



Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 09:07 PM UTC

PDB ID : 8G54 / pdb_00008g54
BMRB ID : 31074
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

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>.

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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

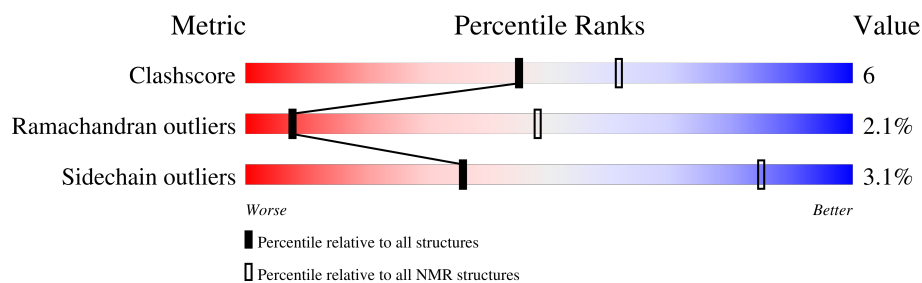
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 7%.

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



Metric	Whole archive (#Entries)	NMR archive (#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 ≥ 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	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:319, B:274-B:319, C:274-C:319, D:274-D:319, E:274-E:319 (230)	2.74	1

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 and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 9, 10
2	3, 7, 8
Single-model clusters	5; 6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4030 atoms, of which 2100 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	52	Total	C	H	N	O	S	0
			806	242	420	69	73	2	
1	B	52	Total	C	H	N	O	S	0
			806	242	420	69	73	2	
1	C	52	Total	C	H	N	O	S	0
			806	242	420	69	73	2	
1	D	52	Total	C	H	N	O	S	0
			806	242	420	69	73	2	
1	E	52	Total	C	H	N	O	S	0
			806	242	420	69	73	2	

- [illegible]

Chain B: 19% • • 74%

SER SER
PRO PRO
GLY GLY
SER SER
PRO PRO
GLY GLY
THR THR
PRO PRO
GLY GLY
SER SER
ARG ARG
SER SER
ARG ARG
THR THR
PRO PRO
SER SER
LEU LEU
PRO PRO
THR THR

SER
LYS
ILE
GLY
SER
THR
GLY
ASN
LEU
LYS
HIS
GLN
PRO
GLY
GLY
K274
V275
1278
S285
S289
D295
1308
L315
S320
K321
C322
G323
S324
L325
GLY
ASN
ILE
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ALA
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GLY
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THR
ALA
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PHE
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ASN
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LYS
HIS
GLN
PRO
GLY
GLY
K274
V275
1278
S285
S289
D295
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L315
S320
K321
C322
G323
S324
L325
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ASN
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GLY
GLN
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PRO
VAL
VAL
LYS
MET
SER
GLU
LYS
LEU
ASP
PHE
LYS
VAL
LYS
ASP

• Molecule 1: Microtubule-associated protein tau

Chain C: 19% 74%

SER SER
PRO PRO
GLY GLY
SER SER
PRO PRO
GLY GLY
THR THR
PRO PRO
GLY GLY
SER SER
ASP ASP
HIS HIS
GLN GLN
ARG ARG
SER SER
ARG ARG
THR THR
PRO PRO
SER SER
LEU LEU
PRO PRO
THR THR

SER
LYS
ILE
GLY
SER
THR
GLY
ASN
LEU
LYS
HIS
GLN
PRO
GLY
GLY
K274
V275
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S320
K321
C322
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S324
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GLY
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LEU
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HIS
GLN
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K274
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D295
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K321
C322
G323
S324
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ASP
PHE
LYS
VAL
LYS
ASP

• Molecule 1: Microtubule-associated protein tau

Chain D: 19% 74%

SER SER
PRO PRO
GLY GLY
SER SER
PRO PRO
GLY GLY
THR THR
PRO PRO
GLY GLY
SER SER
ASP ASP
HIS HIS
GLN GLN
ARG ARG
SER SER
ARG ARG
THR THR
PRO PRO
SER SER
LEU LEU
PRO PRO
THR THR

SER
LYS
ILE
GLY
SER
THR
GLY
ASN
LEU
LYS
HIS
GLN
PRO
GLY
GLY
K274
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S289
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S320
K321
C322
G323
S324
L325
GLY
ASN
ILE
HIS
HIS
ALA
LYS
PRO
GLY
GLY
GLN
THR
ALA
PRO
VAL
VAL
LYS
MET
SER
GLU
LYS
LEU
ASP
PHE
LYS
VAL
LYS
ASP

ARG
VAL
GLN
SER
LYS
ILE
GLY
SER
THR
GLY
ASN
LEU
LYS
HIS
GLN
PRO
GLY
GLY
K274
V275
1278
S285
S289
D295
1308
L315
S320
K321
C322
G323
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L325
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THR
ALA
PRO
VAL
VAL
LYS
MET
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GLU
LYS
LEU
ASP
PHE
LYS
VAL
LYS
ASP

• Molecule 1: Microtubule-associated protein tau

Chain E: 19% 74%

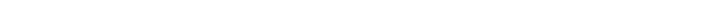
SER SER
PRO PRO
GLY GLY
SER SER
PRO PRO
GLY GLY
THR THR
PRO PRO
GLY GLY
SER SER
ASP ASP
HIS HIS
GLN GLN
ARG ARG
SER SER
ARG ARG
THR THR
PRO PRO
SER SER
LEU LEU
PRO PRO
THR THR

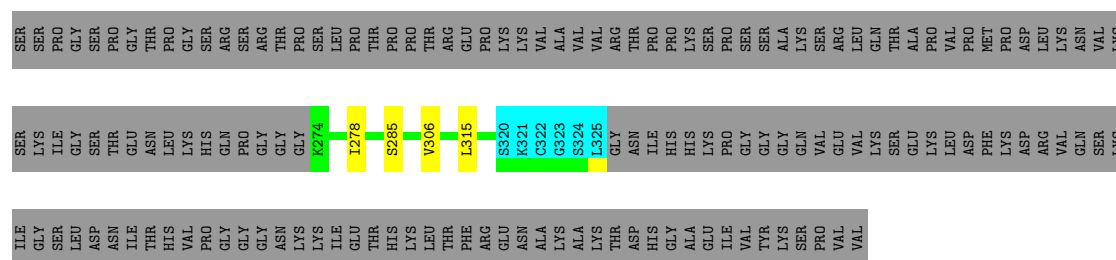
SER
LYS
ILE
GLY
SER
THR
GLY
ASN
LEU
LYS
HIS
GLN
PRO
GLY
GLY
K274
V275
1278
S285
S289
D295
1308
L315
S320
K321
C322
G323
S324
L325
GLY
ASN
ILE
HIS
HIS
ALA
LYS
PRO
GLY
GLY
GLN
THR
ALA
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MET
SER
GLU
LYS
LEU
ASP
PHE
LYS
VAL
LYS
ASP

ARG
VAL
GLN
SER
LYS
ILE
GLY
SER
THR
GLY
ASN
LEU
LYS
HIS
GLN
PRO
GLY
GLY
K274
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K321
C322
G323
S324
L325
GLY
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GLY
GLY
GLN
THR
ALA
PRO
VAL
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LYS
MET
SER
GLU
LYS
LEU
ASP
PHE
LYS
VAL
LYS
ASP

4.2.2 Score per residue for model 2

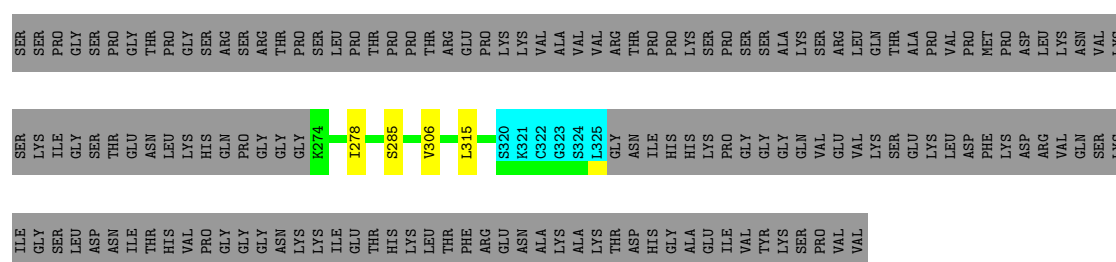
• Molecule 1: Microtubule-associated protein tau

