.43 |
| 1:N:210:PRO:HA | 1:N:211:PRO:HD3 | 1.89 | 0.43 |
| 1:O:256:GLN:HA | 1:O:261:ARG:HH12 | 1.83 | 0.43 |
| 1:P:394:LEU:HD11 | 1:P:487:ASP:HB2 | 2.00 | 0.43 |
| 1:C:197:SER:HA | 1:C:200:HIS:CD2 | 2.53 | 0.43 |
| 1:E:197:SER:HA | 1:E:200:HIS:CD2 | 2.53 | 0.43 |
| 1:E:437:LEU:HB2 | 1:E:445:LEU:HD11 | 2.01 | 0.43 |
| 1:E:486:LYS:HE2 | 1:E:486:LYS:HB3 | 1.91 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:515:PRO:HA | 1:E:518:LYS:HE2 | 2.00 | 0.43 |
| 1:I:437:LEU:HB2 | 1:I:445:LEU:HD11 | 2.01 | 0.43 |
| 1:K:437:LEU:HB2 | 1:K:445:LEU:HD11 | 2.01 | 0.43 |
| 1:M:394:LEU:HD11 | 1:M:487:ASP:HB2 | 2.00 | 0.43 |
| 1:N:437:LEU:HB2 | 1:N:445:LEU:HD11 | 2.01 | 0.43 |
| 1:P:437:LEU:HB2 | 1:P:445:LEU:HD11 | 2.01 | 0.43 |
| 1:B:515:PRO:HA | 1:B:518:LYS:HE2 | 2.00 | 0.43 |
| 1:E:167:THR:HA | 1:E:181:ALA:HA | 1.99 | 0.43 |
| 1:E:394:LEU:HD11 | 1:E:487:ASP:HB2 | 2.00 | 0.43 |
| 1:F:152:GLU:O | 1:F:163:ALA:N | 2.45 | 0.43 |
| 1:F:438:TRP:HD1 | 1:G:435:ARG:HH21 | 1.66 | 0.43 |
| 1:G:437:LEU:HB2 | 1:G:445:LEU:HD11 | 2.01 | 0.43 |
| 1:G:515:PRO:HA | 1:G:518:LYS:HE2 | 2.00 | 0.43 |
| 1:J:394:LEU:HD11 | 1:J:487:ASP:HB2 | 2.00 | 0.43 |
| 1:R:437:LEU:HB2 | 1:R:445:LEU:HD11 | 2.01 | 0.43 |
| 1:D:437:LEU:HB2 | 1:D:445:LEU:HD11 | 2.01 | 0.43 |
| 1:L:437:LEU:HB2 | 1:L:445:LEU:HD11 | 2.01 | 0.43 |
| 1:N:256:GLN:HA | 1:N:261:ARG:HH12 | 1.83 | 0.43 |
| 1:P:515:PRO:HA | 1:P:518:LYS:HE2 | 2.00 | 0.43 |
| 1:A:196:LEU:HD21 | 1:A:260:VAL:HG11 | 2.01 | 0.43 |
| 1:F:196:LEU:HD21 | 1:F:260:VAL:HG11 | 2.01 | 0.43 |
| 1:F:515:PRO:HA | 1:F:518:LYS:HE2 | 2.00 | 0.43 |
| 1:I:460:THR:O | 1:I:464:ARG:NE | 2.37 | 0.43 |
| 1:M:515:PRO:HA | 1:M:518:LYS:HE2 | 2.00 | 0.43 |
| 1:Q:197:SER:HA | 1:Q:200:HIS:CD2 | 2.53 | 0.43 |
| 1:C:437:LEU:HB2 | 1:C:445:LEU:HD11 | 2.01 | 0.43 |
| 1:D:196:LEU:HD21 | 1:D:260:VAL:HG11 | 2.01 | 0.43 |
| 1:J:515:PRO:HA | 1:J:518:LYS:HE2 | 2.00 | 0.43 |
| 1:L:515:PRO:HA | 1:L:518:LYS:HE2 | 2.00 | 0.43 |
| 1:O:196:LEU:HD21 | 1:O:260:VAL:HG11 | 2.01 | 0.43 |
| 1:E:196:LEU:HD21 | 1:E:260:VAL:HG11 | 2.01 | 0.42 |
| 1:F:394:LEU:HD11 | 1:F:487:ASP:HB2 | 2.00 | 0.42 |
| 1:G:501:HIS:HA | 1:G:504:GLN:HG3 | 2.01 | 0.42 |
| 1:N:322:LEU:HD13 | 1:N:395:LEU:HB2 | 2.01 | 0.42 |
| 1:P:197:SER:HA | 1:P:200:HIS:CD2 | 2.53 | 0.42 |
| 1:Q:196:LEU:HD21 | 1:Q:260:VAL:HG11 | 2.01 | 0.42 |
| 1:Q:437:LEU:HB2 | 1:Q:445:LEU:HD11 | 2.01 | 0.42 |
| 1:R:196:LEU:HD21 | 1:R:260:VAL:HG11 | 2.01 | 0.42 |
| 1:R:208:PRO:HB2 | 1:R:244:TYR:HA | 2.01 | 0.42 |
| 1:A:477:VAL:HA | 1:A:480:PHE:CE2 | 2.55 | 0.42 |
| 1:B:197:SER:HA | 1:B:200:HIS:CD2 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:208:PRO:HB2 | 1:B:244:TYR:HA | 2.01 | 0.42 |
| 1:C:196:LEU:HD21 | 1:C:260:VAL:HG11 | 2.01 | 0.42 |
| 1:F:437:LEU:HB2 | 1:F:445:LEU:HD11 | 2.01 | 0.42 |
| 1:H:196:LEU:HD21 | 1:H:260:VAL:HG11 | 2.01 | 0.42 |
| 1:L:210:PRO:HA | 1:L:211:PRO:HD3 | 1.89 | 0.42 |
| 1:M:197:SER:HA | 1:M:200:HIS:CD2 | 2.53 | 0.42 |
| 1:M:437:LEU:HB2 | 1:M:445:LEU:HD11 | 2.01 | 0.42 |
| 1:N:438:TRP:HD1 | 1:O:435:ARG:HH21 | 1.66 | 0.42 |
| 1:R:501:HIS:HA | 1:R:504:GLN:HG3 | 2.01 | 0.42 |
| 1:F:210:PRO:HA | 1:F:211:PRO:HD3 | 1.89 | 0.42 |
| 1:H:477:VAL:HA | 1:H:480:PHE:CE2 | 2.55 | 0.42 |
| 1:J:437:LEU:HB2 | 1:J:445:LEU:HD11 | 2.01 | 0.42 |
| 1:K:256:GLN:HA | 1:K:261:ARG:HH12 | 1.83 | 0.42 |
| 1:O:477:VAL:HA | 1:O:480:PHE:CE2 | 2.55 | 0.42 |
| 1:Q:208:PRO:HB2 | 1:Q:244:TYR:HA | 2.01 | 0.42 |
| 1:Q:515:PRO:HA | 1:Q:518:LYS:HE2 | 2.00 | 0.42 |
| 1:R:197:SER:HA | 1:R:200:HIS:CD2 | 2.53 | 0.42 |
| 1:C:515:PRO:HA | 1:C:518:LYS:HE2 | 2.00 | 0.42 |
| 1:D:209:PRO:HG2 | 1:D:243:ARG:HB3 | 2.01 | 0.42 |
| 1:D:501:HIS:HA | 1:D:504:GLN:HG3 | 2.01 | 0.42 |
| 1:E:501:HIS:HA | 1:E:504:GLN:HG3 | 2.01 | 0.42 |
| 1:J:477:VAL:HA | 1:J:480:PHE:CE2 | 2.55 | 0.42 |
| 1:J:501:HIS:HA | 1:J:504:GLN:HG3 | 2.01 | 0.42 |
| 1:J:509:TYR:O | 1:J:513:PHE:HB2 | 2.20 | 0.42 |
| 1:K:515:PRO:HA | 1:K:518:LYS:HE2 | 2.00 | 0.42 |
| 1:N:376:ILE:O | 1:N:380:HIS:ND1 | 2.51 | 0.42 |
| 1:O:208:PRO:HB2 | 1:O:244:TYR:HA | 2.01 | 0.42 |
| 1:O:437:LEU:HB2 | 1:O:445:LEU:HD11 | 2.01 | 0.42 |
| 1:P:509:TYR:O | 1:P:513:PHE:HB2 | 2.20 | 0.42 |
| 1:A:437:LEU:HB2 | 1:A:445:LEU:HD11 | 2.01 | 0.42 |
| 1:B:196:LEU:HD21 | 1:B:260:VAL:HG11 | 2.01 | 0.42 |
| 1:B:501:HIS:HA | 1:B:504:GLN:HG3 | 2.01 | 0.42 |
| 1:B:509:TYR:O | 1:B:513:PHE:HB2 | 2.20 | 0.42 |
| 1:D:197:SER:HA | 1:D:200:HIS:CD2 | 2.53 | 0.42 |
| 1:D:394:LEU:HD11 | 1:D:487:ASP:HB2 | 2.00 | 0.42 |
| 1:F:208:PRO:HB2 | 1:F:244:TYR:HA | 2.01 | 0.42 |
| 1:G:509:TYR:O | 1:G:513:PHE:HB2 | 2.20 | 0.42 |
| 1:J:196:LEU:HD21 | 1:J:260:VAL:HG11 | 2.01 | 0.42 |
| 1:M:477:VAL:HA | 1:M:480:PHE:CE2 | 2.55 | 0.42 |
| 1:M:509:TYR:O | 1:M:513:PHE:HB2 | 2.20 | 0.42 |
| 1:P:196:LEU:HD21 | 1:P:260:VAL:HG11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:501:HIS:HA | 1:P:504:GLN:HG3 | 2.01 | 0.42 |
| 1:D:509:TYR:O | 1:D:513:PHE:HB2 | 2.20 | 0.42 |
| 1:F:176:ARG:NH2 | 1:F:262:GLU:OE2 | 2.53 | 0.42 |
| 1:H:509:TYR:O | 1:H:513:PHE:HB2 | 2.20 | 0.42 |
| 1:I:509:TYR:O | 1:I:513:PHE:HB2 | 2.20 | 0.42 |
| 1:M:486:LYS:HE2 | 1:M:486:LYS:HB3 | 1.91 | 0.42 |
| 1:M:501:HIS:HA | 1:M:504:GLN:HG3 | 2.01 | 0.42 |
| 1:R:334:ASN:HA | 1:R:337:LYS:HE2 | 2.02 | 0.42 |
| 1:R:394:LEU:HD11 | 1:R:487:ASP:HB2 | 2.00 | 0.42 |
| 1:C:208:PRO:HB2 | 1:C:244:TYR:HA | 2.02 | 0.42 |
| 1:C:477:VAL:HA | 1:C:480:PHE:CE2 | 2.55 | 0.42 |
| 1:D:334:ASN:HA | 1:D:337:LYS:HE2 | 2.02 | 0.42 |
| 1:E:208:PRO:HB2 | 1:E:244:TYR:HA | 2.02 | 0.42 |
| 1:G:208:PRO:HB2 | 1:G:244:TYR:HA | 2.02 | 0.42 |
| 1:G:334:ASN:HA | 1:G:337:LYS:HE2 | 2.02 | 0.42 |
| 1:H:394:LEU:HD11 | 1:H:487:ASP:HB2 | 2.00 | 0.42 |
| 1:H:437:LEU:HB2 | 1:H:445:LEU:HD11 | 2.01 | 0.42 |
| 1:K:509:TYR:O | 1:K:513:PHE:HB2 | 2.20 | 0.42 |
| 1:M:196:LEU:HD21 | 1:M:260:VAL:HG11 | 2.01 | 0.42 |
| 1:O:509:TYR:O | 1:O:513:PHE:HB2 | 2.20 | 0.42 |
| 1:P:208:PRO:HB2 | 1:P:244:TYR:HA | 2.02 | 0.42 |
| 1:Q:477:VAL:HA | 1:Q:480:PHE:CE2 | 2.55 | 0.42 |
| 1:R:509:TYR:O | 1:R:513:PHE:HB2 | 2.20 | 0.42 |
| 1:C:501:HIS:HA | 1:C:504:GLN:HG3 | 2.01 | 0.42 |
| 1:E:210:PRO:HA | 1:E:211:PRO:HD3 | 1.90 | 0.42 |
| 1:G:196:LEU:HD21 | 1:G:260:VAL:HG11 | 2.01 | 0.42 |
| 1:I:501:HIS:HA | 1:I:504:GLN:HG3 | 2.01 | 0.42 |
| 1:L:509:TYR:O | 1:L:513:PHE:HB2 | 2.20 | 0.42 |
| 1:N:509:TYR:O | 1:N:513:PHE:HB2 | 2.20 | 0.42 |
| 1:Q:501:HIS:HA | 1:Q:504:GLN:HG3 | 2.01 | 0.42 |
| 1:A:176:ARG:NH2 | 1:A:262:GLU:OE2 | 2.53 | 0.42 |
| 1:A:501:HIS:HA | 1:A:504:GLN:HG3 | 2.01 | 0.42 |
| 1:A:509:TYR:O | 1:A:513:PHE:HB2 | 2.20 | 0.42 |
| 1:C:334:ASN:HA | 1:C:337:LYS:HE2 | 2.02 | 0.42 |
| 1:F:501:HIS:HA | 1:F:504:GLN:HG3 | 2.01 | 0.42 |
| 1:F:509:TYR:O | 1:F:513:PHE:HB2 | 2.20 | 0.42 |
| 1:G:477:VAL:HA | 1:G:480:PHE:CE2 | 2.55 | 0.42 |
| 1:H:334:ASN:HA | 1:H:337:LYS:HE2 | 2.02 | 0.42 |
| 1:I:269:LEU:HA | 1:I:270:PRO:HD3 | 1.95 | 0.42 |
| 1:I:515:PRO:HA | 1:I:518:LYS:HE2 | 2.00 | 0.42 |
| 1:K:196:LEU:HD21 | 1:K:260:VAL:HG11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:196:LEU:HD21 | 1:L:260:VAL:HG11 | 2.01 | 0.42 |
| 1:L:477:VAL:HA | 1:L:480:PHE:CE2 | 2.55 | 0.42 |
| 1:N:196:LEU:HD21 | 1:N:260:VAL:HG11 | 2.01 | 0.42 |
| 1:O:334:ASN:HA | 1:O:337:LYS:HE2 | 2.02 | 0.42 |
| 1:Q:334:ASN:HA | 1:Q:337:LYS:HE2 | 2.02 | 0.42 |
| 1:A:334:ASN:HA | 1:A:337:LYS:HE2 | 2.02 | 0.42 |
| 1:F:477:VAL:HA | 1:F:480:PHE:CE2 | 2.55 | 0.42 |
| 1:G:269:LEU:HA | 1:G:270:PRO:HD3 | 1.95 | 0.42 |
| 1:L:501:HIS:HA | 1:L:504:GLN:HG3 | 2.01 | 0.42 |
| 1:N:477:VAL:HA | 1:N:480:PHE:CE2 | 2.55 | 0.42 |
| 1:O:176:ARG:NH2 | 1:O:262:GLU:OE2 | 2.53 | 0.42 |
| 1:R:515:PRO:HA | 1:R:518:LYS:HE2 | 2.00 | 0.42 |
| 1:B:477:VAL:HA | 1:B:480:PHE:CE2 | 2.55 | 0.41 |
| 1:D:269:LEU:HA | 1:D:270:PRO:HD3 | 1.95 | 0.41 |
| 1:E:509:TYR:O | 1:E:513:PHE:HB2 | 2.20 | 0.41 |
| 1:G:175:PHE:HB3 | 1:G:178:ARG:HH21 | 1.85 | 0.41 |
| 1:H:501:HIS:HA | 1:H:504:GLN:HG3 | 2.01 | 0.41 |
| 1:I:477:VAL:HA | 1:I:480:PHE:CE2 | 2.55 | 0.41 |
| 1:N:175:PHE:HB3 | 1:N:178:ARG:HH21 | 1.85 | 0.41 |
| 1:N:501:HIS:HA | 1:N:504:GLN:HG3 | 2.01 | 0.41 |
| 1:O:501:HIS:HA | 1:O:504:GLN:HG3 | 2.01 | 0.41 |
| 1:A:208:PRO:HB2 | 1:A:244:TYR:HA | 2.02 | 0.41 |
| 1:B:334:ASN:HA | 1:B:337:LYS:HE2 | 2.02 | 0.41 |
| 1:E:477:VAL:HA | 1:E:480:PHE:CE2 | 2.55 | 0.41 |
| 1:I:196:LEU:HD21 | 1:I:260:VAL:HG11 | 2.01 | 0.41 |
| 1:K:210:PRO:HA | 1:K:211:PRO:HD3 | 1.90 | 0.41 |
| 1:R:269:LEU:HA | 1:R:270:PRO:HD3 | 1.95 | 0.41 |
| 1:C:144:LEU:HD11 | 1:C:245:LEU:HD13 | 2.03 | 0.41 |
| 1:D:175:PHE:HB3 | 1:D:178:ARG:HH21 | 1.85 | 0.41 |
| 1:E:334:ASN:HA | 1:E:337:LYS:HE2 | 2.02 | 0.41 |
| 1:G:210:PRO:HA | 1:G:211:PRO:HD3 | 1.89 | 0.41 |
| 1:K:144:LEU:HD11 | 1:K:245:LEU:HD13 | 2.03 | 0.41 |
| 1:P:334:ASN:HA | 1:P:337:LYS:HE2 | 2.02 | 0.41 |
| 1:P:477:VAL:HA | 1:P:480:PHE:CE2 | 2.55 | 0.41 |
| 1:R:477:VAL:HA | 1:R:480:PHE:CE2 | 2.55 | 0.41 |
