



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 04:42 PM UTC

PDB ID : 8G55 / pdb\_00008g55  
BMRB ID : 31075  
Title : Temperature-dependent structures of tau aggregates  
Authors : El Mammeri, N.; Duan, P.; Dregni, A.J.; Hong, M.  
Deposited on : 2023-02-11

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

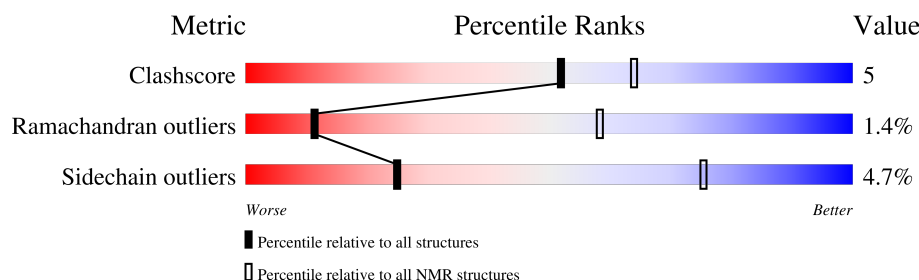
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 3%.

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<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 202    |                  |
| 1   | B     | 202    |                  |
| 1   | C     | 202    |                  |
| 1   | D     | 202    |                  |
| 1   | E     | 202    |                  |
| 1   | F     | 202    |                  |
| 1   | G     | 202    |                  |
| 1   | H     | 202    |                  |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 1   | I     | 202    |  24% 7% 69% |
| 1   | J     | 202    |  24% 7% 69% |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *medoid*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |                                                                                                                                                       |                   |              |
|--------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                                                                                                                                 | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:274-A:322, B:274-B:322,<br>C:274-C:322, D:274-D:322,<br>E:274-E:322, F:274-F:322,<br>G:274-G:322, H:274-H:322,<br>I:274-I:322, J:274-J:322<br>(490) | 3.48              | 4            |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

| Cluster number | Models           |
|----------------|------------------|
| 1              | 1, 4, 5, 6, 7, 9 |
| 2              | 2, 3, 8, 10      |

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 9530 atoms, of which 4910 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Microtubule-associated protein tau.

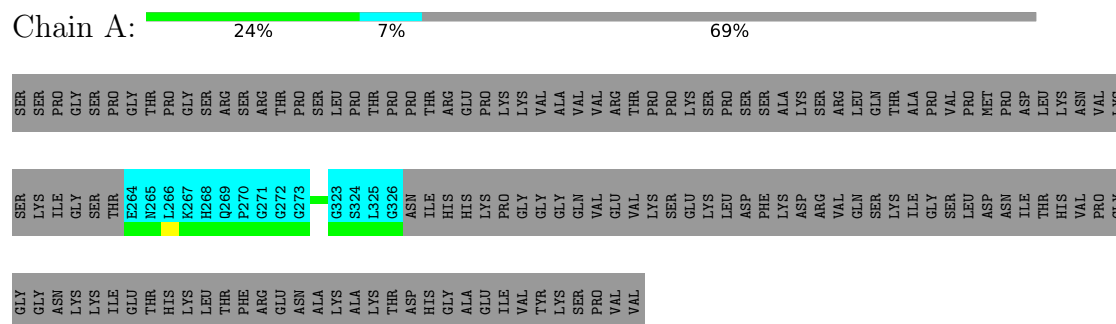
| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | B     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | C     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | D     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | E     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | F     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | G     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | H     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | I     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |
| 1   | J     | 63       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 953   | 287 | 491 | 85 | 88 | 2 |       |

## 4 Residue-property plots

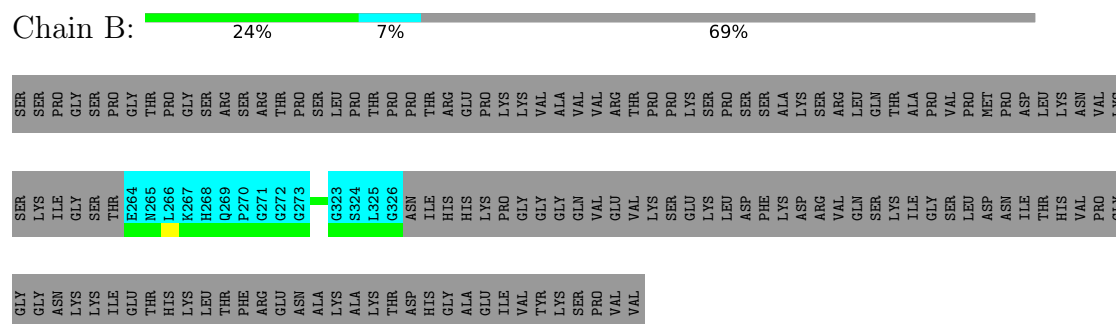
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

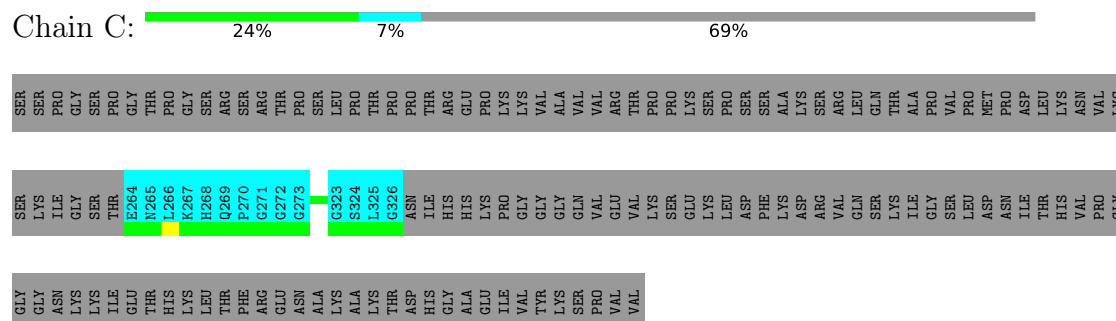
- Molecule 1: Microtubule-associated protein tau



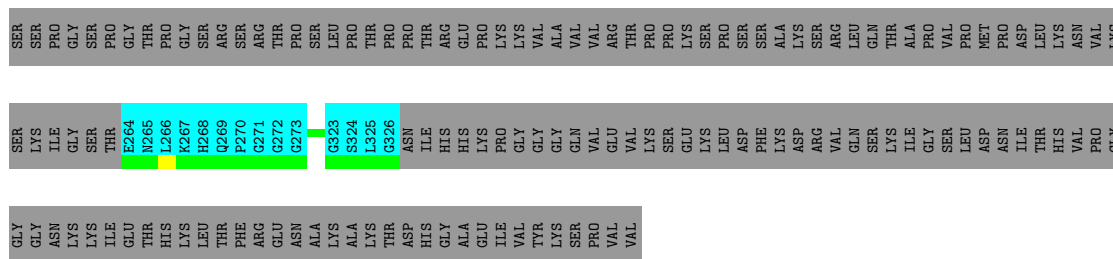
- Molecule 1: Microtubule-associated protein tau



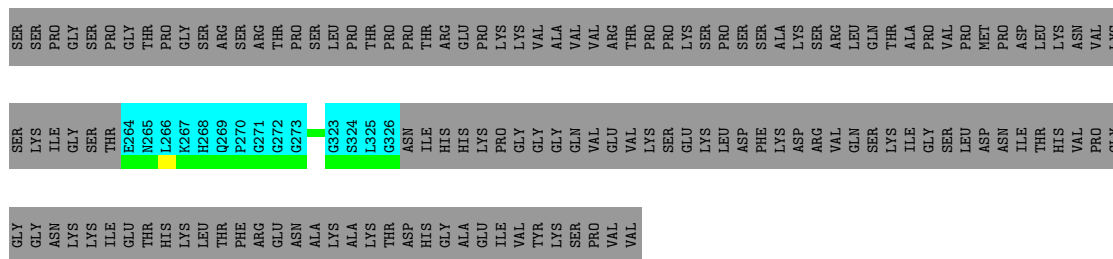
- Molecule 1: Microtubule-associated protein tau



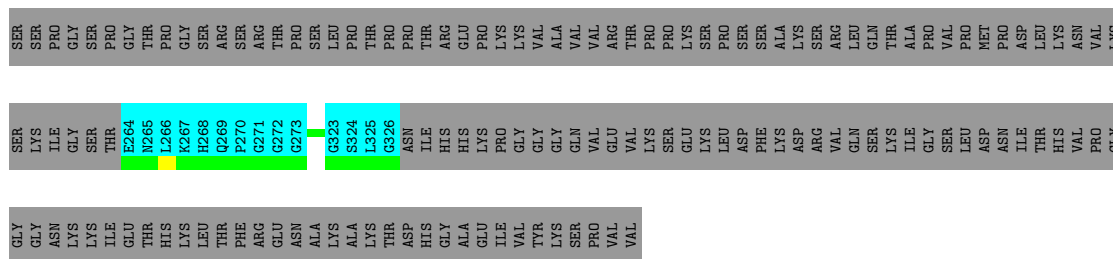
Chain D:  24% 7% 69%



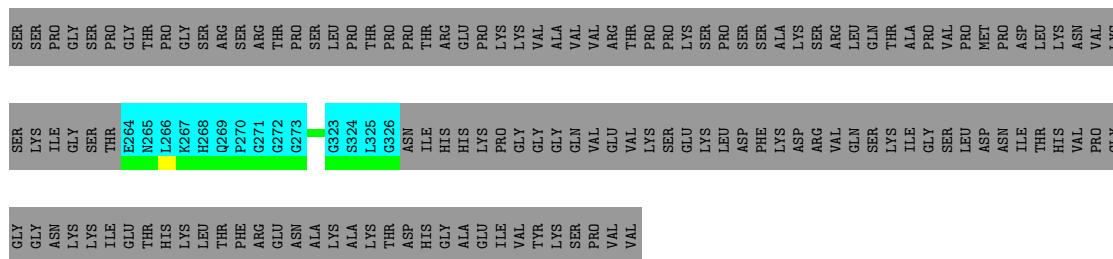
Chain E:  24% 7% 69%



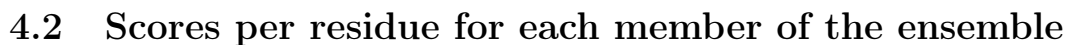
Chain F:  24% 7% 69%



Chain G:  24% 7% 69%



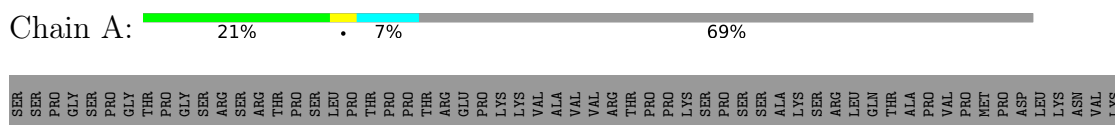
WORLD WIDE  
PDB  
PROTEIN DATA BANK



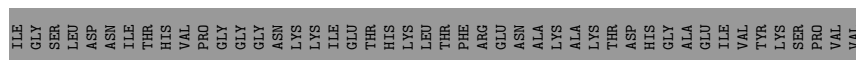
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

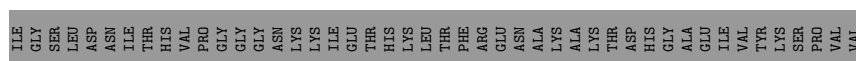
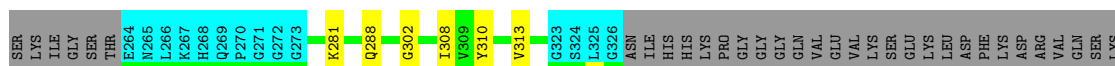
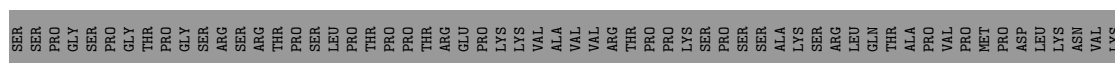
- Molecule 1: Microtubule-associated protein tau



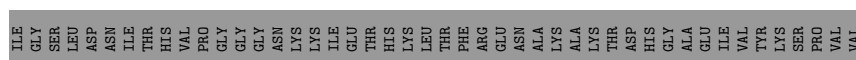
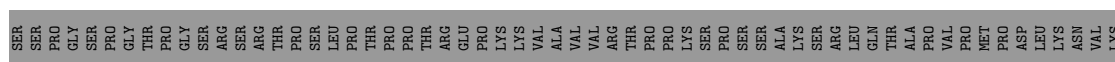




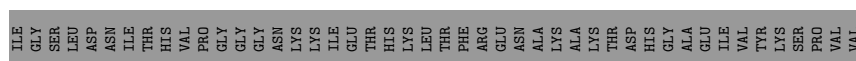
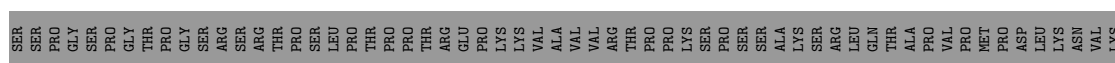
• Molecule 1: Microtubule-associated protein tau



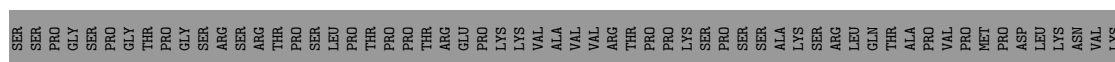
• Molecule 1: Microtubule-associated protein tau



• Molecule 1: Microtubule-associated protein tau



• Molecule 1: Microtubule-associated protein tau



|     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | LYS | ILE | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | ILE | HIS | PRO | GLY | ALA | LYS | LYS | GLN | VAL | GLU | VAL | LYS | SER | THR | GLN | ASP | PHE | LYS | ASP | ARG | VAL | GLN | ASN | VAL | LYS |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
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| ILE | GLY | SER | ILE | GLY | LEU | ASP | ASN | ILE | THR | HIS | VAL | GLY | PRO | ARG | GLY | GLY | ASN | LYS | LYS | ILE | GLU | THR | HIS | LYS | LEU | THR | PHE | ARG | GLU | ASN | ALA | LYS | LYS | ALA | VAL | VAL | VAL | ARG | THR | ASP | ILE | HIS | PRO | GLY | ALA | GLU | ILE | VAL | TYR | LYS | SER | GLN | VAL | PRO | VAL | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 1: Microtubule-associated protein tau

Chain F:  21% 7% 69%

|     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | SER | PRO | GLY | SER | PRO | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | THR | ILE | PRO | LYS | LYS | SER | PRO | GLY | VAL | TYR | LYS | SER | GLN | VAL | VAL | GLU | ARG | LEU | GLN | THR | THR | VAL | PRO | ASP | MET | PRO | PRO | ASP | LEU | LYS | ASN | VAL | SER | VAL | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | LYS | ILE | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | ILE | HIS | PRO | GLY | LYS | LYS | GLN | VAL | VAL | GLU | VAL | VAL | LYS | SER | THR | GLN | VAL | GLU | LYS | LEU | VAL | PRO | ASP | PHE | LYS | ASP | ARG | VAL | GLN | SER | VAL | LYS |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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| ILE | GLY | SER | ILE | GLY | LEU | ASP | ASN | ILE | THR | HIS | VAL | GLY | PRO | ARG | GLY | GLY | ASN | LYS | LYS | ILE | GLU | THR | HIS | LYS | LEU | THR | PHE | ARG | GLU | ASN | ALA | LYS | LYS | ALA | VAL | VAL | VAL | ARG | THR | ASP | ILE | HIS | PRO | GLY | ALA | GLU | ILE | VAL | TYR | LYS | SER | PRO | VAL | VAL | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 1: Microtubule-associated protein tau

Chain G:  21% 7% 69%

|     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | SER | PRO | GLY | SER | PRO | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | THR | ILE | PRO | LYS | LYS | SER | PRO | GLY | VAL | TYR | LYS | SER | GLN | VAL | VAL | GLU | ARG | LEU | GLN | THR | THR | VAL | PRO | ASP | MET | PRO | PRO | ASP | LEU | LYS | ASN | VAL | SER | VAL | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | LYS | ILE | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | ILE | HIS | PRO | GLY | LYS | LYS | GLN | VAL | VAL | GLU | VAL | VAL | LYS | SER | THR | GLN | VAL | GLU | LYS | LEU | VAL | PRO | ASP | PHE | LYS | ASP | ARG | VAL | GLN | SER | VAL | LYS |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ILE | GLY | SER | ILE | GLY | LEU | ASP | ASN | ILE | THR | HIS | VAL | GLY | PRO | ARG | GLY | GLY | ASN | LYS | LYS | ILE | GLU | THR | HIS | LYS | LEU | THR | PHE | ARG | GLU | ASN | ALA | LYS | LYS | ALA | VAL | VAL | VAL | ARG | THR | ASP | ILE | HIS | PRO | GLY | ALA | GLU | ILE | VAL | TYR | LYS | SER | PRO | VAL | VAL | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 1: Microtubule-associated protein tau

Chain H:  21% 7% 69%

|     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | SER | PRO | GLY | SER | PRO | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | THR | ILE | PRO | LYS | LYS | SER | PRO | GLY | VAL | TYR | LYS | SER | GLN | VAL | VAL | GLU | ARG | LEU | GLN | THR | THR | VAL | PRO | ASP | MET | PRO | PRO | ASP | LEU | LYS | ASN | VAL | SER | VAL | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

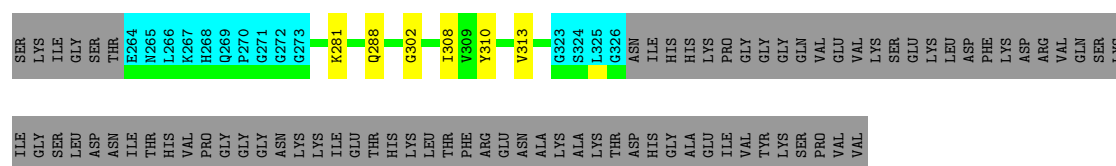
|     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | LYS | ILE | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | ILE | HIS | PRO | GLY | LYS | LYS | GLN | VAL | VAL | GLU | VAL | VAL | LYS | SER | THR | GLN | VAL | GLU | LYS | LEU | VAL | PRO | ASP | PHE | LYS | ASP | ARG | VAL | GLN | SER | VAL | LYS |
|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ILE | GLY | SER | ILE | GLY | LEU | ASP | ASN | ILE | THR | HIS | VAL | GLY | PRO | ARG | GLY | GLY | ASN | LYS | LYS | ILE | GLU | THR | HIS | LYS | LEU | THR | PHE | ARG | GLU | ASN | ALA | LYS | LYS | ALA | VAL | VAL | VAL | ARG | THR | ASP | ILE | HIS | PRO | GLY | ALA | GLU | ILE | VAL | TYR | LYS | SER | PRO | VAL | VAL | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

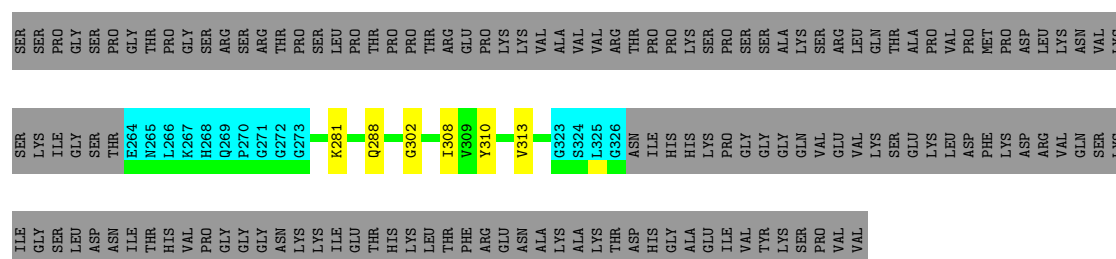
- Molecule 1: Microtubule-associated protein tau

Chain I:  21% 7% 69%

|     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | SER | PRO | GLY | SER | PRO | GLY | THR | E264 | N265 | L266 | K267 | H268 | Q269 | P270 | G271 | G272 | G273 | K281 | Q288 | G302 | I308 | V309 | Y310 | V313 | G323 | S324 | L325 | G326 | ASN | THR | ILE | PRO | LYS | LYS | SER | PRO | GLY | VAL | TYR | LYS | SER | GLN | VAL | VAL | GLU | ARG | LEU | GLN | THR | THR | VAL | PRO | ASP | MET | PRO | PRO | ASP | LEU | LYS | ASN | VAL | SER | VAL | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