Chain A:  21% 74%

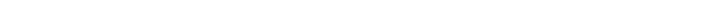


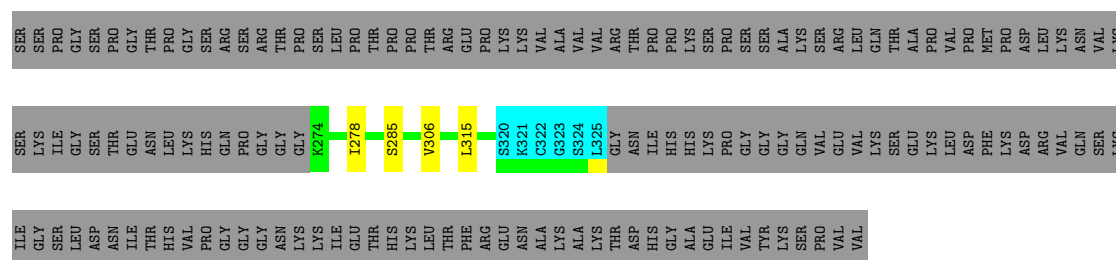
- Molecule 1: Microtubule-associated protein tau

Chain B: 21% • • 74%



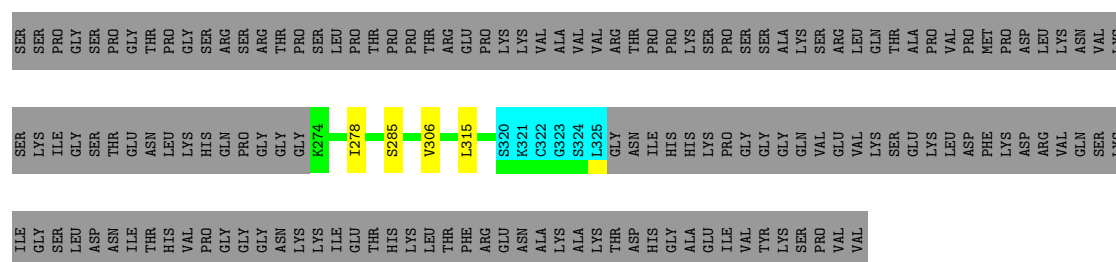
- Molecule 1: Microtubule-associated protein tau

Chain C:  21% • • 74%

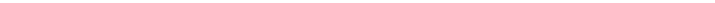


- Molecule 1: Microtubule-associated protein tau

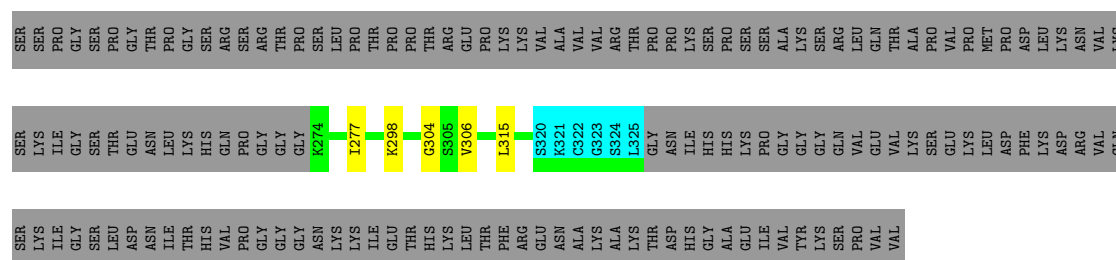
Chain D: 21% 74%



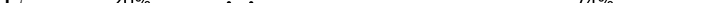
- Molecule 1: Microtubule-associated protein tau

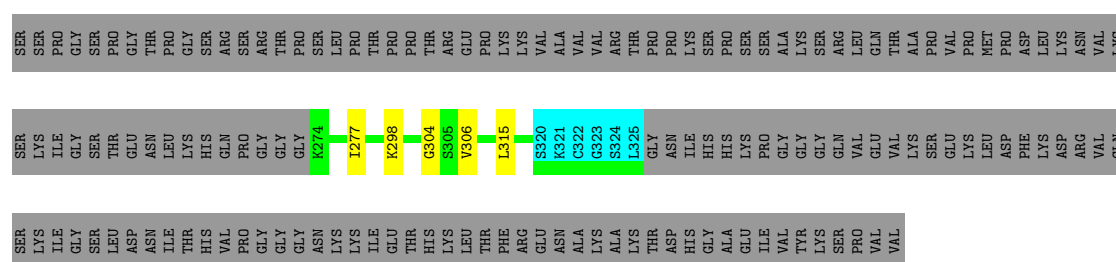
Chain E:  21% • • 74%

Chain D: 20% . . 74%



- Molecule 1: Microtubule-associated protein tau

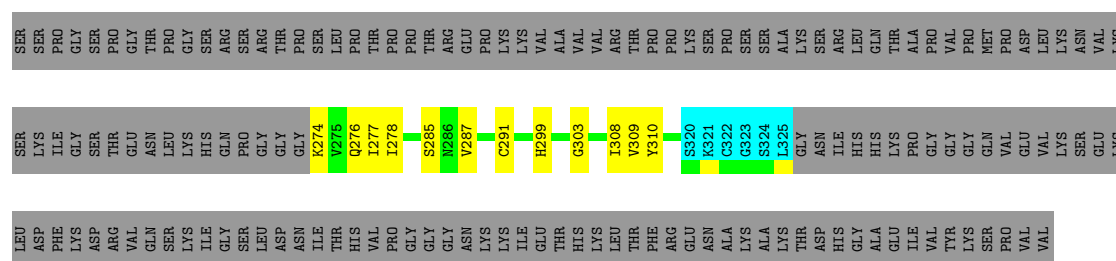
Chain E:  20% 74%



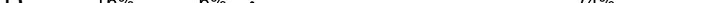
4.2.4 Score per residue for model 4

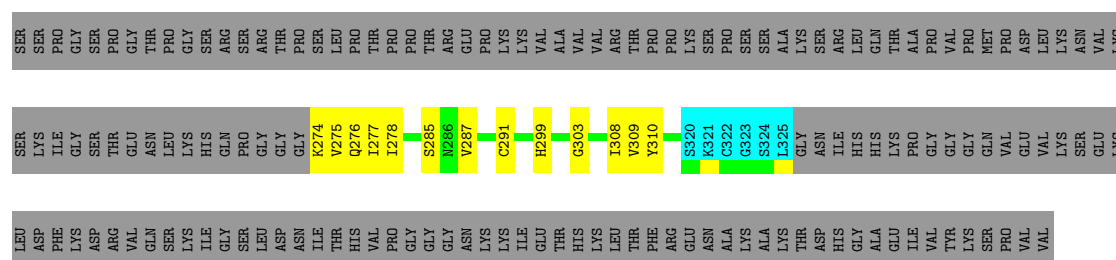
- Molecule 1: Microtubule-associated protein tau

Chain A: 17% 6% 74%



- Molecule 1: Microtubule-associated protein tau

Chain B:  16% 6% 74%



- [illegible]

- [illegible]