| 1:A:144:LEU:HD11 | 1:A:245:LEU:HD13 | 2.03 | 0.41 |
| 1:D:144:LEU:HD11 | 1:D:245:LEU:HD13 | 2.03 | 0.41 |
| 1:D:515:PRO:HA | 1:D:518:LYS:HE2 | 2.00 | 0.41 |
| 1:F:144:LEU:HD11 | 1:F:245:LEU:HD13 | 2.03 | 0.41 |
| 1:H:176:ARG:NH2 | 1:H:262:GLU:OE2 | 2.53 | 0.41 |
| 1:J:144:LEU:HD11 | 1:J:245:LEU:HD13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:501:HIS:HA | 1:K:504:GLN:HG3 | 2.01 | 0.41 |
| 1:Q:144:LEU:HD11 | 1:Q:245:LEU:HD13 | 2.03 | 0.41 |
| 1:Q:509:TYR:O | 1:Q:513:PHE:HB2 | 2.20 | 0.41 |
| 1:R:144:LEU:HD11 | 1:R:245:LEU:HD13 | 2.03 | 0.41 |
| 1:A:495:TYR:CE1 | 1:B:369:LEU:HD21 | 2.56 | 0.41 |
| 1:B:175:PHE:HB3 | 1:B:178:ARG:HH21 | 1.85 | 0.41 |
| 1:B:186:PHE:CE2 | 1:B:214:SER:HB3 | 2.52 | 0.41 |
| 1:D:152:GLU:O | 1:D:163:ALA:N | 2.46 | 0.41 |
| 1:D:208:PRO:HB3 | 1:D:247:ARG:HB2 | 2.01 | 0.41 |
| 1:D:477:VAL:HA | 1:D:480:PHE:CE2 | 2.55 | 0.41 |
| 1:E:376:ILE:O | 1:E:380:HIS:ND1 | 2.51 | 0.41 |
| 1:G:280:GLY:HA2 | 1:G:283:LEU:HB2 | 2.02 | 0.41 |
| 1:H:208:PRO:HB2 | 1:H:244:TYR:HA | 2.01 | 0.41 |
| 1:I:208:PRO:HB2 | 1:I:244:TYR:HA | 2.02 | 0.41 |
| 1:I:210:PRO:HA | 1:I:211:PRO:HD3 | 1.90 | 0.41 |
| 1:K:477:VAL:HA | 1:K:480:PHE:CE2 | 2.55 | 0.41 |
| 1:L:144:LEU:HD11 | 1:L:245:LEU:HD13 | 2.03 | 0.41 |
| 1:M:144:LEU:HD11 | 1:M:245:LEU:HD13 | 2.03 | 0.41 |
| 1:N:208:PRO:HB2 | 1:N:244:TYR:HA | 2.02 | 0.41 |
| 1:O:144:LEU:HD11 | 1:O:245:LEU:HD13 | 2.03 | 0.41 |
| 1:O:495:TYR:CE1 | 1:P:369:LEU:HD21 | 2.56 | 0.41 |
| 1:R:175:PHE:HB3 | 1:R:178:ARG:HH21 | 1.85 | 0.41 |
| 1:B:280:GLY:HA2 | 1:B:283:LEU:HB2 | 2.03 | 0.41 |
| 1:F:269:LEU:HA | 1:F:270:PRO:HD3 | 1.95 | 0.41 |
| 1:H:144:LEU:HD11 | 1:H:245:LEU:HD13 | 2.03 | 0.41 |
| 1:J:334:ASN:HA | 1:J:337:LYS:HE2 | 2.02 | 0.41 |
| 1:K:495:TYR:CE1 | 1:L:369:LEU:HD21 | 2.56 | 0.41 |
| 1:M:495:TYR:CE1 | 1:N:369:LEU:HD21 | 2.56 | 0.41 |
| 1:P:175:PHE:HB3 | 1:P:178:ARG:HH21 | 1.85 | 0.41 |
| 1:P:280:GLY:HA2 | 1:P:283:LEU:HB2 | 2.02 | 0.41 |
| 1:B:376:ILE:O | 1:B:380:HIS:ND1 | 2.51 | 0.41 |
| 1:C:175:PHE:HB3 | 1:C:178:ARG:HH21 | 1.85 | 0.41 |
| 1:C:509:TYR:O | 1:C:513:PHE:HB2 | 2.20 | 0.41 |
| 1:E:144:LEU:HD11 | 1:E:245:LEU:HD13 | 2.03 | 0.41 |
| 1:G:176:ARG:NH2 | 1:G:262:GLU:OE2 | 2.53 | 0.41 |
| 1:L:334:ASN:HA | 1:L:337:LYS:HE2 | 2.02 | 0.41 |
| 1:N:334:ASN:HA | 1:N:337:LYS:HE2 | 2.02 | 0.41 |
| 1:P:144:LEU:HD11 | 1:P:245:LEU:HD13 | 2.03 | 0.41 |
| 1:Q:175:PHE:HB3 | 1:Q:178:ARG:HH21 | 1.85 | 0.41 |
| 1:A:147:GLY:O | 1:A:167:THR:N | 2.44 | 0.41 |
| 1:G:376:ILE:O | 1:G:380:HIS:ND1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:486:LYS:HE2 | 1:H:486:LYS:HB3 | 1.91 | 0.41 |
| 1:I:144:LEU:HD11 | 1:I:245:LEU:HD13 | 2.03 | 0.41 |
| 1:I:175:PHE:HB3 | 1:I:178:ARG:HH21 | 1.85 | 0.41 |
| 1:J:208:PRO:HB2 | 1:J:244:TYR:HA | 2.01 | 0.41 |
| 1:N:269:LEU:HA | 1:N:270:PRO:HD3 | 1.95 | 0.41 |
| 1:A:175:PHE:HB3 | 1:A:178:ARG:HH21 | 1.85 | 0.41 |
| 1:A:387:ASP:CG | 1:A:494:LYS:HG3 | 2.42 | 0.41 |
| 1:B:144:LEU:HD11 | 1:B:245:LEU:HD13 | 2.03 | 0.41 |
| 1:C:326:HIS:CE1 | 1:C:392:ALA:HB1 | 2.56 | 0.41 |
| 1:D:387:ASP:CG | 1:D:494:LYS:HG3 | 2.42 | 0.41 |
| 1:F:334:ASN:HA | 1:F:337:LYS:HE2 | 2.02 | 0.41 |
| 1:H:175:PHE:HB3 | 1:H:178:ARG:HH21 | 1.85 | 0.41 |
| 1:H:280:GLY:HA2 | 1:H:283:LEU:HB2 | 2.03 | 0.41 |
| 1:H:326:HIS:CE1 | 1:H:392:ALA:HB1 | 2.56 | 0.41 |
| 1:H:387:ASP:CG | 1:H:494:LYS:HG3 | 2.42 | 0.41 |
| 1:I:183:LYS:N | 1:I:267:GLU:OE2 | 2.44 | 0.41 |
| 1:I:334:ASN:HA | 1:I:337:LYS:HE2 | 2.02 | 0.41 |
| 1:J:175:PHE:HB3 | 1:J:178:ARG:HH21 | 1.85 | 0.41 |
| 1:J:280:GLY:HA2 | 1:J:283:LEU:HB2 | 2.02 | 0.41 |
| 1:K:326:HIS:CE1 | 1:K:392:ALA:HB1 | 2.56 | 0.41 |
| 1:L:387:ASP:CG | 1:L:494:LYS:HG3 | 2.42 | 0.41 |
| 1:M:175:PHE:HB3 | 1:M:178:ARG:HH21 | 1.85 | 0.41 |
| 1:M:208:PRO:HB2 | 1:M:244:TYR:HA | 2.01 | 0.41 |
| 1:O:175:PHE:HB3 | 1:O:178:ARG:HH21 | 1.85 | 0.41 |
| 1:O:387:ASP:CG | 1:O:494:LYS:HG3 | 2.42 | 0.41 |
| 1:P:376:ILE:O | 1:P:380:HIS:ND1 | 2.51 | 0.41 |
| 1:R:152:GLU:O | 1:R:163:ALA:N | 2.45 | 0.41 |
| 1:B:152:GLU:O | 1:B:163:ALA:N | 2.46 | 0.41 |
| 1:C:387:ASP:CG | 1:C:494:LYS:HG3 | 2.42 | 0.41 |
| 1:D:233:PHE:O | 1:D:237:ARG:HG2 | 2.22 | 0.41 |
| 1:E:326:HIS:CE1 | 1:E:392:ALA:HB1 | 2.56 | 0.41 |
| 1:F:387:ASP:CG | 1:F:494:LYS:HG3 | 2.42 | 0.41 |
| 1:G:326:HIS:CE1 | 1:G:392:ALA:HB1 | 2.56 | 0.41 |
| 1:I:280:GLY:HA2 | 1:I:283:LEU:HB2 | 2.02 | 0.41 |
| 1:I:326:HIS:CE1 | 1:I:392:ALA:HB1 | 2.56 | 0.41 |
| 1:I:376:ILE:O | 1:I:380:HIS:ND1 | 2.51 | 0.41 |
| 1:J:326:HIS:CE1 | 1:J:392:ALA:HB1 | 2.56 | 0.41 |
| 1:J:387:ASP:CG | 1:J:494:LYS:HG3 | 2.42 | 0.41 |
| 1:K:175:PHE:HB3 | 1:K:178:ARG:HH21 | 1.85 | 0.41 |
| 1:K:183:LYS:N | 1:K:267:GLU:OE2 | 2.44 | 0.41 |
| 1:L:208:PRO:HB2 | 1:L:244:TYR:HA | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:387:ASP:CG | 1:M:494:LYS:HG3 | 2.42 | 0.41 |
| 1:N:144:LEU:HD11 | 1:N:245:LEU:HD13 | 2.03 | 0.41 |
| 1:Q:233:PHE:O | 1:Q:237:ARG:HG2 | 2.22 | 0.41 |
| 1:R:387:ASP:CG | 1:R:494:LYS:HG3 | 2.42 | 0.41 |
| 1:A:326:HIS:CE1 | 1:A:392:ALA:HB1 | 2.56 | 0.40 |
| 1:C:233:PHE:O | 1:C:237:ARG:HG2 | 2.22 | 0.40 |
| 1:G:144:LEU:HD11 | 1:G:245:LEU:HD13 | 2.03 | 0.40 |
| 1:H:183:LYS:N | 1:H:267:GLU:OE2 | 2.44 | 0.40 |
| 1:H:233:PHE:O | 1:H:237:ARG:HG2 | 2.22 | 0.40 |
| 1:I:387:ASP:CG | 1:I:494:LYS:HG3 | 2.42 | 0.40 |
| 1:J:486:LYS:HE2 | 1:J:486:LYS:HB3 | 1.91 | 0.40 |
| 1:L:326:HIS:CE1 | 1:L:392:ALA:HB1 | 2.56 | 0.40 |
| 1:M:280:GLY:HA2 | 1:M:283:LEU:HB2 | 2.02 | 0.40 |
| 1:M:334:ASN:HA | 1:M:337:LYS:HE2 | 2.02 | 0.40 |
| 1:O:147:GLY:O | 1:O:167:THR:N | 2.44 | 0.40 |
| 1:O:326:HIS:CE1 | 1:O:392:ALA:HB1 | 2.56 | 0.40 |
| 1:Q:326:HIS:CE1 | 1:Q:392:ALA:HB1 | 2.57 | 0.40 |
| 1:Q:387:ASP:CG | 1:Q:494:LYS:HG3 | 2.42 | 0.40 |
| 1:R:233:PHE:O | 1:R:237:ARG:HG2 | 2.22 | 0.40 |
| 1:A:280:GLY:HA2 | 1:A:283:LEU:HB2 | 2.03 | 0.40 |
| 1:B:176:ARG:NH2 | 1:B:262:GLU:OE2 | 2.53 | 0.40 |
| 1:E:175:PHE:HB3 | 1:E:178:ARG:HH21 | 1.85 | 0.40 |
| 1:E:280:GLY:HA2 | 1:E:283:LEU:HB2 | 2.03 | 0.40 |
| 1:G:147:GLY:O | 1:G:167:THR:N | 2.44 | 0.40 |
| 1:I:495:TYR:CE1 | 1:J:369:LEU:HD21 | 2.56 | 0.40 |
| 1:K:233:PHE:O | 1:K:237:ARG:HG2 | 2.22 | 0.40 |
| 1:M:326:HIS:CE1 | 1:M:392:ALA:HB1 | 2.56 | 0.40 |
| 1:N:233:PHE:O | 1:N:237:ARG:HG2 | 2.22 | 0.40 |
| 1:O:280:GLY:HA2 | 1:O:283:LEU:HB2 | 2.03 | 0.40 |
| 1:P:176:ARG:NH2 | 1:P:262:GLU:OE2 | 2.53 | 0.40 |
| 1:Q:152:GLU:O | 1:Q:163:ALA:N | 2.45 | 0.40 |
| 1:Q:280:GLY:HA2 | 1:Q:283:LEU:HB2 | 2.03 | 0.40 |
| 1:B:147:GLY:O | 1:B:167:THR:N | 2.44 | 0.40 |
| 1:G:183:LYS:N | 1:G:267:GLU:OE2 | 2.44 | 0.40 |
| 1:K:208:PRO:HB2 | 1:K:244:TYR:HA | 2.02 | 0.40 |
| 1:L:152:GLU:O | 1:L:163:ALA:N | 2.45 | 0.40 |
| 1:N:326:HIS:CE1 | 1:N:392:ALA:HB1 | 2.56 | 0.40 |
| 1:P:326:HIS:CE1 | 1:P:392:ALA:HB1 | 2.56 | 0.40 |
| 1:A:233:PHE:O | 1:A:237:ARG:HG2 | 2.22 | 0.40 |
| 1:C:210:PRO:HA | 1:C:211:PRO:HD3 | 1.90 | 0.40 |
| 1:C:280:GLY:HA2 | 1:C:283:LEU:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:376:ILE:O | 1:D:380:HIS:ND1 | 2.51 | 0.40 |
| 1:E:495:TYR:CE1 | 1:F:369:LEU:HD21 | 2.56 | 0.40 |
| 1:I:233:PHE:O | 1:I:237:ARG:HG2 | 2.22 | 0.40 |
| 1:N:152:GLU:O | 1:N:163:ALA:N | 2.46 | 0.40 |
| 1:N:387:ASP:CG | 1:N:494:LYS:HG3 | 2.42 | 0.40 |
| 1:O:233:PHE:O | 1:O:237:ARG:HG2 | 2.22 | 0.40 |
| 1:R:326:HIS:CE1 | 1:R:392:ALA:HB1 | 2.56 | 0.40 |
| 1:B:326:HIS:CE1 | 1:B:392:ALA:HB1 | 2.56 | 0.40 |
| 1:C:152:GLU:O | 1:C:163:ALA:N | 2.46 | 0.40 |
| 1:E:387:ASP:CG | 1:E:494:LYS:HG3 | 2.42 | 0.40 |
| 1:G:233:PHE:O | 1:G:237:ARG:HG2 | 2.22 | 0.40 |
| 1:K:176:ARG:NH2 | 1:K:262:GLU:OE2 | 2.53 | 0.40 |
| 1:N:176:ARG:NH2 | 1:N:262:GLU:OE2 | 2.53 | 0.40 |
| 1:P:152:GLU:O | 1:P:163:ALA:N | 2.46 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | A | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | B | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | C | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | D | 378/529 (72%) | 331 (88%) | 45 (12%) | 2 (0%) | 29 | 69 |
| 1 | E | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | F | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | G | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | H | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | I | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | J | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | K | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | L | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | M | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | N | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | O | 378/529 (72%) | 332 (88%) | 44 (12%) | 2 (0%) | 29 | 69 |
| 1 | P | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | Q | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| 1 | R | 378/529 (72%) | 333 (88%) | 43 (11%) | 2 (0%) | 29 | 69 |
| All | All | 6804/9522 (72%) | 5991 (88%) | 777 (11%) | 36 (0%) | 32 | 69 |