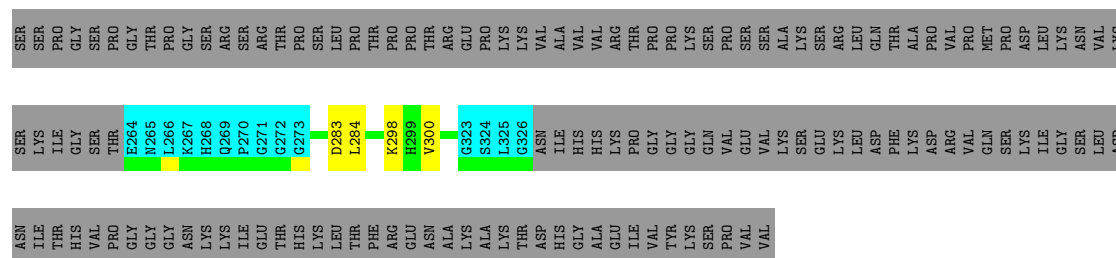


- Molecule 1: Microtubule-associated protein tau

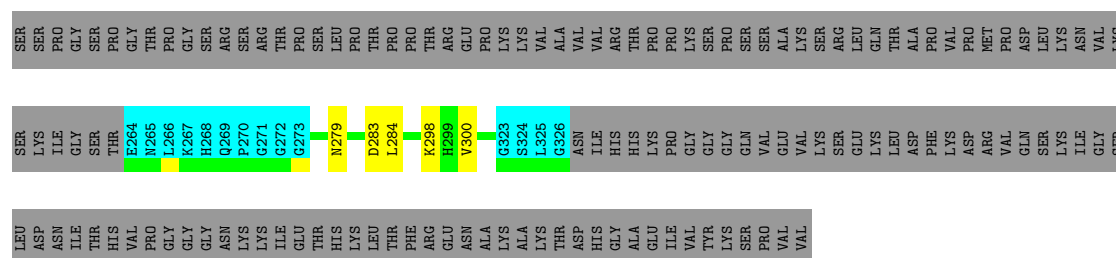


#### 4.2.2 Score per residue for model 2

- Molecule 1: Microtubule-associated protein tau

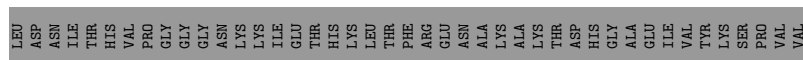


- Molecule 1: Microtubule-associated protein tau

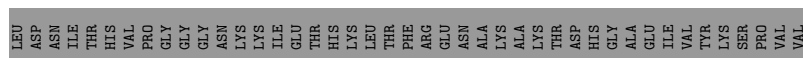


- Molecule 1: Microtubule-associated protein tau

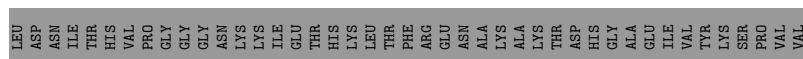




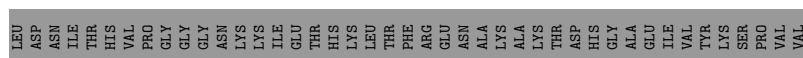
Chain D:  22% • 7% 69%



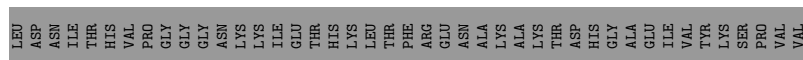
Chain E:  22% • 7% 69%



Chain F:  22% • 7% 69%



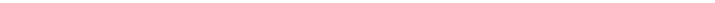
Chain G:  22% 7% 69%

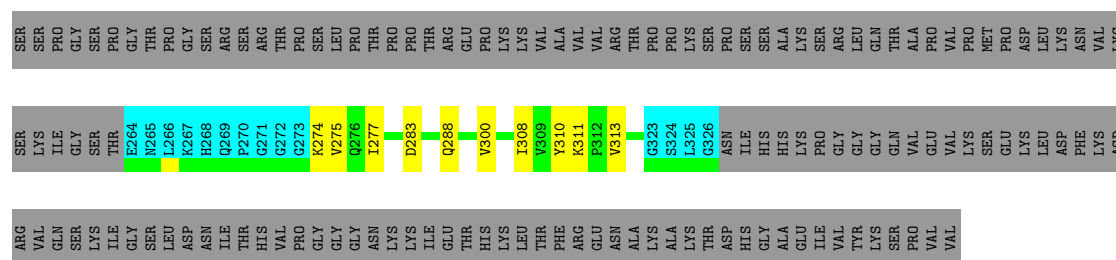


- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LEU | ASP | ASN | ASN | ILE | THR | HIS | VAL | PRO | GLY | GLY | ASN | LYS | LYS | ILE | GLU | THR | HIS | LYS | LEU | THR | PHE | ARG | GLU | ASN | ALA | LYS | ALA | LYS | THR | ASP | HIS | GLY | ALA | GLU | ILE | VAL | TYR | LYS | SER | PRO | VAL | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASN | ILE | THR | HIS | VAL | PRO | GLY | GLY | ASN | LYS | LYS | ILE | GLU | THR | HIS | LYS | LEU | THR | PHE | ARG | GLU | ASN | ALA | LYS | ALA | LYS | THR | ASP | HIS | GLY | ALA | GLU | ILE | VAL | TYR | LYS | SER | PRO | VAL | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

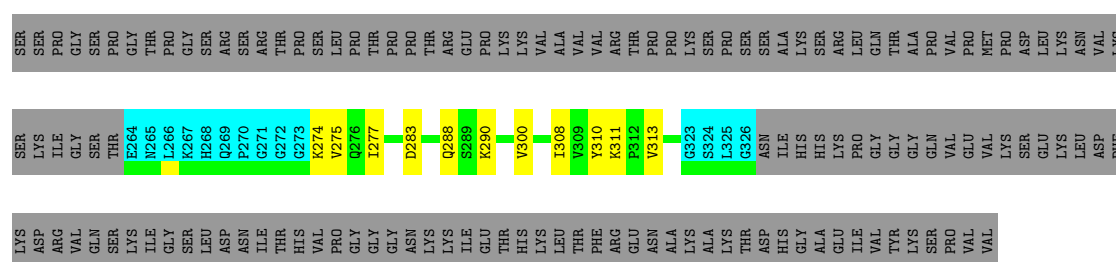
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASN | ILE | THR | HIS | VAL | PRO | GLY | GLY | ASN | LYS | LYS | ILE | GLU | THR | HIS | LYS | LEU | THR | PHE | ARG | GLU | ASN | ALA | LYS | ALA | LYS | THR | ASP | HIS | GLY | ALA | GLU | ILE | VAL | TYR | LYS | SER | PRO | VAL | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

Chain A:  19% 5% 7% 69%



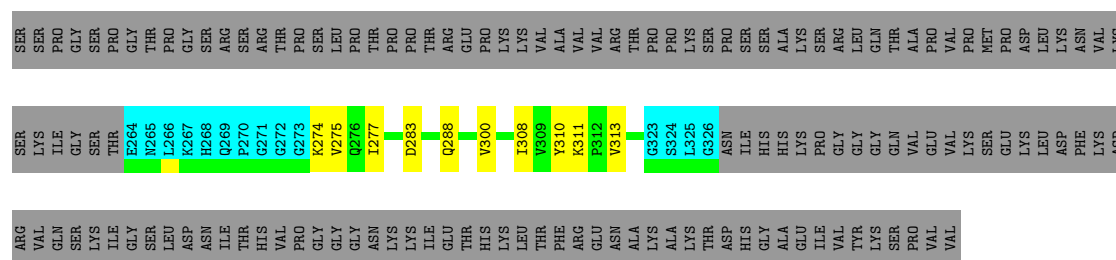
- Molecule 1: Microtubule-associated protein tau

Chain B:  19% 5% 7% 69%



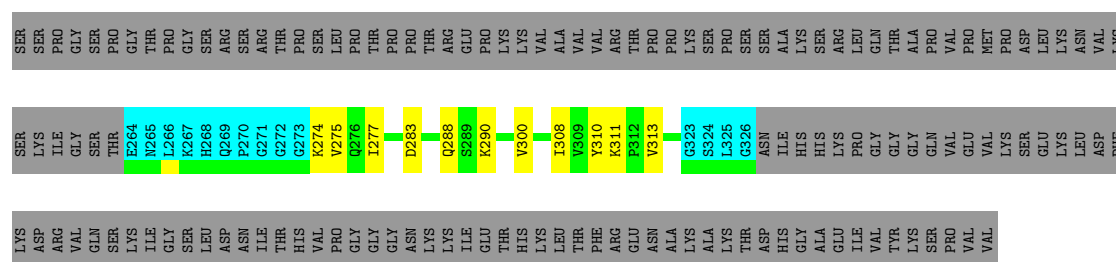
- Molecule 1: Microtubule-associated protein tau

Chain C:  19% 5% 7% 69%

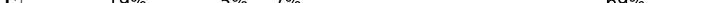


- Molecule 1: Microtubule-associated protein tau

Chain D:  19% 5% 7% 69%



- Molecule 1: Microtubule-associated protein tau

Chain E:  19% 5% 7% 69%

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### • Molecule 1: Microtubule-associated protein tau

Chain F:  19% 5% 7% 69%

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### • Molecule 1: Microtubule-associated protein tau

Chain G:  19% 5% 7% 69%

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### • Molecule 1: Microtubule-associated protein tau

Chain H:  18% 6% 7% 69%

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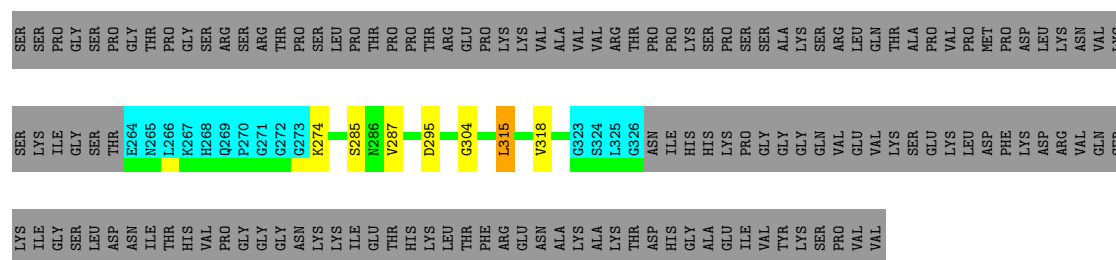
### • Molecule 1: Microtubule-associated protein tau

Chain I:  19% 5% 7% 69%



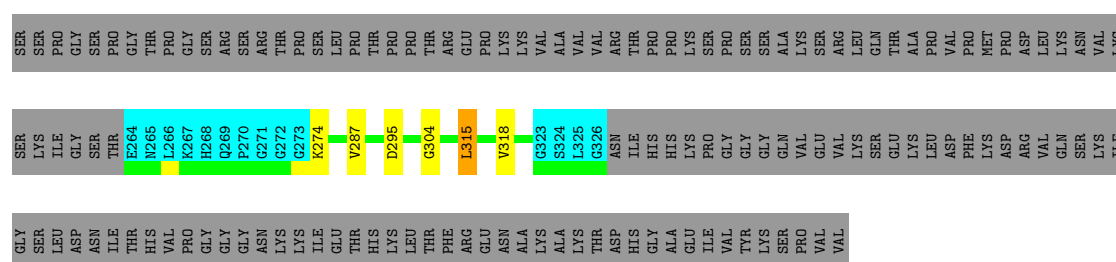


Chain C:  21% • 7% 72%

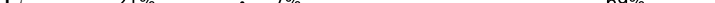


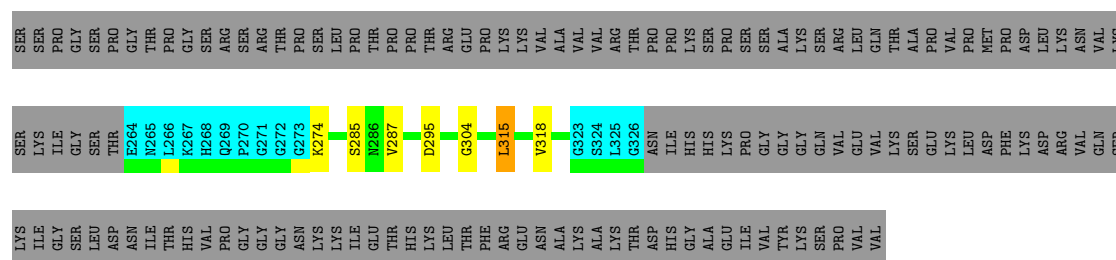
- Molecule 1: Microtubule-associated protein tau

Chain D:  21% • 7% 69%

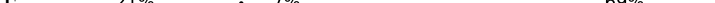


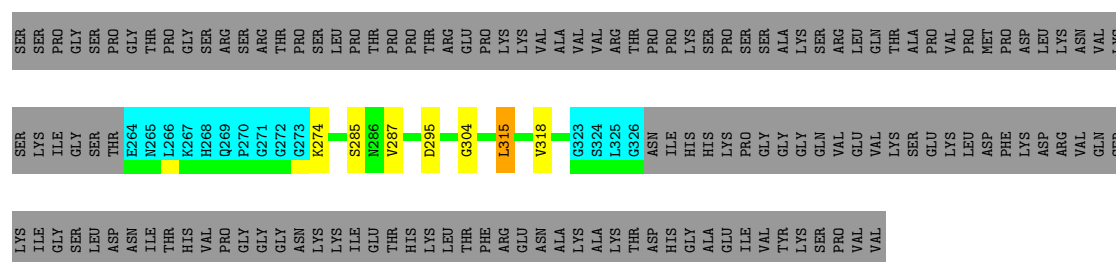
- Molecule 1: Microtubule-associated protein tau

Chain E:  21% • 7% 72%

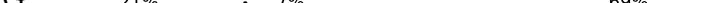


- Molecule 1: Microtubule-associated protein tau

Chain F:  21% 7% 69%



- Molecule 1: Microtubule-associated protein tau

Chain G:  21% • 7% 69%

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THR THR  
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### • Molecule 1: Microtubule-associated protein tau

Chain H:  21% 7% 69%

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### • Molecule 1: Microtubule-associated protein tau

Chain I:  21% 7% 69%

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### • Molecule 1: Microtubule-associated protein tau

Chain J:  21% 7% 69%

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THR THR  
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SER SER  
LEU LEU  
PRO PRO  
THR THR  
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THR THR  
ARG ARG  
GLU GLU  
PRO PRO  
LYS LYS  
VAL VAL  
ALA ALA  
VAL VAL  
VAL VAL  
ARG ARG  
THR THR  
PRO PRO  
PRO PRO  
LYS LYS  
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PRO PRO  
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GLY GLY  
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LYS LYS  
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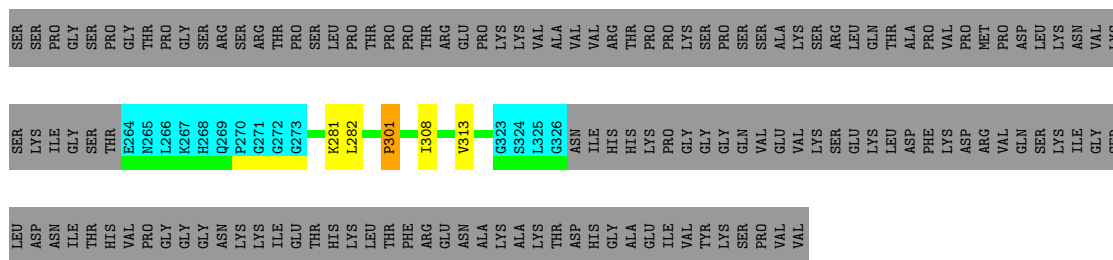
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## 4.2.5 Score per residue for model 5

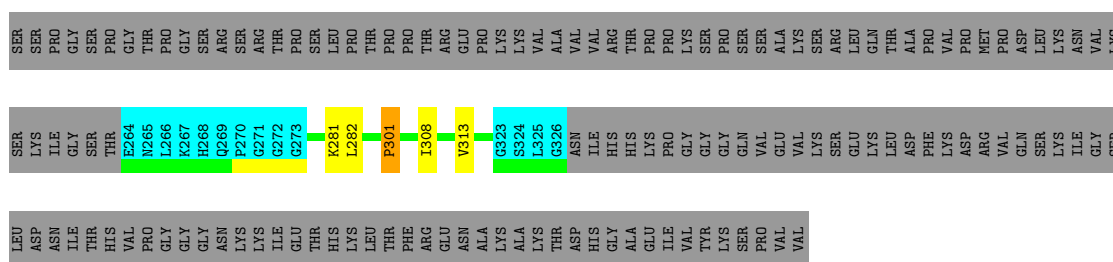
### • Molecule 1: Microtubule-associated protein tau

Chain A:  22% • 7% 69%



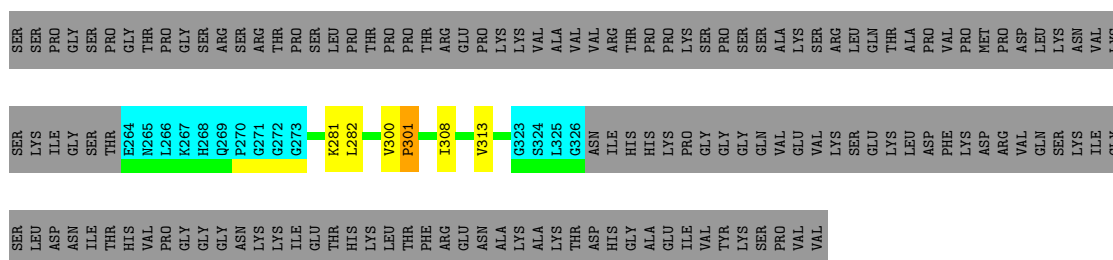
- Molecule 1: Microtubule-associated protein tau

Chain B:  22% • 7% 69%



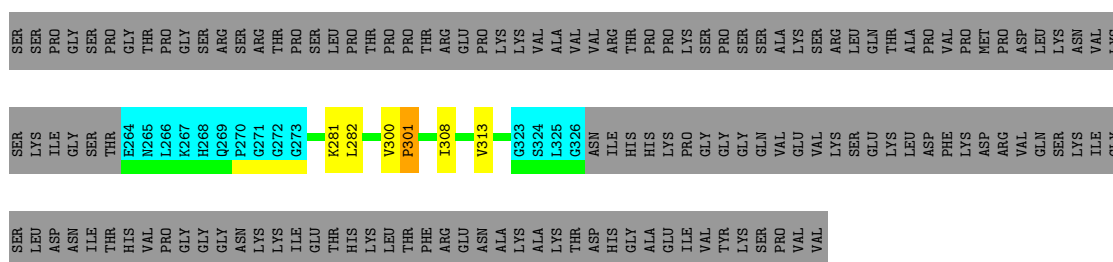
- Molecule 1: Microtubule-associated protein tau

Chain C:  21% • 7% 69%

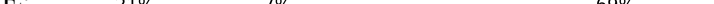


- Molecule 1: Microtubule-associated protein tau

Chain D:  21% • 7% 69%



- Molecule 1: Microtubule-associated protein tau

Chain E:  21% • 7% 69%

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ARG ARG  
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SER SER  
LEU LEU  
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### • Molecule 1: Microtubule-associated protein tau

Chain F: 21% 7% 69%

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### • Molecule 1: Microtubule-associated protein tau

Chain G: 21% 7% 69%

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### • Molecule 1: Microtubule-associated protein tau

Chain H: 21% 7% 69%

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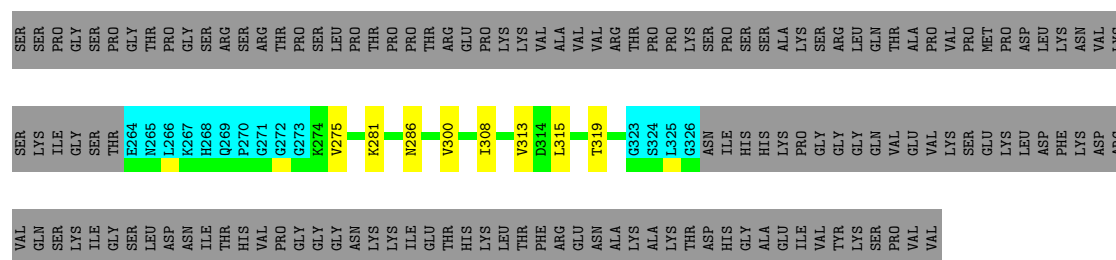
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### • Molecule 1: Microtubule-associated protein tau

Chain I: 21% 7% 69%

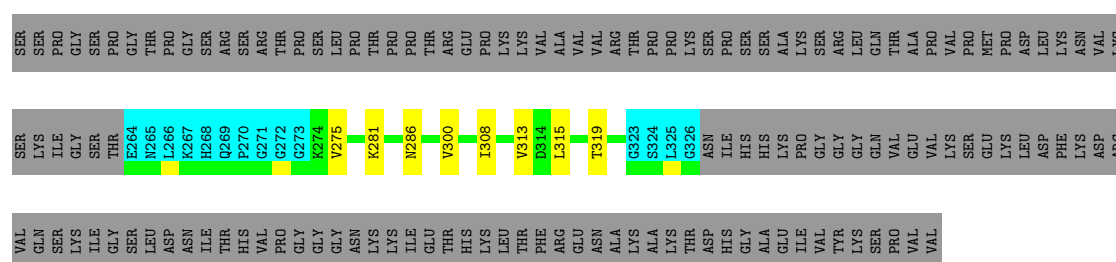


Chain C:  20% 7% 69%

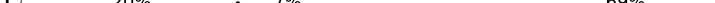


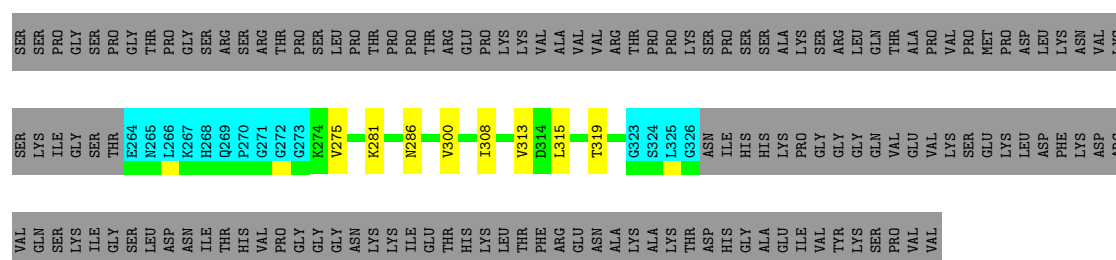
- Molecule 1: Microtubule-associated protein tau