- Chain E: 
- | Chain | Category | Value |
|---------|----------|-------|
| Chain A | LYS | 1 |
| | ASP | 1 |
| | LEU | 1 |
| | PHE | 1 |
| | GLY | 1 |
| | LYS | 1 |
| | ASP | 1 |
| | ARG | 1 |
| | VAL | 1 |
| | GLN | 1 |
| Chain B | LEU | 1 |
| | GLN | 1 |
| | ILE | 1 |
| | LYS | 1 |
| | GLY | 1 |
| | SER | 1 |
| | GLY | 1 |
| | ASP | 1 |
| | ASN | 1 |
| | ILE | 1 |
| Chain C | THR | 1 |
| | HIS | 1 |
| | VAL | 1 |
| | PRO | 1 |
| | GLY | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | LYS | 1 |
| | ILE | 1 |
| | GLU | 1 |
| Chain D | THR | 1 |
| | HIS | 1 |
| | LYS | 1 |
| | LEU | 1 |
| | THR | 1 |
| | PHE | 1 |
| | ARG | 1 |
| | GLU | 1 |
| | ASN | 1 |
| | ALA | 1 |
| Chain E | LYS | 1 |
| | THR | 1 |
| | LEU | 1 |
| | ASP | 1 |
| | HIS | 1 |
| | GLY | 1 |
| | ALA | 1 |
| | GLU | 1 |
| | ILE | 1 |
| | VAL | 1 |
| Chain F | TYR | 1 |
| | LYS | 1 |
| | SER | 1 |
| | PRO | 1 |
| | VAL | 1 |
| | VAL | 1 |
| | LYS | 1 |
| | ASN | 1 |
| | VAL | 1 |
| | LYS | 1 |
| Chain G | THR | 1 |
| | GLN | 1 |
| | HIS | 1 |
| | ILE | 1 |
| | LEU | 1 |
| | ARG | 1 |
| | SER | 1 |
| | LYS | 1 |
| | GLY | 1 |
| | ASP | 1 |
| Chain H | PRO | 1 |
| | MET | 1 |
| | PRO | 1 |
| | ASP | 1 |
| | LEU | 1 |
| | LYS | 1 |
| | ASN | 1 |
| | VAL | 1 |
| | LYS | 1 |
| | VAL | 1 |
| Chain I | THR | 1 |
| | VAL | 1 |
| | ALA | 1 |
| | VAL | 1 |
| | VAL | 1 |
| | ARG | 1 |
| | THR | 1 |
| | PRO | 1 |
| | PRO | 1 |
| | LYS | 1 |
| Chain J | LYS | 1 |
| | THR | 1 |
| | ARG | 1 |
| | GLU | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | PRO | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain K | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLN | 1 |
| | HIS | 1 |
| | LEU | 1 |
| | ARG | 1 |
| | SER | 1 |
| | LYS | 1 |
| Chain L | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | VAL | 1 |
| | GLN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | GLY | 1 |
| | SER | 1 |
| | PRO | 1 |
| Chain M | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain N | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain O | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain P | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain Q | LYS | 1 |
| | THR | 1 |
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| | GLY | 1 |
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| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain R | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
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| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain S | LYS | 1 |
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| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain T | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain U | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |
| | ARG | 1 |
| | LEU | 1 |
| | PRO | 1 |
| | SER | 1 |
| Chain V | LYS | 1 |
| | THR | 1 |
| | GLY | 1 |
| | ASN | 1 |
| | GLY | 1 |
| | THR | 1 |

Chain A: 19% 74%

Chain B: 19% 74%

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

• Molecule 1: Microtubule-associated protein tau

Chain B: 18% 74%

SER SER PRO GLY SER PRO GLY SER ARG ARG THR SER LEU PRO THR PRO PRO THR VAL VAL VAL ARG THR PRO PRO LYS LYS VAL ALA VAL VAL ARG THR PRO PRO LYS SER PRO SER SER SER ALA LYS LYS SER ARG LEU GLN THR VAL PRO VAL MET VAL ASP LEU LYS ASN VAL VAL LYS

SER LYS ILE GLY THR ASN LEU HIS ARG PRO GLY THR K274 L277 L282 D283 L284 V287 C291 V300 V306 Q307 I308 L315 S320 K321 C322 G323 S324 L325 GLY ASN ILE HIS GLN THR PRO GLY GLY GLN VAL GLU VAL LYS SER ASN VAL LYS

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

• Molecule 1: Microtubule-associated protein tau

Chain C: 18% 74%

SER SER PRO GLY THR ASN LEU HIS ARG PRO GLY THR K274 L277 L282 D283 L284 V287 C291 V300 V306 Q307 I308 L315 S320 K321 C322 G323 S324 L325 GLY ASN ILE HIS GLN THR PRO GLY GLY GLN VAL GLU VAL LYS SER ASN VAL VAL LYS

SER LYS ILE GLY THR ASN LEU HIS ARG PRO GLY THR K274 L277 L282 D283 L284 V287 C291 V300 V306 Q307 I308 L315 S320 K321 C322 G323 S324 L325 GLY ASN ILE HIS GLN THR PRO GLY GLY GLN VAL GLU VAL LYS SER ASN VAL VAL LYS

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

• Molecule 1: Microtubule-associated protein tau

Chain D: 18% 74%

SER SER PRO GLY THR ASN LEU HIS ARG PRO GLY THR K274 L277 L282 D283 L284 V287 C291 V300 V306 Q307 I308 L315 S320 K321 C322 G323 S324 L325 GLY ASN ILE HIS GLN THR PRO GLY GLY GLN VAL GLU VAL LYS SER ASN VAL VAL LYS

SER LYS ILE GLY THR ASN LEU HIS ARG PRO GLY THR K274 L277 L282 D283 L284 V287 C291 V300 V306 Q307 I308 L315 S320 K321 C322 G323 S324 L325 GLY ASN ILE HIS GLN THR PRO GLY GLY GLN VAL GLU VAL LYS SER ASN VAL VAL LYS

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

• Molecule 1: Microtubule-associated protein tau

Chain E: 19% 74%

SER SER PRO GLY THR ASN LEU HIS ARG PRO GLY THR K274 L277 L282 D283 L284 V287 V300 V306 Q307 I308 L315 S320 K321 C322 G323 S324 L325 GLY ASN ILE HIS GLN THR PRO GLY GLY GLN VAL VAL VAL MET VAL VAL LYS SER ASP LEU LYS ASN VAL VAL LYS

SER LYS ILE GLY THR ASN LEU HIS ARG PRO GLY THR K274 L277 L282 D283 L284 V287 V300 V306 Q307 I308 L315 S320 K321 C322 G323 S324 L325 GLY ASN ILE HIS GLN THR PRO GLY GLY GLN VAL VAL VAL MET VAL VAL LYS SER ASP LEU LYS ASN VAL VAL LYS

PHE	LYS	ASP	ARG	VAL	GLN	SER	LYS	ILE	GLY	SER	LEU	ASP	ASN	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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4.2.6 Score per residue for model 6

- Molecule 1: Microtubule-associated protein tau



SER	SER	LYS	ILE	THR	GLY	PRO	THR	GLY	ASN	THR	GLY	LYS	PRO	ARG	GLY	THR	PRO	LEU	SER	THR	GLY	GLY	LYS	THR	GLY	LYS	LEU	PRO	THR	PRO	THR	THR	PRO	GLY	ASN	GLU	ALA	ILE	HIS	VAL	VAL	ARG	GLY	LYS	PRO	LYS	GLY	GLN	VAL	PRO	SER	VAL	LYS	ALA	LYS	SER	GLY	LYS	ARG	LEU	GLN	THR	PHE	ASP	LYS	ALA	PRO	VAL	GLN	MET	PRO	PRO	ASP	LYS	ILE	GLY	LYS	ASN	SER	LEU	VAL	LYS
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SER	LYS	ILE	THR	GLY	PRO	THR	GLY	ASN	THR	GLY	LYS	PRO	ARG	GLY	THR	PRO	LEU	SER	THR	GLY	GLY	LYS	THR	GLY	LYS	LEU	PRO	THR	PRO	THR	THR	PRO	GLY	ASN	GLU	ALA	ILE	HIS	VAL	VAL	ARG	GLY	LYS	PRO	LYS	GLY	GLN	VAL	PRO	SER	VAL	LYS	ALA	LYS	SER	GLY	LYS	ARG	LEU	GLN	THR	PHE	ASP	LYS	ALA	PRO	VAL	GLN	MET	PRO	PRO	ASP	LYS	ILE	GLY	LYS	ASN	SER	LEU	VAL	LYS	ASP
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- Molecule 1: Microtubule-associated protein tau