All (36) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 209 | PRO |
| 1 | B | 209 | PRO |
| 1 | C | 209 | PRO |
| 1 | E | 209 | PRO |
| 1 | F | 209 | PRO |
| 1 | G | 209 | PRO |
| 1 | H | 209 | PRO |
| 1 | I | 209 | PRO |
| 1 | J | 209 | PRO |
| 1 | K | 209 | PRO |
| 1 | L | 209 | PRO |
| 1 | N | 209 | PRO |
| 1 | O | 209 | PRO |
| 1 | P | 209 | PRO |
| 1 | R | 209 | PRO |
| 1 | D | 209 | PRO |
| 1 | M | 209 | PRO |
| 1 | Q | 209 | PRO |
| 1 | A | 173 | PRO |
| 1 | B | 173 | PRO |
| 1 | C | 173 | PRO |
| 1 | D | 173 | PRO |
| 1 | E | 173 | PRO |
| 1 | F | 173 | PRO |
| 1 | G | 173 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 173 | PRO |
| 1 | I | 173 | PRO |
| 1 | J | 173 | PRO |
| 1 | K | 173 | PRO |
| 1 | L | 173 | PRO |
| 1 | M | 173 | PRO |
| 1 | N | 173 | PRO |
| 1 | O | 173 | PRO |
| 1 | P | 173 | PRO |
| 1 | Q | 173 | PRO |
| 1 | R | 173 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | B | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | C | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | D | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | E | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | F | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | G | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | H | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | I | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | J | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | K | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | L | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | M | 336/457 (74%) | 322 (96%) | 14 (4%) | 30 | 54 |
| 1 | N | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | O | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | P | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | Q | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| 1 | R | 336/457 (74%) | 321 (96%) | 15 (4%) | 27 | 52 |
| All | All | 6048/8226 (74%) | 5779 (96%) | 269 (4%) | 32 | 53 |