Chain D:  20% 7% 69%

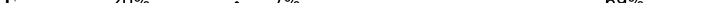


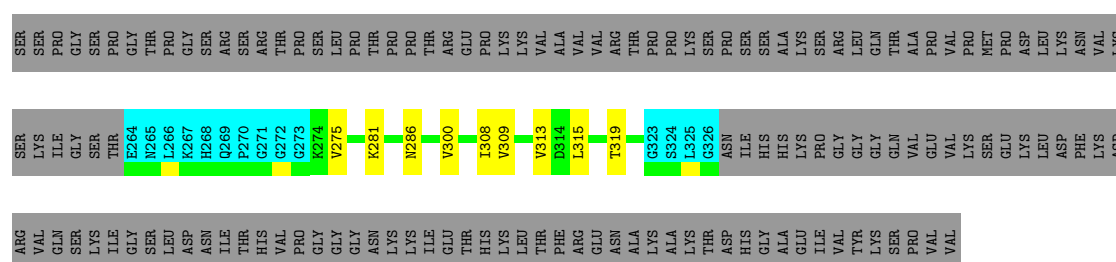
- Molecule 1: Microtubule-associated protein tau

Chain E:  20% 7% 69%

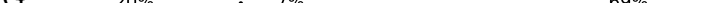


- Molecule 1: Microtubule-associated protein tau

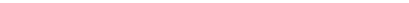
Chain F:  20% 7% 69%



- Molecule 1: Microtubule-associated protein tau

Chain G:  20% 7% 69%



Chain A:  22% • 7% 69%

[illegible]

- Molecule 1: Microtubule-associated protein tau

Chain B:  22% • 7% 69%

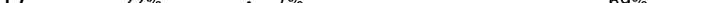
[illegible]

- Molecule 1: Microtubule-associated protein tau

Chain C:  22% • 7% 69%

[illegible]

- Molecule 1: Microtubule-associated protein tau

Chain D:  22% • 7% 69%

[illegible]

- Molecule 1: Microtubule-associated protein tau

Chain E:  22% • 7% 69%



SER SER  
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SER SER  
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PRO GLY  
SER SER  
ARG ARG  
SER ARG  
THR THR  
PRO PRO  
SER SER  
LEU LEU  
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THR THR  
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## • Molecule 1: Microtubule-associated protein tau

Chain F:  21% 7% 69%

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## • Molecule 1: Microtubule-associated protein tau

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## • Molecule 1: Microtubule-associated protein tau

Chain H:  21% 7% 69%

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## • Molecule 1: Microtubule-associated protein tau

Chain I:  22% 7% 69%

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- Molecule 1: Microtubule-associated protein tau

Chain J: 21% 7% 69%

SER SER  
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#### 4.2.8 Score per residue for model 8

- Molecule 1: Microtubule-associated protein tau

Chain A: 21% 7% 69%

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- Molecule 1: Microtubule-associated protein tau

Chain B: 21% 7% 69%

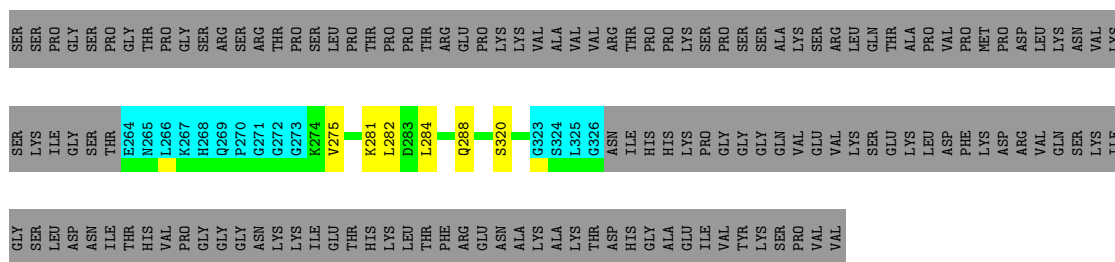
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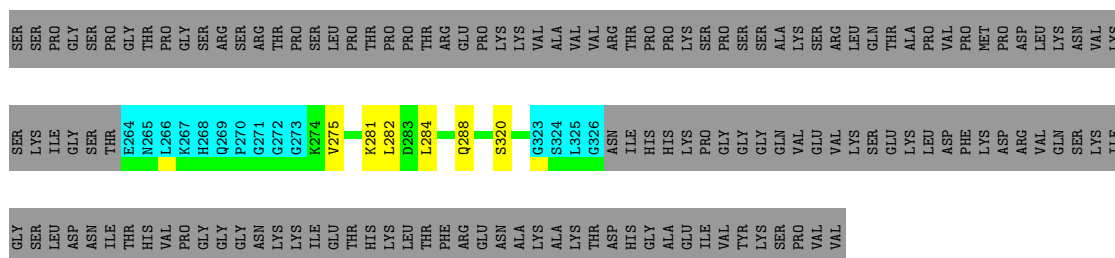
- Molecule 1: Microtubule-associated protein tau





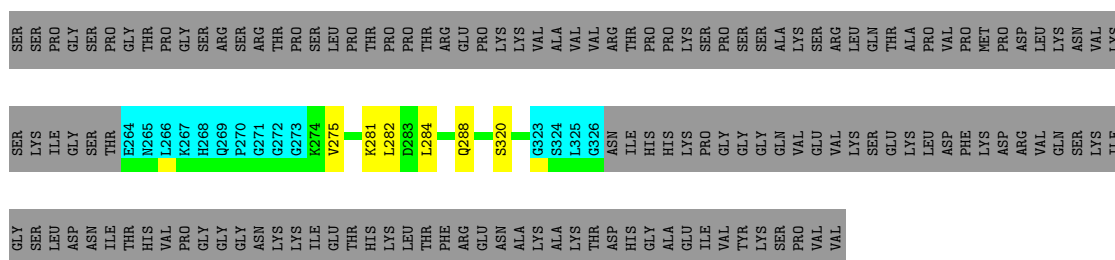
- Molecule 1: Microtubule-associated protein tau

Chain H: 21% 7% 69%



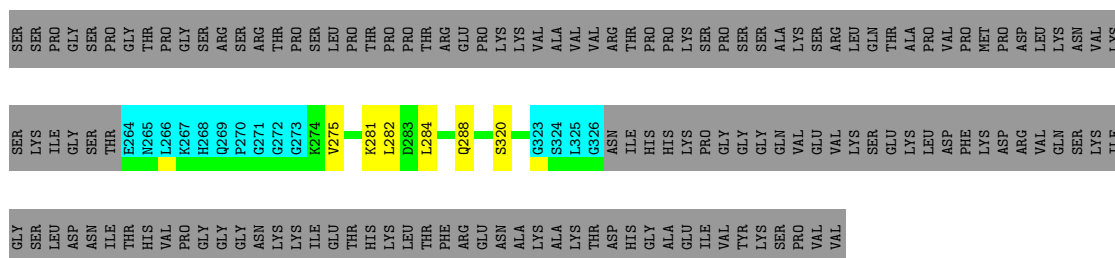
- Molecule 1: Microtubule-associated protein tau

Chain I: 21% 7% 69%



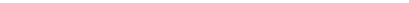
- Molecule 1: Microtubule-associated protein tau

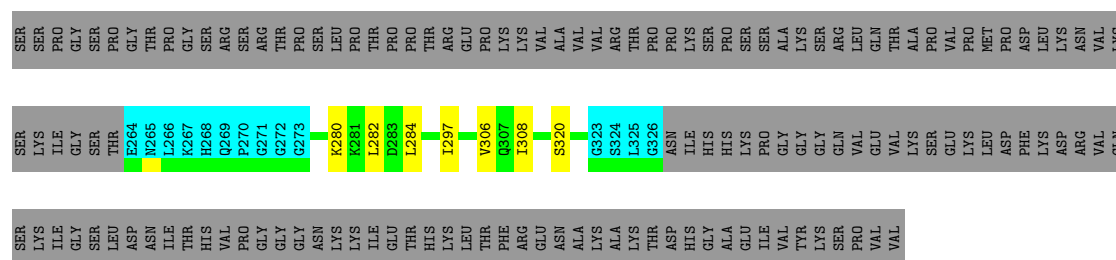
Chain J: 21% 7% 69%



## 4.2.9 Score per residue for model 9

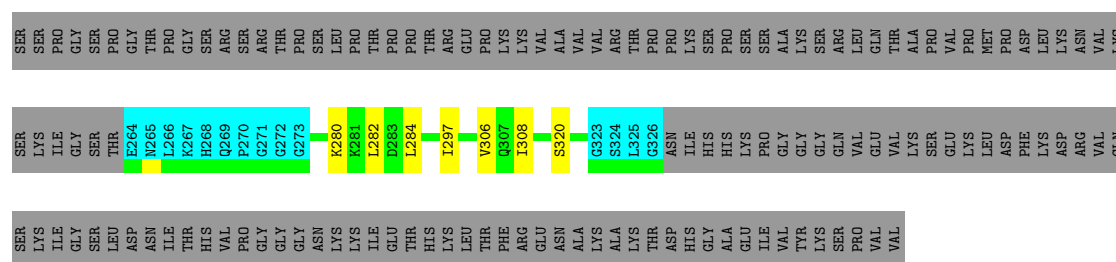
- Molecule 1: Microtubule-associated protein tau

Chain A:  21% • 7% 69%

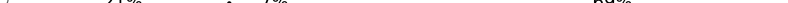


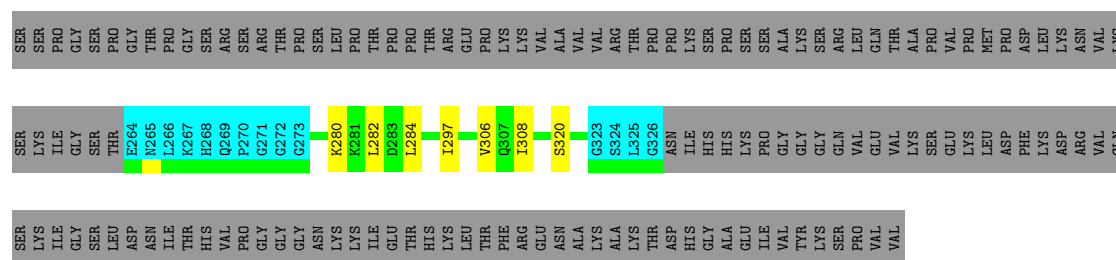
- Molecule 1: Microtubule-associated protein tau

Chain B:  21% • 7% 72%

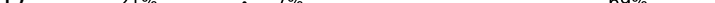


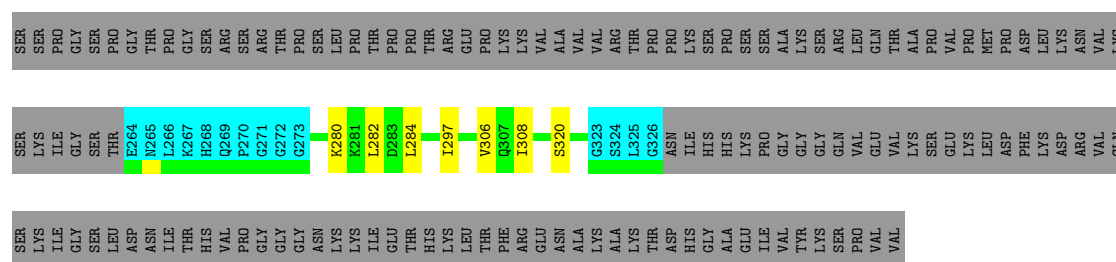
- Molecule 1: Microtubule-associated protein tau

Chain C:  21% 7% 72%

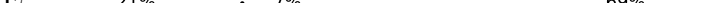


- Molecule 1: Microtubule-associated protein tau

Chain D:  21% 7% 69%



- Molecule 1: Microtubule-associated protein tau

Chain E:  21% • 7% 72%

SER SER  
PRO PRO  
GLY GLY  
SER SER  
PRO PRO  
GLY GLY  
THR THR

SER  
LYS  
ILE  
GLY  
SER  
THR  
E264  
N285  
L286  
K267  
H268  
Q269  
P270  
G271  
G272  
G273  
K280  
K281  
L282  
D283  
L284  
L297  
V306  
Q307  
L308  
S320  
G323  
S324  
L325  
G326  
ASN  
ILE  
HIS  
HIS  
HIS  
PRO  
ILE  
GLY  
GLY  
GLN  
VAL  
VAL  
LYS  
SER  
GLU  
VAL  
PRO  
MET  
LEU  
PRO  
ASP  
PHE  
LYS  
ASP  
ARG  
VAL  
GLN  
LYS

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

### • Molecule 1: Microtubule-associated protein tau

Chain F: 21% 7% 69%

SER SER  
PRO PRO  
GLY GLY  
SER SER  
PRO PRO  
GLY GLY  
THR THR

SER  
LYS  
ILE  
GLY  
SER  
THR  
E264  
N285  
L286  
K267  
H268  
Q269  
P270  
G271  
G272  
G273  
K280  
K281  
L282  
D283  
L284  
L297  
V306  
Q307  
L308  
S320  
G323  
S324  
L325  
G326  
ASN  
ILE  
HIS  
HIS  
HIS  
PRO  
ILE  
GLY  
GLY  
GLN  
VAL  
VAL  
LYS  
SER  
GLU  
VAL  
PRO  
MET  
LEU  
PRO  
ASP  
PHE  
LYS  
ASP  
ARG  
VAL  
GLN  
LYS

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

### • Molecule 1: Microtubule-associated protein tau

Chain G: 21% 7% 69%

SER SER  
PRO PRO  
GLY GLY  
SER SER  
PRO PRO  
GLY GLY  
THR THR

SER  
LYS  
ILE  
GLY  
SER  
THR  
E264  
N285  
L286  
K267  
H268  
Q269  
P270  
G271  
G272  
G273  
K280  
K281  
L282  
D283  
L284  
L297  
V306  
Q307  
L308  
S320  
G323  
S324  
L325  
G326  
ASN  
ILE  
HIS  
HIS  
HIS  
PRO  
ILE  
GLY  
GLY  
GLN  
VAL  
VAL  
LYS  
SER  
GLU  
VAL  
PRO  
MET  
LEU  
PRO  
ASP  
PHE  
LYS  
ASP  
ARG  
VAL  
GLN  
LYS

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

### • Molecule 1: Microtubule-associated protein tau

Chain H: 21% 7% 69%

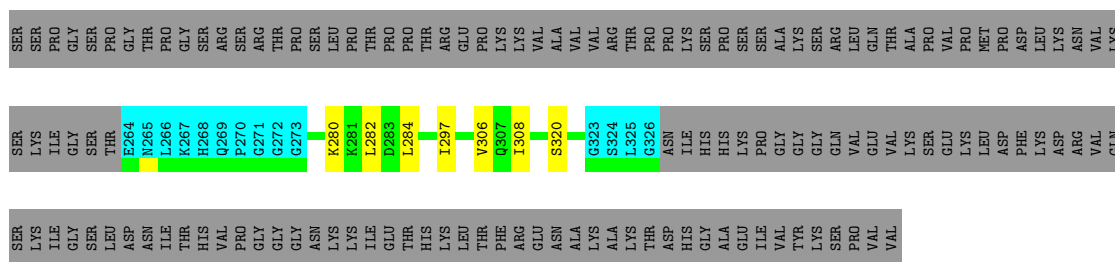
SER SER  
PRO PRO  
GLY GLY  
SER SER  
PRO PRO  
GLY GLY  
THR THR

SER  
LYS  
ILE  
GLY  
SER  
THR  
E264  
N285  
L286  
K267  
H268  
Q269  
P270  
G271  
G272  
G273  
K280  
K281  
L282  
D283  
L284  
L297  
V306  
Q307  
L308  
S320  
G323  
S324  
L325  
G326  
ASN  
ILE  
HIS  
HIS  
HIS  
PRO  
ILE  
GLY  
GLY  
GLN  
VAL  
VAL  
LYS  
SER  
GLU  
VAL  
PRO  
MET  
LEU  
PRO  
ASP  
PHE  
LYS  
ASP  
ARG  
VAL  
GLN  
LYS

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

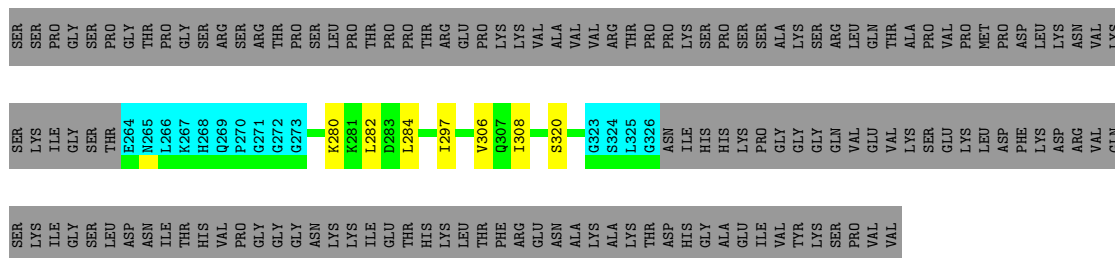
### • Molecule 1: Microtubule-associated protein tau

Chain I: 21% 7% 69%



- Molecule 1: Microtubule-associated protein tau

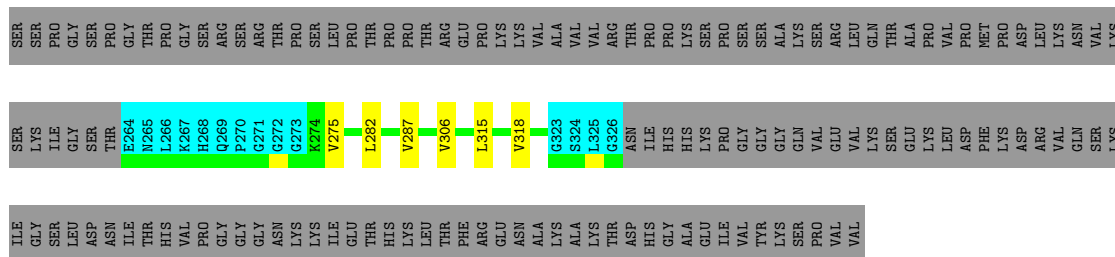
Chain J: 21% 7% 69%



#### 4.2.10 Score per residue for model 10

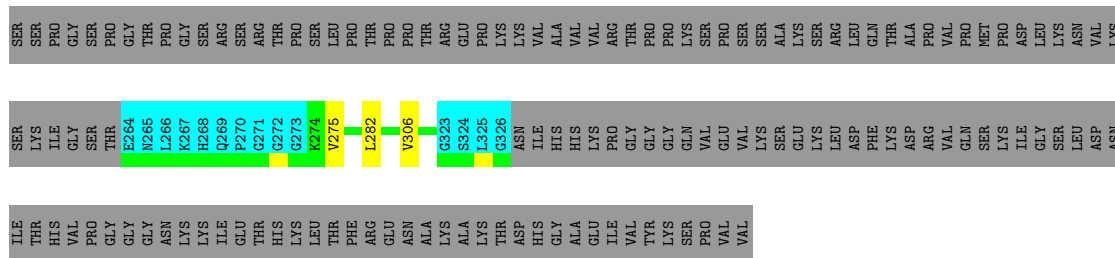
- Molecule 1: Microtubule-associated protein tau