SER	SER	LYS	ILE	THR	GLY	PRO	THR	GLY	ASN	THR	GLY	LYS	PRO	ARG	GLY	THR	PRO	LEU	SER	THR	GLY	GLY	LYS	THR	GLY	LYS	LEU	PRO	THR	PRO	THR	THR	PRO	GLY	ASN	GLU	ALA	ILE	HIS	VAL	VAL	ARG	GLY	LYS	PRO	LYS	GLY	GLN	VAL	PRO	SER	VAL	LYS	ALA	LYS	SER	GLY	LYS	ARG	LEU	GLN	THR	PHE	ASP	LYS	ALA	PRO	VAL	GLN	MET	PRO	PRO	ASP	LYS	ILE	GLY	LYS	ASN	SER	LEU	VAL	LYS	ASP
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SER	LYS	ILE	THR	GLY	PRO	THR	GLY	ASN	THR	GLY	LYS	PRO	ARG	GLY	THR	PRO	LEU	SER	THR	GLY	GLY	LYS	THR	GLY	LYS	LEU	PRO	THR	PRO	THR	THR	PRO	GLY	ASN	GLU	ALA	ILE	HIS	VAL	VAL	ARG	GLY	LYS	PRO	LYS	GLY	GLN	VAL	PRO	SER	VAL	LYS	ALA	LYS	SER	GLY	LYS	ARG	LEU	GLN	THR	PHE	ASP	LYS	ALA	PRO	VAL	GLN	MET	PRO	PRO	ASP	LYS	ILE	GLY	LYS	ASN	SER	LEU	VAL	LYS	ASP
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ASN	ILE	THR	HIS	VAL	GLY	GLY	ASN	LYS	LYS	ILE	GLY	THR	HIS	LYS	LEU	THR	PHE	ARG	GLU	ASN	ALA	LYS	LYS	ALA	THR	ASP	HIS	ILE	GLY	ALA	GLY	LYS	THR	ASP	VAL	PRO	VAL	VAL
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- Molecule 1: Microtubule-associated protein tau



SER	SER	LYS	ILE	THR	GLY	PRO	THR	GLY	ASN	THR	GLY	LYS	PRO	ARG	GLY	THR	PRO	LEU	SER	THR	GLY	GLY	LYS	THR	GLY	LYS	LEU	PRO	THR	PRO	THR	THR	PRO	GLY	ASN	GLU	ALA	ILE	HIS	VAL	VAL	ARG	GLY	LYS	PRO	LYS	GLY	GLN	VAL	PRO	SER	VAL	LYS	ALA	LYS	SER	GLY	LYS	ARG	LEU	GLN	THR	PHE	ASP	LYS	ALA	PRO	VAL	GLN	MET	PRO	PRO	ASP	LYS	ILE	GLY	LYS	ASN	SER	LEU	VAL	LYS	ASP
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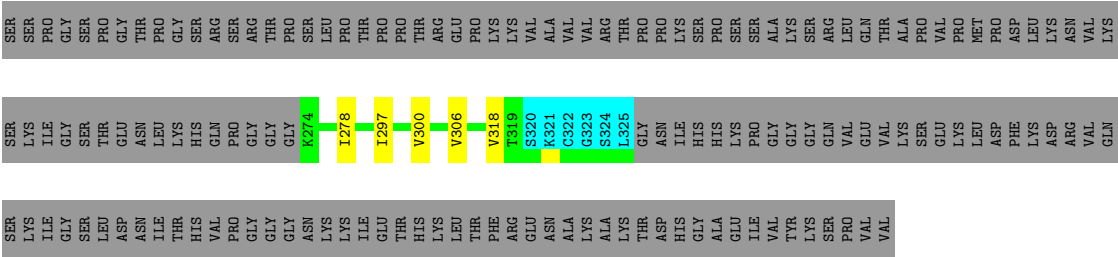
SER	LYS	ILE	THR	GLY	PRO	THR	GLY	ASN	THR	GLY	LYS	PRO	ARG	GLY	THR	PRO	LEU	SER	THR	GLY	GLY	LYS	THR	GLY	LYS	LEU	PRO	THR	PRO	THR	THR	PRO	GLY	ASN	GLU	ALA	ILE	HIS	VAL	VAL	ARG	GLY	LYS	PRO	LYS	GLY	GLN	VAL	PRO	SER	VAL	LYS	ALA	LYS	SER	GLY	LYS	ARG	LEU	GLN	THR	PHE	ASP	LYS	ALA	PRO	VAL	GLN	MET	PRO	PRO	ASP	LYS	ILE	GLY	LYS	ASN	SER	LEU	VAL	LYS	ASP
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ASN	ILE	THR	HIS	VAL	GLY	GLY	ASN	LYS	LYS	ILE	GLY	THR	HIS	LYS	LEU	THR	PHE	ARG	GLU	ASN	ALA	LYS	LYS	ALA	THR	ASP	HIS	ILE	GLY	ALA	GLY	LYS	THR	ASP	VAL	PRO	VAL	VAL
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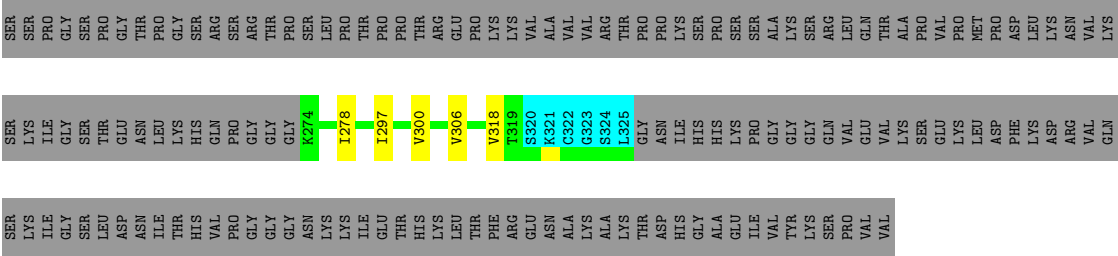
- Molecule 1: Microtubule-associated protein tau



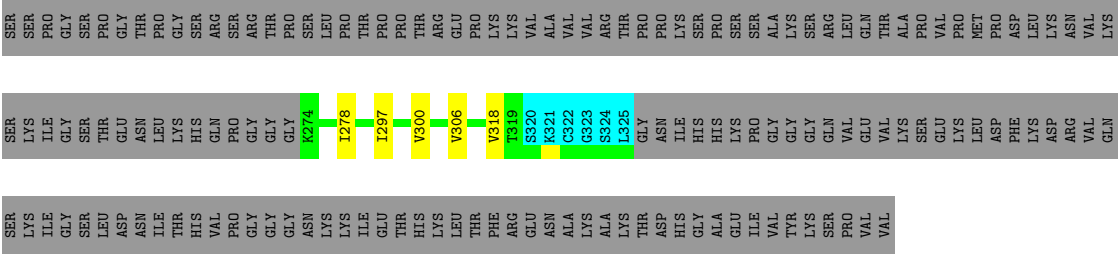
SER	SER	PRO	GLY	SER	PRO	PRO	GLY	THR	PRO	GLY	SER	ARG	ARG	THR	THR	SER	SER	LEU	PRO	THR	GLY	GLY	LYS	THR	GLY	LYS	LEU	PRO	THR	PRO	THR	THR	PRO	GLY	ASN	GLU	ALA	ILE	HIS	VAL	VAL	ARG	GLY	LYS	PRO	LYS	GLY	GLN	VAL	PRO	SER	VAL	LYS	ALA	LYS	SER	GLY	LYS	ARG	LEU	GLN	THR	PHE	ASP	LYS	ALA	PRO	VAL	GLN	MET	PRO	PRO	ASP	LYS	ILE	GLY	LYS	ASN	SER	LEU	VAL	LYS	ASP
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• Molecule 1: Microtubule-associated protein tau