All (269) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 153 | LYS |
| 1 | A | 202 | GLN |
| 1 | A | 209 | PRO |
| 1 | A | 213 | LYS |
| 1 | A | 250 | ASN |
| 1 | A | 271 | ARG |
| 1 | A | 323 | ARG |
| 1 | A | 334 | ASN |
| 1 | A | 336 | ARG |
| 1 | A | 364 | ARG |
| 1 | A | 389 | PHE |
| 1 | A | 390 | LEU |
| 1 | A | 391 | LEU |
| 1 | A | 464 | ARG |
| 1 | A | 494 | LYS |
| 1 | B | 153 | LYS |
| 1 | B | 202 | GLN |
| 1 | B | 209 | PRO |
| 1 | B | 213 | LYS |
| 1 | B | 250 | ASN |
| 1 | B | 271 | ARG |
| 1 | B | 323 | ARG |
| 1 | B | 334 | ASN |
| 1 | B | 336 | ARG |
| 1 | B | 364 | ARG |
| 1 | B | 389 | PHE |
| 1 | B | 390 | LEU |
| 1 | B | 391 | LEU |
| 1 | B | 464 | ARG |
| 1 | B | 494 | LYS |
| 1 | C | 153 | LYS |
| 1 | C | 202 | GLN |
| 1 | C | 209 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 213 | LYS |
| 1 | C | 250 | ASN |
| 1 | C | 271 | ARG |
| 1 | C | 323 | ARG |
| 1 | C | 334 | ASN |
| 1 | C | 336 | ARG |
| 1 | C | 364 | ARG |
| 1 | C | 389 | PHE |
| 1 | C | 390 | LEU |
| 1 | C | 391 | LEU |
| 1 | C | 464 | ARG |
| 1 | C | 494 | LYS |
| 1 | D | 153 | LYS |
| 1 | D | 202 | GLN |
| 1 | D | 209 | PRO |
| 1 | D | 213 | LYS |
| 1 | D | 250 | ASN |
| 1 | D | 271 | ARG |
| 1 | D | 323 | ARG |
| 1 | D | 334 | ASN |
| 1 | D | 336 | ARG |
| 1 | D | 364 | ARG |
| 1 | D | 389 | PHE |
| 1 | D | 390 | LEU |
| 1 | D | 391 | LEU |
| 1 | D | 464 | ARG |
| 1 | D | 494 | LYS |
| 1 | E | 153 | LYS |
| 1 | E | 202 | GLN |
| 1 | E | 209 | PRO |
| 1 | E | 213 | LYS |
| 1 | E | 250 | ASN |
| 1 | E | 271 | ARG |
| 1 | E | 323 | ARG |
| 1 | E | 334 | ASN |
| 1 | E | 336 | ARG |
| 1 | E | 364 | ARG |
| 1 | E | 389 | PHE |
| 1 | E | 390 | LEU |
| 1 | E | 391 | LEU |
| 1 | E | 464 | ARG |
| 1 | E | 494 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 153 | LYS |
| 1 | F | 202 | GLN |
| 1 | F | 209 | PRO |
| 1 | F | 213 | LYS |
| 1 | F | 250 | ASN |
| 1 | F | 271 | ARG |
| 1 | F | 323 | ARG |
| 1 | F | 334 | ASN |
| 1 | F | 336 | ARG |
| 1 | F | 364 | ARG |
| 1 | F | 389 | PHE |
| 1 | F | 390 | LEU |
| 1 | F | 391 | LEU |
| 1 | F | 464 | ARG |
| 1 | F | 494 | LYS |
| 1 | G | 153 | LYS |
| 1 | G | 202 | GLN |
| 1 | G | 209 | PRO |
| 1 | G | 213 | LYS |
| 1 | G | 250 | ASN |
| 1 | G | 271 | ARG |
| 1 | G | 323 | ARG |
| 1 | G | 334 | ASN |
| 1 | G | 336 | ARG |
| 1 | G | 364 | ARG |
| 1 | G | 389 | PHE |
| 1 | G | 390 | LEU |
| 1 | G | 391 | LEU |
| 1 | G | 464 | ARG |
| 1 | G | 494 | LYS |
| 1 | H | 153 | LYS |
| 1 | H | 202 | GLN |
| 1 | H | 209 | PRO |
| 1 | H | 213 | LYS |
| 1 | H | 250 | ASN |
| 1 | H | 271 | ARG |
| 1 | H | 323 | ARG |
| 1 | H | 334 | ASN |
| 1 | H | 336 | ARG |
| 1 | H | 364 | ARG |
| 1 | H | 389 | PHE |
| 1 | H | 390 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 391 | LEU |
| 1 | H | 464 | ARG |
| 1 | H | 494 | LYS |
| 1 | I | 153 | LYS |
| 1 | I | 202 | GLN |
| 1 | I | 209 | PRO |
| 1 | I | 213 | LYS |
| 1 | I | 250 | ASN |
| 1 | I | 271 | ARG |
| 1 | I | 323 | ARG |
| 1 | I | 334 | ASN |
| 1 | I | 336 | ARG |
| 1 | I | 364 | ARG |
| 1 | I | 389 | PHE |
| 1 | I | 390 | LEU |
| 1 | I | 391 | LEU |
| 1 | I | 464 | ARG |
| 1 | I | 494 | LYS |
| 1 | J | 153 | LYS |
| 1 | J | 202 | GLN |
| 1 | J | 209 | PRO |
| 1 | J | 213 | LYS |
| 1 | J | 250 | ASN |
| 1 | J | 271 | ARG |
| 1 | J | 323 | ARG |
| 1 | J | 334 | ASN |
| 1 | J | 336 | ARG |
| 1 | J | 364 | ARG |
| 1 | J | 389 | PHE |
| 1 | J | 390 | LEU |
| 1 | J | 391 | LEU |
| 1 | J | 464 | ARG |
| 1 | J | 494 | LYS |
| 1 | K | 153 | LYS |
| 1 | K | 202 | GLN |
| 1 | K | 209 | PRO |
| 1 | K | 213 | LYS |
| 1 | K | 250 | ASN |
| 1 | K | 271 | ARG |
| 1 | K | 323 | ARG |
| 1 | K | 334 | ASN |
| 1 | K | 336 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 364 | ARG |
| 1 | K | 389 | PHE |
| 1 | K | 390 | LEU |
| 1 | K | 391 | LEU |
| 1 | K | 464 | ARG |
| 1 | K | 494 | LYS |
| 1 | L | 153 | LYS |
| 1 | L | 202 | GLN |
| 1 | L | 209 | PRO |
| 1 | L | 213 | LYS |
| 1 | L | 250 | ASN |
| 1 | L | 271 | ARG |
| 1 | L | 323 | ARG |
| 1 | L | 334 | ASN |
| 1 | L | 336 | ARG |
| 1 | L | 364 | ARG |
| 1 | L | 389 | PHE |
| 1 | L | 390 | LEU |
| 1 | L | 391 | LEU |
| 1 | L | 464 | ARG |
| 1 | L | 494 | LYS |
| 1 | M | 153 | LYS |
| 1 | M | 202 | GLN |
| 1 | M | 209 | PRO |
| 1 | M | 250 | ASN |
| 1 | M | 271 | ARG |
| 1 | M | 323 | ARG |
| 1 | M | 334 | ASN |
| 1 | M | 336 | ARG |
| 1 | M | 364 | ARG |
| 1 | M | 389 | PHE |
| 1 | M | 390 | LEU |
| 1 | M | 391 | LEU |
| 1 | M | 464 | ARG |
| 1 | M | 494 | LYS |
| 1 | N | 153 | LYS |
| 1 | N | 202 | GLN |
| 1 | N | 209 | PRO |
| 1 | N | 213 | LYS |
| 1 | N | 250 | ASN |
| 1 | N | 271 | ARG |
| 1 | N | 323 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 334 | ASN |
| 1 | N | 336 | ARG |
| 1 | N | 364 | ARG |
| 1 | N | 389 | PHE |
| 1 | N | 390 | LEU |
| 1 | N | 391 | LEU |
| 1 | N | 464 | ARG |
| 1 | N | 494 | LYS |
| 1 | O | 153 | LYS |
| 1 | O | 202 | GLN |
| 1 | O | 209 | PRO |
| 1 | O | 213 | LYS |
| 1 | O | 250 | ASN |
| 1 | O | 271 | ARG |
| 1 | O | 323 | ARG |
| 1 | O | 334 | ASN |
| 1 | O | 336 | ARG |
| 1 | O | 364 | ARG |
| 1 | O | 389 | PHE |
| 1 | O | 390 | LEU |
| 1 | O | 391 | LEU |
| 1 | O | 464 | ARG |
| 1 | O | 494 | LYS |
| 1 | P | 153 | LYS |
| 1 | P | 202 | GLN |
| 1 | P | 209 | PRO |
| 1 | P | 213 | LYS |
| 1 | P | 250 | ASN |
| 1 | P | 271 | ARG |
| 1 | P | 323 | ARG |
| 1 | P | 334 | ASN |
| 1 | P | 336 | ARG |
| 1 | P | 364 | ARG |
| 1 | P | 389 | PHE |
| 1 | P | 390 | LEU |
| 1 | P | 391 | LEU |
| 1 | P | 464 | ARG |
| 1 | P | 494 | LYS |
| 1 | Q | 153 | LYS |
| 1 | Q | 202 | GLN |
| 1 | Q | 209 | PRO |
| 1 | Q | 213 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 250 | ASN |
| 1 | Q | 271 | ARG |
| 1 | Q | 323 | ARG |
| 1 | Q | 334 | ASN |
| 1 | Q | 336 | ARG |
| 1 | Q | 364 | ARG |
| 1 | Q | 389 | PHE |
| 1 | Q | 390 | LEU |
| 1 | Q | 391 | LEU |
| 1 | Q | 464 | ARG |
| 1 | Q | 494 | LYS |
| 1 | R | 153 | LYS |
| 1 | R | 202 | GLN |
| 1 | R | 209 | PRO |
| 1 | R | 213 | LYS |
| 1 | R | 250 | ASN |
| 1 | R | 271 | ARG |
| 1 | R | 323 | ARG |
| 1 | R | 334 | ASN |
| 1 | R | 336 | ARG |
| 1 | R | 364 | ARG |
| 1 | R | 389 | PHE |
| 1 | R | 390 | LEU |
| 1 | R | 391 | LEU |
| 1 | R | 464 | ARG |
| 1 | R | 494 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 334 | ASN |
| 1 | A | 427 | GLN |
| 1 | B | 334 | ASN |
| 1 | B | 427 | GLN |
| 1 | B | 503 | GLN |
| 1 | C | 334 | ASN |
| 1 | C | 427 | GLN |
| 1 | D | 334 | ASN |
| 1 | D | 427 | GLN |
| 1 | D | 503 | GLN |
| 1 | E | 334 | ASN |
| 1 | E | 427 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 334 | ASN |
| 1 | F | 427 | GLN |
| 1 | F | 503 | GLN |
| 1 | G | 334 | ASN |
| 1 | G | 427 | GLN |
| 1 | H | 334 | ASN |
| 1 | H | 427 | GLN |
| 1 | H | 503 | GLN |
| 1 | I | 334 | ASN |
| 1 | I | 427 | GLN |
| 1 | J | 334 | ASN |
| 1 | J | 427 | GLN |
| 1 | J | 503 | GLN |
| 1 | K | 334 | ASN |
| 1 | K | 427 | GLN |
| 1 | L | 334 | ASN |
| 1 | L | 427 | GLN |
| 1 | L | 503 | GLN |
| 1 | M | 334 | ASN |
| 1 | M | 427 | GLN |
| 1 | N | 334 | ASN |
| 1 | N | 427 | GLN |
| 1 | N | 503 | GLN |
| 1 | O | 334 | ASN |
| 1 | O | 427 | GLN |
| 1 | P | 334 | ASN |
| 1 | P | 427 | GLN |
| 1 | P | 503 | GLN |
| 1 | Q | 334 | ASN |
| 1 | Q | 427 | GLN |
| 1 | R | 334 | ASN |
| 1 | R | 427 | GLN |
| 1 | R | 503 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