Chain A: 21% 7% 69%

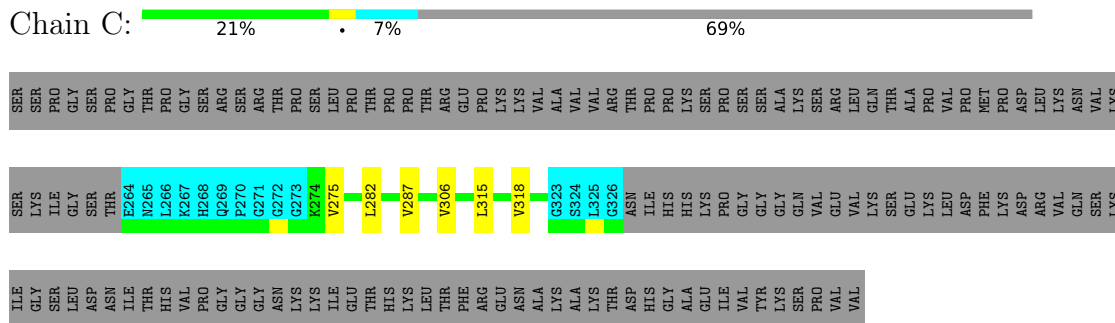


- Molecule 1: Microtubule-associated protein tau

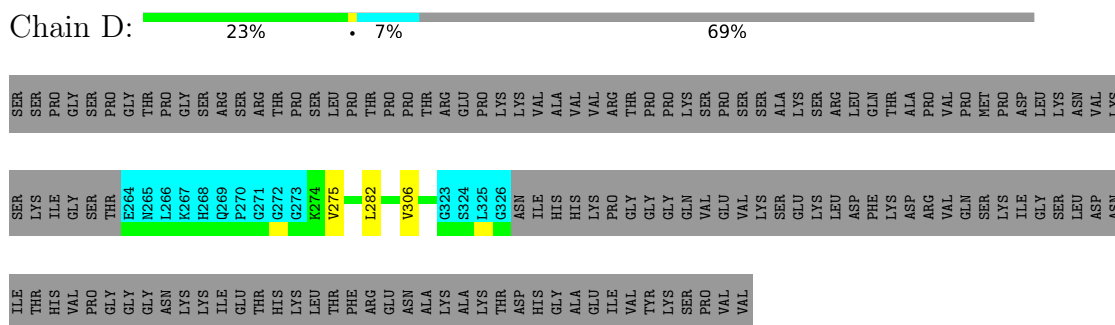
Chain B: 23% 7% 69%



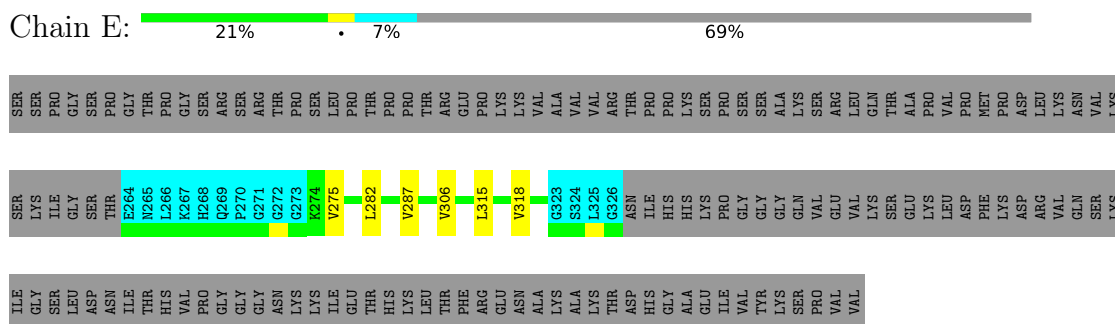
- Molecule 1: Microtubule-associated protein tau



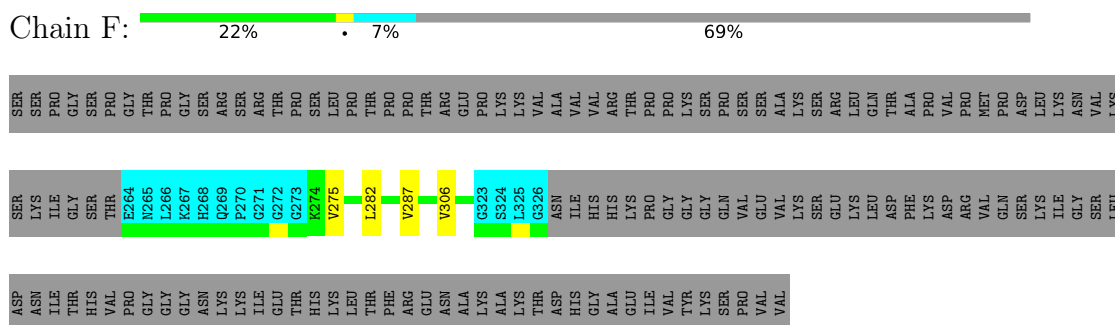
- Molecule 1: Microtubule-associated protein tau



- Molecule 1: Microtubule-associated protein tau



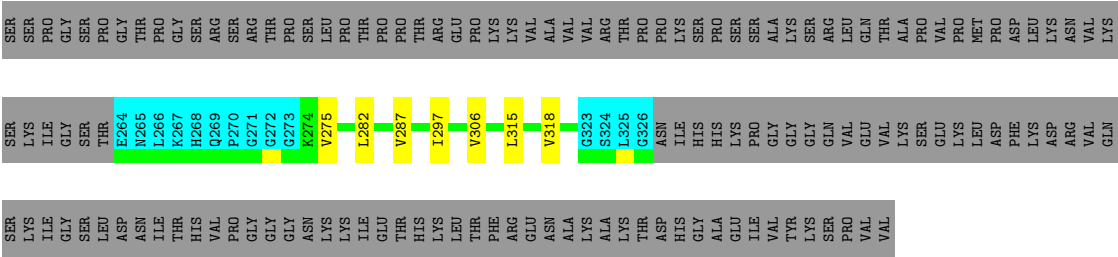
- Molecule 1: Microtubule-associated protein tau



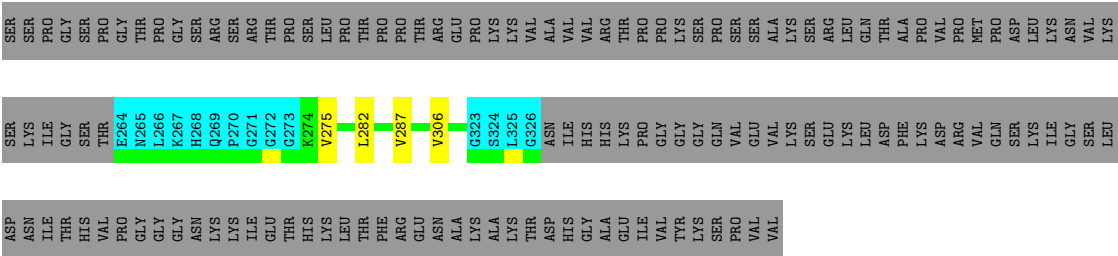
- Molecule 1: Microtubule-associated protein tau



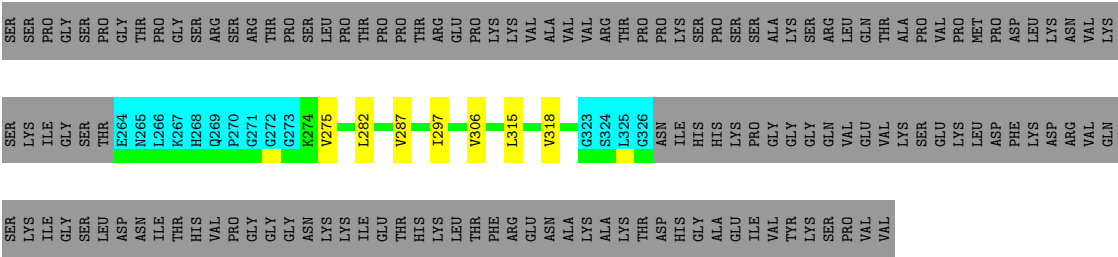




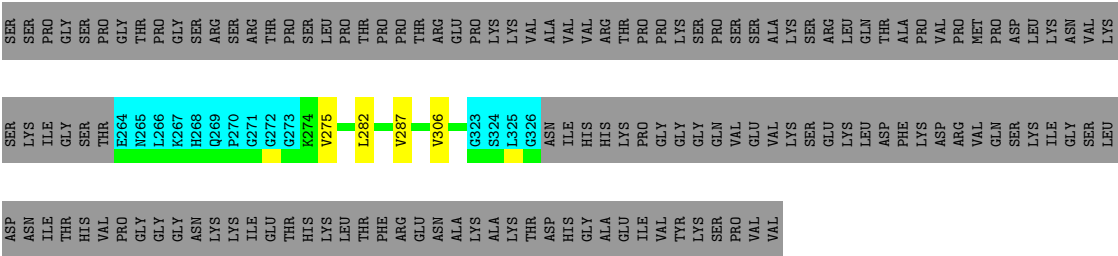
• Molecule 1: Microtubule-associated protein tau



• Molecule 1: Microtubule-associated protein tau



• Molecule 1: Microtubule-associated protein tau



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH    | refinement            |         |
| X-PLOR NIH    | structure calculation |         |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 329            |
| Number of shifts mapped to atoms             | 227            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 102            |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 3%             |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 6 Model quality

### 6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 368   | 401      | 400      | 4±1     |
| 1   | B     | 368   | 401      | 400      | 5±2     |
| 1   | C     | 368   | 401      | 400      | 7±2     |
| 1   | D     | 368   | 401      | 400      | 7±3     |
| 1   | E     | 368   | 401      | 400      | 7±2     |
| 1   | F     | 368   | 401      | 400      | 7±2     |
| 1   | G     | 368   | 401      | 400      | 7±3     |
| 1   | H     | 368   | 401      | 400      | 7±3     |
| 1   | I     | 368   | 401      | 400      | 4±2     |
| 1   | J     | 368   | 401      | 400      | 5±2     |
| All | All   | 36800 | 40100    | 40000    | 414     |