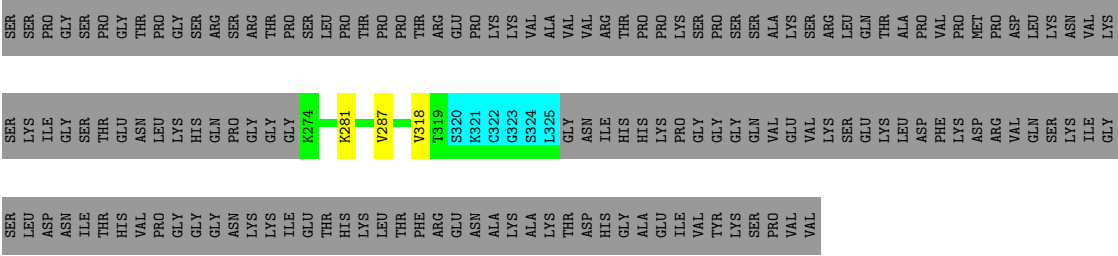


• Molecule 1: Microtubule-associated protein tau



4.2.8 Score per residue for model 8

• Molecule 1: Microtubule-associated protein tau



• Molecule 1: Microtubule-associated protein tau

Chain B: 21% • • 74%

[illegible]

- Molecule 1: Microtubule-associated protein tau

Chain C:  21% • • 74%

GLY	LEU	ASP	ASN	ILE	THR	HIS	VAL	PRO	GLY	GLY	ASN	LYS	ILE	GLU	THR	HIS	THR	PHE	ARG	GLU	ASN	ALA	LYS	ALA	LYS	THR	ASP	GLY	ALA	GLU	ILE	VAL	TYR	LYS	SER	PRO	VAL	VAL									
SER	SER	ILE	GLY	SER	THR	GLU	LEU	HIS	GLN	GLY	PRO	K274	K281	L282	V287	V318	T319	S320	K321	C322	G323	S324	L325	GLY	ASN	ARG	THR	PRO	PRO	SER	PRO	GLY	SER	SER	ALA	LYS	SER	ARG	LEU	GLN	THR	ALA	VAL	PRO	ASN	LYS	VAL

- Molecule 1: Microtubule-associated protein tau

Chain D: 21% 74%

[illegible]

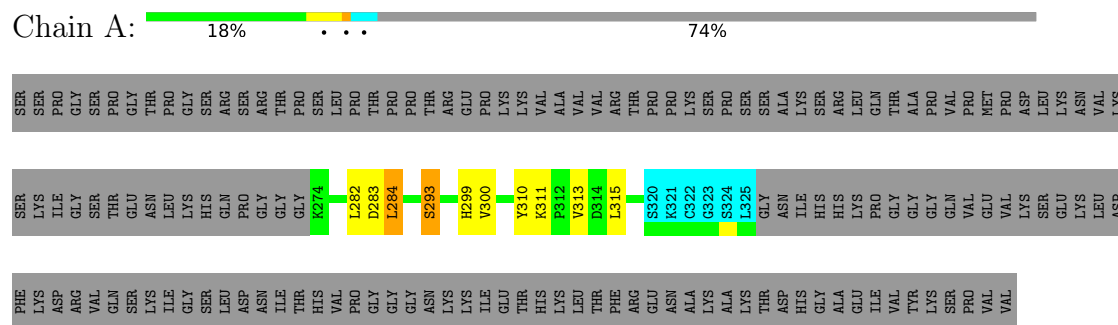
- Molecule 1: Microtubule-associated protein tau

Chain E: 21% 74%

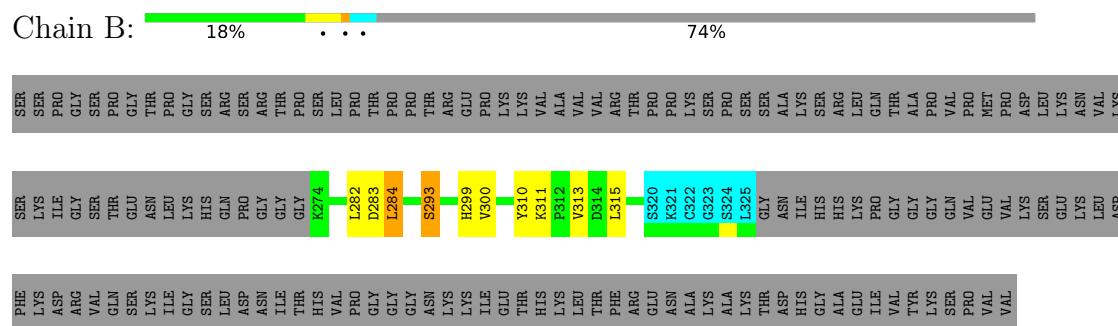
[illegible]

4.2.9 Score per residue for model 9

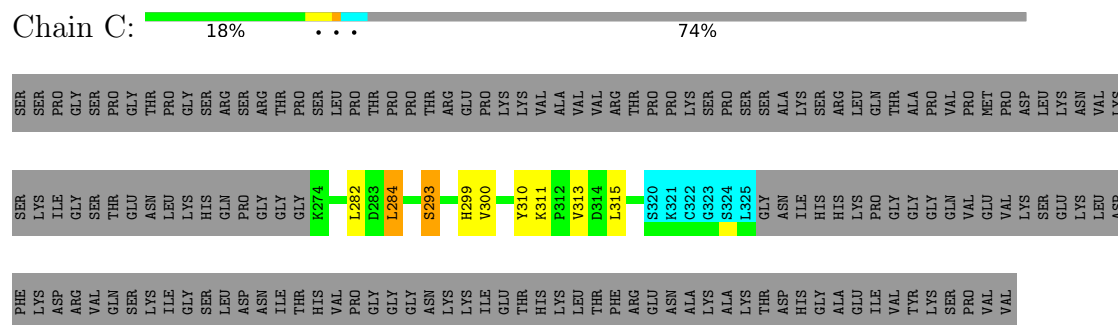
• Molecule 1: Microtubule-associated protein tau



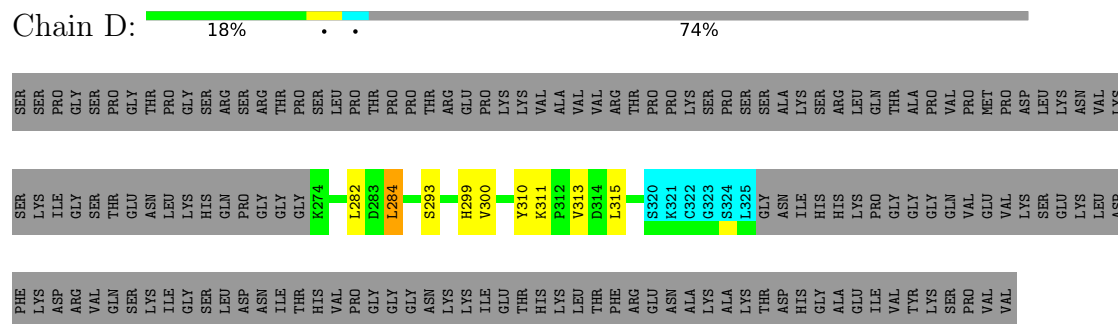
• Molecule 1: Microtubule-associated protein tau



• Molecule 1: Microtubule-associated protein tau

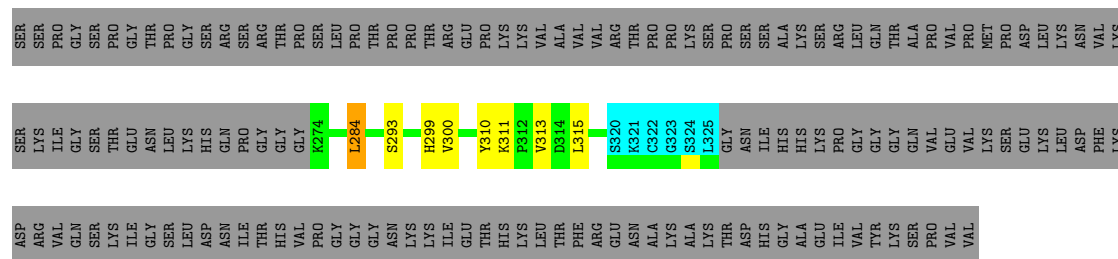


• Molecule 1: Microtubule-associated protein tau



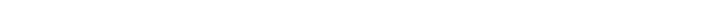
- Molecule 1: Microtubule-associated protein tau