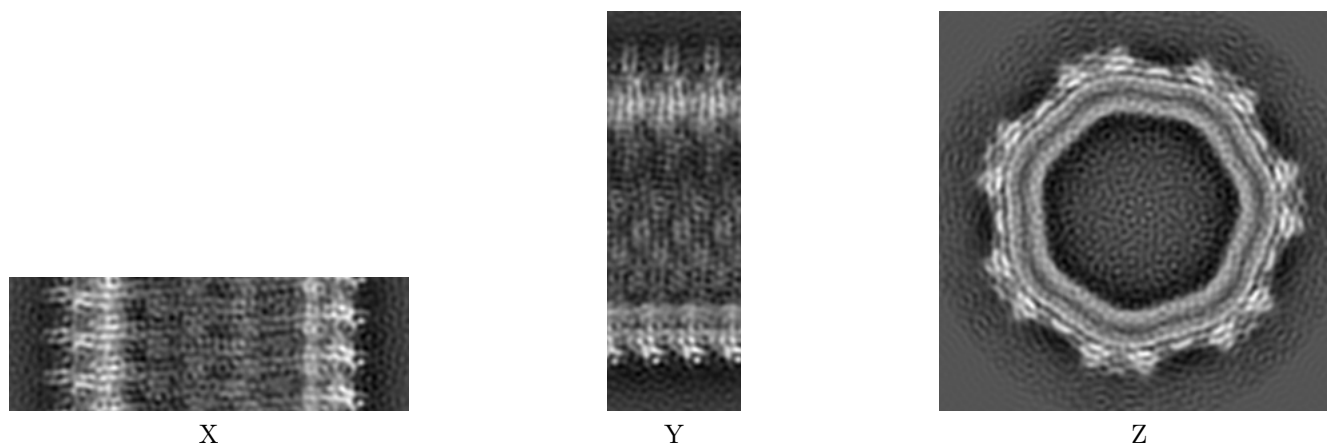
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30593. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