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 5.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:G:300:VAL:HG12 | 1:I:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |
| 1:A:300:VAL:HG12 | 1:C:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |
| 1:H:300:VAL:HG12 | 1:J:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |
| 1:E:300:VAL:HG12 | 1:G:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |
| 1:B:300:VAL:HG12 | 1:D:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:300:VAL:HG12 | 1:E:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |
| 1:D:300:VAL:HG12 | 1:F:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |
| 1:F:300:VAL:HG12 | 1:H:300:VAL:HG22 | 0.76     | 1.58        | 6      | 4     |
| 1:A:313:VAL:HG23 | 1:C:313:VAL:HG13 | 0.71     | 1.62        | 1      | 3     |
| 1:C:313:VAL:HG23 | 1:E:313:VAL:HG13 | 0.71     | 1.62        | 1      | 3     |
| 1:E:313:VAL:HG23 | 1:G:313:VAL:HG13 | 0.71     | 1.63        | 1      | 3     |
| 1:G:313:VAL:HG23 | 1:I:313:VAL:HG13 | 0.71     | 1.63        | 1      | 3     |
| 1:B:313:VAL:HG23 | 1:D:313:VAL:HG13 | 0.71     | 1.62        | 1      | 3     |
| 1:D:313:VAL:HG23 | 1:F:313:VAL:HG13 | 0.71     | 1.62        | 1      | 3     |
| 1:H:313:VAL:HG23 | 1:J:313:VAL:HG13 | 0.71     | 1.62        | 1      | 3     |
| 1:F:313:VAL:HG23 | 1:H:313:VAL:HG13 | 0.71     | 1.63        | 1      | 3     |
| 1:A:275:VAL:HG23 | 1:C:275:VAL:HG13 | 0.61     | 1.71        | 3      | 2     |
| 1:B:275:VAL:HG23 | 1:D:275:VAL:HG13 | 0.61     | 1.71        | 3      | 2     |
| 1:D:275:VAL:HG23 | 1:F:275:VAL:HG13 | 0.61     | 1.71        | 3      | 2     |
| 1:C:275:VAL:HG23 | 1:E:275:VAL:HG13 | 0.61     | 1.71        | 3      | 2     |
| 1:F:275:VAL:HG23 | 1:H:275:VAL:HG13 | 0.61     | 1.71        | 3      | 2     |
| 1:H:275:VAL:HG23 | 1:J:275:VAL:HG13 | 0.60     | 1.72        | 3      | 2     |
| 1:E:275:VAL:HG23 | 1:G:275:VAL:HG13 | 0.60     | 1.71        | 3      | 2     |
| 1:G:275:VAL:HG23 | 1:I:275:VAL:HG13 | 0.60     | 1.72        | 3      | 2     |
| 1:G:308:ILE:O    | 1:G:308:ILE:HD12 | 0.55     | 2.02        | 1      | 1     |
| 1:I:308:ILE:HD12 | 1:I:308:ILE:O    | 0.55     | 2.02        | 1      | 1     |
| 1:E:308:ILE:HD12 | 1:E:308:ILE:O    | 0.55     | 2.02        | 1      | 1     |
| 1:C:308:ILE:O    | 1:C:308:ILE:HD12 | 0.55     | 2.02        | 1      | 1     |
| 1:A:308:ILE:HD12 | 1:A:308:ILE:O    | 0.55     | 2.02        | 1      | 1     |
| 1:J:308:ILE:HD12 | 1:J:308:ILE:O    | 0.54     | 2.02        | 1      | 1     |
| 1:D:308:ILE:HD12 | 1:D:308:ILE:O    | 0.54     | 2.02        | 1      | 1     |
| 1:H:308:ILE:HD12 | 1:H:308:ILE:O    | 0.54     | 2.02        | 1      | 1     |
| 1:F:308:ILE:HD12 | 1:F:308:ILE:O    | 0.54     | 2.02        | 1      | 1     |
| 1:B:308:ILE:HD12 | 1:B:308:ILE:O    | 0.54     | 2.02        | 1      | 1     |
| 1:H:306:VAL:HG23 | 1:J:306:VAL:HG13 | 0.50     | 1.83        | 9      | 1     |
| 1:J:300:VAL:O    | 1:J:300:VAL:HG23 | 0.50     | 2.06        | 2      | 4     |
| 1:B:300:VAL:O    | 1:B:300:VAL:HG23 | 0.50     | 2.06        | 2      | 4     |
| 1:F:300:VAL:O    | 1:F:300:VAL:HG23 | 0.50     | 2.06        | 2      | 4     |
| 1:I:300:VAL:HG23 | 1:I:300:VAL:O    | 0.50     | 2.06        | 2      | 4     |
| 1:D:300:VAL:HG23 | 1:D:300:VAL:O    | 0.50     | 2.06        | 2      | 4     |
| 1:H:300:VAL:HG23 | 1:H:300:VAL:O    | 0.50     | 2.06        | 2      | 4     |
| 1:G:300:VAL:O    | 1:G:300:VAL:HG23 | 0.50     | 2.06        | 2      | 4     |
| 1:E:300:VAL:HG23 | 1:E:300:VAL:O    | 0.50     | 2.06        | 2      | 4     |
| 1:C:300:VAL:O    | 1:C:300:VAL:HG23 | 0.49     | 2.06        | 2      | 4     |
| 1:F:306:VAL:HG23 | 1:H:306:VAL:HG13 | 0.49     | 1.84        | 9      | 1     |
| 1:A:300:VAL:HG23 | 1:A:300:VAL:O    | 0.49     | 2.06        | 2      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:301:PRO:HD3  | 1:C:300:VAL:HG12 | 0.49     | 1.84        | 5      | 1     |
| 1:B:301:PRO:HD3  | 1:D:300:VAL:HG12 | 0.49     | 1.84        | 5      | 1     |
| 1:H:301:PRO:HD3  | 1:J:300:VAL:HG12 | 0.49     | 1.85        | 5      | 1     |
| 1:C:301:PRO:HD3  | 1:E:300:VAL:HG12 | 0.49     | 1.85        | 5      | 1     |
| 1:G:301:PRO:HD3  | 1:I:300:VAL:HG12 | 0.49     | 1.85        | 5      | 1     |
| 1:D:306:VAL:HG23 | 1:F:306:VAL:HG13 | 0.49     | 1.85        | 9      | 1     |
| 1:D:301:PRO:HD3  | 1:F:300:VAL:HG12 | 0.48     | 1.85        | 5      | 1     |
| 1:F:301:PRO:HD3  | 1:H:300:VAL:HG12 | 0.48     | 1.85        | 5      | 1     |
| 1:E:301:PRO:HD3  | 1:G:300:VAL:HG12 | 0.48     | 1.85        | 5      | 1     |
| 1:A:284:LEU:HD21 | 1:B:279:ASN:ND2  | 0.48     | 2.24        | 2      | 1     |
| 1:B:275:VAL:HG13 | 1:D:275:VAL:HG23 | 0.48     | 1.85        | 7      | 1     |
| 1:B:306:VAL:HG23 | 1:D:306:VAL:HG13 | 0.48     | 1.85        | 9      | 1     |
| 1:G:306:VAL:HG23 | 1:I:306:VAL:HG13 | 0.48     | 1.84        | 9      | 1     |
| 1:B:315:LEU:HD11 | 1:B:318:VAL:HG13 | 0.48     | 1.85        | 4      | 1     |
| 1:D:315:LEU:HD11 | 1:D:318:VAL:HG13 | 0.48     | 1.85        | 4      | 1     |
| 1:A:275:VAL:HG13 | 1:C:275:VAL:HG23 | 0.48     | 1.85        | 7      | 1     |
| 1:D:275:VAL:HG13 | 1:F:275:VAL:HG23 | 0.48     | 1.86        | 7      | 1     |
| 1:F:315:LEU:HD11 | 1:F:318:VAL:HG13 | 0.48     | 1.85        | 4      | 1     |
| 1:C:275:VAL:HG13 | 1:E:275:VAL:HG23 | 0.47     | 1.85        | 7      | 1     |
| 1:E:306:VAL:HG23 | 1:G:306:VAL:HG13 | 0.47     | 1.85        | 9      | 1     |
| 1:H:315:LEU:HD11 | 1:H:318:VAL:HG13 | 0.47     | 1.85        | 4      | 1     |
| 1:B:284:LEU:HD21 | 1:C:279:ASN:ND2  | 0.47     | 2.24        | 2      | 1     |
| 1:E:275:VAL:HG13 | 1:G:275:VAL:HG23 | 0.47     | 1.86        | 7      | 1     |
| 1:C:284:LEU:HD21 | 1:D:279:ASN:ND2  | 0.47     | 2.25        | 2      | 1     |
| 1:H:308:ILE:N    | 1:H:308:ILE:HD12 | 0.47     | 2.25        | 9      | 2     |
| 1:J:308:ILE:HD13 | 1:J:310:TYR:HE1  | 0.47     | 1.69        | 1      | 1     |
| 1:B:287:VAL:HG22 | 1:D:287:VAL:HG12 | 0.47     | 1.86        | 4      | 1     |
| 1:C:315:LEU:HD11 | 1:C:318:VAL:HG13 | 0.47     | 1.85        | 4      | 1     |
| 1:E:315:LEU:HD11 | 1:E:318:VAL:HG13 | 0.47     | 1.85        | 4      | 1     |
| 1:D:308:ILE:N    | 1:D:308:ILE:HD12 | 0.47     | 2.25        | 9      | 2     |
| 1:F:308:ILE:HD12 | 1:F:308:ILE:N    | 0.47     | 2.25        | 9      | 2     |
| 1:J:308:ILE:HD12 | 1:J:308:ILE:N    | 0.47     | 2.25        | 9      | 2     |
| 1:F:275:VAL:HG13 | 1:H:275:VAL:HG23 | 0.47     | 1.86        | 7      | 1     |
| 1:G:275:VAL:HG13 | 1:I:275:VAL:HG23 | 0.47     | 1.86        | 7      | 1     |
| 1:H:275:VAL:HG13 | 1:J:275:VAL:HG23 | 0.47     | 1.86        | 7      | 1     |
| 1:A:306:VAL:HG23 | 1:C:306:VAL:HG13 | 0.47     | 1.86        | 9      | 1     |
| 1:C:306:VAL:HG23 | 1:E:306:VAL:HG13 | 0.47     | 1.85        | 9      | 1     |
| 1:H:308:ILE:HD13 | 1:H:310:TYR:HE1  | 0.47     | 1.70        | 1      | 1     |
| 1:J:308:ILE:HD12 | 1:J:310:TYR:CE2  | 0.47     | 2.45        | 3      | 1     |
| 1:G:315:LEU:HD11 | 1:G:318:VAL:HG13 | 0.47     | 1.85        | 4      | 1     |
| 1:J:315:LEU:HD11 | 1:J:318:VAL:HG13 | 0.47     | 1.86        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:308:ILE:HD12 | 1:B:308:ILE:N    | 0.47     | 2.25        | 9      | 2     |
| 1:D:308:ILE:HD12 | 1:D:310:TYR:CE2  | 0.47     | 2.45        | 3      | 1     |
| 1:F:308:ILE:HD12 | 1:F:310:TYR:CE2  | 0.47     | 2.45        | 3      | 1     |
| 1:H:308:ILE:HD12 | 1:H:310:TYR:CE2  | 0.47     | 2.45        | 3      | 1     |
| 1:D:287:VAL:HG22 | 1:F:287:VAL:HG12 | 0.47     | 1.86        | 4      | 1     |
| 1:F:308:ILE:HD13 | 1:F:310:TYR:HE1  | 0.47     | 1.70        | 1      | 1     |
| 1:A:315:LEU:HD11 | 1:A:318:VAL:HG13 | 0.47     | 1.85        | 4      | 1     |
| 1:C:287:VAL:HG22 | 1:E:287:VAL:HG12 | 0.46     | 1.85        | 4      | 1     |
| 1:D:308:ILE:HD13 | 1:D:310:TYR:HE1  | 0.46     | 1.70        | 1      | 1     |
| 1:F:287:VAL:HG22 | 1:H:287:VAL:HG12 | 0.46     | 1.86        | 4      | 1     |
| 1:H:287:VAL:HG22 | 1:J:287:VAL:HG12 | 0.46     | 1.86        | 4      | 1     |
| 1:A:287:VAL:HG22 | 1:C:287:VAL:HG12 | 0.46     | 1.85        | 4      | 1     |
| 1:E:287:VAL:HG22 | 1:G:287:VAL:HG12 | 0.46     | 1.86        | 4      | 1     |
| 1:I:315:LEU:HD11 | 1:I:318:VAL:HG13 | 0.46     | 1.86        | 4      | 1     |
| 1:B:308:ILE:HD13 | 1:B:310:TYR:HE1  | 0.46     | 1.70        | 1      | 1     |
| 1:B:308:ILE:HD12 | 1:B:310:TYR:CE2  | 0.46     | 2.46        | 3      | 1     |
| 1:I:308:ILE:HD12 | 1:I:310:TYR:CE2  | 0.46     | 2.45        | 3      | 1     |
| 1:G:308:ILE:HD12 | 1:G:310:TYR:CE2  | 0.46     | 2.45        | 3      | 1     |
| 1:E:308:ILE:HD12 | 1:E:310:TYR:CE2  | 0.46     | 2.45        | 3      | 1     |
| 1:G:287:VAL:HG22 | 1:I:287:VAL:HG12 | 0.46     | 1.86        | 4      | 1     |
| 1:A:308:ILE:HD12 | 1:A:308:ILE:N    | 0.46     | 2.25        | 9      | 2     |
| 1:A:308:ILE:HD12 | 1:A:310:TYR:CE2  | 0.46     | 2.46        | 3      | 1     |
| 1:C:308:ILE:HD12 | 1:C:310:TYR:CE2  | 0.46     | 2.45        | 3      | 1     |
| 1:C:308:ILE:HD12 | 1:C:308:ILE:N    | 0.46     | 2.25        | 9      | 2     |
| 1:A:306:VAL:HG12 | 1:C:306:VAL:HG22 | 0.46     | 1.87        | 10     | 1     |
| 1:E:308:ILE:HD12 | 1:E:308:ILE:N    | 0.46     | 2.25        | 9      | 2     |
| 1:I:308:ILE:HD13 | 1:I:310:TYR:HE1  | 0.46     | 1.70        | 1      | 1     |
| 1:D:284:LEU:HD21 | 1:E:279:ASN:ND2  | 0.46     | 2.26        | 2      | 1     |
| 1:G:308:ILE:HD12 | 1:G:308:ILE:N    | 0.46     | 2.25        | 9      | 2     |
| 1:I:308:ILE:HD12 | 1:I:308:ILE:N    | 0.46     | 2.25        | 9      | 2     |
| 1:G:308:ILE:HD13 | 1:G:310:TYR:HE1  | 0.45     | 1.70        | 1      | 1     |
| 1:E:284:LEU:HD21 | 1:F:279:ASN:ND2  | 0.45     | 2.27        | 2      | 1     |
| 1:E:282:LEU:HD12 | 1:E:282:LEU:N    | 0.45     | 2.27        | 5      | 1     |
| 1:I:282:LEU:HD12 | 1:I:282:LEU:N    | 0.45     | 2.27        | 5      | 1     |
| 1:B:306:VAL:HG12 | 1:D:306:VAL:HG22 | 0.45     | 1.88        | 10     | 1     |
| 1:C:282:LEU:HD12 | 1:C:282:LEU:N    | 0.45     | 2.27        | 5      | 1     |
| 1:G:282:LEU:HD12 | 1:G:282:LEU:N    | 0.45     | 2.27        | 5      | 1     |
| 1:C:306:VAL:HG12 | 1:E:306:VAL:HG22 | 0.45     | 1.88        | 10     | 1     |
| 1:D:306:VAL:HG12 | 1:F:306:VAL:HG22 | 0.45     | 1.88        | 10     | 1     |
| 1:E:308:ILE:HD13 | 1:E:310:TYR:HE1  | 0.45     | 1.70        | 1      | 1     |
| 1:J:284:LEU:HD12 | 1:J:284:LEU:O    | 0.45     | 2.11        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:D:282:LEU:HD12 | 1:D:282:LEU:N    | 0.45     | 2.27        | 5      | 1     |
| 1:F:282:LEU:N    | 1:F:282:LEU:HD12 | 0.45     | 2.27        | 5      | 1     |
| 1:D:308:ILE:HD12 | 1:D:308:ILE:C    | 0.45     | 2.37        | 6      | 2     |
| 1:H:282:LEU:HD12 | 1:H:282:LEU:N    | 0.45     | 2.27        | 5      | 1     |
| 1:B:308:ILE:C    | 1:B:308:ILE:HD12 | 0.45     | 2.37        | 6      | 1     |
| 1:A:297:ILE:HD12 | 1:A:297:ILE:N    | 0.45     | 2.26        | 9      | 1     |
| 1:E:306:VAL:HG12 | 1:G:306:VAL:HG22 | 0.45     | 1.88        | 10     | 1     |
| 1:H:284:LEU:O    | 1:H:284:LEU:HD12 | 0.45     | 2.11        | 2      | 1     |
| 1:A:282:LEU:HD12 | 1:A:282:LEU:N    | 0.45     | 2.27        | 5      | 1     |
| 1:J:282:LEU:N    | 1:J:282:LEU:HD12 | 0.45     | 2.27        | 5      | 1     |
| 1:C:297:ILE:N    | 1:C:297:ILE:HD12 | 0.45     | 2.26        | 9      | 1     |
| 1:E:297:ILE:HD12 | 1:E:297:ILE:N    | 0.45     | 2.26        | 9      | 1     |
| 1:I:297:ILE:HD12 | 1:I:297:ILE:N    | 0.45     | 2.26        | 9      | 1     |
| 1:C:308:ILE:HD13 | 1:C:310:TYR:HE1  | 0.45     | 1.70        | 1      | 1     |
| 1:F:284:LEU:HD12 | 1:F:284:LEU:O    | 0.45     | 2.11        | 2      | 1     |
| 1:B:282:LEU:N    | 1:B:282:LEU:HD12 | 0.45     | 2.27        | 5      | 1     |
| 1:F:308:ILE:C    | 1:F:308:ILE:HD12 | 0.45     | 2.37        | 6      | 1     |
| 1:J:308:ILE:C    | 1:J:308:ILE:HD12 | 0.45     | 2.37        | 6      | 1     |
| 1:G:297:ILE:N    | 1:G:297:ILE:HD12 | 0.45     | 2.26        | 9      | 1     |
| 1:F:306:VAL:HG12 | 1:H:306:VAL:HG22 | 0.45     | 1.88        | 10     | 1     |
| 1:G:306:VAL:HG12 | 1:I:306:VAL:HG22 | 0.45     | 1.88        | 10     | 1     |
| 1:H:306:VAL:HG12 | 1:J:306:VAL:HG22 | 0.45     | 1.88        | 10     | 1     |
| 1:I:284:LEU:HD12 | 1:I:284:LEU:O    | 0.45     | 2.11        | 2      | 1     |
| 1:F:297:ILE:HD12 | 1:F:297:ILE:N    | 0.45     | 2.26        | 9      | 1     |
| 1:A:308:ILE:HD13 | 1:A:310:TYR:HE1  | 0.45     | 1.70        | 1      | 1     |
| 1:H:308:ILE:HD12 | 1:H:308:ILE:C    | 0.45     | 2.37        | 6      | 2     |
| 1:C:308:ILE:C    | 1:C:308:ILE:HD12 | 0.45     | 2.37        | 6      | 1     |
| 1:H:313:VAL:CG2  | 1:J:313:VAL:HG13 | 0.45     | 2.39        | 1      | 3     |
| 1:A:308:ILE:C    | 1:A:308:ILE:HD12 | 0.45     | 2.37        | 6      | 1     |
| 1:B:297:ILE:HD12 | 1:B:297:ILE:N    | 0.45     | 2.26        | 9      | 1     |
| 1:G:284:LEU:HD12 | 1:G:284:LEU:O    | 0.44     | 2.11        | 2      | 1     |
| 1:E:308:ILE:C    | 1:E:308:ILE:HD12 | 0.44     | 2.37        | 6      | 1     |
| 1:G:308:ILE:C    | 1:G:308:ILE:HD12 | 0.44     | 2.37        | 6      | 1     |
| 1:D:297:ILE:HD12 | 1:D:297:ILE:N    | 0.44     | 2.26        | 9      | 1     |
| 1:H:297:ILE:HD12 | 1:H:297:ILE:N    | 0.44     | 2.26        | 9      | 1     |
| 1:D:313:VAL:CG2  | 1:F:313:VAL:HG13 | 0.44     | 2.39        | 1      | 3     |
| 1:F:313:VAL:CG2  | 1:H:313:VAL:HG13 | 0.44     | 2.39        | 1      | 3     |
| 1:I:308:ILE:C    | 1:I:308:ILE:HD12 | 0.44     | 2.37        | 6      | 1     |
| 1:J:297:ILE:N    | 1:J:297:ILE:HD12 | 0.44     | 2.26        | 9      | 1     |
| 1:B:313:VAL:CG2  | 1:D:313:VAL:HG13 | 0.44     | 2.39        | 3      | 3     |
| 1:C:284:LEU:HD23 | 1:E:283:ASP:OD2  | 0.44     | 2.13        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:E:284:LEU:HD23 | 1:G:283:ASP:OD2  | 0.44     | 2.13        | 2      | 1     |
| 1:A:284:LEU:HD23 | 1:C:283:ASP:OD2  | 0.44     | 2.13        | 2      | 1     |
| 1:G:284:LEU:HD23 | 1:I:283:ASP:OD2  | 0.44     | 2.13        | 2      | 1     |
| 1:D:284:LEU:O    | 1:D:284:LEU:HD12 | 0.44     | 2.12        | 2      | 1     |
| 1:E:284:LEU:HD12 | 1:E:284:LEU:O    | 0.44     | 2.12        | 2      | 1     |
| 1:H:284:LEU:C    | 1:H:284:LEU:HD23 | 0.44     | 2.38        | 9      | 2     |
| 1:F:284:LEU:C    | 1:F:284:LEU:HD23 | 0.44     | 2.38        | 9      | 2     |
| 1:J:284:LEU:C    | 1:J:284:LEU:HD23 | 0.44     | 2.38        | 9      | 2     |
| 1:J:308:ILE:HD13 | 1:J:310:TYR:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:H:308:ILE:HD13 | 1:H:310:TYR:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:I:308:ILE:HD13 | 1:I:310:TYR:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:D:290:LYS:HZ3  | 1:E:275:VAL:HG11 | 0.43     | 1.73        | 3      | 1     |
| 1:B:284:LEU:C    | 1:B:284:LEU:HD23 | 0.43     | 2.38        | 9      | 2     |
| 1:D:284:LEU:HD23 | 1:D:284:LEU:C    | 0.43     | 2.38        | 9      | 2     |
| 1:A:284:LEU:C    | 1:A:284:LEU:HD23 | 0.43     | 2.38        | 9      | 2     |
| 1:C:284:LEU:C    | 1:C:284:LEU:HD23 | 0.43     | 2.38        | 9      | 2     |
| 1:J:277:ILE:HG23 | 1:J:277:ILE:O    | 0.43     | 2.14        | 3      | 1     |
| 1:F:308:ILE:HD13 | 1:F:310:TYR:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:G:308:ILE:HD13 | 1:G:310:TYR:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:H:277:ILE:O    | 1:H:277:ILE:HG23 | 0.43     | 2.14        | 3      | 1     |
| 1:E:284:LEU:C    | 1:E:284:LEU:HD23 | 0.43     | 2.38        | 9      | 2     |
| 1:G:284:LEU:C    | 1:G:284:LEU:HD23 | 0.43     | 2.38        | 9      | 2     |
| 1:G:287:VAL:O    | 1:I:287:VAL:HG23 | 0.43     | 2.13        | 10     | 1     |
| 1:F:277:ILE:HG23 | 1:F:277:ILE:O    | 0.43     | 2.14        | 3      | 1     |
| 1:I:284:LEU:C    | 1:I:284:LEU:HD23 | 0.43     | 2.38        | 9      | 2     |
| 1:E:308:ILE:HD13 | 1:E:310:TYR:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:B:277:ILE:HG23 | 1:B:277:ILE:O    | 0.43     | 2.14        | 3      | 1     |
| 1:D:277:ILE:O    | 1:D:277:ILE:HG23 | 0.43     | 2.14        | 3      | 1     |
| 1:H:287:VAL:O    | 1:J:287:VAL:HG23 | 0.43     | 2.12        | 10     | 1     |
| 1:D:308:ILE:HD13 | 1:D:310:TYR:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:G:313:VAL:CG2  | 1:I:313:VAL:HG13 | 0.43     | 2.39        | 1      | 3     |
| 1:F:284:LEU:HD21 | 1:G:279:ASN:ND2  | 0.43     | 2.28        | 2      | 1     |
| 1:A:282:LEU:HD23 | 1:A:282:LEU:C    | 0.43     | 2.39        | 10     | 3     |
| 1:A:313:VAL:CG2  | 1:C:313:VAL:HG13 | 0.43     | 2.39        | 1      | 3     |
| 1:C:313:VAL:CG2  | 1:E:313:VAL:HG13 | 0.43     | 2.39        | 1      | 3     |
| 1:E:313:VAL:CG2  | 1:G:313:VAL:HG13 | 0.43     | 2.39        | 1      | 3     |
| 1:H:284:LEU:HD23 | 1:J:283:ASP:OD2  | 0.43     | 2.13        | 2      | 1     |
| 1:F:290:LYS:HZ3  | 1:G:275:VAL:HG11 | 0.43     | 1.74        | 3      | 1     |
| 1:C:282:LEU:C    | 1:C:282:LEU:HD23 | 0.43     | 2.39        | 10     | 3     |
| 1:E:282:LEU:C    | 1:E:282:LEU:HD23 | 0.43     | 2.39        | 10     | 3     |
| 1:G:277:ILE:O    | 1:G:277:ILE:HG23 | 0.43     | 2.14        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:G:282:LEU:C    | 1:G:282:LEU:HD23 | 0.43     | 2.39        | 10     | 3     |
| 1:I:282:LEU:HD23 | 1:I:282:LEU:C    | 0.43     | 2.39        | 10     | 3     |
| 1:I:277:ILE:HG23 | 1:I:277:ILE:O    | 0.42     | 2.14        | 3      | 1     |
| 1:B:282:LEU:C    | 1:B:282:LEU:HD23 | 0.42     | 2.39        | 9      | 3     |
| 1:F:282:LEU:C    | 1:F:282:LEU:HD23 | 0.42     | 2.39        | 9      | 3     |
| 1:B:308:ILE:HD13 | 1:B:310:TYR:CE1  | 0.42     | 2.48        | 1      | 1     |
| 1:C:308:ILE:HD13 | 1:C:310:TYR:CE1  | 0.42     | 2.48        | 1      | 1     |
| 1:C:284:LEU:HD12 | 1:C:284:LEU:O    | 0.42     | 2.13        | 2      | 1     |
| 1:J:282:LEU:C    | 1:J:282:LEU:HD23 | 0.42     | 2.40        | 9      | 3     |
| 1:B:284:LEU:HD23 | 1:D:283:ASP:OD2  | 0.42     | 2.13        | 2      | 1     |
| 1:G:284:LEU:HD21 | 1:H:279:ASN:ND2  | 0.42     | 2.30        | 2      | 1     |
| 1:C:277:ILE:O    | 1:C:277:ILE:HG23 | 0.42     | 2.14        | 3      | 1     |
| 1:E:277:ILE:HG23 | 1:E:277:ILE:O    | 0.42     | 2.14        | 3      | 1     |
| 1:D:282:LEU:C    | 1:D:282:LEU:HD23 | 0.42     | 2.40        | 9      | 3     |
| 1:H:282:LEU:C    | 1:H:282:LEU:HD23 | 0.42     | 2.40        | 9      | 3     |
| 1:A:277:ILE:HG23 | 1:A:277:ILE:O    | 0.42     | 2.14        | 3      | 1     |
| 1:D:284:LEU:HD23 | 1:F:283:ASP:OD2  | 0.42     | 2.13        | 2      | 1     |
| 1:F:284:LEU:HD23 | 1:H:283:ASP:OD2  | 0.42     | 2.13        | 2      | 1     |
| 1:A:308:ILE:HD13 | 1:A:310:TYR:CE1  | 0.42     | 2.49        | 1      | 1     |
| 1:E:287:VAL:O    | 1:G:287:VAL:HG23 | 0.41     | 2.14        | 10     | 1     |
| 1:F:287:VAL:O    | 1:H:287:VAL:HG23 | 0.41     | 2.14        | 10     | 1     |
| 1:B:290:LYS:HZ3  | 1:C:275:VAL:HG11 | 0.41     | 1.75        | 3      | 1     |
| 1:B:284:LEU:HD12 | 1:B:284:LEU:O    | 0.41     | 2.15        | 2      | 1     |
| 1:G:285:SER:C    | 1:I:285:SER:CB   | 0.41     | 2.94        | 4      | 1     |
| 1:J:308:ILE:HD12 | 1:J:308:ILE:C    | 0.41     | 2.41        | 1      | 1     |
| 1:A:285:SER:C    | 1:C:285:SER:CB   | 0.41     | 2.94        | 4      | 1     |
| 1:A:313:VAL:HG13 | 1:C:313:VAL:O    | 0.41     | 2.16        | 6      | 1     |
| 1:B:313:VAL:HG12 | 1:B:315:LEU:CD1  | 0.41     | 2.46        | 6      | 1     |
| 1:C:313:VAL:HG12 | 1:C:315:LEU:CD1  | 0.41     | 2.46        | 6      | 1     |
| 1:F:313:VAL:HG12 | 1:F:315:LEU:CD1  | 0.41     | 2.46        | 6      | 1     |
| 1:H:277:ILE:CG2  | 1:J:277:ILE:HD12 | 0.41     | 2.46        | 7      | 1     |
| 1:F:308:ILE:HD12 | 1:F:308:ILE:C    | 0.41     | 2.41        | 1      | 1     |
| 1:H:290:LYS:HZ3  | 1:I:275:VAL:HG11 | 0.41     | 1.76        | 3      | 1     |
| 1:E:285:SER:C    | 1:G:285:SER:CB   | 0.41     | 2.94        | 4      | 1     |
| 1:H:285:SER:C    | 1:J:285:SER:CB   | 0.41     | 2.94        | 4      | 1     |
| 1:C:313:VAL:HG13 | 1:E:313:VAL:O    | 0.41     | 2.16        | 6      | 1     |
| 1:D:313:VAL:HG12 | 1:D:315:LEU:CD1  | 0.41     | 2.46        | 6      | 1     |
| 1:D:313:VAL:HG13 | 1:F:313:VAL:O    | 0.41     | 2.16        | 6      | 1     |
| 1:E:313:VAL:HG12 | 1:E:315:LEU:CD1  | 0.41     | 2.46        | 6      | 1     |
| 1:H:313:VAL:HG12 | 1:H:315:LEU:CD1  | 0.41     | 2.46        | 6      | 1     |
| 1:J:313:VAL:HG12 | 1:J:315:LEU:CD1  | 0.41     | 2.46        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:287:VAL:O    | 1:E:287:VAL:HG23 | 0.41     | 2.16        | 10     | 1     |
| 1:A:313:VAL:HG12 | 1:A:315:LEU:CD1  | 0.40     | 2.46        | 6      | 1     |
| 1:B:313:VAL:HG13 | 1:D:313:VAL:O    | 0.40     | 2.16        | 6      | 1     |
| 1:G:313:VAL:HG12 | 1:G:315:LEU:CD1  | 0.40     | 2.46        | 6      | 1     |
| 1:H:309:VAL:HG11 | 1:J:297:ILE:HD12 | 0.40     | 1.93        | 6      | 1     |
| 1:I:313:VAL:HG12 | 1:I:315:LEU:CD1  | 0.40     | 2.46        | 6      | 1     |
| 1:B:287:VAL:HG22 | 1:D:287:VAL:CG1  | 0.40     | 2.47        | 4      | 1     |
| 1:D:287:VAL:HG22 | 1:F:287:VAL:CG1  | 0.40     | 2.47        | 4      | 1     |
| 1:F:277:ILE:CG2  | 1:H:277:ILE:HD12 | 0.40     | 2.47        | 7      | 1     |
| 1:A:315:LEU:HD23 | 1:A:318:VAL:HG21 | 0.40     | 1.93        | 10     | 1     |
| 1:E:315:LEU:HD23 | 1:E:318:VAL:HG21 | 0.40     | 1.93        | 10     | 1     |
| 1:C:285:SER:C    | 1:E:285:SER:CB   | 0.40     | 2.94        | 4      | 1     |
| 1:F:287:VAL:HG22 | 1:H:287:VAL:CG1  | 0.40     | 2.47        | 4      | 1     |
| 1:H:287:VAL:HG22 | 1:J:287:VAL:CG1  | 0.40     | 2.47        | 4      | 1     |
| 1:E:313:VAL:HG13 | 1:G:313:VAL:O    | 0.40     | 2.16        | 6      | 1     |
| 1:C:315:LEU:HD23 | 1:C:318:VAL:HG21 | 0.40     | 1.93        | 10     | 1     |
| 1:I:315:LEU:HD23 | 1:I:318:VAL:HG21 | 0.40     | 1.94        | 10     | 1     |
| 1:H:281:LYS:O    | 1:J:281:LYS:CB   | 0.40     | 2.70        | 5      | 1     |
| 1:F:313:VAL:HG13 | 1:H:313:VAL:O    | 0.40     | 2.16        | 6      | 1     |
| 1:A:287:VAL:O    | 1:C:287:VAL:HG23 | 0.40     | 2.16        | 10     | 1     |
| 1:G:297:ILE:HG23 | 1:G:297:ILE:O    | 0.40     | 2.17        | 10     | 1     |
| 1:G:315:LEU:HD23 | 1:G:318:VAL:HG21 | 0.40     | 1.94        | 10     | 1     |
| 1:B:308:ILE:HD12 | 1:B:308:ILE:C    | 0.40     | 2.42        | 1      | 1     |
| 1:H:297:ILE:HG12 | 1:J:297:ILE:HG22 | 0.40     | 1.92        | 3      | 1     |
| 1:F:285:SER:C    | 1:H:285:SER:CB   | 0.40     | 2.94        | 4      | 1     |
| 1:F:309:VAL:HG11 | 1:H:297:ILE:HD12 | 0.40     | 1.94        | 6      | 1     |
| 1:I:297:ILE:HG23 | 1:I:297:ILE:O    | 0.40     | 2.17        | 10     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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 NMR 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     | 49/202 (24%) | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | B     | 49/202 (24%) | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |

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| Mol | Chain | Analysed         | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|------------------|--------------|------------|------------|-------------|----|
| 1   | C     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | D     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | E     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | F     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | G     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | H     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | I     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| 1   | J     | 49/202 (24%)     | 45±1 (92±2%) | 3±1 (6±2%) | 1±1 (1±1%) | 11          | 58 |
| All | All   | 4900/20200 (24%) | 4530 (92%)   | 300 (6%)   | 70 (1%)    | 11          | 58 |

All 50 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 274 | LYS  | 2              |
| 1   | B     | 274 | LYS  | 2              |
| 1   | C     | 274 | LYS  | 2              |
| 1   | D     | 274 | LYS  | 2              |
| 1   | E     | 274 | LYS  | 2              |
| 1   | F     | 274 | LYS  | 2              |
| 1   | G     | 274 | LYS  | 2              |
| 1   | H     | 274 | LYS  | 2              |
| 1   | I     | 274 | LYS  | 2              |
| 1   | J     | 274 | LYS  | 2              |
| 1   | A     | 275 | VAL  | 2              |
| 1   | B     | 275 | VAL  | 2              |
| 1   | C     | 275 | VAL  | 2              |
| 1   | D     | 275 | VAL  | 2              |
| 1   | E     | 275 | VAL  | 2              |
| 1   | F     | 275 | VAL  | 2              |
| 1   | G     | 275 | VAL  | 2              |
| 1   | H     | 275 | VAL  | 2              |
| 1   | I     | 275 | VAL  | 2              |
| 1   | J     | 275 | VAL  | 2              |
| 1   | A     | 302 | GLY  | 1              |
| 1   | B     | 302 | GLY  | 1              |
| 1   | C     | 302 | GLY  | 1              |
| 1   | D     | 302 | GLY  | 1              |
| 1   | E     | 302 | GLY  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | F     | 302 | GLY  | 1              |
| 1   | G     | 302 | GLY  | 1              |
| 1   | H     | 302 | GLY  | 1              |
| 1   | I     | 302 | GLY  | 1              |
| 1   | J     | 302 | GLY  | 1              |
| 1   | A     | 304 | GLY  | 1              |
| 1   | B     | 304 | GLY  | 1              |
| 1   | C     | 304 | GLY  | 1              |
| 1   | D     | 304 | GLY  | 1              |
| 1   | E     | 304 | GLY  | 1              |
| 1   | F     | 304 | GLY  | 1              |
| 1   | G     | 304 | GLY  | 1              |
| 1   | H     | 304 | GLY  | 1              |
| 1   | I     | 304 | GLY  | 1              |
| 1   | J     | 304 | GLY  | 1              |
| 1   | A     | 301 | PRO  | 1              |
| 1   | B     | 301 | PRO  | 1              |
| 1   | C     | 301 | PRO  | 1              |
| 1   | D     | 301 | PRO  | 1              |
| 1   | E     | 301 | PRO  | 1              |
| 1   | F     | 301 | PRO  | 1              |
| 1   | G     | 301 | PRO  | 1              |
| 1   | H     | 301 | PRO  | 1              |
| 1   | I     | 301 | PRO  | 1              |
| 1   | J     | 301 | PRO  | 1              |

### 6.3.2 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 NMR 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     | 45/175 (26%) | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | B     | 45/175 (26%) | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | C     | 45/175 (26%) | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | D     | 45/175 (26%) | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | E     | 45/175 (26%) | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | F     | 45/175 (26%) | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |

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| Mol | Chain | Analysed         | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|------------------|--------------|------------|-------------|----|
| 1   | G     | 45/175 (26%)     | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | H     | 45/175 (26%)     | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | I     | 45/175 (26%)     | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| 1   | J     | 45/175 (26%)     | 43±1 (95±2%) | 2±1 (5±2%) | 25          | 75 |
| All | All   | 4500/17500 (26%) | 4290 (95%)   | 210 (5%)   | 25          | 75 |

All 130 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 281 | LYS  | 4              |
| 1   | A     | 288 | GLN  | 4              |
| 1   | B     | 281 | LYS  | 4              |
| 1   | B     | 288 | GLN  | 4              |
| 1   | C     | 281 | LYS  | 4              |
| 1   | C     | 288 | GLN  | 4              |
| 1   | D     | 281 | LYS  | 4              |
| 1   | D     | 288 | GLN  | 4              |
| 1   | E     | 281 | LYS  | 4              |
| 1   | E     | 288 | GLN  | 4              |
| 1   | F     | 281 | LYS  | 4              |
| 1   | F     | 288 | GLN  | 4              |
| 1   | G     | 281 | LYS  | 4              |
| 1   | G     | 288 | GLN  | 4              |
| 1   | H     | 281 | LYS  | 4              |
| 1   | H     | 288 | GLN  | 4              |
| 1   | I     | 281 | LYS  | 4              |
| 1   | I     | 288 | GLN  | 4              |
| 1   | J     | 281 | LYS  | 4              |
| 1   | J     | 288 | GLN  | 4              |
| 1   | A     | 283 | ASP  | 2              |
| 1   | B     | 283 | ASP  | 2              |
| 1   | C     | 283 | ASP  | 2              |
| 1   | D     | 283 | ASP  | 2              |
| 1   | E     | 283 | ASP  | 2              |
| 1   | F     | 283 | ASP  | 2              |
| 1   | G     | 283 | ASP  | 2              |
| 1   | H     | 283 | ASP  | 2              |
| 1   | I     | 283 | ASP  | 2              |
| 1   | J     | 283 | ASP  | 2              |
| 1   | A     | 320 | SER  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 320 | SER  | 2              |
| 1   | C     | 320 | SER  | 2              |
| 1   | D     | 320 | SER  | 2              |
| 1   | E     | 320 | SER  | 2              |
| 1   | F     | 320 | SER  | 2              |
| 1   | G     | 320 | SER  | 2              |
| 1   | H     | 320 | SER  | 2              |
| 1   | I     | 320 | SER  | 2              |
| 1   | J     | 320 | SER  | 2              |
| 1   | A     | 298 | LYS  | 1              |
| 1   | B     | 298 | LYS  | 1              |
| 1   | C     | 298 | LYS  | 1              |
| 1   | D     | 298 | LYS  | 1              |
| 1   | E     | 298 | LYS  | 1              |
| 1   | F     | 298 | LYS  | 1              |
| 1   | G     | 298 | LYS  | 1              |
| 1   | H     | 298 | LYS  | 1              |
| 1   | I     | 298 | LYS  | 1              |
| 1   | J     | 298 | LYS  | 1              |
| 1   | A     | 311 | LYS  | 1              |
| 1   | B     | 311 | LYS  | 1              |
| 1   | C     | 311 | LYS  | 1              |
| 1   | D     | 311 | LYS  | 1              |
| 1   | E     | 311 | LYS  | 1              |
| 1   | F     | 311 | LYS  | 1              |
| 1   | G     | 311 | LYS  | 1              |
| 1   | H     | 311 | LYS  | 1              |
| 1   | I     | 311 | LYS  | 1              |
| 1   | J     | 311 | LYS  | 1              |
| 1   | A     | 295 | ASP  | 1              |
| 1   | A     | 315 | LEU  | 1              |
| 1   | B     | 295 | ASP  | 1              |
| 1   | B     | 315 | LEU  | 1              |
| 1   | C     | 295 | ASP  | 1              |
| 1   | C     | 315 | LEU  | 1              |
| 1   | D     | 295 | ASP  | 1              |
| 1   | D     | 315 | LEU  | 1              |
| 1   | E     | 295 | ASP  | 1              |
| 1   | E     | 315 | LEU  | 1              |
| 1   | F     | 295 | ASP  | 1              |
| 1   | F     | 315 | LEU  | 1              |
| 1   | G     | 295 | ASP  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | G     | 315 | LEU  | 1              |
| 1   | H     | 295 | ASP  | 1              |
| 1   | H     | 315 | LEU  | 1              |
| 1   | I     | 295 | ASP  | 1              |
| 1   | I     | 315 | LEU  | 1              |
| 1   | J     | 295 | ASP  | 1              |
| 1   | J     | 315 | LEU  | 1              |
| 1   | A     | 286 | ASN  | 1              |
| 1   | A     | 319 | THR  | 1              |
| 1   | B     | 286 | ASN  | 1              |
| 1   | B     | 319 | THR  | 1              |
| 1   | C     | 286 | ASN  | 1              |
| 1   | C     | 319 | THR  | 1              |
| 1   | D     | 286 | ASN  | 1              |
| 1   | D     | 319 | THR  | 1              |
| 1   | E     | 286 | ASN  | 1              |
| 1   | E     | 319 | THR  | 1              |
| 1   | F     | 286 | ASN  | 1              |
| 1   | F     | 319 | THR  | 1              |
| 1   | G     | 286 | ASN  | 1              |
| 1   | G     | 319 | THR  | 1              |
| 1   | H     | 286 | ASN  | 1              |
| 1   | H     | 319 | THR  | 1              |
| 1   | I     | 286 | ASN  | 1              |
| 1   | I     | 319 | THR  | 1              |
| 1   | J     | 286 | ASN  | 1              |
| 1   | J     | 319 | THR  | 1              |
| 1   | A     | 282 | LEU  | 1              |
| 1   | A     | 284 | LEU  | 1              |
| 1   | B     | 282 | LEU  | 1              |
| 1   | B     | 284 | LEU  | 1              |
| 1   | C     | 282 | LEU  | 1              |
| 1   | C     | 284 | LEU  | 1              |
| 1   | D     | 282 | LEU  | 1              |
| 1   | D     | 284 | LEU  | 1              |
| 1   | E     | 282 | LEU  | 1              |
| 1   | E     | 284 | LEU  | 1              |
| 1   | F     | 282 | LEU  | 1              |
| 1   | F     | 284 | LEU  | 1              |
| 1   | G     | 282 | LEU  | 1              |
| 1   | G     | 284 | LEU  | 1              |
| 1   | H     | 282 | LEU  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | H     | 284 | LEU  | 1              |
| 1   | I     | 282 | LEU  | 1              |
| 1   | I     | 284 | LEU  | 1              |
| 1   | J     | 282 | LEU  | 1              |
| 1   | J     | 284 | LEU  | 1              |
| 1   | A     | 280 | LYS  | 1              |
| 1   | B     | 280 | LYS  | 1              |
| 1   | C     | 280 | LYS  | 1              |
| 1   | D     | 280 | LYS  | 1              |
| 1   | E     | 280 | LYS  | 1              |
| 1   | F     | 280 | LYS  | 1              |
| 1   | G     | 280 | LYS  | 1              |
| 1   | H     | 280 | LYS  | 1              |
| 1   | I     | 280 | LYS  | 1              |
| 1   | J     | 280 | LYS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 329 |
| Number of shifts mapped to atoms        | 227 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 102 |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 102 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 329 | HIS  | C    | 171.312    | .           | 1         |
| 1       | A     | 329 | HIS  | CA   | 53.017     | .           | 1         |
| 1       | A     | 329 | HIS  | CB   | 33.177     | .           | 1         |
| 1       | A     | 329 | HIS  | CD2  | 114.657    | .           | 1         |
| 1       | A     | 329 | HIS  | CE1  | 134.415    | .           | 1         |
| 1       | A     | 329 | HIS  | N    | 126.468    | .           | 1         |
| 1       | A     | 330 | HIS  | C    | 170.615    | .           | 1         |
| 1       | A     | 330 | HIS  | CA   | 54.85      | .           | 1         |
| 1       | A     | 330 | HIS  | CB   | 29.771     | .           | 1         |
| 1       | A     | 330 | HIS  | CD2  | 114.139    | .           | 1         |
| 1       | A     | 330 | HIS  | CE1  | 132.203    | .           | 1         |
| 1       | A     | 330 | HIS  | N    | 126.386    | .           | 1         |
| 1       | A     | 331 | LYS  | C    | 173.087    | .           | 1         |
| 1       | A     | 331 | LYS  | CA   | 52.602     | .           | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 331 | LYS  | CB   | 31.039     | .           | 1         |
| 1       | A     | 331 | LYS  | CD   | 28.661     | .           | 1         |
| 1       | A     | 331 | LYS  | CG   | 23.905     | .           | 1         |
| 1       | A     | 331 | LYS  | N    | 126.423    | .           | 1         |
| 1       | A     | 355 | GLY  | C    | 172.8      | .           | 1         |
| 1       | A     | 355 | GLY  | CA   | 46.259     | .           | 1         |
| 1       | A     | 355 | GLY  | N    | 119.144    | .           | 1         |
| 1       | A     | 356 | SER  | C    | 169.267    | .           | 1         |
| 1       | A     | 356 | SER  | CA   | 56.825     | .           | 1         |
| 1       | A     | 356 | SER  | CB   | 66.356     | .           | 1         |
| 1       | A     | 356 | SER  | N    | 111.365    | .           | 1         |
| 1       | A     | 361 | THR  | C    | 171.314    | .           | 1         |
| 1       | A     | 361 | THR  | CA   | 54.681     | .           | 1         |
| 1       | A     | 361 | THR  | CB   | 64.461     | .           | 1         |
| 1       | A     | 361 | THR  | N    | 117.933    | .           | 1         |
| 1       | A     | 362 | HIS  | C    | 172.025    | .           | 1         |
| 1       | A     | 362 | HIS  | CA   | 53.107     | .           | 1         |
| 1       | A     | 362 | HIS  | CB   | 33.183     | .           | 1         |
| 1       | A     | 362 | HIS  | CD2  | 114.554    | .           | 1         |
| 1       | A     | 362 | HIS  | CE1  | 135.843    | .           | 1         |
| 1       | A     | 362 | HIS  | CG   | 134.97     | .           | 1         |
| 1       | A     | 362 | HIS  | N    | 123.797    | .           | 1         |
| 1       | A     | 367 | GLY  | C    | 172.227    | .           | 1         |
| 1       | A     | 367 | GLY  | CA   | 45.757     | .           | 1         |
| 1       | A     | 367 | GLY  | N    | 106.945    | .           | 1         |
| 1       | A     | 368 | ASN  | CA   | 51.188     | .           | 1         |
| 1       | A     | 368 | ASN  | CB   | 40.099     | .           | 1         |
| 1       | A     | 368 | ASN  | N    | 117.029    | .           | 1         |
| 1       | A     | 372 | GLU  | C    | 174.186    | .           | 1         |
| 1       | A     | 372 | GLU  | CA   | 51.814     | .           | 1         |
| 1       | A     | 372 | GLU  | CB   | 29.264     | .           | 1         |
| 1       | A     | 372 | GLU  | CD   | 181.675    | .           | 1         |
| 1       | A     | 372 | GLU  | CG   | 35.812     | .           | 1         |
| 1       | A     | 372 | GLU  | N    | 123.093    | .           | 1         |
| 1       | A     | 373 | THR  | C    | 174.257    | .           | 1         |
| 1       | A     | 373 | THR  | CA   | 59.601     | .           | 1         |
| 1       | A     | 373 | THR  | CB   | 66.186     | .           | 1         |
| 1       | A     | 373 | THR  | CG2  | 21.498     | .           | 1         |
| 1       | A     | 373 | THR  | N    | 113.907    | .           | 1         |
| 1       | A     | 374 | HIS  | C    | 171.584    | .           | 1         |
| 1       | A     | 374 | HIS  | CA   | 53.443     | .           | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 374 | HIS  | CB   | 34.63      | .           | 1         |
| 1       | A     | 374 | HIS  | CD2  | 113.796    | .           | 1         |
| 1       | A     | 374 | HIS  | CE1  | 134.765    | .           | 1         |
| 1       | A     | 374 | HIS  | N    | 125.721    | .           | 1         |
| 1       | A     | 375 | LYS  | CA   | 52.269     | .           | 1         |
| 1       | A     | 375 | LYS  | CB   | 29.148     | .           | 1         |
| 1       | A     | 375 | LYS  | CD   | 25.333     | .           | 1         |
| 1       | A     | 375 | LYS  | CE   | 44.057     | .           | 1         |
| 1       | A     | 375 | LYS  | CG   | 21.855     | .           | 1         |
| 1       | A     | 375 | LYS  | N    | 126.043    | .           | 1         |
| 1       | A     | 382 | ALA  | C    | 173.006    | .           | 1         |
| 1       | A     | 382 | ALA  | CA   | 48.654     | .           | 1         |
| 1       | A     | 382 | ALA  | CB   | 20.786     | .           | 1         |
| 1       | A     | 382 | ALA  | N    | 128.749    | .           | 1         |
| 1       | A     | 383 | LYS  | C    | 172.364    | .           | 1         |
| 1       | A     | 383 | LYS  | CA   | 53.08      | .           | 1         |
| 1       | A     | 383 | LYS  | CB   | 32.179     | .           | 1         |
| 1       | A     | 383 | LYS  | N    | 118.358    | .           | 1         |
| 1       | A     | 384 | ALA  | C    | 173.198    | .           | 1         |
| 1       | A     | 384 | ALA  | CA   | 48.714     | .           | 1         |
| 1       | A     | 384 | ALA  | CB   | 20.673     | .           | 1         |
| 1       | A     | 384 | ALA  | N    | 127.074    | .           | 1         |
| 1       | A     | 385 | LYS  | C    | 174.91     | .           | 1         |
| 1       | A     | 385 | LYS  | CA   | 53.63      | .           | 1         |
| 1       | A     | 385 | LYS  | CB   | 31.227     | .           | 1         |
| 1       | A     | 385 | LYS  | N    | 119.634    | .           | 1         |
| 1       | A     | 386 | THR  | C    | 172.605    | .           | 1         |
| 1       | A     | 386 | THR  | CA   | 57.703     | .           | 1         |
| 1       | A     | 386 | THR  | CB   | 67.055     | .           | 1         |
| 1       | A     | 386 | THR  | CG2  | 19.744     | .           | 1         |
| 1       | A     | 386 | THR  | N    | 108.507    | .           | 1         |
| 1       | A     | 388 | HIS  | CA   | 50.481     | .           | 1         |
| 1       | A     | 388 | HIS  | CB   | 29.717     | .           | 1         |
| 1       | A     | 388 | HIS  | CE1  | 135.106    | .           | 1         |
| 1       | A     | 388 | HIS  | CG   | 127.2      | .           | 1         |
| 1       | A     | 388 | HIS  | N    | 128.229    | .           | 1         |
| 1       | A     | 389 | GLY  | C    | 170.969    | .           | 1         |
| 1       | A     | 389 | GLY  | CA   | 44.943     | .           | 1         |
| 1       | A     | 389 | GLY  | N    | 108.718    | .           | 1         |
| 1       | A     | 390 | ALA  | C    | 174.544    | .           | 1         |
| 1       | A     | 390 | ALA  | CA   | 49.537     | .           | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 390 | ALA  | CB   | 18.01      | .           | 1         |
| 1       | A     | 390 | ALA  | N    | 121.808    | .           | 1         |
| 1       | A     | 391 | GLU  | CA   | 53.637     | .           | 1         |
| 1       | A     | 391 | GLU  | CB   | 31.744     | .           | 1         |
| 1       | A     | 391 | GLU  | CG   | 34.681     | .           | 1         |
| 1       | A     | 391 | GLU  | N    | 121.829    | .           | 1         |

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action  |
|------------------------|----------|---------------------------------|-------------------|
| $^{13}\text{C}_\alpha$ | 68       | $2.06 \pm 0.30$                 | Should be checked |
| $^{13}\text{C}_\beta$  | 56       | $0.92 \pm 0.28$                 | Should be checked |
| $^{13}\text{C}'$       | 59       | $2.28 \pm 0.33$                 | Should be applied |
| $^{15}\text{N}$        | 67       | $-1.96 \pm 0.69$                | Should be applied |

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 220 atoms were assigned a chemical shift out of a possible 6570. 0 out of 100 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|--------------|-----------------|-----------------|
| Backbone  | 126/2450 (5%) | 0/1000 (0%)  | 85/980 (9%)     | 41/470 (9%)     |
| Sidechain | 92/3950 (2%)  | 0/2560 (0%)  | 89/1240 (7%)    | 3/150 (2%)      |
| Aromatic  | 2/170 (1%)    | 0/80 (0%)    | 2/70 (3%)       | 0/20 (0%)       |
| Overall   | 220/6570 (3%) | 0/3640 (0%)  | 176/2290 (8%)   | 44/640 (7%)     |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 225 atoms were assigned a chemical shift out of a possible 8160. 0 out of 120 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|--------------|-----------------|-----------------|
| Backbone  | 130/3180 (4%) | 0/1320 (0%)  | 87/1260 (7%)    | 43/600 (7%)     |
| Sidechain | 93/4730 (2%)  | 0/3060 (0%)  | 90/1490 (6%)    | 3/180 (2%)      |
| Aromatic  | 2/250 (1%)    | 0/120 (0%)   | 2/90 (2%)       | 0/40 (0%)       |

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|         | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|---------|---------------|----------------|-----------------|-----------------|
| Overall | 225/8160 (3%) | 0/4500 (0%)    | 179/2840 (6%)   | 46/820 (6%)     |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