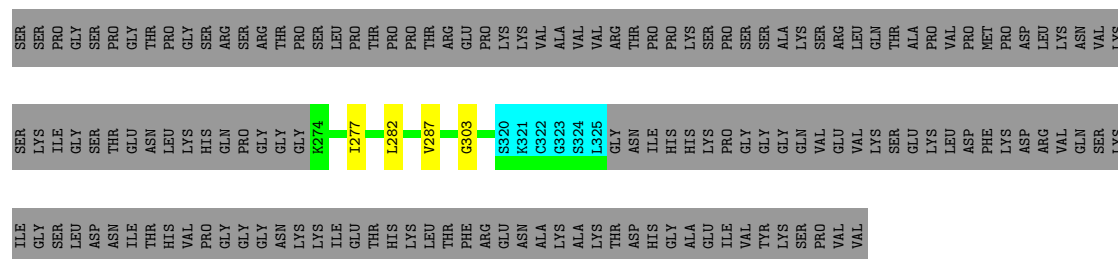
Chain E: 19% . . 74%



4.2.10 Score per residue for model 10

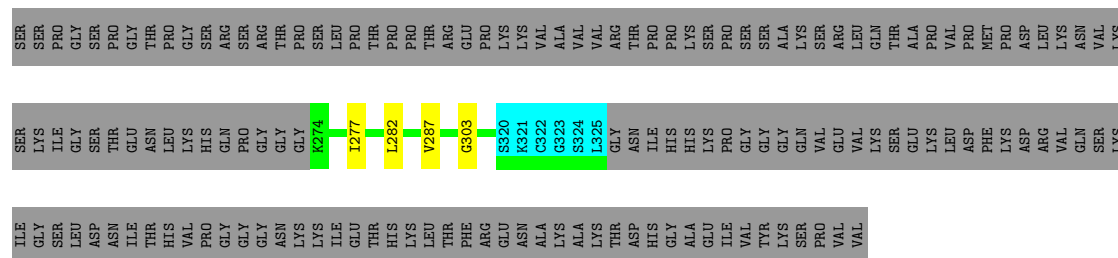
- Molecule 1: Microtubule-associated protein tau

Chain A:  21% 74%



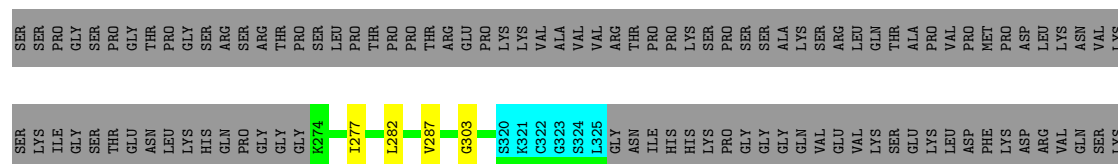
- Molecule 1: Microtubule-associated protein tau

Chain B:  21% 74%



- Molecule 1: Microtubule-associated protein tau

Chain C: 21% • • 74%



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● Molecule 1: Microtubule-associated protein tau



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● Molecule 1: Microtubule-associated protein tau



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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	223
Number of shifts mapped to atoms	219
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	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.

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	347	378	376	5±4
1	B	347	378	376	8±6
1	C	347	378	376	7±5
1	D	347	378	376	7±5
1	E	347	378	376	5±4
All	All	17350	18900	18800	229