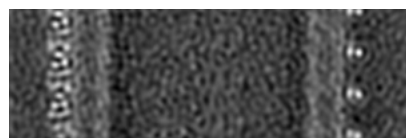
6.1.1 Primary map



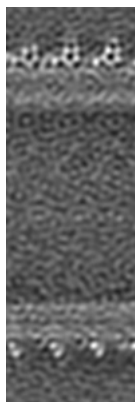
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

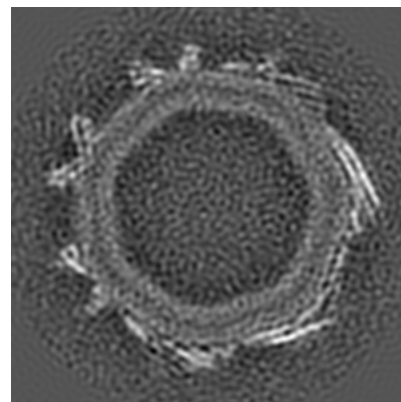
6.2.1 Primary map



X Index: 180



Y Index:
180



Z Index: 60

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

6.3 Largest variance slices [i](#)

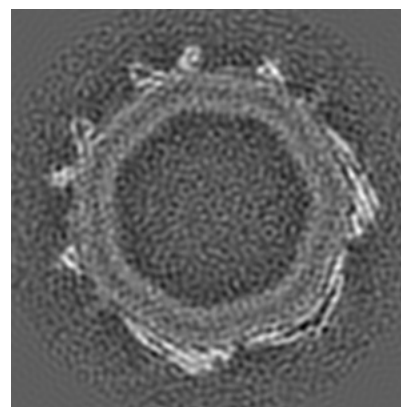
6.3.1 Primary map



X Index: 54



Y Index:
306



Z Index: 62

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

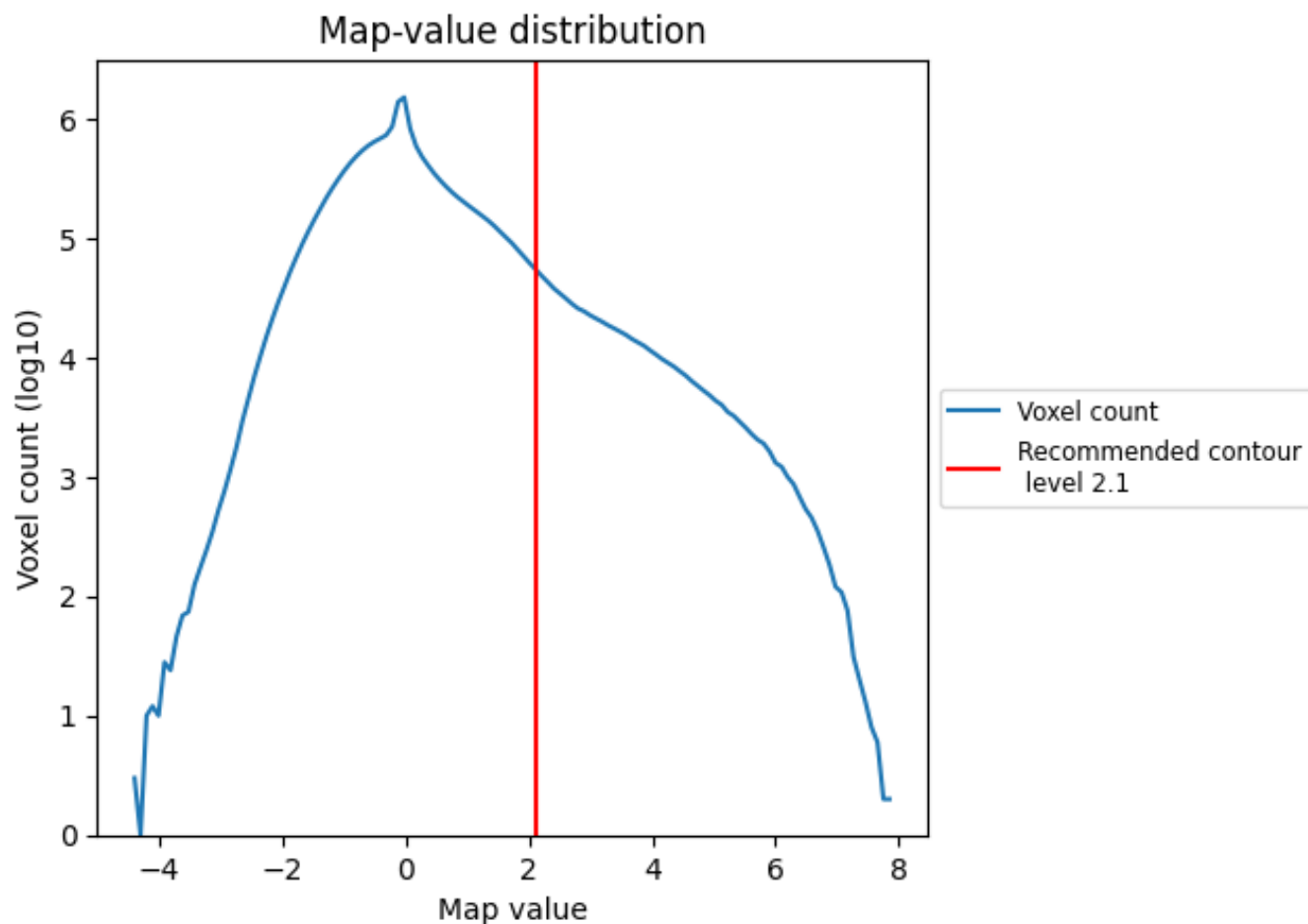
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