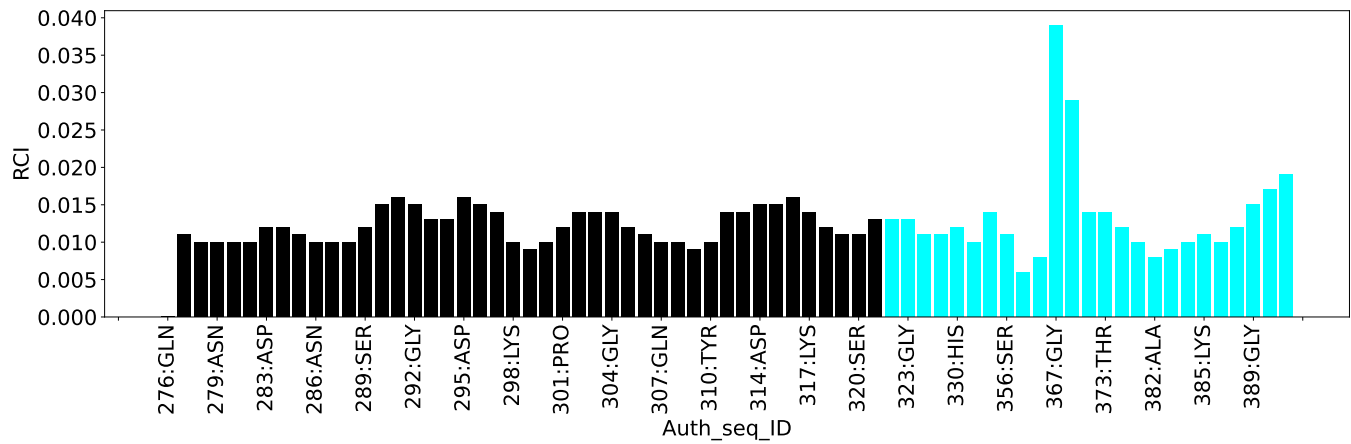
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 46    |
| Intra-residue ( $ i-j =0$ )                              | 0     |
| Sequential ( $ i-j =1$ )                                 | 0     |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 0     |
| Long range ( $ i-j \geq 5$ )                             | 46    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 0.0   |
| Number of long range restraints per residue <sup>1</sup> | 0.0   |

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 1.0                                    | 0.2     |
| 0.2-0.5 (Medium) | 1.4                                    | 0.46    |
| >0.5 (Large)     | 11.6                                   | 4.34    |

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

### 9.1 Summary of distance violations ⓘ

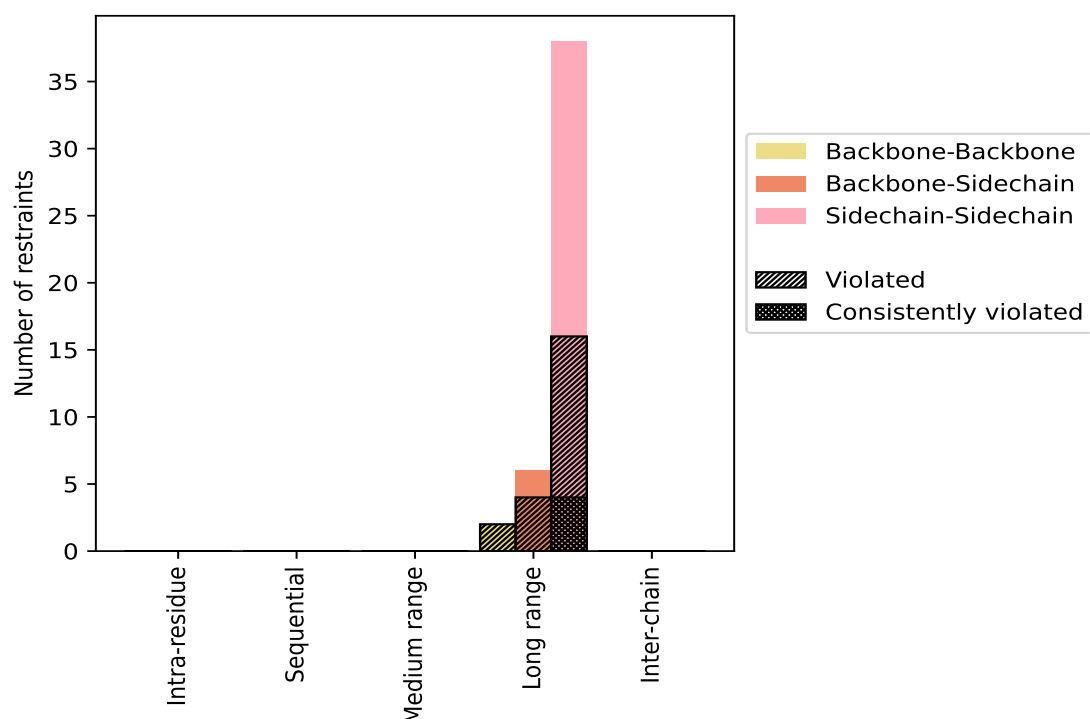
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type                         | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|----------------------------------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                        |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| Intra-residue ( $ i-j =0$ )            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sequential ( $ i-j =1$ )               | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Long range ( $ i-j \geq 5$ )           | 46    | 100.0          | 22                    | 47.8           | 47.8           | 4                                  | 8.7            | 8.7            |
| Backbone-Backbone                      | 2     | 4.3            | 2                     | 100.0          | 4.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 6     | 13.0           | 4                     | 66.7           | 8.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 38    | 82.6           | 16                    | 42.1           | 34.8           | 4                                  | 10.5           | 8.7            |
| Inter-chain                            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Hydrogen bond                          | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Disulfide bond                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 46    | 100.0          | 22                    | 47.8           | 47.8           | 4                                  | 8.7            | 8.7            |
| Backbone-Backbone                      | 2     | 4.3            | 2                     | 100.0          | 4.3            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 6     | 13.0           | 4                     | 66.7           | 8.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 38    | 82.6           | 16                    | 42.1           | 34.8           | 4                                  | 10.5           | 8.7            |

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models



### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

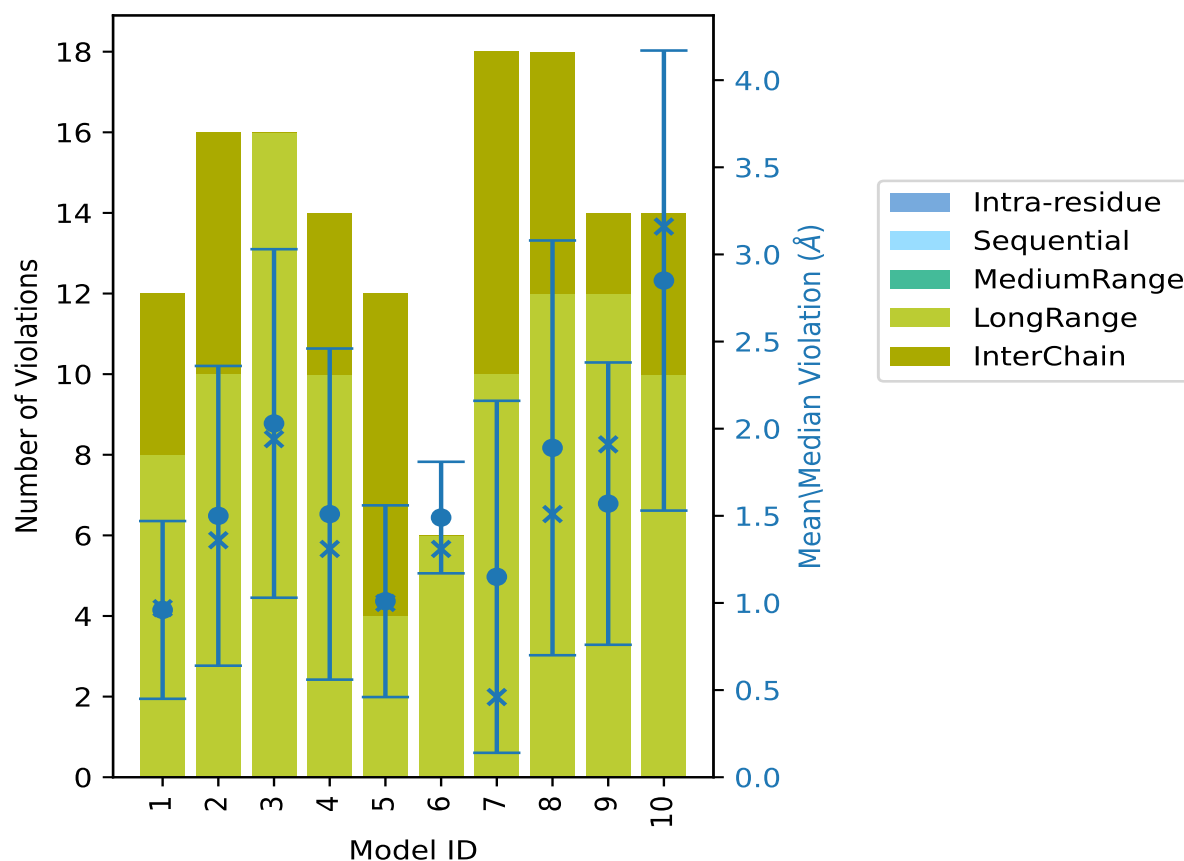
## 9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 0               | 0               | 8               | 4               | 12    | 0.96     | 1.86    | 0.51                | 0.97       |
| 2        | 0                    | 0               | 0               | 10              | 6               | 16    | 1.5      | 3.17    | 0.86                | 1.36       |
| 3        | 0                    | 0               | 0               | 16              | 0               | 16    | 2.03     | 3.58    | 1.0                 | 1.94       |
| 4        | 0                    | 0               | 0               | 10              | 4               | 14    | 1.51     | 3.2     | 0.95                | 1.31       |
| 5        | 0                    | 0               | 0               | 4               | 8               | 12    | 1.01     | 2.03    | 0.55                | 1.0        |
| 6        | 0                    | 0               | 0               | 6               | 0               | 6     | 1.49     | 1.94    | 0.32                | 1.31       |
| 7        | 0                    | 0               | 0               | 10              | 8               | 18    | 1.15     | 3.11    | 1.01                | 0.46       |
| 8        | 0                    | 0               | 0               | 12              | 6               | 18    | 1.89     | 4.09    | 1.19                | 1.51       |
| 9        | 0                    | 0               | 0               | 12              | 2               | 14    | 1.57     | 2.93    | 0.81                | 1.91       |
| 10       | 0                    | 0               | 0               | 10              | 4               | 14    | 2.85     | 4.34    | 1.32                | 3.16       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 24(IR:0, SQ:0, MR:0, LR:24, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |      |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %    |
| 0                             | 0               | 0               | 2               | 0               | 2     | 1                        | 10.0 |
| 0                             | 0               | 0               | 2               | 0               | 2     | 2                        | 20.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 3                        | 30.0 |

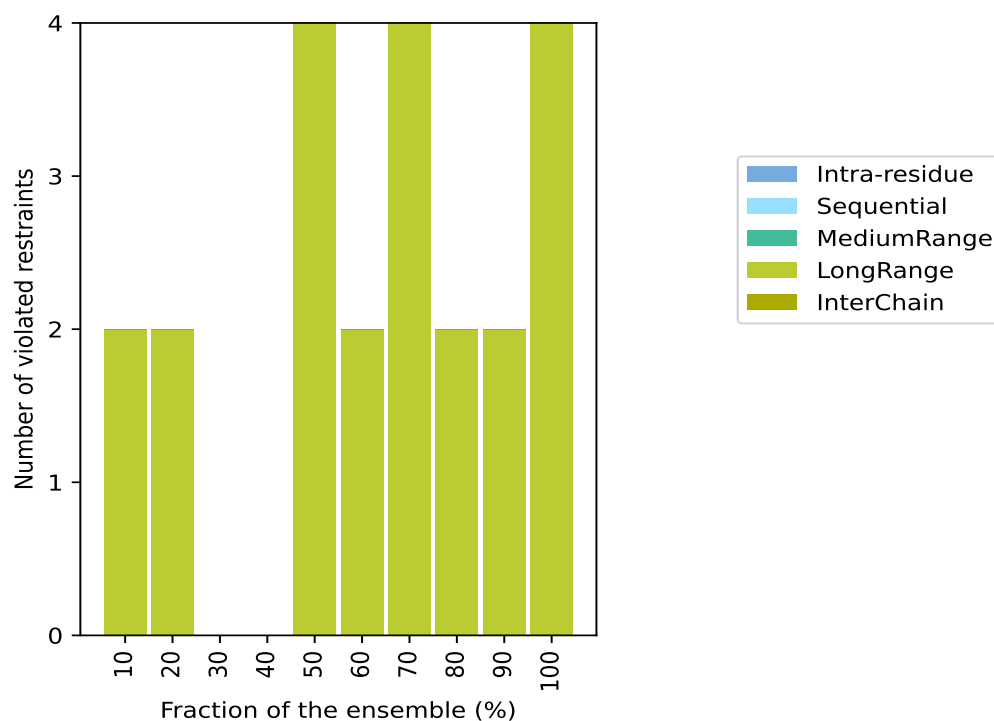
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 0               | 0               | 0               | 0               | 0     | 4                        | 40.0  |
| 0                             | 0               | 0               | 4               | 0               | 4     | 5                        | 50.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 6                        | 60.0  |
| 0                             | 0               | 0               | 4               | 0               | 4     | 7                        | 70.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 8                        | 80.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 9                        | 90.0  |
| 0                             | 0               | 0               | 4               | 0               | 4     | 10                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)

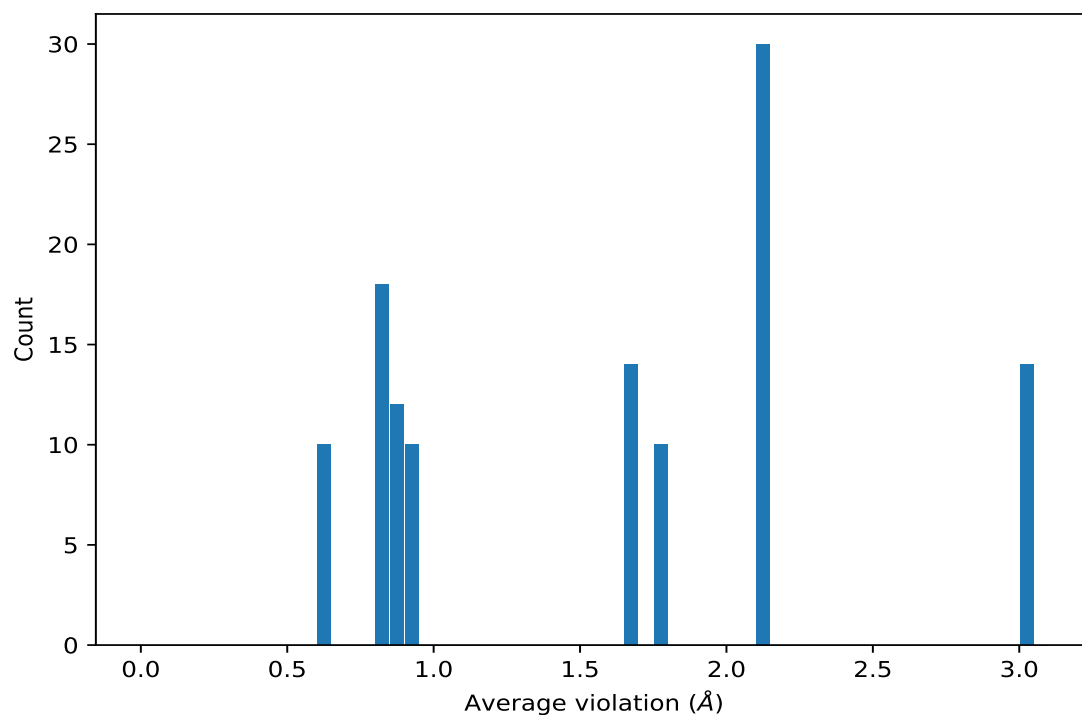


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key    | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,17) | 1:297:I:ILE:CB  | 1:308:I:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (1,17) | 1:297:J:ILE:CB  | 1:308:J:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (1,17) | 1:297:G:ILE:CB  | 1:308:G:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (1,17) | 1:297:G:ILE:CB  | 1:308:I:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (1,17) | 1:297:E:ILE:CB  | 1:308:E:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (1,17) | 1:297:D:ILE:CB  | 1:308:D:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (1,17) | 1:297:H:ILE:CB  | 1:308:H:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (2,17) | 1:297:I:ILE:CB  | 1:308:I:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (2,17) | 1:297:J:ILE:CB  | 1:308:J:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (2,17) | 1:297:G:ILE:CB  | 1:308:G:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (2,17) | 1:297:G:ILE:CB  | 1:308:I:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (2,17) | 1:297:E:ILE:CB  | 1:308:E:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (2,17) | 1:297:D:ILE:CB  | 1:308:D:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (2,17) | 1:297:H:ILE:CB  | 1:308:H:ILE:CD1 | 10                  | 3.02     | 0.82                | 3.14       |
| (1,16) | 1:297:J:ILE:CG1 | 1:308:J:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |

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| Key    | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,16) | 1:297:J:ILE:CG2 | 1:308:J:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,16) | 1:297:C:ILE:CG1 | 1:308:C:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,16) | 1:297:A:ILE:CG1 | 1:308:A:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,16) | 1:297:E:ILE:CG2 | 1:308:E:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,16) | 1:297:D:ILE:CG1 | 1:308:D:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,16) | 1:297:C:ILE:CG2 | 1:308:C:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,16) | 1:297:H:ILE:CG2 | 1:308:F:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,16) | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:J:ILE:CG1 | 1:308:J:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:J:ILE:CG2 | 1:308:J:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:C:ILE:CG1 | 1:308:C:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:A:ILE:CG1 | 1:308:A:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:E:ILE:CG2 | 1:308:E:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:D:ILE:CG1 | 1:308:D:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:C:ILE:CG2 | 1:308:C:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:H:ILE:CG2 | 1:308:F:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (2,16) | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 10                  | 2.12     | 0.75                | 2.16       |
| (1,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (1,2)  | 1:310:A:TYR:CB  | 1:297:A:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (1,2)  | 1:310:J:TYR:CB  | 1:297:J:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (1,2)  | 1:310:I:TYR:CB  | 1:297:G:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (1,2)  | 1:310:F:TYR:CB  | 1:297:F:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (1,2)  | 1:310:D:TYR:CB  | 1:297:D:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (1,2)  | 1:310:C:TYR:CB  | 1:297:C:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (2,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (2,2)  | 1:310:A:TYR:CB  | 1:297:A:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (2,2)  | 1:310:J:TYR:CB  | 1:297:J:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (2,2)  | 1:310:I:TYR:CB  | 1:297:G:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (2,2)  | 1:310:F:TYR:CB  | 1:297:F:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (2,2)  | 1:310:D:TYR:CB  | 1:297:D:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (2,2)  | 1:310:C:TYR:CB  | 1:297:C:ILE:CD1 | 9                   | 0.82     | 0.39                | 0.78       |
| (1,5)  | 1:297:J:ILE:CD1 | 1:308:J:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (1,5)  | 1:297:F:ILE:CD1 | 1:308:F:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (1,5)  | 1:297:A:ILE:CD1 | 1:308:A:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (1,5)  | 1:297:G:ILE:CD1 | 1:308:I:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (1,5)  | 1:297:C:ILE:CD1 | 1:308:C:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (1,5)  | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (1,5)  | 1:297:H:ILE:CD1 | 1:308:H:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (2,5)  | 1:297:J:ILE:CD1 | 1:308:J:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (2,5)  | 1:297:F:ILE:CD1 | 1:308:F:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (2,5)  | 1:297:A:ILE:CD1 | 1:308:A:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (2,5)  | 1:297:G:ILE:CD1 | 1:308:I:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |

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| Key    | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,5)  | 1:297:C:ILE:CD1 | 1:308:C:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (2,5)  | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (2,5)  | 1:297:H:ILE:CD1 | 1:308:H:ILE:CD1 | 8                   | 1.7      | 0.6                 | 1.7        |
| (1,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (1,19) | 1:283:A:ASP:CB  | 1:316:A:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (1,19) | 1:283:D:ASP:CB  | 1:316:D:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (1,19) | 1:283:D:ASP:CB  | 1:316:B:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (1,19) | 1:283:I:ASP:CB  | 1:316:I:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (2,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (2,19) | 1:283:A:ASP:CB  | 1:316:A:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (2,19) | 1:283:D:ASP:CB  | 1:316:D:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (2,19) | 1:283:D:ASP:CB  | 1:316:B:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (2,19) | 1:283:I:ASP:CB  | 1:316:I:SER:CB  | 7                   | 1.79     | 1.05                | 1.34       |
| (1,20) | 1:283:D:ASP:CA  | 1:316:B:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (1,20) | 1:283:H:ASP:CA  | 1:316:J:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (1,20) | 1:283:D:ASP:CA  | 1:316:D:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (1,20) | 1:283:C:ASP:CA  | 1:316:A:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (1,20) | 1:283:A:ASP:CA  | 1:316:A:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (1,20) | 1:288:G:GLN:CA  | 1:316:G:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (2,20) | 1:283:D:ASP:CA  | 1:316:B:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (2,20) | 1:283:H:ASP:CA  | 1:316:J:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (2,20) | 1:283:D:ASP:CA  | 1:316:D:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (2,20) | 1:283:C:ASP:CA  | 1:316:A:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (2,20) | 1:283:A:ASP:CA  | 1:316:A:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (2,20) | 1:288:G:GLN:CA  | 1:316:G:SER:CB  | 7                   | 0.88     | 0.66                | 1.09       |
| (1,18) | 1:282:J:LEU:CG  | 1:316:J:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (1,18) | 1:282:A:LEU:CG  | 1:316:C:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (1,18) | 1:282:F:LEU:CG  | 1:316:F:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (1,18) | 1:283:C:ASP:CG  | 1:316:A:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (1,18) | 1:282:J:LEU:CG  | 1:316:H:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (1,18) | 1:282:C:LEU:CG  | 1:316:A:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (2,18) | 1:282:J:LEU:CG  | 1:316:J:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (2,18) | 1:282:A:LEU:CG  | 1:316:C:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (2,18) | 1:282:F:LEU:CG  | 1:316:F:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (2,18) | 1:283:C:ASP:CG  | 1:316:A:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (2,18) | 1:282:J:LEU:CG  | 1:316:H:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (2,18) | 1:282:C:LEU:CG  | 1:316:A:SER:CB  | 6                   | 2.12     | 1.11                | 1.64       |
| (1,22) | 1:312:J:PRO:CA  | 1:293:H:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (1,22) | 1:312:J:PRO:CA  | 1:293:J:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (1,22) | 1:312:G:PRO:CA  | 1:293:E:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (1,22) | 1:312:A:PRO:CA  | 1:293:C:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (1,22) | 1:312:H:PRO:CA  | 1:293:J:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |