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:300:VAL:HG13	1:B:300:VAL:HG23	0.78	1.55	7	2
1:C:300:VAL:HG13	1:D:300:VAL:HG23	0.78	1.55	7	2
1:D:300:VAL:HG13	1:E:300:VAL:HG23	0.78	1.55	7	2
1:B:300:VAL:HG13	1:C:300:VAL:HG23	0.78	1.55	7	2
1:A:287:VAL:HG12	1:B:287:VAL:HG22	0.61	1.73	5	4
1:B:287:VAL:HG12	1:C:287:VAL:HG22	0.60	1.73	5	4
1:C:287:VAL:HG12	1:D:287:VAL:HG22	0.60	1.73	5	4
1:D:287:VAL:HG12	1:E:287:VAL:HG22	0.60	1.73	5	4
1:A:277:ILE:HD11	1:A:291:CYS:SG	0.59	2.38	4	1
1:B:277:ILE:HD11	1:B:291:CYS:SG	0.59	2.38	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:277:ILE:HD11	1:C:291:CYS:SG	0.59	2.38	4	1
1:D:277:ILE:HD11	1:D:291:CYS:SG	0.58	2.38	4	1
1:E:277:ILE:HD11	1:E:291:CYS:SG	0.58	2.38	4	1
1:A:306:VAL:HG12	1:B:306:VAL:HG22	0.57	1.76	2	1
1:D:306:VAL:HG12	1:E:306:VAL:HG22	0.57	1.76	2	1
1:B:306:VAL:HG12	1:C:306:VAL:HG22	0.57	1.76	2	1
1:C:306:VAL:HG12	1:D:306:VAL:HG22	0.57	1.76	2	1
1:A:291:CYS:CB	1:B:277:ILE:HD11	0.56	2.31	5	1
1:D:291:CYS:CB	1:E:277:ILE:HD11	0.56	2.31	5	1
1:B:291:CYS:CB	1:C:277:ILE:HD11	0.56	2.31	5	1
1:C:291:CYS:CB	1:D:277:ILE:HD11	0.56	2.31	5	1
1:A:309:VAL:CG1	1:B:309:VAL:HG23	0.55	2.31	4	1
1:B:309:VAL:CG1	1:C:309:VAL:HG23	0.55	2.31	4	1
1:D:309:VAL:CG1	1:E:309:VAL:HG23	0.55	2.31	4	1
1:C:309:VAL:CG1	1:D:309:VAL:HG23	0.54	2.31	4	1
1:D:291:CYS:SG	1:E:277:ILE:HD11	0.53	2.44	5	1
1:B:291:CYS:SG	1:C:277:ILE:HD11	0.53	2.44	5	1
1:C:291:CYS:SG	1:D:277:ILE:HD11	0.53	2.44	5	1
1:A:291:CYS:SG	1:B:277:ILE:HD11	0.53	2.44	5	1
1:A:275:VAL:HG23	1:B:275:VAL:HG13	0.53	1.80	1	1
1:B:275:VAL:HG23	1:C:275:VAL:HG13	0.53	1.80	1	1
1:C:275:VAL:HG23	1:D:275:VAL:HG13	0.53	1.80	1	1
1:D:275:VAL:HG23	1:E:275:VAL:HG13	0.52	1.80	1	1
1:A:276:GLN:O	1:A:277:ILE:HD13	0.52	2.04	4	1
1:B:276:GLN:O	1:B:277:ILE:HD13	0.52	2.04	4	1
1:D:276:GLN:O	1:D:277:ILE:HD13	0.52	2.04	4	1
1:C:276:GLN:O	1:C:277:ILE:HD13	0.52	2.04	4	1
1:E:276:GLN:O	1:E:277:ILE:HD13	0.52	2.05	4	1
1:D:306:VAL:CG1	1:E:306:VAL:HG22	0.48	2.38	2	1
1:B:306:VAL:CG1	1:C:306:VAL:HG22	0.48	2.39	2	1
1:A:306:VAL:CG1	1:B:306:VAL:HG22	0.48	2.39	2	1
1:C:306:VAL:CG1	1:D:306:VAL:HG22	0.48	2.39	2	1
1:A:284:LEU:HD21	1:B:284:LEU:HB3	0.48	1.85	9	1
1:B:284:LEU:HD21	1:C:284:LEU:HB3	0.48	1.85	9	1
1:B:287:VAL:CG1	1:C:287:VAL:HG22	0.48	2.38	5	2
1:C:287:VAL:CG1	1:D:287:VAL:HG22	0.48	2.38	5	2
1:D:287:VAL:CG1	1:E:287:VAL:HG22	0.48	2.38	5	2
1:C:284:LEU:HD21	1:D:284:LEU:HB3	0.48	1.85	9	1
1:A:287:VAL:CG1	1:B:287:VAL:HG22	0.47	2.38	5	2
1:D:284:LEU:HD21	1:E:284:LEU:HB3	0.47	1.86	9	1
1:E:277:ILE:HD11	1:E:291:CYS:HB2	0.47	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:ILE:HD11	1:A:291:CYS:HB2	0.47	1.87	4	1
1:B:277:ILE:HD11	1:B:291:CYS:HB2	0.47	1.87	4	1
1:C:277:ILE:HD11	1:C:291:CYS:HB2	0.47	1.87	4	1
1:D:277:ILE:HD11	1:D:291:CYS:HB2	0.47	1.87	4	1
1:D:277:ILE:N	1:D:277:ILE:HD12	0.46	2.25	3	2
1:E:277:ILE:HD12	1:E:277:ILE:N	0.46	2.25	3	3
1:B:277:ILE:HD12	1:B:277:ILE:N	0.46	2.26	3	3
1:C:277:ILE:N	1:C:277:ILE:HD12	0.46	2.26	3	3
1:A:277:ILE:HD12	1:A:277:ILE:N	0.46	2.26	3	3
1:A:309:VAL:HG13	1:B:309:VAL:HG23	0.46	1.87	4	1
1:B:309:VAL:HG13	1:C:309:VAL:HG23	0.46	1.87	4	1
1:E:300:VAL:HG23	1:E:300:VAL:O	0.46	2.12	9	1
1:A:300:VAL:HG23	1:A:300:VAL:O	0.45	2.11	9	1
1:C:300:VAL:O	1:C:300:VAL:HG23	0.45	2.11	9	1
1:D:300:VAL:HG23	1:D:300:VAL:O	0.45	2.12	9	1
1:C:309:VAL:HG13	1:D:309:VAL:HG23	0.45	1.87	4	1
1:D:309:VAL:HG13	1:E:309:VAL:HG23	0.45	1.87	4	1
1:B:300:VAL:O	1:B:300:VAL:HG23	0.45	2.11	9	1
1:C:308:ILE:HD12	1:C:308:ILE:N	0.45	2.27	1	1
1:D:308:ILE:N	1:D:308:ILE:HD12	0.45	2.27	1	1
1:E:308:ILE:HD12	1:E:308:ILE:N	0.45	2.27	1	1
1:A:308:ILE:HD12	1:A:308:ILE:N	0.45	2.27	1	1
1:B:308:ILE:HD12	1:B:308:ILE:N	0.45	2.27	1	1
1:A:291:CYS:SG	1:B:275:VAL:HG12	0.45	2.52	4	1
1:B:291:CYS:SG	1:C:275:VAL:HG12	0.45	2.52	4	1
1:D:318:VAL:HG12	1:E:318:VAL:HG22	0.45	1.89	8	2
1:C:291:CYS:SG	1:D:275:VAL:HG12	0.45	2.52	4	1
1:D:291:CYS:SG	1:E:275:VAL:HG12	0.45	2.52	4	1
1:C:318:VAL:HG12	1:D:318:VAL:HG22	0.44	1.89	8	2
1:A:318:VAL:HG12	1:B:318:VAL:HG22	0.44	1.89	8	2
1:D:284:LEU:HD21	1:E:284:LEU:CB	0.44	2.42	9	1
1:C:276:GLN:CD	1:C:278:ILE:HD11	0.44	2.37	4	1
1:B:276:GLN:CD	1:B:278:ILE:HD11	0.44	2.37	4	1
1:E:276:GLN:CD	1:E:278:ILE:HD11	0.44	2.37	4	1
1:B:318:VAL:HG12	1:C:318:VAL:HG22	0.44	1.89	8	2
1:A:276:GLN:CD	1:A:278:ILE:HD11	0.44	2.37	4	1
1:D:276:GLN:CD	1:D:278:ILE:HD11	0.44	2.37	4	1
1:A:297:ILE:HD12	1:A:297:ILE:N	0.44	2.28	7	1
1:B:284:LEU:HD21	1:C:284:LEU:CB	0.44	2.42	9	1
1:C:284:LEU:HD21	1:D:284:LEU:CB	0.44	2.42	9	1
1:B:297:ILE:HD12	1:B:297:ILE:N	0.44	2.28	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:284:LEU:HD21	1:B:284:LEU:CB	0.44	2.42	9	1
1:C:297:ILE:N	1:C:297:ILE:HD12	0.44	2.28	7	1
1:D:278:ILE:O	1:E:278:ILE:HA	0.43	2.13	1	1
1:D:297:ILE:HD12	1:D:297:ILE:N	0.43	2.28	7	1
1:E:297:ILE:HD12	1:E:297:ILE:N	0.43	2.27	7	1
1:A:300:VAL:HG11	1:B:306:VAL:HG23	0.43	1.89	5	1
1:B:300:VAL:HG11	1:C:306:VAL:HG23	0.43	1.89	5	1
1:E:277:ILE:HD11	1:E:291:CYS:CB	0.43	2.43	4	1
1:A:278:ILE:O	1:B:278:ILE:HA	0.43	2.14	1	1
1:A:315:LEU:N	1:A:315:LEU:HD23	0.43	2.29	2	2
1:B:315:LEU:HD23	1:B:315:LEU:N	0.43	2.29	2	2
1:C:315:LEU:HD23	1:C:315:LEU:N	0.43	2.29	2	2
1:E:315:LEU:HD23	1:E:315:LEU:N	0.43	2.29	2	1
1:C:277:ILE:HD11	1:C:291:CYS:CB	0.43	2.43	4	1
1:D:277:ILE:HD11	1:D:291:CYS:CB	0.43	2.43	4	1
1:B:277:ILE:HD11	1:B:291:CYS:CB	0.43	2.43	4	1
1:B:278:ILE:O	1:C:278:ILE:HA	0.43	2.14	1	1
1:D:315:LEU:N	1:D:315:LEU:HD23	0.43	2.29	2	1
1:A:277:ILE:HD11	1:A:291:CYS:CB	0.43	2.43	4	1
1:C:278:ILE:O	1:D:278:ILE:HA	0.43	2.14	1	1
1:A:278:ILE:HG23	1:A:278:ILE:O	0.43	2.13	7	2
1:C:300:VAL:HG11	1:D:306:VAL:HG23	0.43	1.89	5	1
1:E:278:ILE:HG23	1:E:278:ILE:O	0.42	2.14	7	2
1:B:278:ILE:O	1:B:278:ILE:HG23	0.42	2.13	7	3
1:C:278:ILE:O	1:C:278:ILE:HG23	0.42	2.13	7	3
1:D:277:ILE:HD12	1:D:277:ILE:N	0.42	2.29	5	1
1:D:278:ILE:HG23	1:D:278:ILE:O	0.42	2.14	7	2
1:D:300:VAL:HG11	1:E:306:VAL:HG23	0.42	1.89	5	1
1:B:308:ILE:HD11	1:B:310:TYR:CE1	0.42	2.50	4	1
1:A:308:ILE:HD11	1:A:310:TYR:CE1	0.42	2.50	4	1
1:B:315:LEU:C	1:B:315:LEU:HD23	0.42	2.40	5	3
1:D:308:ILE:HD11	1:D:310:TYR:CE1	0.42	2.50	4	1
1:C:308:ILE:HD11	1:C:310:TYR:CE1	0.42	2.50	4	1
1:A:315:LEU:C	1:A:315:LEU:HD23	0.42	2.40	5	3
1:C:315:LEU:C	1:C:315:LEU:HD23	0.42	2.40	5	3
1:D:315:LEU:C	1:D:315:LEU:HD23	0.42	2.40	5	3
1:E:308:ILE:HD11	1:E:310:TYR:CE1	0.42	2.50	4	1
1:E:300:VAL:HG13	1:E:300:VAL:O	0.42	2.15	7	2
1:E:308:ILE:HG23	1:E:308:ILE:O	0.42	2.15	5	1
1:E:315:LEU:C	1:E:315:LEU:HD23	0.42	2.40	5	3
1:D:308:ILE:HG23	1:D:308:ILE:O	0.41	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:308:ILE:HG23	1:C:308:ILE:O	0.41	2.15	5	1
1:B:308:ILE:HG23	1:B:308:ILE:O	0.41	2.15	5	1
1:A:300:VAL:CG1	1:B:300:VAL:HG23	0.41	2.39	5	1
1:D:300:VAL:HG13	1:D:300:VAL:O	0.41	2.15	7	2
1:A:308:ILE:HG23	1:A:308:ILE:O	0.41	2.15	5	1
1:B:284:LEU:N	1:B:284:LEU:HD12	0.41	2.31	5	1
1:B:300:VAL:HG13	1:B:300:VAL:O	0.41	2.15	7	2
1:D:284:LEU:N	1:D:284:LEU:HD12	0.41	2.31	5	1
1:C:284:LEU:N	1:C:284:LEU:HD12	0.41	2.31	5	2
1:E:284:LEU:N	1:E:284:LEU:HD12	0.41	2.31	5	2
1:A:284:LEU:N	1:A:284:LEU:HD12	0.41	2.31	5	1
1:A:300:VAL:HG13	1:A:300:VAL:O	0.41	2.16	7	2
1:C:300:VAL:HG13	1:C:300:VAL:O	0.41	2.16	7	2
1:A:282:LEU:C	1:A:282:LEU:HD23	0.41	2.41	9	1
1:B:282:LEU:C	1:B:282:LEU:HD23	0.41	2.41	9	1
1:A:278:ILE:O	1:A:278:ILE:HG23	0.41	2.16	1	1
1:E:282:LEU:C	1:E:282:LEU:HD23	0.41	2.41	8	1
1:A:283:ASP:HA	1:B:283:ASP:O	0.41	2.15	9	1
1:C:282:LEU:C	1:C:282:LEU:HD23	0.41	2.41	9	1
1:D:315:LEU:HD23	1:D:315:LEU:N	0.40	2.31	3	1
1:A:291:CYS:HB2	1:B:277:ILE:HD11	0.40	1.93	5	1
1:E:315:LEU:N	1:E:315:LEU:HD23	0.40	2.31	3	1
1:B:291:CYS:HB2	1:C:277:ILE:HD11	0.40	1.94	5	1
1:D:282:LEU:C	1:D:282:LEU:HD23	0.40	2.41	8	2
1:C:310:TYR:CZ	1:C:313:VAL:HG21	0.40	2.51	9	1
1:D:310:TYR:CZ	1:D:313:VAL:HG21	0.40	2.51	9	1
1:E:310:TYR:CZ	1:E:313:VAL:HG21	0.40	2.51	9	1
1:D:278:ILE:O	1:D:278:ILE:HG23	0.40	2.17	1	1
1:C:291:CYS:HB2	1:D:277:ILE:HD11	0.40	1.94	5	1
1:C:282:LEU:HD23	1:C:282:LEU:C	0.40	2.41	8	1
1:A:310:TYR:CZ	1:A:313:VAL:HG21	0.40	2.51	9	1
1:B:310:TYR:CZ	1:B:313:VAL:HG21	0.40	2.51	9	1
1:D:284:LEU:HD12	1:D:284:LEU:N	0.40	2.31	4	1
1:D:291:CYS:HB2	1:E:277:ILE:HD11	0.40	1.94	5	1
1:B:282:LEU:HD23	1:B:282:LEU:C	0.40	2.41	8	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	45/202 (22%)	40±1 (89±2%)	4±1 (8±2%)	1±1 (2±2%)	7	47
1	B	45/202 (22%)	40±1 (89±2%)	4±1 (8±2%)	1±1 (2±2%)	7	47
1	C	45/202 (22%)	40±1 (89±2%)	4±1 (9±2%)	1±1 (2±2%)	7	47
1	D	45/202 (22%)	40±1 (89±2%)	4±1 (9±2%)	1±1 (2±2%)	8	49
1	E	45/202 (22%)	40±1 (89±2%)	4±1 (9±2%)	1±1 (2±2%)	8	49
All	All	2250/10100 (22%)	2007 (89%)	195 (9%)	48 (2%)	8	48