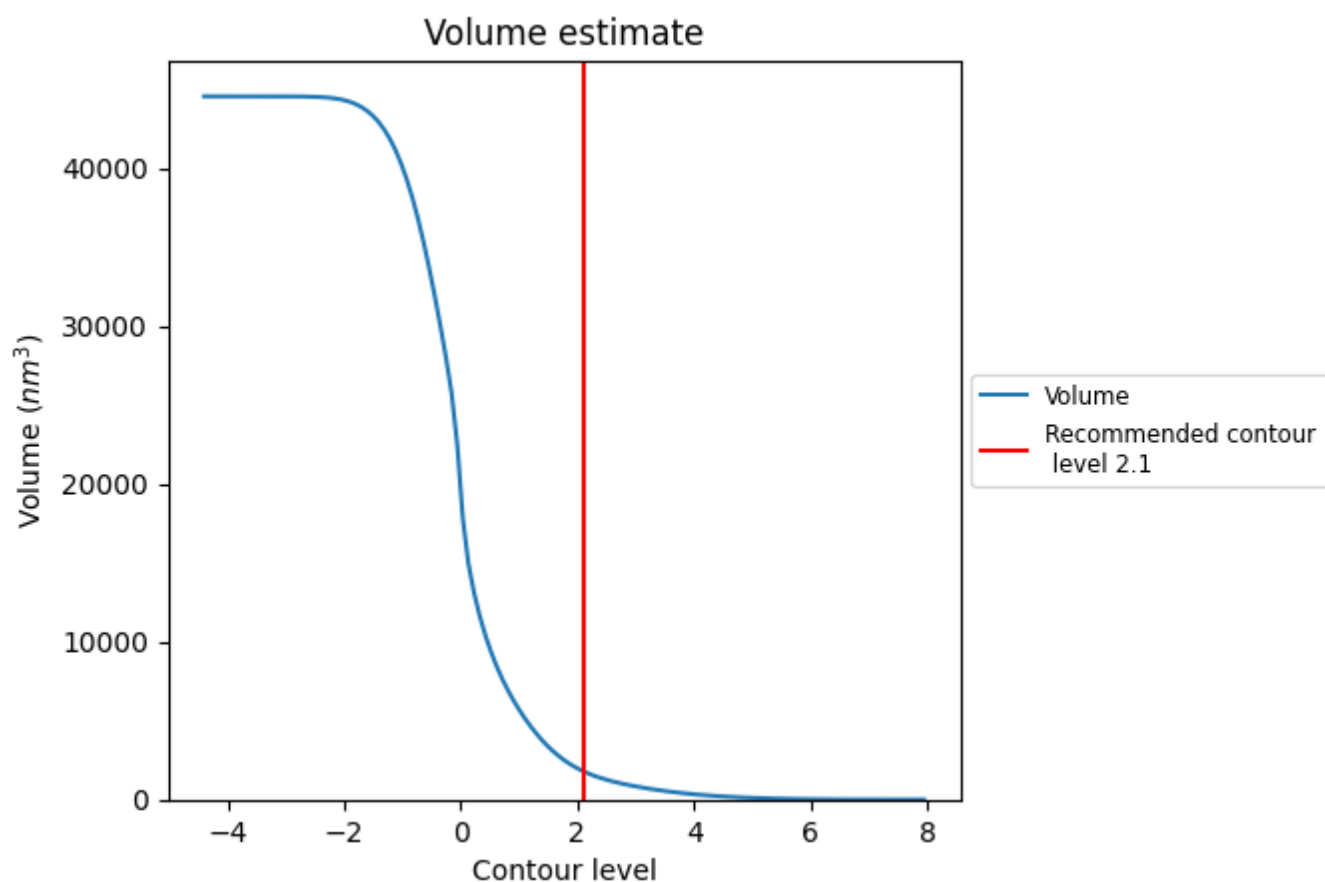
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1800 nm³; this corresponds to an approximate mass of 1626 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

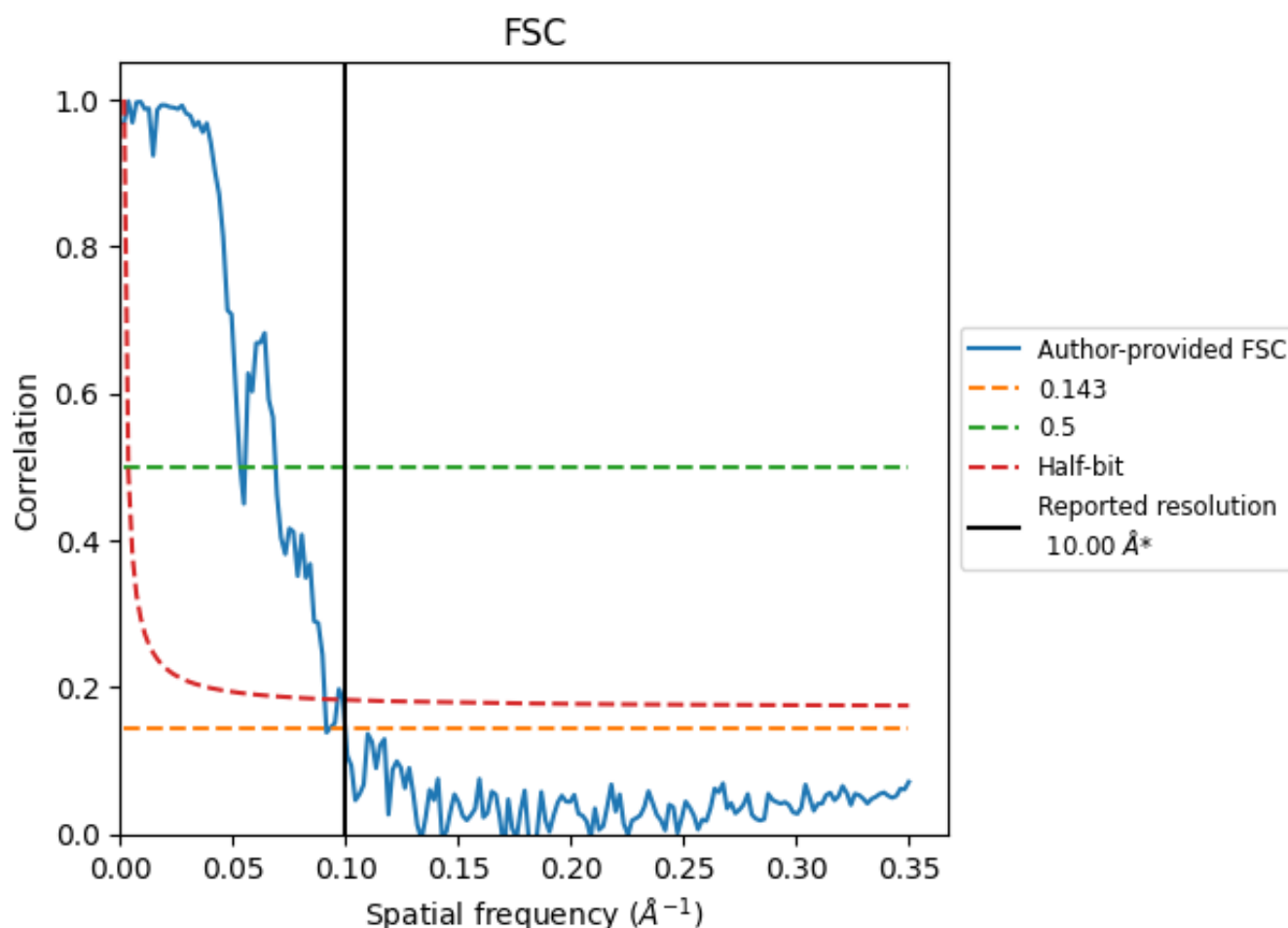
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

8.2 Resolution estimates [i](#)

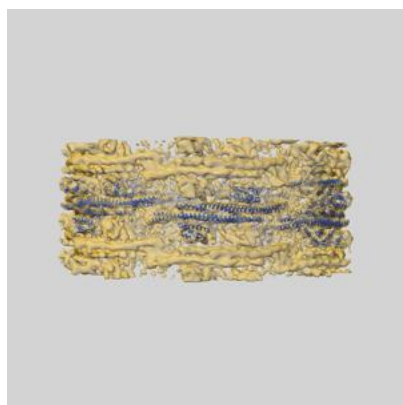
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 10.00 | - | - |
| Author-provided FSC curve | 10.92 | 18.73 | 11.00 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30593 and PDB model 7D6E. Per-residue inclusion information can be found in section [3](#) on page [9](#).

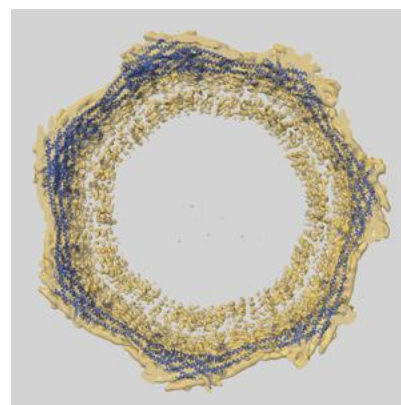
9.1 Map-model overlay [i](#)



X



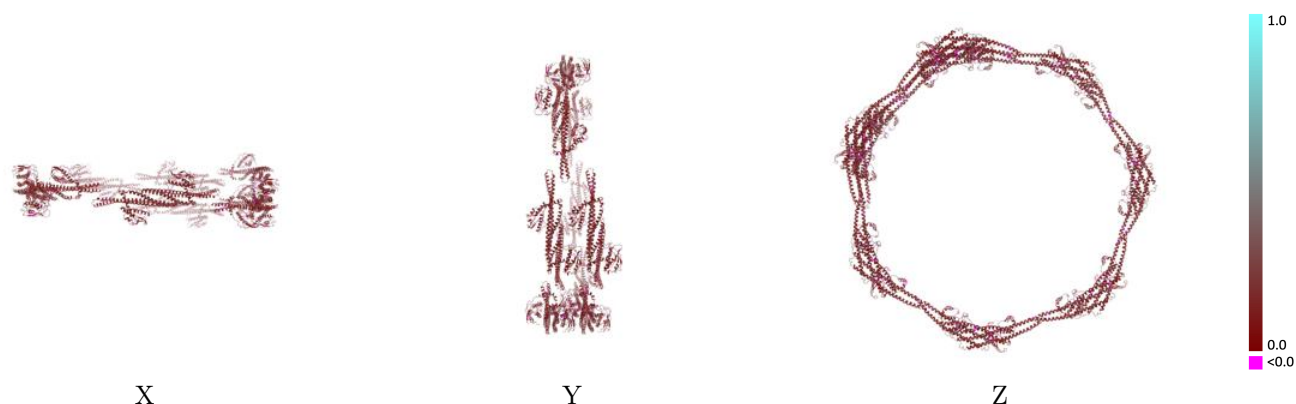
Y



Z

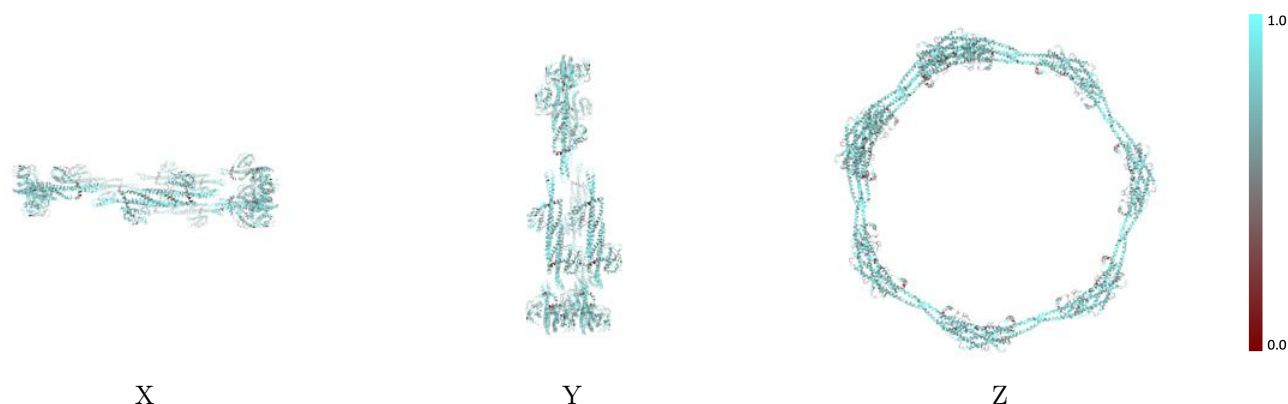
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



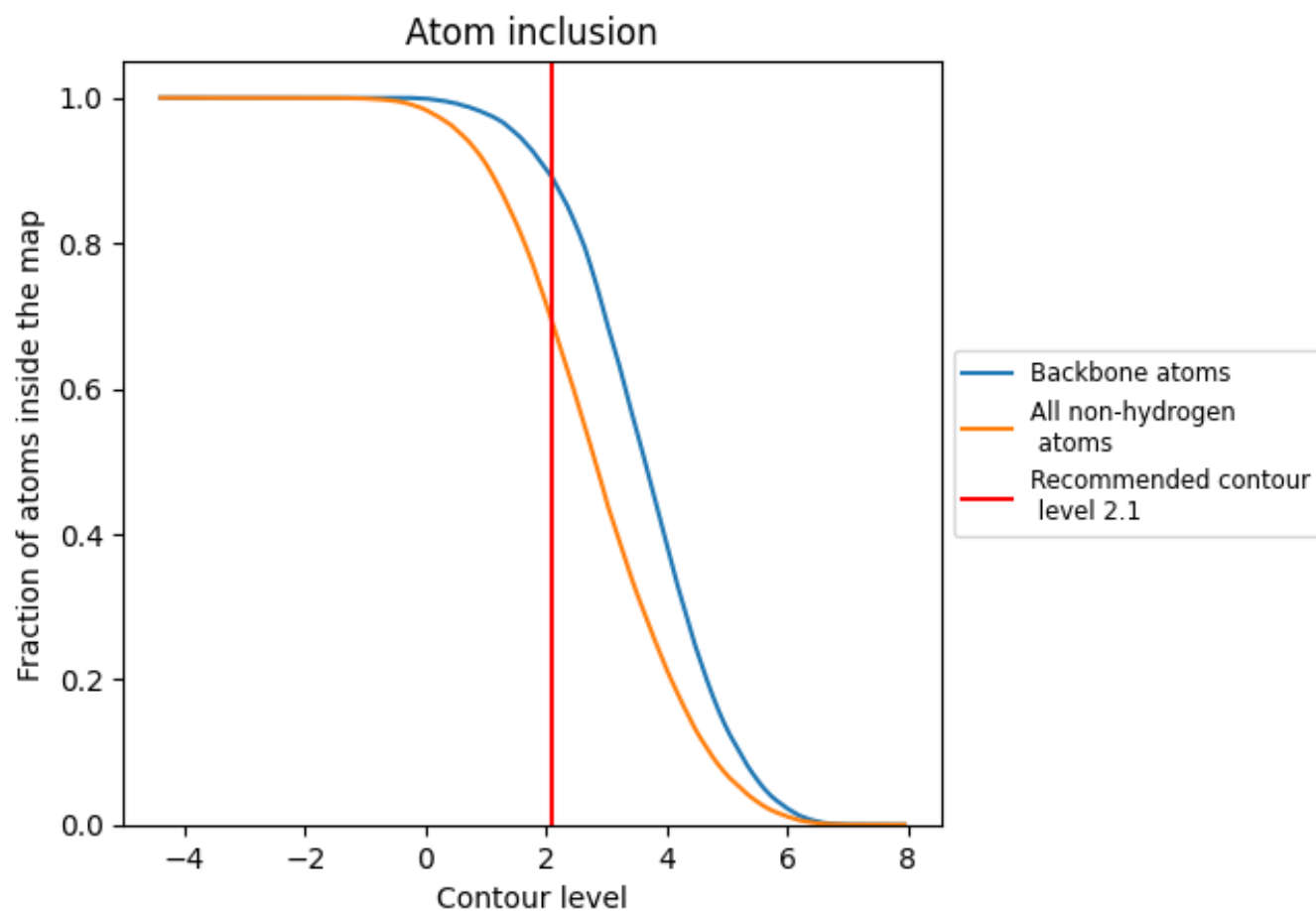
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.1).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.6914 |  0.1740 |
| A |  0.6836 |  0.1740 |
| B |  0.6717 |  0.1700 |
| C |  0.6885 |  0.1760 |
| D |  0.6760 |  0.1710 |
| E |  0.6974 |  0.1770 |
| F |  0.6799 |  0.1720 |
| G |  0.6997 |  0.1770 |
| H |  0.6878 |  0.1710 |
| I |  0.7128 |  0.1790 |
| J |  0.6908 |  0.1750 |
| K |  0.7082 |  0.1790 |
| L |  0.6911 |  0.1710 |
| M |  0.7013 |  0.1760 |
| N |  0.6908 |  0.1720 |
| O |  0.7013 |  0.1780 |
| P |  0.6852 |  0.1720 |
| Q |  0.6993 |  0.1810 |
| R |  0.6796 |  0.1710 |