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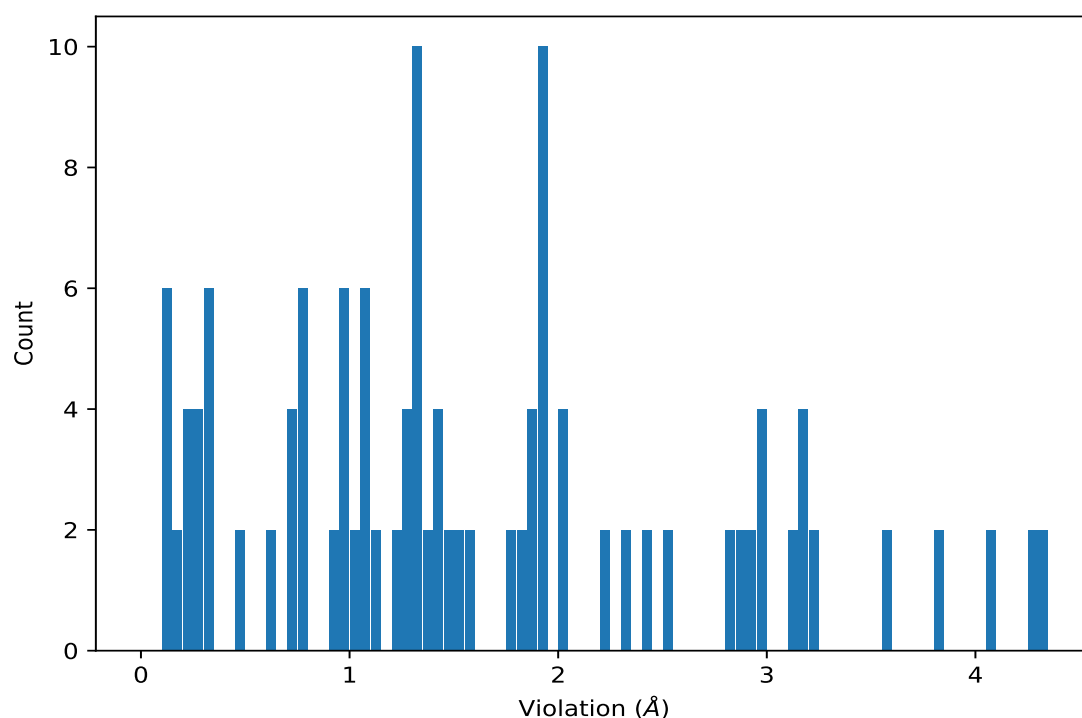
| Key    | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|--------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,22) | 1:312:J:PRO:CA  | 1:293:H:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (2,22) | 1:312:J:PRO:CA  | 1:293:J:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (2,22) | 1:312:G:PRO:CA  | 1:293:E:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (2,22) | 1:312:A:PRO:CA  | 1:293:C:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (2,22) | 1:312:H:PRO:CA  | 1:293:J:SER:CA  | 5                   | 0.91     | 0.36                | 1.07       |
| (1,4)  | 1:308:J:ILE:CG1 | 1:297:J:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (1,4)  | 1:308:H:ILE:CG2 | 1:297:H:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (1,4)  | 1:308:C:ILE:CG2 | 1:297:C:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (1,4)  | 1:308:F:ILE:CG2 | 1:297:F:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (1,4)  | 1:308:D:ILE:CG2 | 1:297:D:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (2,4)  | 1:308:J:ILE:CG1 | 1:297:J:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (2,4)  | 1:308:H:ILE:CG2 | 1:297:H:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (2,4)  | 1:308:C:ILE:CG2 | 1:297:C:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (2,4)  | 1:308:F:ILE:CG2 | 1:297:F:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (2,4)  | 1:308:D:ILE:CG2 | 1:297:D:ILE:CD1 | 5                   | 0.63     | 0.67                | 0.23       |
| (1,21) | 1:285:H:SER:CB  | 1:316:F:SER:CB  | 2                   | 0.8      | 0.49                | 0.8        |
| (1,21) | 1:285:A:SER:CB  | 1:316:A:SER:CB  | 2                   | 0.8      | 0.49                | 0.8        |
| (2,21) | 1:285:H:SER:CB  | 1:316:F:SER:CB  | 2                   | 0.8      | 0.49                | 0.8        |
| (2,21) | 1:285:A:SER:CB  | 1:316:A:SER:CB  | 2                   | 0.8      | 0.49                | 0.8        |

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key    | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|--------|-----------------|-----------------|----------|---------------|
| (2,17) | 1:297:H:ILE:CB  | 1:308:H:ILE:CD1 | 10       | 4.34          |
| (1,17) | 1:297:H:ILE:CB  | 1:308:H:ILE:CD1 | 10       | 4.34          |
| (2,18) | 1:282:C:LEU:CG  | 1:316:A:SER:CB  | 10       | 4.26          |
| (1,18) | 1:282:C:LEU:CG  | 1:316:A:SER:CB  | 10       | 4.26          |
| (2,17) | 1:297:E:ILE:CB  | 1:308:E:ILE:CD1 | 8        | 4.09          |
| (1,17) | 1:297:E:ILE:CB  | 1:308:E:ILE:CD1 | 8        | 4.09          |
| (2,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 10       | 3.84          |
| (1,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 10       | 3.84          |
| (2,17) | 1:297:G:ILE:CB  | 1:308:G:ILE:CD1 | 3        | 3.58          |
| (1,17) | 1:297:G:ILE:CB  | 1:308:G:ILE:CD1 | 3        | 3.58          |
| (2,17) | 1:297:G:ILE:CB  | 1:308:G:ILE:CD1 | 4        | 3.2           |
| (1,17) | 1:297:G:ILE:CB  | 1:308:G:ILE:CD1 | 4        | 3.2           |
| (2,17) | 1:297:J:ILE:CB  | 1:308:J:ILE:CD1 | 2        | 3.17          |
| (1,17) | 1:297:J:ILE:CB  | 1:308:J:ILE:CD1 | 2        | 3.17          |
| (2,16) | 1:297:J:ILE:CG1 | 1:308:J:ILE:CD1 | 10       | 3.16          |
| (1,16) | 1:297:J:ILE:CG1 | 1:308:J:ILE:CD1 | 10       | 3.16          |

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| Key    | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|--------|-----------------|-----------------|----------|---------------|
| (2,17) | 1:297:D:ILE:CB  | 1:308:D:ILE:CD1 | 7        | 3.11          |
| (1,17) | 1:297:D:ILE:CB  | 1:308:D:ILE:CD1 | 7        | 3.11          |
| (2,16) | 1:297:H:ILE:CG2 | 1:308:F:ILE:CD1 | 8        | 2.99          |
| (1,16) | 1:297:H:ILE:CG2 | 1:308:F:ILE:CD1 | 8        | 2.99          |
| (2,5)  | 1:297:F:ILE:CD1 | 1:308:F:ILE:CD1 | 8        | 2.95          |
| (1,5)  | 1:297:F:ILE:CD1 | 1:308:F:ILE:CD1 | 8        | 2.95          |
| (2,17) | 1:297:H:ILE:CB  | 1:308:H:ILE:CD1 | 9        | 2.93          |
| (1,17) | 1:297:H:ILE:CB  | 1:308:H:ILE:CD1 | 9        | 2.93          |
| (2,16) | 1:297:C:ILE:CG1 | 1:308:C:ILE:CD1 | 3        | 2.89          |
| (1,16) | 1:297:C:ILE:CG1 | 1:308:C:ILE:CD1 | 3        | 2.89          |
| (2,18) | 1:282:F:LEU:CG  | 1:316:F:SER:CB  | 3        | 2.82          |
| (1,18) | 1:282:F:LEU:CG  | 1:316:F:SER:CB  | 3        | 2.82          |
| (2,16) | 1:297:A:ILE:CG1 | 1:308:A:ILE:CD1 | 4        | 2.51          |
| (1,16) | 1:297:A:ILE:CG1 | 1:308:A:ILE:CD1 | 4        | 2.51          |
| (2,19) | 1:283:D:ASP:CB  | 1:316:D:SER:CB  | 3        | 2.42          |
| (1,19) | 1:283:D:ASP:CB  | 1:316:D:SER:CB  | 3        | 2.42          |
| (2,16) | 1:297:J:ILE:CG2 | 1:308:J:ILE:CD1 | 2        | 2.32          |
| (1,16) | 1:297:J:ILE:CG2 | 1:308:J:ILE:CD1 | 2        | 2.32          |
| (2,19) | 1:283:I:ASP:CB  | 1:316:I:SER:CB  | 8        | 2.2           |
| (1,19) | 1:283:I:ASP:CB  | 1:316:I:SER:CB  | 8        | 2.2           |
| (2,17) | 1:297:G:ILE:CB  | 1:308:I:ILE:CD1 | 5        | 2.03          |
| (1,17) | 1:297:G:ILE:CB  | 1:308:I:ILE:CD1 | 5        | 2.03          |
| (2,16) | 1:297:C:ILE:CG2 | 1:308:C:ILE:CD1 | 7        | 2.01          |
| (1,16) | 1:297:C:ILE:CG2 | 1:308:C:ILE:CD1 | 7        | 2.01          |
| (2,17) | 1:297:E:ILE:CB  | 1:308:E:ILE:CD1 | 6        | 1.94          |
| (1,17) | 1:297:E:ILE:CB  | 1:308:E:ILE:CD1 | 6        | 1.94          |
| (2,5)  | 1:297:C:ILE:CD1 | 1:308:C:ILE:CD1 | 7        | 1.93          |
| (1,5)  | 1:297:C:ILE:CD1 | 1:308:C:ILE:CD1 | 7        | 1.93          |
| (2,16) | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 9        | 1.92          |
| (2,5)  | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 9        | 1.92          |
| (1,16) | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 9        | 1.92          |
| (1,5)  | 1:297:I:ILE:CG2 | 1:308:I:ILE:CD1 | 9        | 1.92          |
| (2,4)  | 1:308:D:ILE:CG2 | 1:297:D:ILE:CD1 | 9        | 1.91          |
| (1,4)  | 1:308:D:ILE:CG2 | 1:297:D:ILE:CD1 | 9        | 1.91          |
| (2,20) | 1:288:G:GLN:CA  | 1:316:G:SER:CB  | 10       | 1.87          |
| (1,20) | 1:288:G:GLN:CA  | 1:316:G:SER:CB  | 10       | 1.87          |
| (2,17) | 1:297:I:ILE:CB  | 1:308:I:ILE:CD1 | 1        | 1.86          |
| (1,17) | 1:297:I:ILE:CB  | 1:308:I:ILE:CD1 | 1        | 1.86          |
| (2,5)  | 1:297:H:ILE:CD1 | 1:308:H:ILE:CD1 | 10       | 1.84          |
| (1,5)  | 1:297:H:ILE:CD1 | 1:308:H:ILE:CD1 | 10       | 1.84          |
| (2,18) | 1:283:C:ASP:CG  | 1:316:A:SER:CB  | 7        | 1.77          |
| (1,18) | 1:283:C:ASP:CG  | 1:316:A:SER:CB  | 7        | 1.77          |

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| Key    | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|--------|-----------------|-----------------|----------|---------------|
| (2,5)  | 1:297:J:ILE:CD1 | 1:308:J:ILE:CD1 | 2        | 1.56          |
| (1,5)  | 1:297:J:ILE:CD1 | 1:308:J:ILE:CD1 | 2        | 1.56          |
| (2,18) | 1:282:J:LEU:CG  | 1:316:H:SER:CB  | 8        | 1.51          |
| (1,18) | 1:282:J:LEU:CG  | 1:316:H:SER:CB  | 8        | 1.51          |
| (2,5)  | 1:297:F:ILE:CD1 | 1:308:F:ILE:CD1 | 3        | 1.45          |
| (1,5)  | 1:297:F:ILE:CD1 | 1:308:F:ILE:CD1 | 3        | 1.45          |
| (2,20) | 1:283:D:ASP:CA  | 1:316:D:SER:CB  | 3        | 1.4           |
| (2,18) | 1:282:A:LEU:CG  | 1:316:C:SER:CB  | 2        | 1.4           |
| (1,20) | 1:283:D:ASP:CA  | 1:316:D:SER:CB  | 3        | 1.4           |
| (1,18) | 1:282:A:LEU:CG  | 1:316:C:SER:CB  | 2        | 1.4           |
| (2,2)  | 1:310:A:TYR:CB  | 1:297:A:ILE:CD1 | 3        | 1.37          |
| (1,2)  | 1:310:A:TYR:CB  | 1:297:A:ILE:CD1 | 3        | 1.37          |
| (2,19) | 1:283:D:ASP:CB  | 1:316:B:SER:CB  | 4        | 1.34          |
| (1,19) | 1:283:D:ASP:CB  | 1:316:B:SER:CB  | 4        | 1.34          |
| (2,20) | 1:283:H:ASP:CA  | 1:316:J:SER:CB  | 2        | 1.32          |
| (1,20) | 1:283:H:ASP:CA  | 1:316:J:SER:CB  | 2        | 1.32          |
| (2,16) | 1:297:D:ILE:CG1 | 1:308:D:ILE:CD1 | 6        | 1.31          |
| (2,2)  | 1:310:J:TYR:CB  | 1:297:J:ILE:CD1 | 4        | 1.31          |
| (1,16) | 1:297:D:ILE:CG1 | 1:308:D:ILE:CD1 | 6        | 1.31          |
| (1,2)  | 1:310:J:TYR:CB  | 1:297:J:ILE:CD1 | 4        | 1.31          |
| (2,22) | 1:312:H:PRO:CA  | 1:293:J:SER:CA  | 9        | 1.3           |
| (1,22) | 1:312:H:PRO:CA  | 1:293:J:SER:CA  | 9        | 1.3           |
| (2,21) | 1:285:H:SER:CB  | 1:316:F:SER:CB  | 8        | 1.29          |
| (2,19) | 1:283:A:ASP:CB  | 1:316:A:SER:CB  | 2        | 1.29          |
| (1,21) | 1:285:H:SER:CB  | 1:316:F:SER:CB  | 8        | 1.29          |
| (1,19) | 1:283:A:ASP:CB  | 1:316:A:SER:CB  | 2        | 1.29          |
| (2,2)  | 1:310:F:TYR:CB  | 1:297:F:ILE:CD1 | 6        | 1.22          |
| (1,2)  | 1:310:F:TYR:CB  | 1:297:F:ILE:CD1 | 6        | 1.22          |
| (2,22) | 1:312:J:PRO:CA  | 1:293:J:SER:CA  | 4        | 1.12          |
| (1,22) | 1:312:J:PRO:CA  | 1:293:J:SER:CA  | 4        | 1.12          |
| (2,20) | 1:283:A:ASP:CA  | 1:316:A:SER:CB  | 8        | 1.09          |
| (2,16) | 1:297:E:ILE:CG2 | 1:308:E:ILE:CD1 | 5        | 1.09          |
| (1,20) | 1:283:A:ASP:CA  | 1:316:A:SER:CB  | 8        | 1.09          |
| (1,16) | 1:297:E:ILE:CG2 | 1:308:E:ILE:CD1 | 5        | 1.09          |
| (2,22) | 1:312:G:PRO:CA  | 1:293:E:SER:CA  | 5        | 1.07          |
| (1,22) | 1:312:G:PRO:CA  | 1:293:E:SER:CA  | 5        | 1.07          |
| (2,16) | 1:297:J:ILE:CG1 | 1:308:J:ILE:CD1 | 1        | 1.03          |
| (1,16) | 1:297:J:ILE:CG1 | 1:308:J:ILE:CD1 | 1        | 1.03          |
| (2,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 1        | 0.98          |
| (2,5)  | 1:297:A:ILE:CD1 | 1:308:A:ILE:CD1 | 4        | 0.98          |
| (1,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 1        | 0.98          |
| (1,5)  | 1:297:A:ILE:CD1 | 1:308:A:ILE:CD1 | 4        | 0.98          |

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| Key    | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|--------|-----------------|-----------------|----------|---------------|
| (2,18) | 1:282:J:LEU:CG  | 1:316:J:SER:CB  | 1        | 0.96          |
| (1,18) | 1:282:J:LEU:CG  | 1:316:J:SER:CB  | 1        | 0.96          |
| (2,5)  | 1:297:G:ILE:CD1 | 1:308:I:ILE:CD1 | 5        | 0.94          |
| (1,5)  | 1:297:G:ILE:CD1 | 1:308:I:ILE:CD1 | 5        | 0.94          |
| (2,22) | 1:312:J:PRO:CA  | 1:293:H:SER:CA  | 2        | 0.78          |
| (2,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 1        | 0.78          |
| (2,2)  | 1:310:I:TYR:CB  | 1:297:G:ILE:CD1 | 5        | 0.78          |
| (1,22) | 1:312:J:PRO:CA  | 1:293:H:SER:CA  | 2        | 0.78          |
| (1,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 1        | 0.78          |
| (1,2)  | 1:310:I:TYR:CB  | 1:297:G:ILE:CD1 | 5        | 0.78          |
| (2,2)  | 1:310:C:TYR:CB  | 1:297:C:ILE:CD1 | 9        | 0.72          |
| (1,2)  | 1:310:C:TYR:CB  | 1:297:C:ILE:CD1 | 9        | 0.72          |
| (2,4)  | 1:308:F:ILE:CG2 | 1:297:F:ILE:CD1 | 8        | 0.71          |
| (1,4)  | 1:308:F:ILE:CG2 | 1:297:F:ILE:CD1 | 8        | 0.71          |
| (2,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 10       | 0.62          |
| (1,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 10       | 0.62          |
| (2,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 7        | 0.46          |
| (1,19) | 1:283:C:ASP:CB  | 1:316:A:SER:CB  | 7        | 0.46          |
| (2,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 7        | 0.34          |
| (1,2)  | 1:310:B:TYR:CB  | 1:297:B:ILE:CD1 | 7        | 0.34          |
| (2,21) | 1:285:A:SER:CB  | 1:316:A:SER:CB  | 3        | 0.32          |
| (2,1)  | 1:308:B:ILE:CA  | 1:297:B:ILE:CD1 | 9        | 0.32          |
| (1,21) | 1:285:A:SER:CB  | 1:316:A:SER:CB  | 3        | 0.32          |
| (1,1)  | 1:308:B:ILE:CA  | 1:297:B:ILE:CD1 | 9        | 0.32          |
| (2,22) | 1:312:A:PRO:CA  | 1:293:C:SER:CA  | 7        | 0.27          |
| (1,22) | 1:312:A:PRO:CA  | 1:293:C:SER:CA  | 7        | 0.27          |
| (2,20) | 1:283:C:ASP:CA  | 1:316:A:SER:CB  | 7        | 0.26          |
| (1,20) | 1:283:C:ASP:CA  | 1:316:A:SER:CB  | 7        | 0.26          |
| (2,4)  | 1:308:C:ILE:CG2 | 1:297:C:ILE:CD1 | 7        | 0.23          |
| (1,4)  | 1:308:C:ILE:CG2 | 1:297:C:ILE:CD1 | 7        | 0.23          |
| (2,2)  | 1:310:D:TYR:CB  | 1:297:D:ILE:CD1 | 8        | 0.2           |
| (1,2)  | 1:310:D:TYR:CB  | 1:297:D:ILE:CD1 | 8        | 0.2           |
| (2,4)  | 1:308:H:ILE:CG2 | 1:297:H:ILE:CD1 | 5        | 0.17          |
| (1,4)  | 1:308:H:ILE:CG2 | 1:297:H:ILE:CD1 | 5        | 0.17          |
| (2,4)  | 1:308:J:ILE:CG1 | 1:297:J:ILE:CD1 | 2        | 0.14          |
| (1,4)  | 1:308:J:ILE:CG1 | 1:297:J:ILE:CD1 | 2        | 0.14          |
| (2,20) | 1:283:D:ASP:CA  | 1:316:B:SER:CB  | 1        | 0.12          |
| (2,20) | 1:283:D:ASP:CA  | 1:316:B:SER:CB  | 4        | 0.12          |
| (1,20) | 1:283:D:ASP:CA  | 1:316:B:SER:CB  | 1        | 0.12          |
| (1,20) | 1:283:D:ASP:CA  | 1:316:B:SER:CB  | 4        | 0.12          |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found