All 28 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	299	HIS	3
1	B	299	HIS	3
1	C	299	HIS	3
1	D	299	HIS	3
1	E	299	HIS	3
1	A	306	VAL	2
1	B	306	VAL	2
1	C	306	VAL	2
1	D	306	VAL	2
1	E	306	VAL	2
1	A	303	GLY	2
1	B	303	GLY	2
1	C	303	GLY	2
1	D	303	GLY	2
1	E	303	GLY	2
1	A	298	LYS	1
1	A	304	GLY	1
1	B	298	LYS	1
1	B	304	GLY	1
1	C	298	LYS	1
1	C	304	GLY	1
1	D	298	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	D	304	GLY	1
1	E	298	LYS	1
1	E	304	GLY	1
1	A	293	SER	1
1	B	293	SER	1
1	C	293	SER	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	42/175 (24%)	41±1 (97±2%)	1±1 (3±2%)	36	85
1	B	42/175 (24%)	41±1 (97±2%)	1±1 (3±2%)	36	85
1	C	42/175 (24%)	41±1 (97±2%)	1±1 (3±2%)	36	85
1	D	42/175 (24%)	41±1 (97±2%)	1±1 (3±2%)	36	85
1	E	42/175 (24%)	41±1 (97±2%)	1±1 (3±2%)	36	85
All	All	2100/8750 (24%)	2035 (97%)	65 (3%)	36	85

All 50 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	285	SER	3
1	B	285	SER	3
1	C	285	SER	3
1	D	285	SER	3
1	E	285	SER	3
1	A	282	LEU	2
1	B	282	LEU	2
1	C	282	LEU	2
1	D	282	LEU	2
1	E	282	LEU	2
1	A	289	SER	1
1	A	295	ASP	1
1	B	289	SER	1
1	B	295	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	C	289	SER	1
1	C	295	ASP	1
1	D	289	SER	1
1	D	295	ASP	1
1	E	289	SER	1
1	E	295	ASP	1
1	A	274	LYS	1
1	B	274	LYS	1
1	C	274	LYS	1
1	D	274	LYS	1
1	E	274	LYS	1
1	A	300	VAL	1
1	B	300	VAL	1
1	C	300	VAL	1
1	D	300	VAL	1
1	E	300	VAL	1
1	A	281	LYS	1
1	B	281	LYS	1
1	C	281	LYS	1
1	D	281	LYS	1
1	E	281	LYS	1
1	A	284	LEU	1
1	A	293	SER	1
1	A	311	LYS	1
1	B	284	LEU	1
1	B	293	SER	1
1	B	311	LYS	1
1	C	284	LEU	1
1	C	293	SER	1
1	C	311	LYS	1
1	D	284	LEU	1
1	D	293	SER	1
1	D	311	LYS	1
1	E	284	LEU	1
1	E	293	SER	1
1	E	311	LYS	1

6.3.3 RNA ⓘ

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 7% for the well-defined parts and 6% 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	223
Number of shifts mapped to atoms	219
Number of unparsed shifts	0
Number of shifts with mapping errors	4
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 4 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	369	LYS	C	173.583	?	1
1	A	370	LYS	C	171.766	?	1
1	A	370	LYS	N	118.991	?	1
1	A	371	ILE	N	119.925	?	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	40	1.92 ± 0.17	Should be checked
$^{13}\text{C}_\beta$	38	0.55 ± 0.21	Should be checked
$^{13}\text{C}'$	40	2.84 ± 0.26	Should be applied
^{15}N	44	-2.12 ± 0.38	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 7%, i.e. 212 atoms were assigned a chemical shift out of a possible 3115. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	115/1150 (10%)	0/470 (0%)	76/460 (17%)	39/220 (18%)
Sidechain	96/1880 (5%)	0/1220 (0%)	93/590 (16%)	3/70 (4%)
Aromatic	1/85 (1%)	0/40 (0%)	1/35 (3%)	0/10 (0%)
Overall	212/3115 (7%)	0/1730 (0%)	170/1085 (16%)	42/300 (14%)

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 6%, i.e. 216 atoms were assigned a chemical shift out of a possible 3445. 0 out of 55 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	118/1305 (9%)	0/535 (0%)	78/520 (15%)	40/250 (16%)
Sidechain	97/2055 (5%)	0/1335 (0%)	94/645 (15%)	3/75 (4%)
Aromatic	1/85 (1%)	0/40 (0%)	1/35 (3%)	0/10 (0%)
Overall	216/3445 (6%)	0/1910 (0%)	173/1200 (14%)	43/335 (13%)

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 [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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:

