Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 12:07 PM EST

PDB ID	:	6XFM
EMDB ID	:	EMD-22169
Title	:	Molecular structure of the core of amyloid-like fibrils formed by residues 111-214 of FUS
Authors	:	Tycko, R.; Lee, M.; Ghosh, U.; Thurber, K.; Kato, M.
Deposited on	:	2020-06-15
Resolution	:	2.62 Å(reported)

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

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

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

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

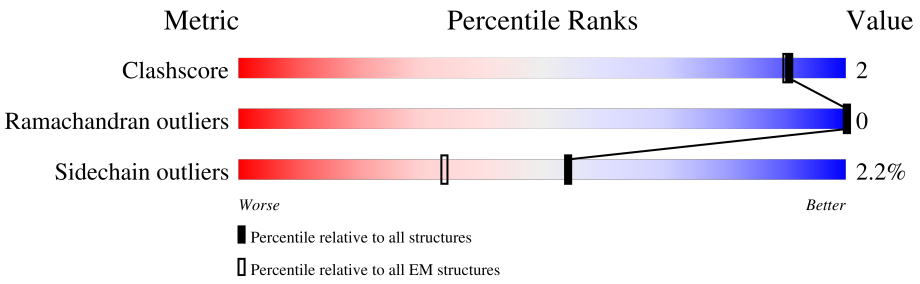
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	1-1	104	38% 62%
1	1-2	104	38% 62%
1	1-3	104	38% 62%
1	1-4	104	38% 62%
1	1-5	104	38% 62%
1	1-6	104	38% 62%
1	1-7	104	38% 62%
1	1-8	104	38% 62%

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Mol	Chain	Length	Quality of chain
1	10-1	104	36% • 62%
1	10-2	104	36% • 62%
1	10-3	104	36% • 62%
1	10-4	104	36% • 62%
1	10-5	104	36% • 62%
1	10-6	104	36% • 62%
1	10-7	104	36% • 62%
1	10-8	104	37% • 62%
1	11-1	104	37% • 62%
1	11-2	104	37% • 62%
1	11-3	104	36% • 62%
1	11-4	104	37% • 62%
1	11-5	104	37% • 62%
1	11-6	104	37% • 62%
1	11-7	104	36% • 62%
1	11-8	104	37% • 62%
1	12-1	104	36% • 62%
1	12-2	104	36% • 62%
1	12-3	104	36% • 62%
1	12-4	104	36% • 62%
1	12-5	104	36% • 62%
1	12-6	104	36% • 62%
1	12-7	104	36% • 62%
1	12-8	104	37% • 62%
1	13-1	104	36% • 62%

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Mol	Chain	Length	Quality of chain
1	13-2	104	35% • 62%
1	13-3	104	35% • 62%
1	13-4	104	36% • 62%
1	13-5	104	36% • 62%
1	13-6	104	36% • 62%
1	13-7	104	36% • 62%
1	13-8	104	36% • 62%
1	14-1	104	38% 62%
1	14-2	104	38% 62%
1	14-3	104	38% 62%
1	14-4	104	38% 62%
1	14-5	104	38% 62%
1	14-6	104	38% 62%
1	14-7	104	38% 62%
1	14-8	104	38% 62%
1	2-1	104	37% • 62%
1	2-2	104	37% • 62%
1	2-3	104	37% • 62%
1	2-4	104	38% 62%
1	2-5	104	38% 62%
1	2-6	104	37% • 62%
1	2-7	104	38% 62%
1	2-8	104	38% 62%
1	3-1	104	35% • 62%
1	3-2	104	35% • 62%

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Mol	Chain	Length	Quality of chain
1	3-3	104	35% • 62%
1	3-4	104	36% • 62%
1	3-5	104	35% • 62%
1	3-6	104	35% • 62%
1	3-7	104	36% • 62%
1	3-8	104	36% • 62%
1	4-1	104	37% • 62%
1	4-2	104	37% • 62%
1	4-3	104	37% • 62%
1	4-4	104	37% • 62%
1	4-5	104	37% • 62%
1	4-6	104	37% • 62%
1	4-7	104	37% • 62%
1	4-8	104	37% • 62%
1	5-1	104	35% • 62%
1	5-2	104	35% • 62%
1	5-3	104	35% • 62%
1	5-4	104	35% • 62%
1	5-5	104	35% • 62%
1	5-6	104	35% • 62%
1	5-7	104	35% • 62%
1	5-8	104	35% • 62%
1	6-1	104	37% • 62%
1	6-2	104	37% • 62%
1	6-3	104	37% • 62%

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Mol	Chain	Length	Quality of chain
1	6-4	104	37% • 62%
1	6-5	104	37% • 62%
1	6-6	104	37% • 62%
1	6-7	104	37% • 62%
1	6-8	104	37% • 62%
1	7-1	104	35% • 62%
1	7-2	104	34% • 62%
1	7-3	104	34% • 62%
1	7-4	104	35% • 62%
1	7-5	104	34% • 62%
1	7-6	104	34% • 62%
1	7-7	104	35% • 62%
1	7-8	104	35% • 62%
1	8-1	104	35% • 62%
1	8-2	104	36% • 62%
1	8-3	104	36% • 62%
1	8-4	104	36% • 62%
1	8-5	104	37% • 62%
1	8-6	104	35% • 62%
1	8-7	104	36% • 62%
1	8-8	104	37% • 62%
1	9-1	104	35% • 62%
1	9-2	104	34% • 62%
1	9-3	104	34% • 62%
1	9-4	104	35% • 62%

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Mol	Chain	Length	Quality of chain
1	9-5	104	35% • 62%
1	9-6	104	34% • 62%
1	9-7	104	32% 6% 62%
1	9-8	104	35% • 62%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 57680 atoms, of which 24640 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-binding protein FUS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	1-1	39	515	174	220	51	70	0	0
1	2-1	39	515	174	220	51	70	0	0
1	3-1	39	515	174	220	51	70	0	0
1	4-1	39	515	174	220	51	70	0	0
1	5-1	39	515	174	220	51	70	0	0
1	6-1	39	515	174	220	51	70	0	0
1	7-1	39	515	174	220	51	70	0	0
1	8-1	39	515	174	220	51	70	0	0
1	9-1	39	515	174	220	51	70	0	0
1	10-1	39	515	174	220	51	70	0	0
1	11-1	39	515	174	220	51	70	0	0
1	12-1	39	515	174	220	51	70	0	0
1	13-1	39	515	174	220	51	70	0	0
1	14-1	39	515	174	220	51	70	0	0
1	1-2	39	515	174	220	51	70	0	0
1	2-2	39	515	174	220	51	70	0	0
1	3-2	39	515	174	220	51	70	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	4-2	39	515	174	220	51	70	0	0
1	5-2	39	515	174	220	51	70	0	0
1	6-2	39	515	174	220	51	70	0	0
1	7-2	39	515	174	220	51	70	0	0
1	8-2	39	515	174	220	51	70	0	0
1	9-2	39	515	174	220	51	70	0	0
1	10-2	39	515	174	220	51	70	0	0
1	11-2	39	515	174	220	51	70	0	0
1	12-2	39	515	174	220	51	70	0	0
1	13-2	39	515	174	220	51	70	0	0
1	14-2	39	515	174	220	51	70	0	0
1	1-3	39	515	174	220	51	70	0	0
1	2-3	39	515	174	220	51	70	0	0
1	3-3	39	515	174	220	51	70	0	0
1	4-3	39	515	174	220	51	70	0	0
1	5-3	39	515	174	220	51	70	0	0
1	6-3	39	515	174	220	51	70	0	0
1	7-3	39	515	174	220	51	70	0	0
1	8-3	39	515	174	220	51	70	0	0
1	9-3	39	515	174	220	51	70	0	0
1	10-3	39	515	174	220	51	70	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	11-3	39	515	174	220	51	70	0	0
1	12-3	39	515	174	220	51	70	0	0
1	13-3	39	515	174	220	51	70	0	0
1	14-3	39	515	174	220	51	70	0	0
1	1-4	39	515	174	220	51	70	0	0
1	2-4	39	515	174	220	51	70	0	0
1	3-4	39	515	174	220	51	70	0	0
1	4-4	39	515	174	220	51	70	0	0
1	5-4	39	515	174	220	51	70	0	0
1	6-4	39	515	174	220	51	70	0	0
1	7-4	39	515	174	220	51	70	0	0
1	8-4	39	515	174	220	51	70	0	0
1	9-4	39	515	174	220	51	70	0	0
1	10-4	39	515	174	220	51	70	0	0
1	11-4	39	515	174	220	51	70	0	0
1	12-4	39	515	174	220	51	70	0	0
1	13-4	39	515	174	220	51	70	0	0
1	14-4	39	515	174	220	51	70	0	0
1	1-5	39	515	174	220	51	70	0	0
1	2-5	39	515	174	220	51	70	0	0
1	3-5	39	515	174	220	51	70	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	4-5	39	515	174	220	51	70	0	0
1	5-5	39	515	174	220	51	70	0	0
1	6-5	39	515	174	220	51	70	0	0
1	7-5	39	515	174	220	51	70	0	0
1	8-5	39	515	174	220	51	70	0	0
1	9-5	39	515	174	220	51	70	0	0
1	10-5	39	515	174	220	51	70	0	0
1	11-5	39	515	174	220	51	70	0	0
1	12-5	39	515	174	220	51	70	0	0
1	13-5	39	515	174	220	51	70	0	0
1	14-5	39	515	174	220	51	70	0	0
1	1-6	39	515	174	220	51	70	0	0
1	2-6	39	515	174	220	51	70	0	0
1	3-6	39	515	174	220	51	70	0	0
1	4-6	39	515	174	220	51	70	0	0
1	5-6	39	515	174	220	51	70	0	0
1	6-6	39	515	174	220	51	70	0	0
1	7-6	39	515	174	220	51	70	0	0
1	8-6	39	515	174	220	51	70	0	0
1	9-6	39	515	174	220	51	70	0	0
1	10-6	39	515	174	220	51	70	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	11-6	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	12-6	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	13-6	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	14-6	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	1-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	2-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	3-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	4-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	5-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	6-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	7-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	8-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	9-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	10-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	11-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	12-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	13-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	14-7	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	1-8	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	2-8	39	515	174	220	51	70	0	0
			Total	C	H	N	O		
1	3-8	39	515	174	220	51	70	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	4-8	39	515	174	220	51	70	0	0
1	5-8	39	515	174	220	51	70	0	0
1	6-8	39	515	174	220	51	70	0	0
1	7-8	39	515	174	220	51	70	0	0
1	8-8	39	515	174	220	51	70	0	0
1	9-8	39	515	174	220	51	70	0	0
1	10-8	39	515	174	220	51	70	0	0
1	11-8	39	515	174	220	51	70	0	0
1	12-8	39	515	174	220	51	70	0	0
1	13-8	39	515	174	220	51	70	0	0
1	14-8	39	515	174	220	51	70	0	0

There are 8 discrepancies between the modelled and reference sequences:

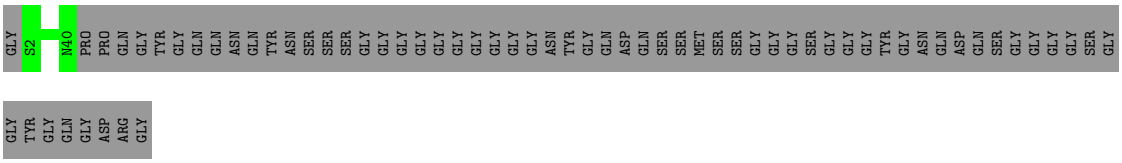
Chain	Residue	Modelled	Actual	Comment	Reference
1	101	GLY	GLN	conflict	UNP P35637
2	101	GLY	GLN	conflict	UNP P35637
3	101	GLY	GLN	conflict	UNP P35637
4	101	GLY	GLN	conflict	UNP P35637
5	101	GLY	GLN	conflict	UNP P35637
6	101	GLY	GLN	conflict	UNP P35637
7	101	GLY	GLN	conflict	UNP P35637
8	101	GLY	GLN	conflict	UNP P35637

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

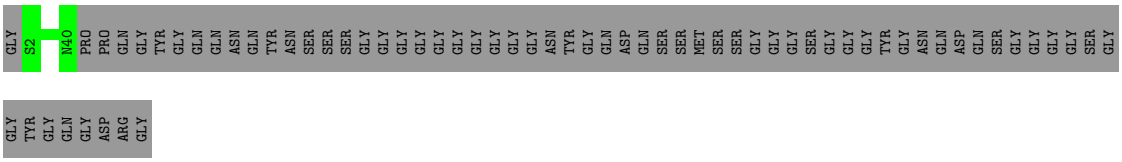
• Molecule 1: RNA-binding protein FUS

Chain 1-1:



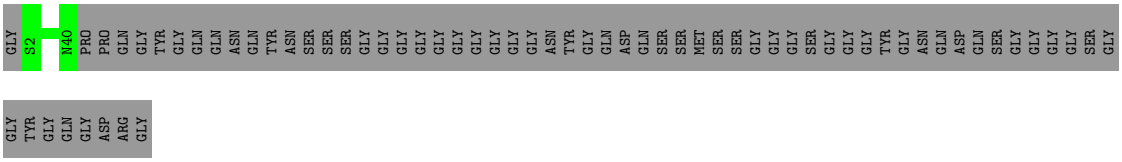
• Molecule 1: RNA-binding protein FUS

Chain 1-2:



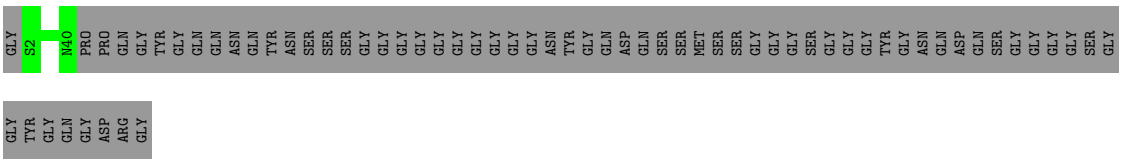
• Molecule 1: RNA-binding protein FUS

Chain 1-3:



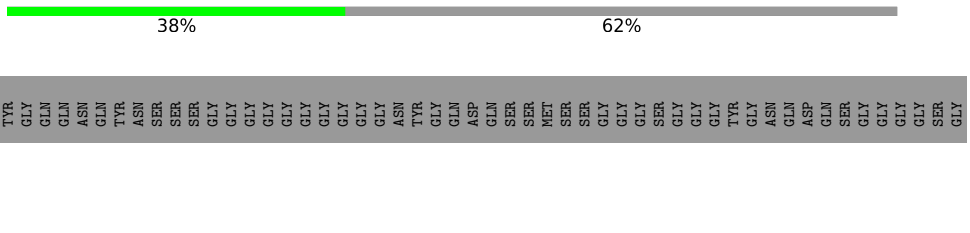
• Molecule 1: RNA-binding protein FUS

Chain 1-4:



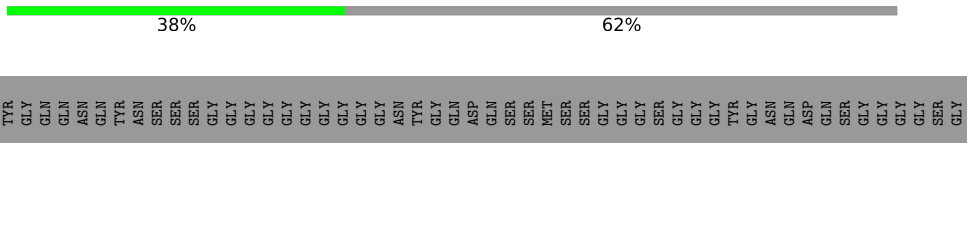
- Molecule 1: RNA-binding protein FUS

Chain 1-5:



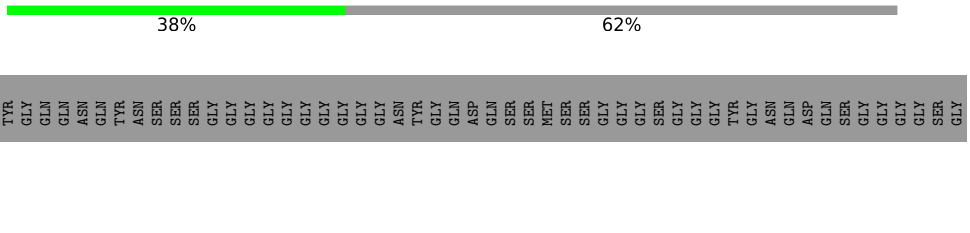
- Molecule 1: RNA-binding protein FUS

Chain 1-6:



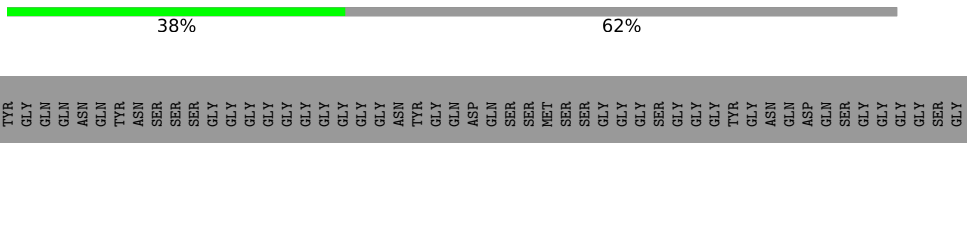
- Molecule 1: RNA-binding protein FUS

Chain 1-7:



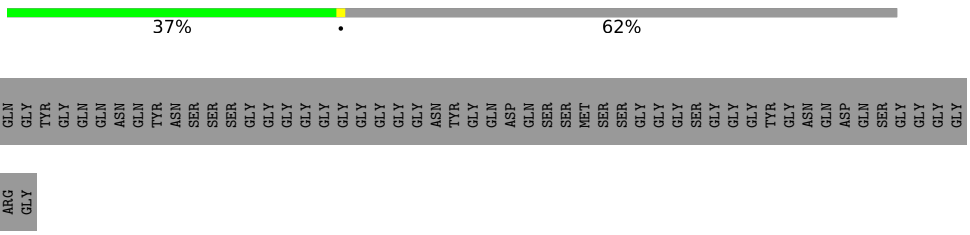
- Molecule 1: RNA-binding protein FUS

Chain 1-8:



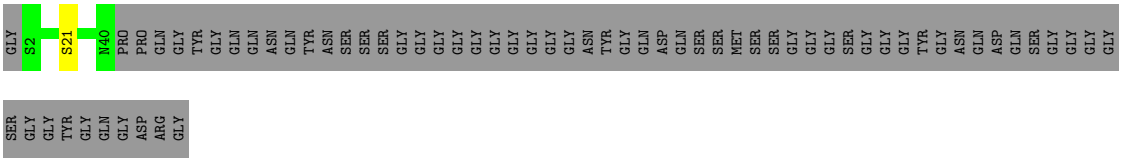
- Molecule 1: RNA-binding protein FUS

Chain 2-1:



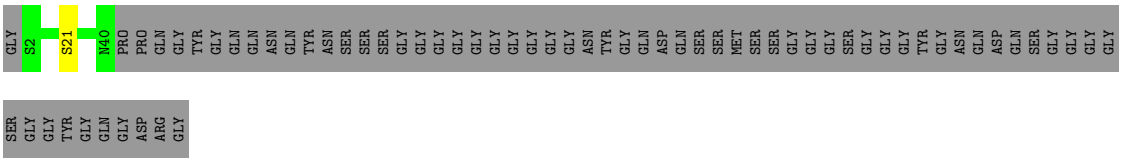
- Molecule 1: RNA-binding protein FUS

Chain 2-2: 37% 62%



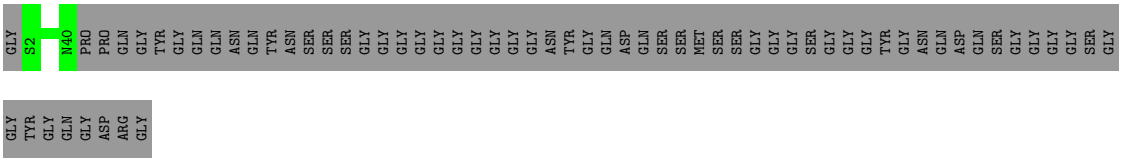
• Molecule 1: RNA-binding protein FUS

Chain 2-3: 37% 62%



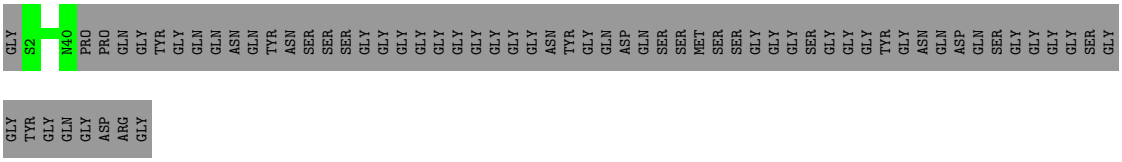
• Molecule 1: RNA-binding protein FUS

Chain 2-4: 38% 62%



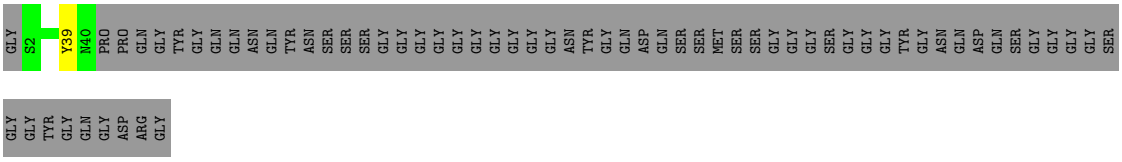
• Molecule 1: RNA-binding protein FUS

Chain 2-5: 38% 62%



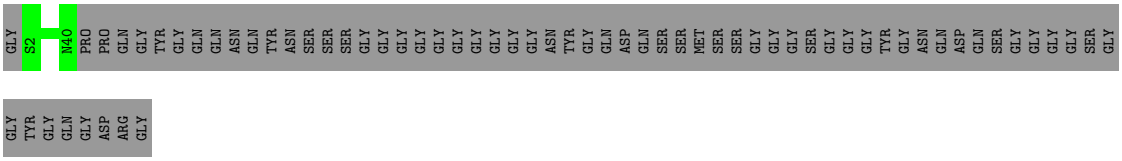
• Molecule 1: RNA-binding protein FUS

Chain 2-6: 37% 62%



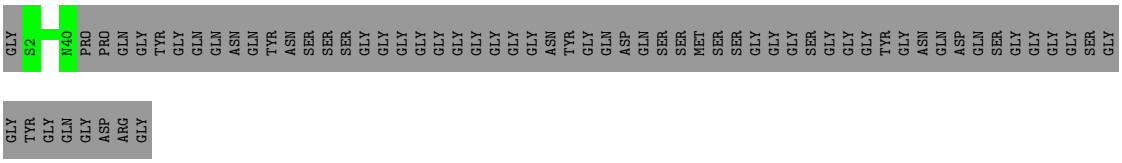
• Molecule 1: RNA-binding protein FUS

Chain 2-7: 38% 62%



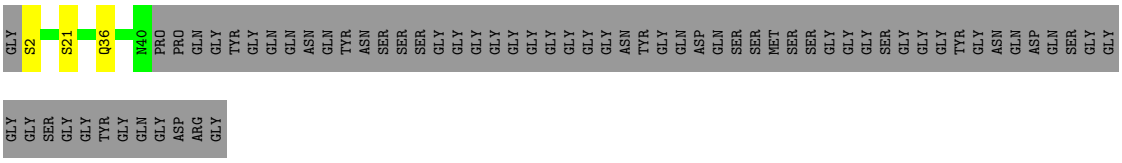
• Molecule 1: RNA-binding protein FUS

Chain 2-8: 38% 62%



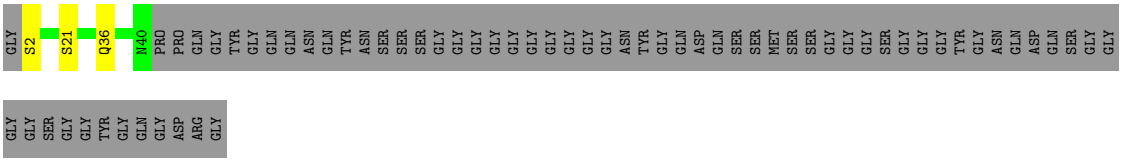
• Molecule 1: RNA-binding protein FUS

Chain 3-1: 35% • 62%



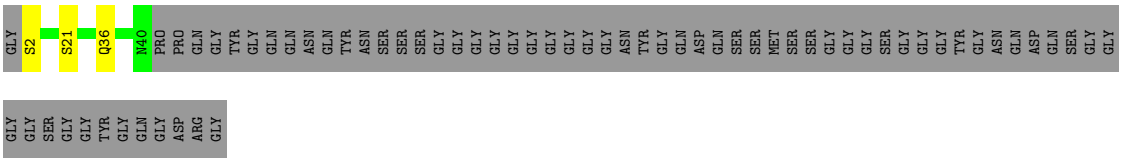
• Molecule 1: RNA-binding protein FUS

Chain 3-2: 35% • 62%



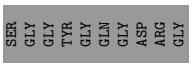
• Molecule 1: RNA-binding protein FUS

Chain 3-3: 35% • 62%



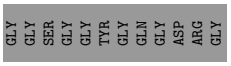
• Molecule 1: RNA-binding protein FUS

Chain 3-4: 36% • 62%



• Molecule 1: RNA-binding protein FUS

Chain 3-5:

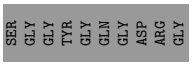


• Molecule 1: RNA-binding protein FUS

Chain 3-6:

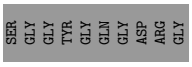
• Molecule 1: RNA-binding protein FUS

Chain 3-7:



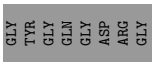
• Molecule 1: RNA-binding protein FUS

Chain 3-8:



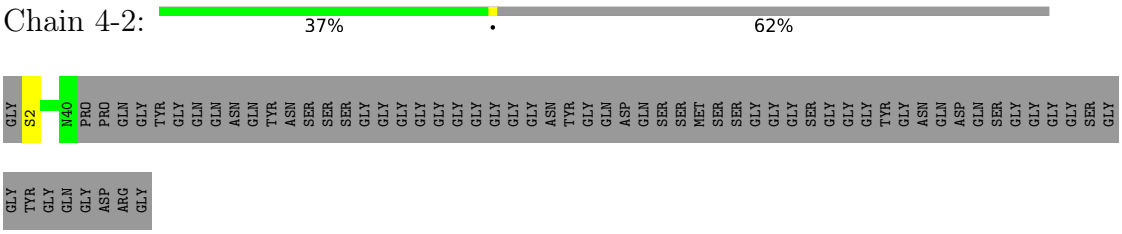
• Molecule 1: RNA-binding protein FUS

Chain 4-1:



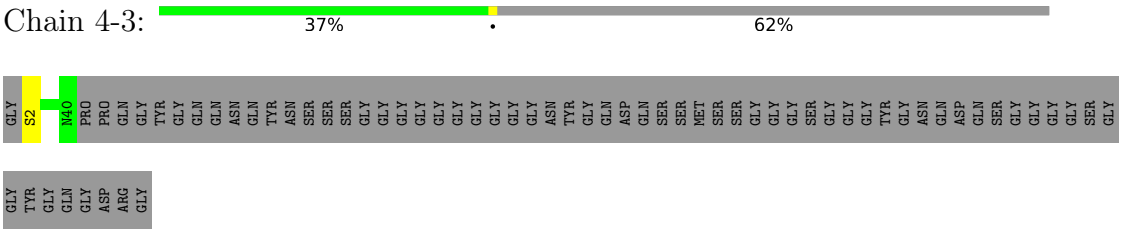
- Molecule 1: RNA-binding protein FUS

Chain 4-2:



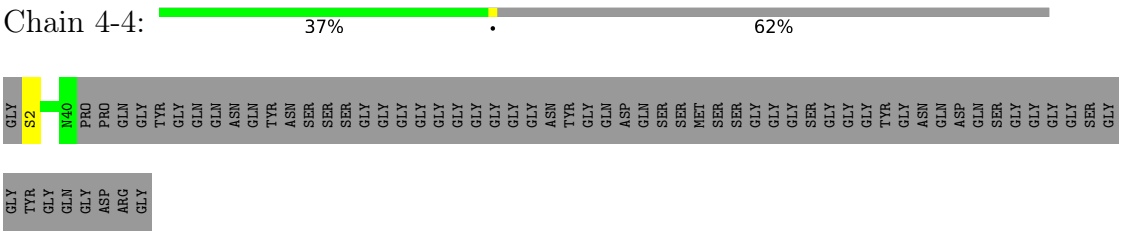
- Molecule 1: RNA-binding protein FUS

Chain 4-3:



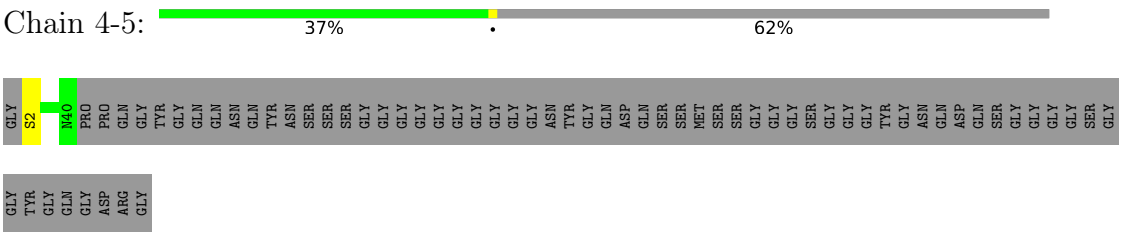
- Molecule 1: RNA-binding protein FUS

Chain 4-4:



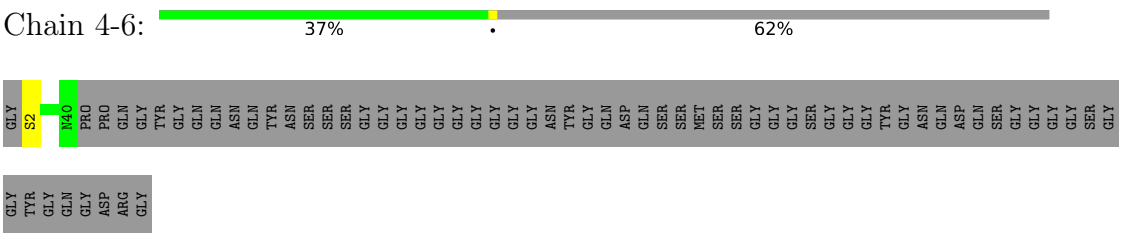
- Molecule 1: RNA-binding protein FUS

Chain 4-5:



- Molecule 1: RNA-binding protein FUS

Chain 4-6:



- Molecule 1: RNA-binding protein FUS

Chain 4-7: 37% • 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 4-8: 37% • 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 5-1: 35% • 62%

GLY S2 S21 Q36 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY

GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 5-2: 35% • 62%

GLY S2 S21 Q36 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY

GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

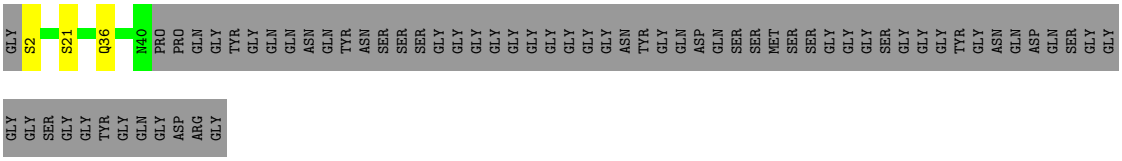
Chain 5-3: 35% • 62%

GLY S2 S21 Q36 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY

GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

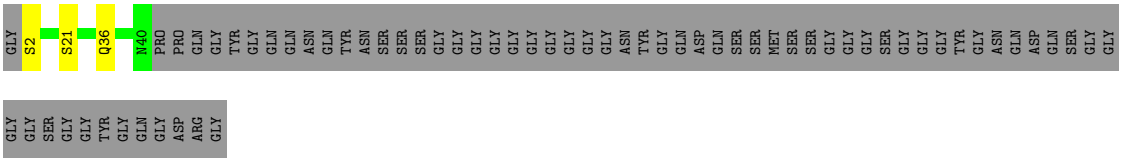
- Molecule 1: RNA-binding protein FUS

Chain 5-4: 35% • 62%



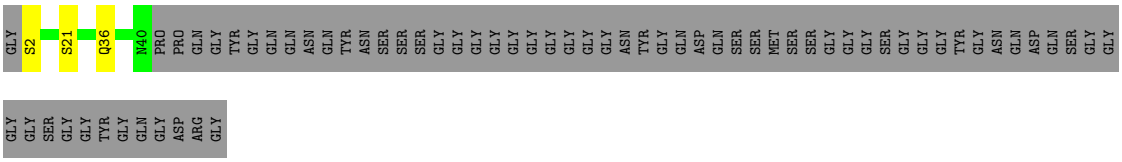
• Molecule 1: RNA-binding protein FUS

Chain 5-5:



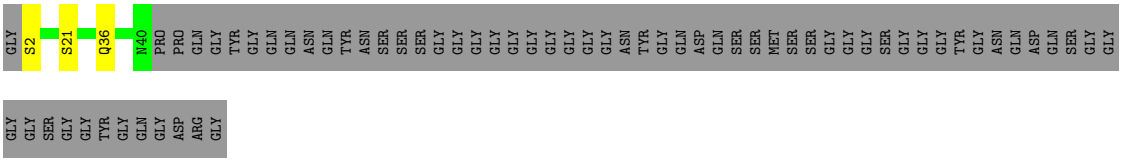
• Molecule 1: RNA-binding protein FUS

Chain 5-6:



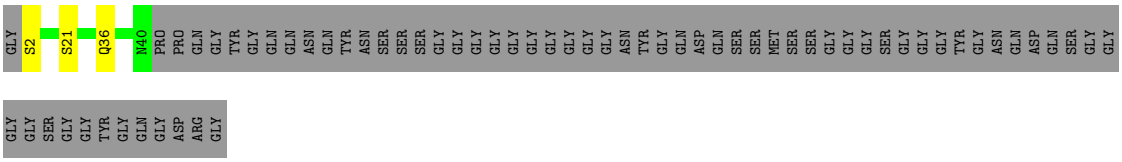
• Molecule 1: RNA-binding protein FUS

Chain 5-7:



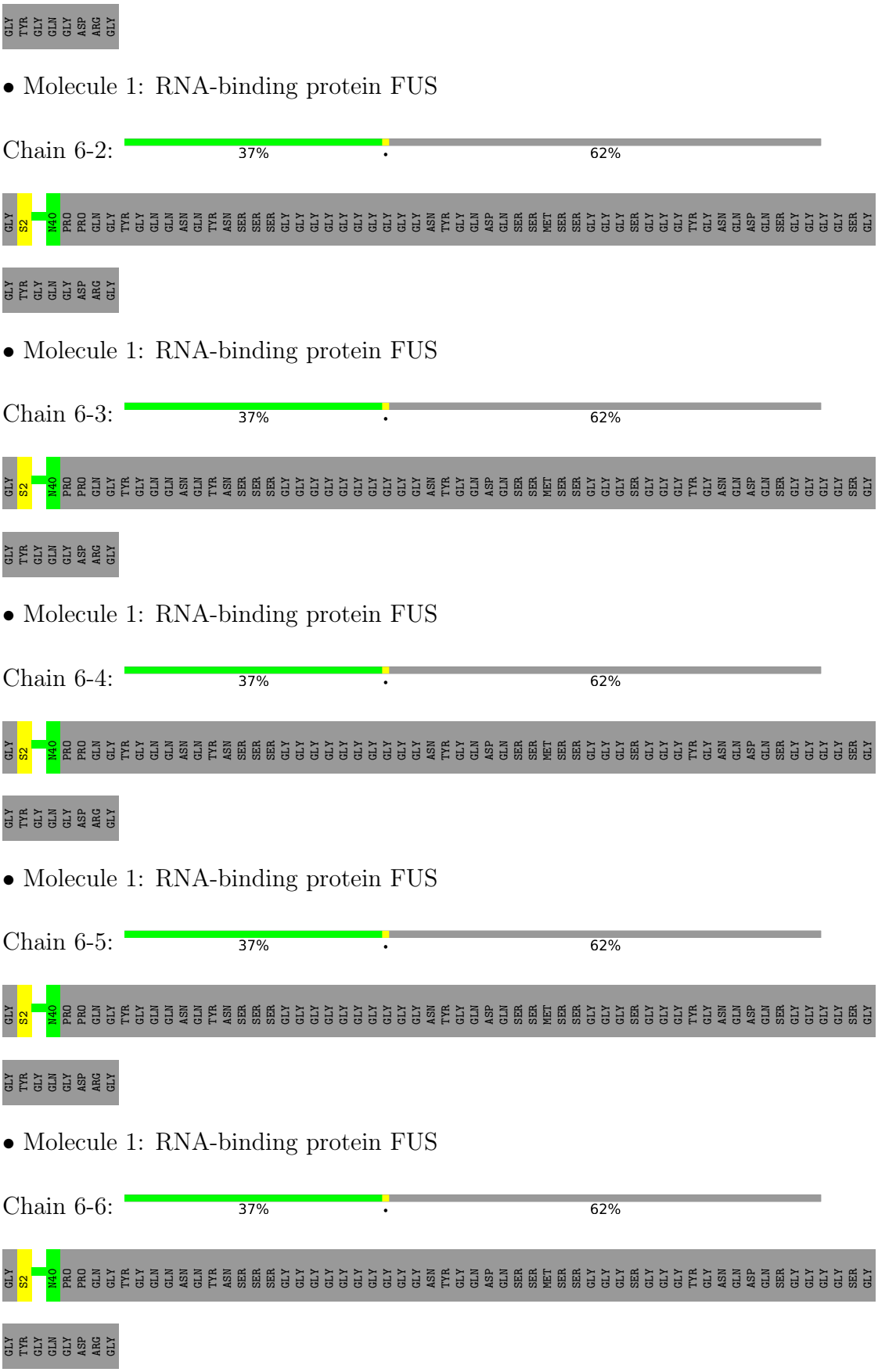
• Molecule 1: RNA-binding protein FUS

Chain 5-8:



• Molecule 1: RNA-binding protein FUS

Chain 6-1:


GLY TYR GLY GLN GLY ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain 6-2:
37%
62%
GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY
GLY TYR GLY GLN GLY ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain 6-3:
37%
62%
GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY
GLY TYR GLY GLN GLY ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain 6-4:
37%
62%
GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY
GLY TYR GLY GLN GLY ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain 6-5:
37%
62%
GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY
GLY TYR GLY GLN GLY ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain 6-6:
37%
62%
GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY
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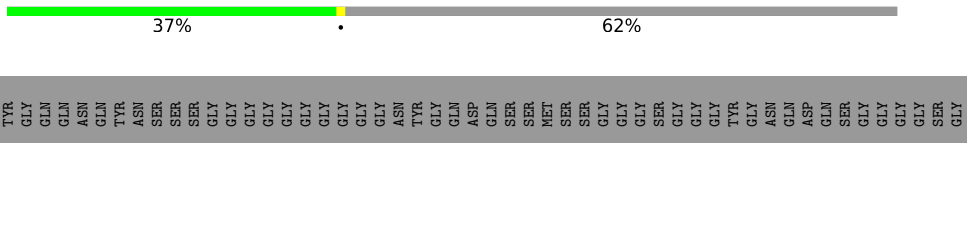
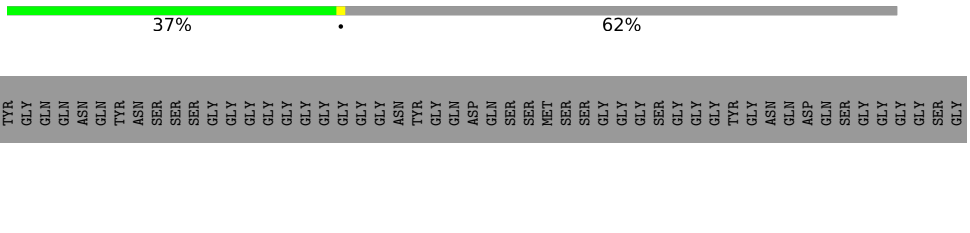
• Molecule 1: RNA-binding protein FUS

Chain 6-7:



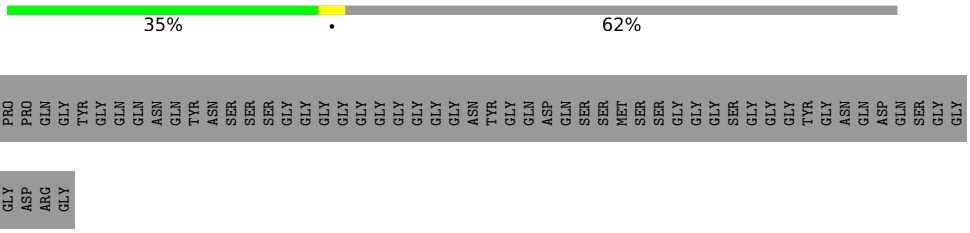
• Molecule 1: RNA-binding protein FUS

Chain 6-8:



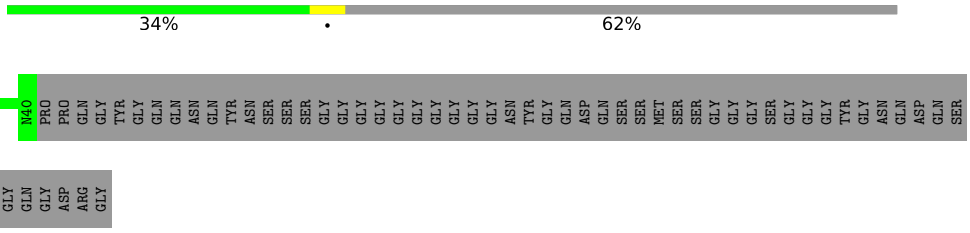
• Molecule 1: RNA-binding protein FUS

Chain 7-1:



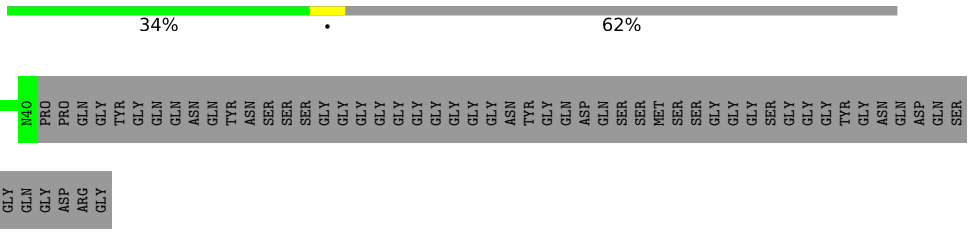
• Molecule 1: RNA-binding protein FUS

Chain 7-2:



• Molecule 1: RNA-binding protein FUS

Chain 7-3:



• Molecule 1: RNA-binding protein FUS

Chain 7-4: 35% • 62%

GLY S2 G18 Q23 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY

GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain 7-5: 34% • 62%

GLY S2 G18 S21 Q22 Q23 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER

GLY GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain 7-6: 34% • 62%

GLY S2 G18 S21 Q22 Q23 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER

GLY GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain 7-7: 35% • 62%

GLY S2 G18 Q23 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY

GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

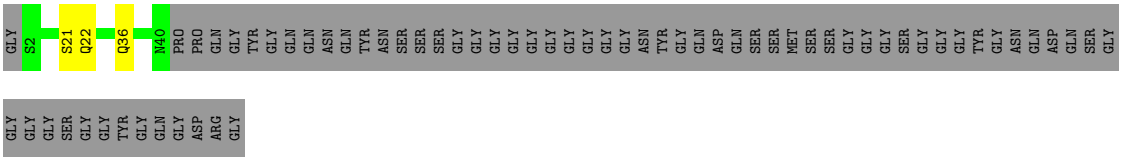
Chain 7-8: 35% • 62%

GLY S2 G18 Q23 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY

GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

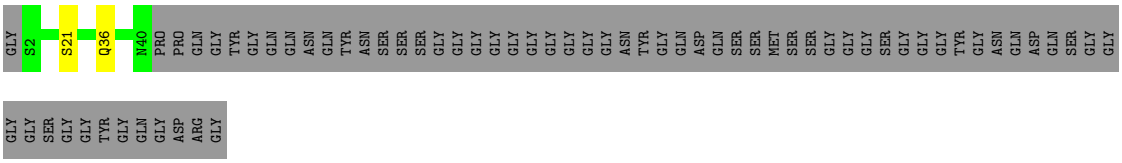
• Molecule 1: RNA-binding protein FUS

Chain 8-1: 35% • 62%



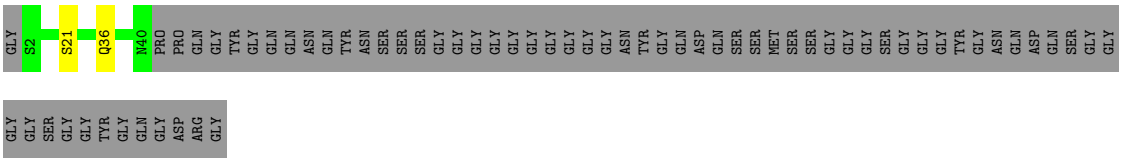
• Molecule 1: RNA-binding protein FUS

Chain 8-2:



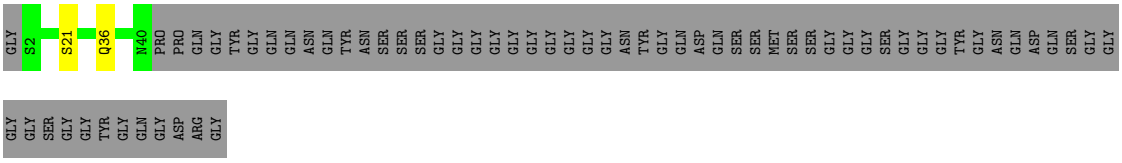
• Molecule 1: RNA-binding protein FUS

Chain 8-3:



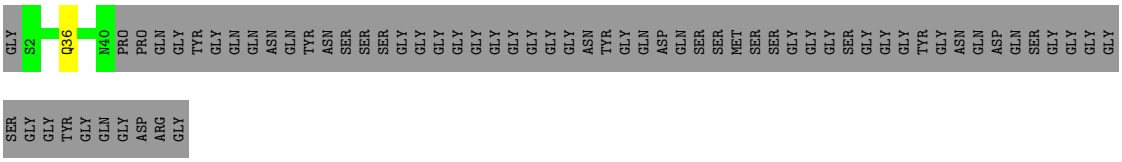
• Molecule 1: RNA-binding protein FUS

Chain 8-4:



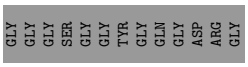
• Molecule 1: RNA-binding protein FUS

Chain 8-5:



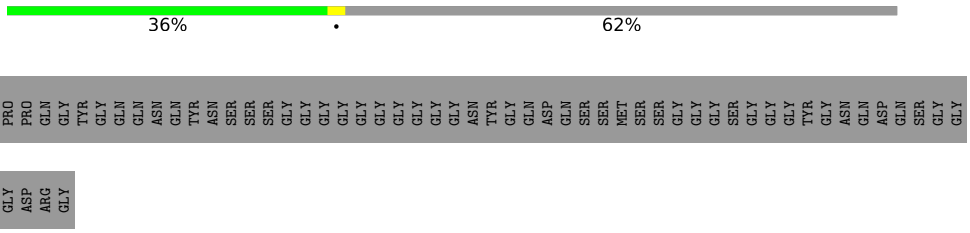
• Molecule 1: RNA-binding protein FUS

Chain 8-6:



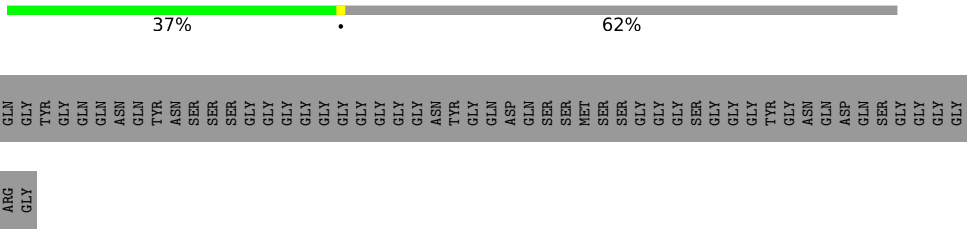
• Molecule 1: RNA-binding protein FUS

Chain 8-7:



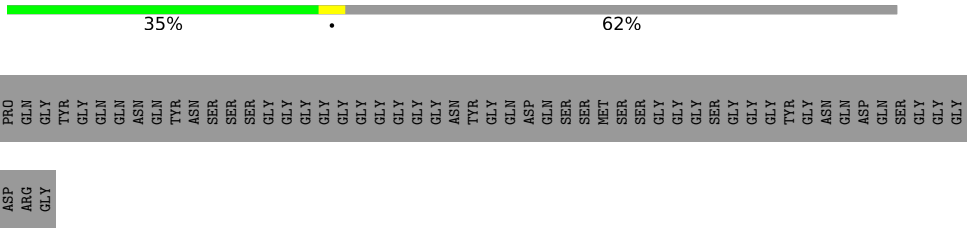
• Molecule 1: RNA-binding protein FUS

Chain 8-8:



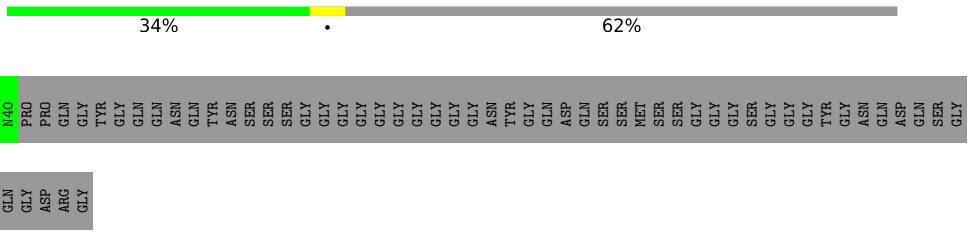
• Molecule 1: RNA-binding protein FUS

Chain 9-1:



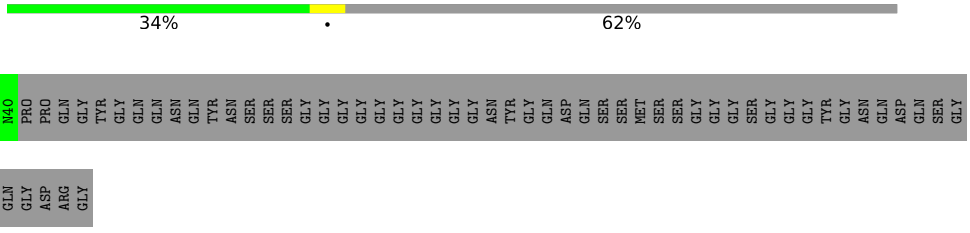
• Molecule 1: RNA-binding protein FUS

Chain 9-2:



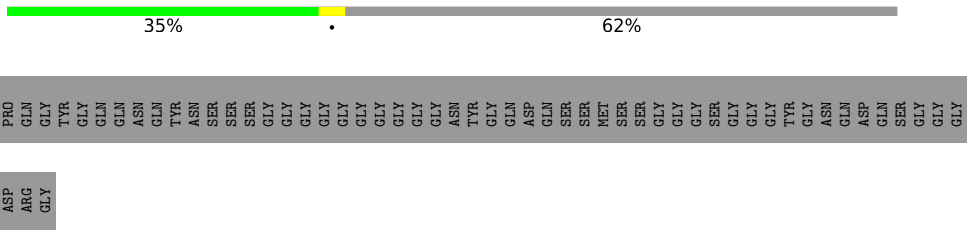
• Molecule 1: RNA-binding protein FUS

Chain 9-3:



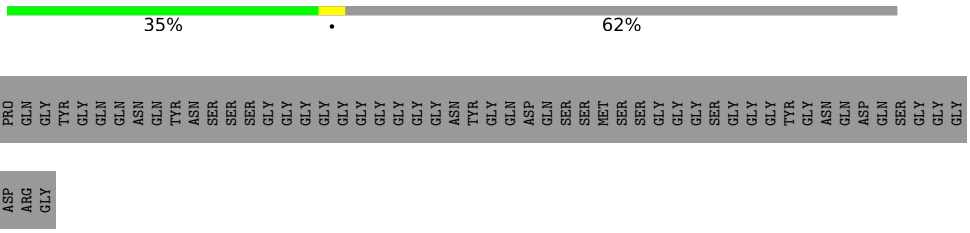
• Molecule 1: RNA-binding protein FUS

Chain 9-4:



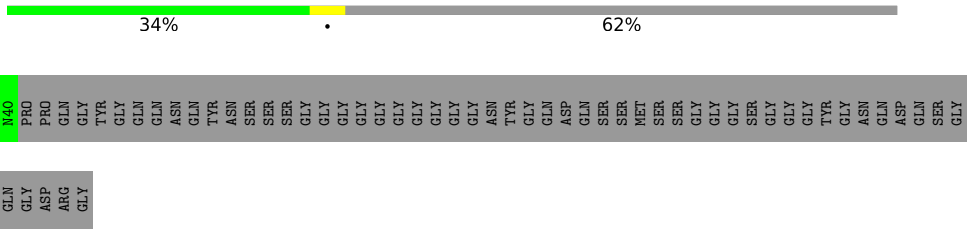
• Molecule 1: RNA-binding protein FUS

Chain 9-5:



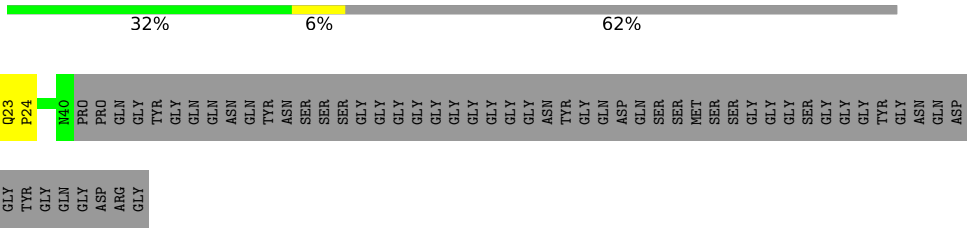
• Molecule 1: RNA-binding protein FUS

Chain 9-6:



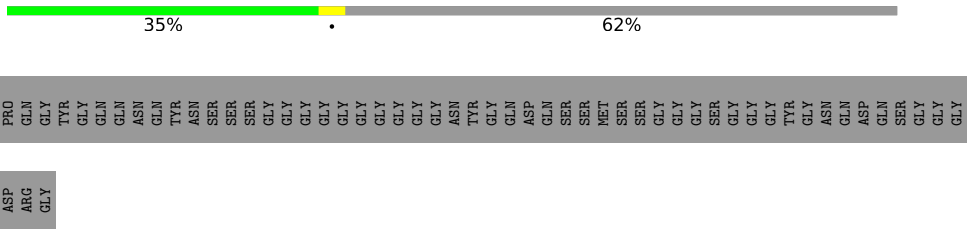
• Molecule 1: RNA-binding protein FUS

Chain 9-7:



• Molecule 1: RNA-binding protein FUS

Chain 9-8:



• Molecule 1: RNA-binding protein FUS

Chain 10-1: 36% • 62%

GLY S2 S21 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 10-2: 36% • 62%

GLY S2 S21 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 10-3: 36% • 62%

GLY S2 S21 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 10-4: 36% • 62%

GLY S2 S21 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

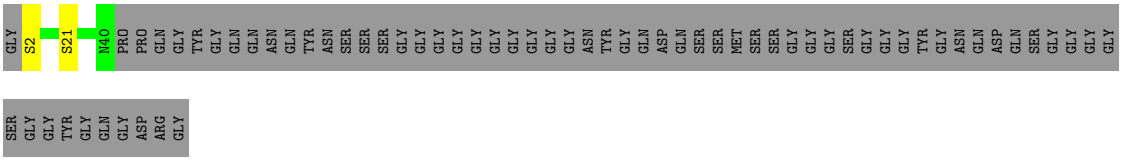
Chain 10-5: 36% • 62%

GLY S2 S21 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

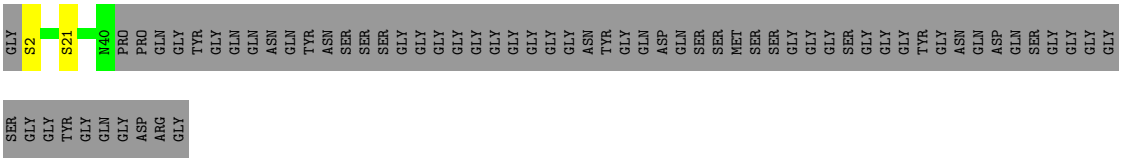
- Molecule 1: RNA-binding protein FUS

Chain 10-6: 36% • 62%



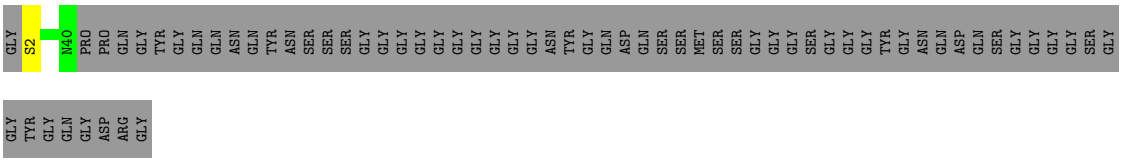
• Molecule 1: RNA-binding protein FUS

Chain 10-7:



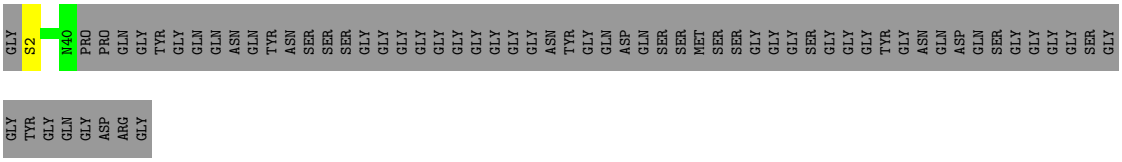
• Molecule 1: RNA-binding protein FUS

Chain 10-8:



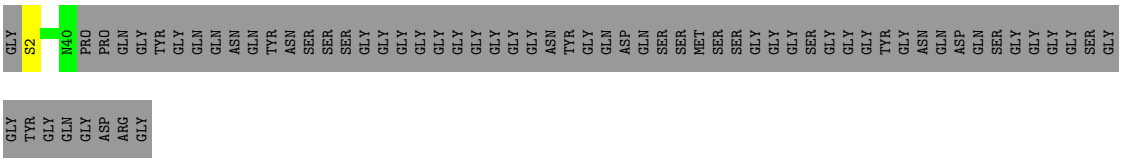
• Molecule 1: RNA-binding protein FUS

Chain 11-1:



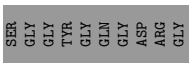
• Molecule 1: RNA-binding protein FUS

Chain 11-2:



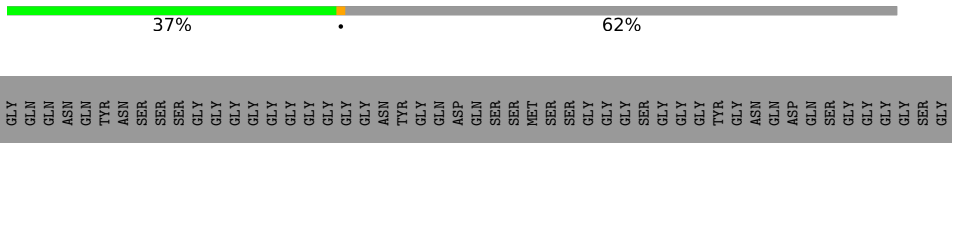
• Molecule 1: RNA-binding protein FUS

Chain 11-3:



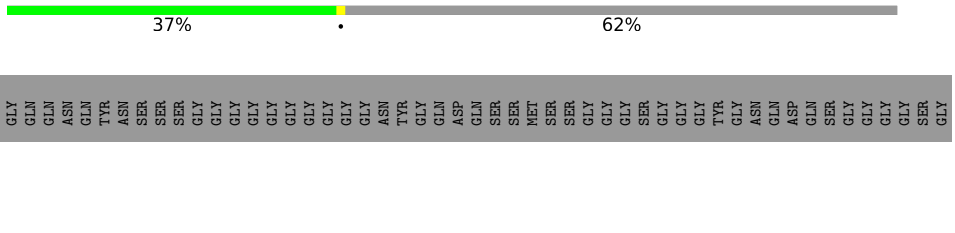
• Molecule 1: RNA-binding protein FUS

Chain 11-4:



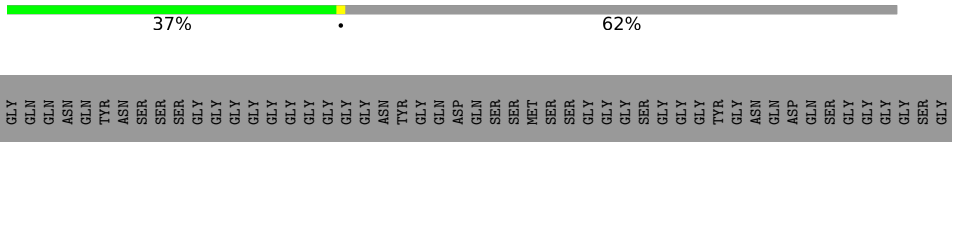
• Molecule 1: RNA-binding protein FUS

Chain 11-5:



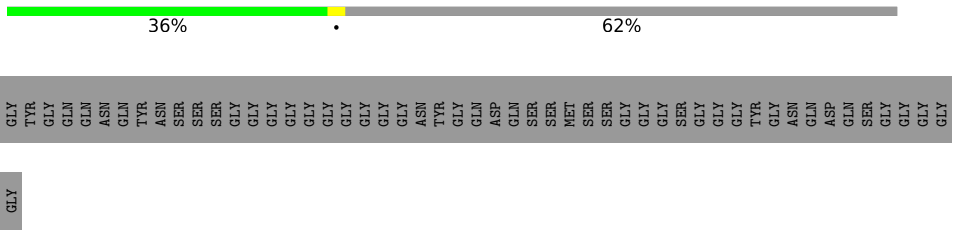
• Molecule 1: RNA-binding protein FUS

Chain 11-6:



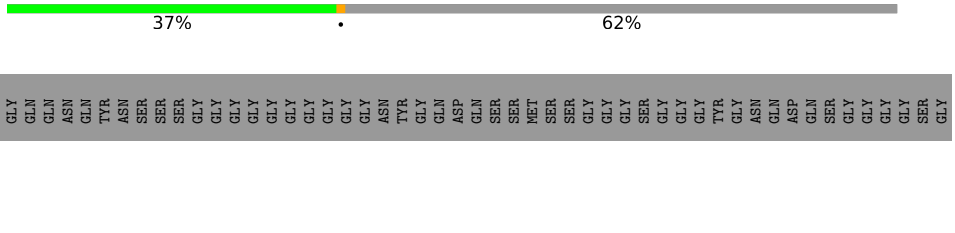
• Molecule 1: RNA-binding protein FUS

Chain 11-7:



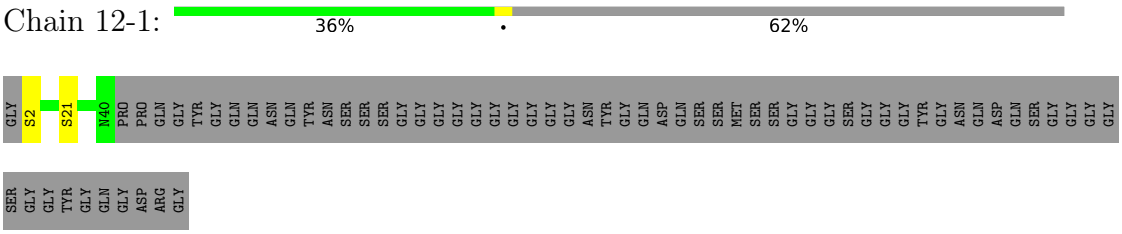
• Molecule 1: RNA-binding protein FUS

Chain 11-8:



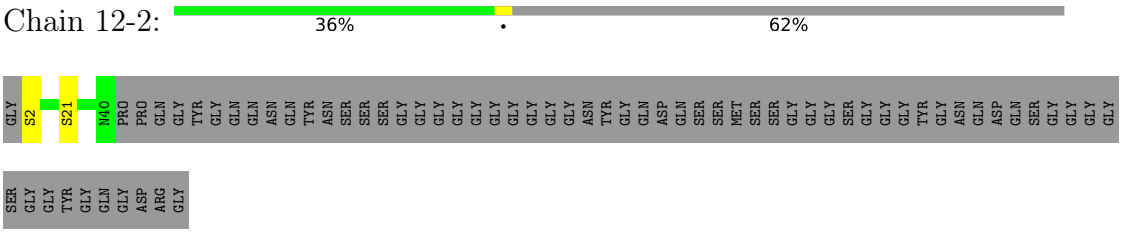
• Molecule 1: RNA-binding protein FUS

Chain 12-1:



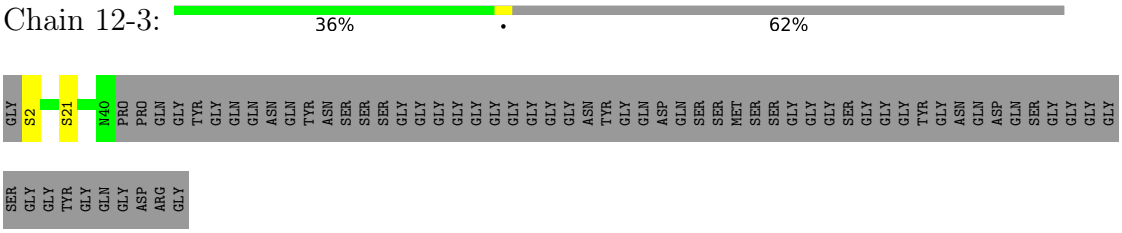
• Molecule 1: RNA-binding protein FUS

Chain 12-2:



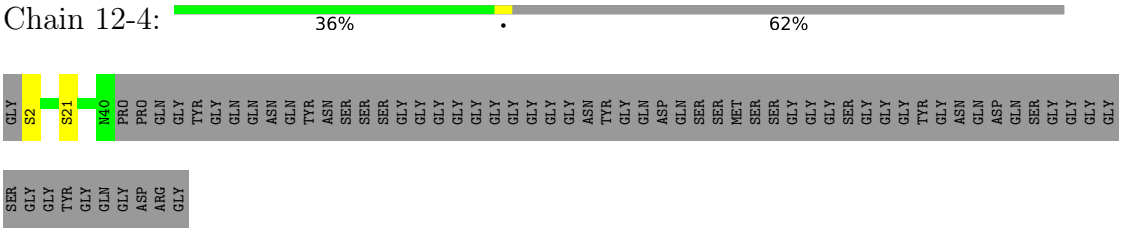
• Molecule 1: RNA-binding protein FUS

Chain 12-3:



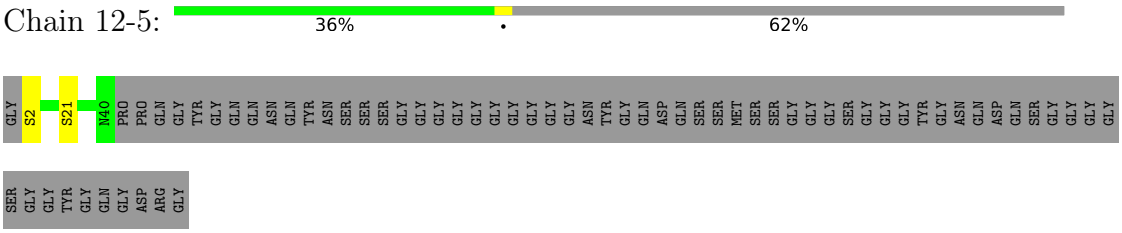
• Molecule 1: RNA-binding protein FUS

Chain 12-4:



• Molecule 1: RNA-binding protein FUS

Chain 12-5:



• Molecule 1: RNA-binding protein FUS

Chain 12-6: 36% • 62%

GLY S2 S21 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 12-7: 36% • 62%

GLY S2 S21 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 12-8: 37% • 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain 13-1: 36% • 62%

GLY S2 Q36 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

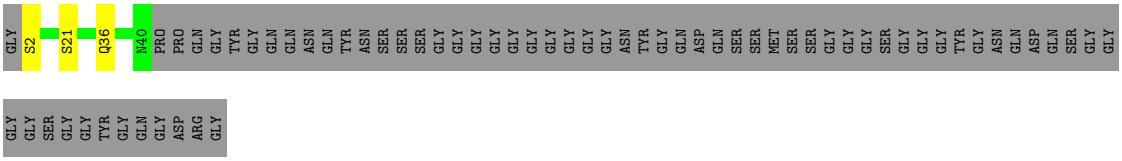
Chain 13-2: 35% • 62%

GLY S2 S21 Q36 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY

GLY GLY SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

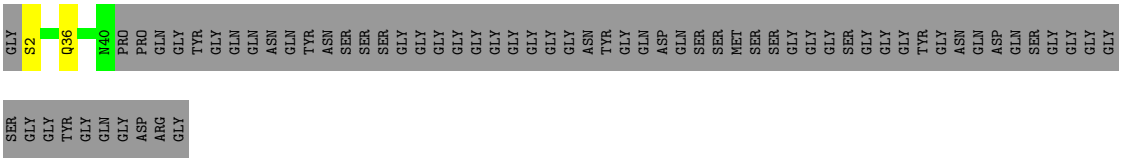
- Molecule 1: RNA-binding protein FUS

Chain 13-3: 35% • 62%



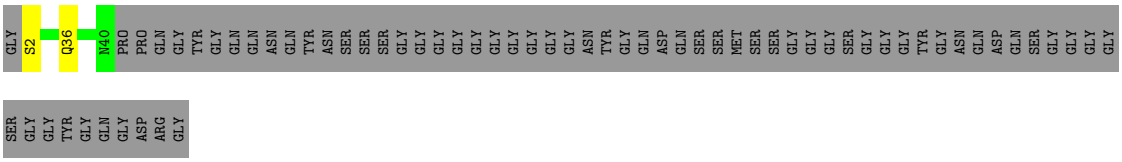
• Molecule 1: RNA-binding protein FUS

Chain 13-4:



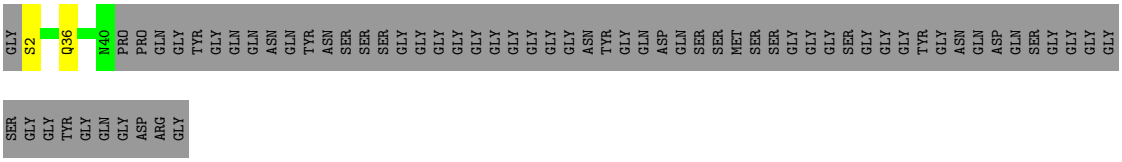
• Molecule 1: RNA-binding protein FUS

Chain 13-5:



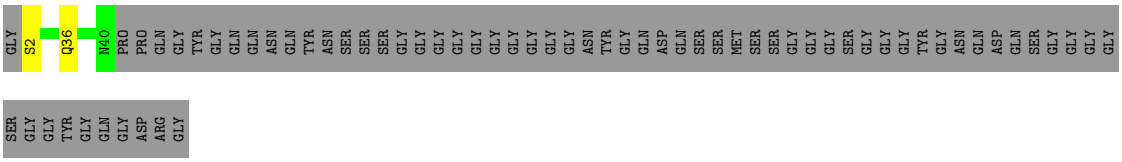
• Molecule 1: RNA-binding protein FUS

Chain 13-6:



• Molecule 1: RNA-binding protein FUS

Chain 13-7:



• Molecule 1: RNA-binding protein FUS

Chain 13-8:

SER GLY GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain 14-1: 38% 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain 14-2: 38% 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain 14-3: 38% 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain 14-4: 38% 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

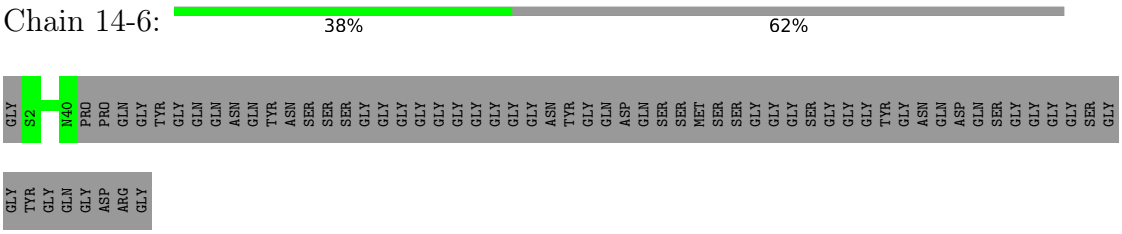
Chain 14-5: 38% 62%

GLY S2 N40 PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY

GLY TYR GLY GLN GLY ASP ARG GLY

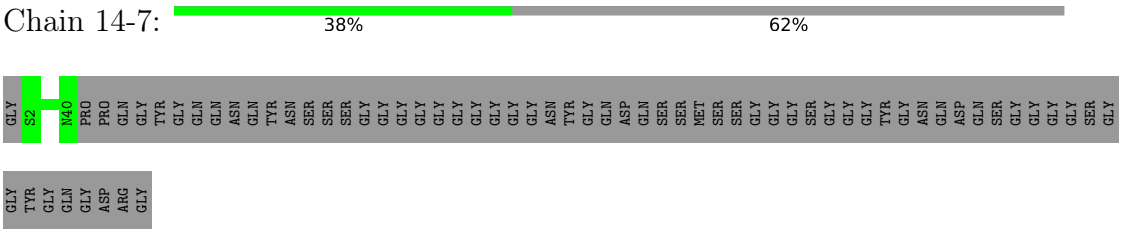
• Molecule 1: RNA-binding protein FUS

Chain 14-6:



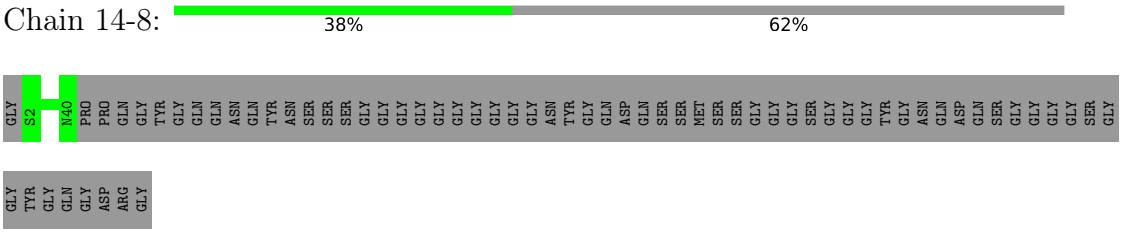
• Molecule 1: RNA-binding protein FUS

Chain 14-7:



• Molecule 1: RNA-binding protein FUS

Chain 14-8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	275520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Gctf	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	429.6, 429.6, 429.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	1-1	0.54	0/302	0.77	0/406
1	1-2	0.54	0/302	0.77	0/406
1	1-3	0.54	0/302	0.77	0/406
1	1-4	0.54	0/302	0.77	0/406
1	1-5	0.55	0/302	0.77	0/406
1	1-6	0.55	0/302	0.78	0/406
1	1-7	0.55	0/302	0.78	0/406
1	1-8	0.55	0/302	0.77	0/406
1	2-1	0.57	0/302	0.77	0/406
1	2-2	0.58	0/302	0.78	0/406
1	2-3	0.57	0/302	0.78	0/406
1	2-4	0.57	0/302	0.77	0/406
1	2-5	0.57	0/302	0.77	0/406
1	2-6	0.57	0/302	0.78	0/406
1	2-7	0.57	0/302	0.78	0/406
1	2-8	0.57	0/302	0.78	0/406
1	3-1	0.55	0/302	0.78	0/406
1	3-2	0.55	0/302	0.79	0/406
1	3-3	0.55	0/302	0.79	0/406
1	3-4	0.55	0/302	0.79	0/406
1	3-5	0.55	0/302	0.79	0/406
1	3-6	0.55	0/302	0.79	0/406
1	3-7	0.55	0/302	0.79	0/406
1	3-8	0.55	0/302	0.78	0/406
1	4-1	0.54	0/302	0.77	0/406
1	4-2	0.54	0/302	0.77	0/406
1	4-3	0.54	0/302	0.77	0/406
1	4-4	0.54	0/302	0.77	0/406
1	4-5	0.54	0/302	0.77	0/406
1	4-6	0.54	0/302	0.78	0/406
1	4-7	0.54	0/302	0.78	0/406
1	4-8	0.53	0/302	0.77	0/406
1	5-1	0.57	0/302	0.78	0/406
1	5-2	0.58	0/302	0.78	0/406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	5-3	0.58	0/302	0.79	0/406
1	5-4	0.58	0/302	0.78	0/406
1	5-5	0.58	0/302	0.78	0/406
1	5-6	0.58	0/302	0.79	0/406
1	5-7	0.58	0/302	0.78	0/406
1	5-8	0.58	0/302	0.78	0/406
1	6-1	0.55	0/302	0.77	0/406
1	6-2	0.55	0/302	0.77	0/406
1	6-3	0.55	0/302	0.78	0/406
1	6-4	0.55	0/302	0.77	0/406
1	6-5	0.55	0/302	0.77	0/406
1	6-6	0.55	0/302	0.77	0/406
1	6-7	0.55	0/302	0.77	0/406
1	6-8	0.55	0/302	0.77	0/406
1	7-1	0.58	0/302	0.77	0/406
1	7-2	0.58	0/302	0.77	0/406
1	7-3	0.59	0/302	0.77	0/406
1	7-4	0.59	0/302	0.77	0/406
1	7-5	0.58	0/302	0.77	0/406
1	7-6	0.58	0/302	0.77	0/406
1	7-7	0.59	0/302	0.78	0/406
1	7-8	0.58	0/302	0.77	0/406
1	8-1	0.55	0/302	0.77	0/406
1	8-2	0.55	0/302	0.78	0/406
1	8-3	0.56	0/302	0.78	0/406
1	8-4	0.55	0/302	0.77	0/406
1	8-5	0.55	0/302	0.77	0/406
1	8-6	0.55	0/302	0.78	0/406
1	8-7	0.55	0/302	0.78	0/406
1	8-8	0.55	0/302	0.77	0/406
1	9-1	0.56	0/302	0.78	0/406
1	9-2	0.56	0/302	0.77	0/406
1	9-3	0.56	0/302	0.77	0/406
1	9-4	0.56	0/302	0.78	0/406
1	9-5	0.56	0/302	0.78	0/406
1	9-6	0.55	0/302	0.78	0/406
1	9-7	0.55	0/302	0.78	0/406
1	9-8	0.55	0/302	0.78	0/406
1	10-1	0.56	0/302	0.78	0/406
1	10-2	0.55	0/302	0.78	0/406
1	10-3	0.56	0/302	0.78	0/406
1	10-4	0.56	0/302	0.78	0/406
1	10-5	0.56	0/302	0.78	0/406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	10-6	0.56	0/302	0.78	0/406
1	10-7	0.56	0/302	0.78	0/406
1	10-8	0.56	0/302	0.78	0/406
1	11-1	0.55	0/302	0.77	0/406
1	11-2	0.54	0/302	0.78	0/406
1	11-3	0.55	0/302	0.78	0/406
1	11-4	0.54	0/302	0.78	0/406
1	11-5	0.55	0/302	0.78	0/406
1	11-6	0.55	0/302	0.78	0/406
1	11-7	0.55	0/302	0.78	0/406
1	11-8	0.55	0/302	0.78	0/406
1	12-1	0.55	0/302	0.78	0/406
1	12-2	0.56	0/302	0.78	0/406
1	12-3	0.56	0/302	0.78	0/406
1	12-4	0.56	0/302	0.78	0/406
1	12-5	0.56	0/302	0.77	0/406
1	12-6	0.56	0/302	0.78	0/406
1	12-7	0.56	0/302	0.78	0/406
1	12-8	0.55	0/302	0.77	0/406
1	13-1	0.55	0/302	0.77	0/406
1	13-2	0.54	0/302	0.77	0/406
1	13-3	0.55	0/302	0.77	0/406
1	13-4	0.54	0/302	0.77	0/406
1	13-5	0.55	0/302	0.76	0/406
1	13-6	0.54	0/302	0.77	0/406
1	13-7	0.55	0/302	0.77	0/406
1	13-8	0.54	0/302	0.76	0/406
1	14-1	0.54	0/302	0.77	0/406
1	14-2	0.54	0/302	0.77	0/406
1	14-3	0.54	0/302	0.77	0/406
1	14-4	0.54	0/302	0.78	0/406
1	14-5	0.54	0/302	0.76	0/406
1	14-6	0.54	0/302	0.77	0/406
1	14-7	0.54	0/302	0.77	0/406
1	14-8	0.54	0/302	0.77	0/406
All	All	0.56	0/33824	0.78	0/45472

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-1	295	220	244	0	0
1	1-2	295	220	244	0	0
1	1-3	295	220	244	0	0
1	1-4	295	220	244	0	0
1	1-5	295	220	244	0	0
1	1-6	295	220	244	0	0
1	1-7	295	220	244	0	0
1	1-8	295	220	244	0	0
1	2-1	295	220	244	1	0
1	2-2	295	220	244	1	0
1	2-3	295	220	244	1	0
1	2-4	295	220	244	0	0
1	2-5	295	220	244	0	0
1	2-6	295	220	244	1	0
1	2-7	295	220	244	0	0
1	2-8	295	220	244	0	0
1	3-1	295	220	244	3	0
1	3-2	295	220	244	6	0
1	3-3	295	220	244	5	0
1	3-4	295	220	244	2	0
1	3-5	295	220	244	3	0
1	3-6	295	220	244	5	0
1	3-7	295	220	244	4	0
1	3-8	295	220	244	2	0
1	4-1	295	220	244	0	0
1	4-2	295	220	244	0	0
1	4-3	295	220	244	0	0
1	4-4	295	220	244	0	0
1	4-5	295	220	244	0	0
1	4-6	295	220	244	0	0
1	4-7	295	220	244	0	0
1	4-8	295	220	244	0	0
1	5-1	295	220	244	3	0
1	5-2	295	220	244	6	0
1	5-3	295	220	244	6	0
1	5-4	295	220	244	3	0
1	5-5	295	220	244	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-6	295	220	244	6	0
1	5-7	295	220	244	6	0
1	5-8	295	220	244	3	0
1	6-1	295	220	244	0	0
1	6-2	295	220	244	0	0
1	6-3	295	220	244	0	0
1	6-4	295	220	244	0	0
1	6-5	295	220	244	0	0
1	6-6	295	220	244	0	0
1	6-7	295	220	244	0	0
1	6-8	295	220	244	0	0
1	7-1	295	220	244	1	0
1	7-2	295	220	244	2	0
1	7-3	295	220	244	2	0
1	7-4	295	220	244	1	0
1	7-5	295	220	244	2	0
1	7-6	295	220	244	2	0
1	7-7	295	220	244	1	0
1	7-8	295	220	244	1	0
1	8-1	295	220	244	4	0
1	8-2	295	220	244	6	0
1	8-3	295	220	244	6	0
1	8-4	295	220	244	3	0
1	8-5	295	220	244	2	0
1	8-6	295	220	244	6	0
1	8-7	295	220	244	5	0
1	8-8	295	220	244	2	0
1	9-1	295	220	244	1	0
1	9-2	295	220	244	2	0
1	9-3	295	220	244	2	0
1	9-4	295	220	244	1	0
1	9-5	295	220	244	1	0
1	9-6	295	220	244	2	0
1	9-7	295	220	244	3	0
1	9-8	295	220	244	1	0
1	10-1	295	220	244	1	0
1	10-2	295	220	244	2	0
1	10-3	295	220	244	2	0
1	10-4	295	220	244	1	0
1	10-5	295	220	244	1	0
1	10-6	295	220	244	2	0
1	10-7	295	220	244	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-8	295	220	244	0	0
1	11-1	295	220	244	0	0
1	11-2	295	220	244	0	0
1	11-3	295	220	244	1	0
1	11-4	295	220	244	1	0
1	11-5	295	220	244	0	0
1	11-6	295	220	244	0	0
1	11-7	295	220	244	1	0
1	11-8	295	220	244	1	0
1	12-1	295	220	244	1	0
1	12-2	295	220	244	2	0
1	12-3	295	220	244	2	0
1	12-4	295	220	244	1	0
1	12-5	295	220	244	1	0
1	12-6	295	220	244	2	0
1	12-7	295	220	244	1	0
1	12-8	295	220	244	0	0
1	13-1	295	220	244	2	0
1	13-2	295	220	244	5	0
1	13-3	295	220	244	5	0
1	13-4	295	220	244	2	0
1	13-5	295	220	244	2	0
1	13-6	295	220	244	4	0
1	13-7	295	220	244	4	0
1	13-8	295	220	244	2	0
1	14-1	295	220	244	0	0
1	14-2	295	220	244	0	0
1	14-3	295	220	244	0	0
1	14-4	295	220	244	0	0
1	14-5	295	220	244	0	0
1	14-6	295	220	244	0	0
1	14-7	295	220	244	0	0
1	14-8	295	220	244	0	0
All	All	33040	24640	27328	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:36:GLN:HG3	1:8:36:GLN:HE22	1.60	0.67
1:6:36:GLN:HG3	1:7:36:GLN:HE22	1.61	0.66
1:5:36:GLN:HG3	1:6:36:GLN:HE22	1.62	0.65
1:2:36:GLN:HG3	1:3:36:GLN:HE22	1.61	0.65
1:5:36:GLN:HG3	1:6:36:GLN:HE22	1.62	0.64
1:7:36:GLN:HG3	1:8:36:GLN:HE22	1.63	0.64
1:1:36:GLN:HG3	1:2:36:GLN:HE22	1.62	0.64
1:3:36:GLN:HG3	1:4:36:GLN:HE22	1.61	0.64
1:2:36:GLN:HG3	1:3:36:GLN:HE22	1.62	0.64
1:5:36:GLN:HG3	1:6:36:GLN:HE22	1.63	0.64
1:3:36:GLN:HG3	1:4:36:GLN:HE22	1.63	0.64
1:2:36:GLN:HG3	1:3:36:GLN:HE22	1.63	0.63
1:1:36:GLN:HG3	1:2:36:GLN:HE22	1.62	0.63
1:3:36:GLN:HG3	1:4:36:GLN:HE22	1.64	0.63
1:7:36:GLN:HG3	1:8:36:GLN:HE22	1.64	0.63
1:7:36:GLN:HG3	1:8:36:GLN:HE22	1.64	0.63
1:6:36:GLN:HG3	1:7:36:GLN:HE22	1.64	0.63
1:1:36:GLN:HG3	1:2:36:GLN:HE22	1.63	0.63
1:6:36:GLN:HG3	1:7:36:GLN:HE22	1.64	0.62
1:2:36:GLN:HG3	1:3:36:GLN:HE22	1.65	0.62
1:6:36:GLN:HG3	1:7:36:GLN:HE22	1.65	0.61
1:1:36:GLN:HG3	1:2:36:GLN:HE22	1.65	0.61
1:5:36:GLN:HG3	1:6:36:GLN:HE22	1.65	0.61
1:3:36:GLN:HG3	1:4:36:GLN:HE22	1.64	0.61
1:3:36:GLN:CG	1:4:36:GLN:HE22	2.16	0.57
1:6:36:GLN:CG	1:7:36:GLN:HE22	2.17	0.57
1:5:36:GLN:CG	1:6:36:GLN:HE22	2.17	0.57
1:5:36:GLN:CG	1:6:36:GLN:HE22	2.17	0.57
1:7:36:GLN:CG	1:8:36:GLN:HE22	2.18	0.56
1:1:36:GLN:CG	1:2:36:GLN:HE22	2.19	0.56
1:7:36:GLN:CG	1:8:36:GLN:HE22	2.18	0.56
1:2:36:GLN:CG	1:3:36:GLN:HE22	2.18	0.56
1:2:36:GLN:CG	1:3:36:GLN:HE22	2.18	0.56
1:1:36:GLN:CG	1:2:36:GLN:HE22	2.18	0.56
1:2:36:GLN:CG	1:3:36:GLN:HE22	2.18	0.56
1:5:36:GLN:CG	1:6:36:GLN:HE22	2.18	0.56
1:6:36:GLN:CG	1:7:36:GLN:HE22	2.18	0.56
1:6:36:GLN:CG	1:7:36:GLN:HE22	2.18	0.56
1:3:36:GLN:CG	1:4:36:GLN:HE22	2.19	0.55
1:3:36:GLN:CG	1:4:36:GLN:HE22	2.19	0.55
1:5:36:GLN:CG	1:6:36:GLN:HE22	2.19	0.55
1:2:36:GLN:CG	1:3:36:GLN:HE22	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:36:GLN:CG	1:2:36:GLN:HE22	2.20	0.54
1:7:36:GLN:CG	1:8:36:GLN:HE22	2.21	0.54
1:2:21:SER:O	1:3:21:SER:HB2	2.08	0.54
1:1:36:GLN:CG	1:2:36:GLN:HE22	2.20	0.53
1:6:36:GLN:CG	1:7:36:GLN:HE22	2.21	0.53
1:7:36:GLN:CG	1:8:36:GLN:HE22	2.22	0.53
1:3:36:GLN:CG	1:4:36:GLN:HE22	2.22	0.52
1:6:21:SER:O	1:7:21:SER:HB2	2.11	0.51
1:7:21:SER:O	1:8:21:SER:HB2	2.11	0.50
1:5:21:SER:O	1:6:21:SER:HB2	2.12	0.50
1:5:18:GLY:N	1:5:23:GLN:HE22	2.10	0.49
1:7:18:GLY:N	1:7:23:GLN:HE22	2.11	0.48
1:8:18:GLY:N	1:8:23:GLN:HE22	2.11	0.48
1:1:18:GLY:N	1:1:23:GLN:HE22	2.11	0.48
1:1:21:SER:O	1:2:21:SER:HB2	2.14	0.48
1:3:21:SER:O	1:4:21:SER:HB2	2.13	0.48
1:2:18:GLY:N	1:2:23:GLN:HE22	2.11	0.48
1:3:18:GLY:N	1:3:23:GLN:HE22	2.12	0.47
1:4:18:GLY:N	1:4:23:GLN:HE22	2.12	0.47
1:6:18:GLY:N	1:6:23:GLN:HE22	2.13	0.47
1:5:14:GLN:N	1:5:15:PRO:HD3	2.32	0.45
1:6:14:GLN:N	1:6:15:PRO:HD3	2.31	0.45
1:2:14:GLN:N	1:2:15:PRO:HD3	2.32	0.45
1:3:14:GLN:N	1:3:15:PRO:HD3	2.32	0.45
1:1:14:GLN:N	1:1:15:PRO:HD3	2.32	0.45
1:7:14:GLN:N	1:7:15:PRO:HD3	2.31	0.45
1:4:14:GLN:N	1:4:15:PRO:HD3	2.32	0.44
1:8:14:GLN:N	1:8:15:PRO:HD3	2.31	0.44
1:2:21:SER:O	1:3:21:SER:HB2	2.19	0.43
1:1:22:GLN:HE21	1:6:39:TYR:HB2	1.84	0.42
1:2:21:SER:O	1:3:21:SER:HB2	2.20	0.42
1:5:21:SER:O	1:6:21:SER:HB2	2.20	0.42
1:1:21:SER:O	1:2:21:SER:HB2	2.20	0.42
1:7:36:GLN:HE21	1:8:2:SER:HB2	1.85	0.42
1:2:21:SER:O	1:3:21:SER:HB2	2.20	0.42
1:2:21:SER:O	1:3:21:SER:HB2	2.20	0.42
1:5:21:SER:O	1:6:21:SER:HB2	2.20	0.41
1:2:21:SER:O	1:3:21:SER:HB2	2.21	0.41
1:6:21:SER:O	1:7:21:SER:HB2	2.21	0.41
1:2:21:SER:O	1:3:21:SER:HB2	2.21	0.41
1:3:21:SER:O	1:4:21:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:21:SER:O	1:3:21:SER:HB2	2.21	0.41
1:1:21:SER:O	1:2:21:SER:HB2	2.21	0.41
1:3:36:GLN:HE21	1:4:2:SER:HB2	1.85	0.41
1:3:21:SER:O	1:4:21:SER:HB2	2.21	0.41
1:6:21:SER:O	1:7:21:SER:HB2	2.22	0.40
1:1:21:SER:O	1:2:21:SER:HB2	2.21	0.40
1:5:21:SER:O	1:6:21:SER:HB2	2.22	0.40
1:6:21:SER:O	1:7:21:SER:HB2	2.21	0.40
1:6:21:SER:O	1:7:21:SER:HB2	2.22	0.40
1:1:22:GLN:HE21	1:6:39:TYR:HB2	1.86	0.40
1:1:21:SER:O	1:2:21:SER:HB2	2.22	0.40
1:5:21:SER:O	1:6:21:SER:HB2	2.22	0.40
1:2:21:SER:O	1:3:21:SER:HB2	2.21	0.40
1:7:23:GLN:N	1:7:24:PRO:HD3	2.37	0.40
1:3:21:SER:O	1:4:21:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	1-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	1-3	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	1-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	1-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	1-6	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	1-7	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	1-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	2-2	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	2-3	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	2-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	2-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	2-6	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	2-7	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	2-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	3-1	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	3-2	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	3-3	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	3-4	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	3-5	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	3-6	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	3-7	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	3-8	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	4-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	4-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	4-3	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	4-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	4-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	4-6	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	4-7	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	4-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	5-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	5-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	5-3	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	5-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	5-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	5-6	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	5-7	37/104 (36%)	35 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-3	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-6	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-7	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	6-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	7-1	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	7-2	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	7-3	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	7-4	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	7-5	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	7-6	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	7-7	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	7-8	37/104 (36%)	33 (89%)	4 (11%)	0	100	100
1	8-1	37/104 (36%)	36 (97%)	1 (3%)	0	100	100
1	8-2	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	8-3	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	8-4	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	8-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	8-6	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	8-7	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	8-8	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	9-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	9-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	9-3	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	9-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	9-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	9-6	37/104 (36%)	35 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-7	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	9-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-3	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-6	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-7	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	10-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	11-1	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	11-2	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	11-3	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	11-4	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	11-5	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	11-6	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	11-7	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	11-8	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	12-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	12-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	12-3	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	12-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	12-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	12-6	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	12-7	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	12-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	13-1	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	13-2	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	13-3	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	13-4	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	13-5	37/104 (36%)	34 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-6	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	13-7	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	13-8	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	14-1	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	14-2	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	14-3	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	14-4	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	14-5	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
1	14-6	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	14-7	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
1	14-8	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
All	All	4144/11648 (36%)	3868 (93%)	276 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-1	33/68 (48%)	33 (100%)	0	100	100
1	1-2	33/68 (48%)	33 (100%)	0	100	100
1	1-3	33/68 (48%)	33 (100%)	0	100	100
1	1-4	33/68 (48%)	33 (100%)	0	100	100
1	1-5	33/68 (48%)	33 (100%)	0	100	100
1	1-6	33/68 (48%)	33 (100%)	0	100	100
1	1-7	33/68 (48%)	33 (100%)	0	100	100
1	1-8	33/68 (48%)	33 (100%)	0	100	100
1	2-1	33/68 (48%)	33 (100%)	0	100	100
1	2-2	33/68 (48%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-3	33/68 (48%)	33 (100%)	0	100	100
1	2-4	33/68 (48%)	33 (100%)	0	100	100
1	2-5	33/68 (48%)	33 (100%)	0	100	100
1	2-6	33/68 (48%)	33 (100%)	0	100	100
1	2-7	33/68 (48%)	33 (100%)	0	100	100
1	2-8	33/68 (48%)	33 (100%)	0	100	100
1	3-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	3-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	3-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	3-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	3-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	3-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	3-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	3-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	4-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	5-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	6-1	33/68 (48%)	32 (97%)	1 (3%)	41	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	6-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	6-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	6-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	6-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	6-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	6-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	7-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	8-1	33/68 (48%)	33 (100%)	0	100	100
1	8-2	33/68 (48%)	33 (100%)	0	100	100
1	8-3	33/68 (48%)	33 (100%)	0	100	100
1	8-4	33/68 (48%)	33 (100%)	0	100	100
1	8-5	33/68 (48%)	33 (100%)	0	100	100
1	8-6	33/68 (48%)	33 (100%)	0	100	100
1	8-7	33/68 (48%)	33 (100%)	0	100	100
1	8-8	33/68 (48%)	33 (100%)	0	100	100
1	9-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	9-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	9-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	9-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	9-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	9-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	9-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	9-8	33/68 (48%)	32 (97%)	1 (3%)	41	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	10-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	10-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	10-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	10-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	10-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	10-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	10-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	11-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-7	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	12-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	13-1	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	13-2	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	13-3	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	13-4	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	13-5	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	13-6	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	13-7	33/68 (48%)	32 (97%)	1 (3%)	41	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	13-8	33/68 (48%)	32 (97%)	1 (3%)	41	66
1	14-1	33/68 (48%)	33 (100%)	0	100	100
1	14-2	33/68 (48%)	33 (100%)	0	100	100
1	14-3	33/68 (48%)	33 (100%)	0	100	100
1	14-4	33/68 (48%)	33 (100%)	0	100	100
1	14-5	33/68 (48%)	33 (100%)	0	100	100
1	14-6	33/68 (48%)	33 (100%)	0	100	100
1	14-7	33/68 (48%)	33 (100%)	0	100	100
1	14-8	33/68 (48%)	33 (100%)	0	100	100
All	All	3696/7616 (48%)	3616 (98%)	80 (2%)	54	74

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3-1	2	SER
1	3-2	2	SER
1	3-3	2	SER
1	3-4	2	SER
1	3-5	2	SER
1	3-6	2	SER
1	3-7	2	SER
1	3-8	2	SER
1	4-1	2	SER
1	4-2	2	SER
1	4-3	2	SER
1	4-4	2	SER
1	4-5	2	SER
1	4-6	2	SER
1	4-7	2	SER
1	4-8	2	SER
1	5-1	2	SER
1	5-2	2	SER
1	5-3	2	SER
1	5-4	2	SER
1	5-5	2	SER
1	5-6	2	SER
1	5-7	2	SER
1	5-8	2	SER
1	6-1	2	SER

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Mol	Chain	Res	Type
1	6-2	2	SER
1	6-3	2	SER
1	6-4	2	SER
1	6-5	2	SER
1	6-6	2	SER
1	6-7	2	SER
1	6-8	2	SER
1	7-1	2	SER
1	7-2	2	SER
1	7-3	2	SER
1	7-4	2	SER
1	7-5	2	SER
1	7-6	2	SER
1	7-7	2	SER
1	7-8	2	SER
1	9-1	2	SER
1	9-2	2	SER
1	9-3	2	SER
1	9-4	2	SER
1	9-5	2	SER
1	9-6	2	SER
1	9-7	2	SER
1	9-8	2	SER
1	10-1	2	SER
1	10-2	2	SER
1	10-3	2	SER
1	10-4	2	SER
1	10-5	2	SER
1	10-6	2	SER
1	10-7	2	SER
1	10-8	2	SER
1	11-1	2	SER
1	11-2	2	SER
1	11-3	2	SER
1	11-4	2	SER
1	11-5	2	SER
1	11-6	2	SER
1	11-7	2	SER
1	11-8	2	SER
1	12-1	2	SER
1	12-2	2	SER
1	12-3	2	SER

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Mol	Chain	Res	Type
1	12-4	2	SER
1	12-5	2	SER
1	12-6	2	SER
1	12-7	2	SER
1	12-8	2	SER
1	13-1	2	SER
1	13-2	2	SER
1	13-3	2	SER
1	13-4	2	SER
1	13-5	2	SER
1	13-6	2	SER
1	13-7	2	SER
1	13-8	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-1	35	GLN
1	1-1	36	GLN
1	1-2	35	GLN
1	1-2	36	GLN
1	1-3	35	GLN
1	1-3	36	GLN
1	1-4	35	GLN
1	1-4	36	GLN
1	1-5	35	GLN
1	1-5	36	GLN
1	1-6	35	GLN
1	1-6	36	GLN
1	1-7	35	GLN
1	1-7	36	GLN
1	1-8	35	GLN
1	1-8	36	GLN
1	2-1	22	GLN
1	2-1	23	GLN
1	2-1	31	GLN
1	2-1	36	GLN
1	2-1	40	ASN
1	2-2	22	GLN
1	2-2	23	GLN
1	2-2	31	GLN
1	2-2	36	GLN

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Mol	Chain	Res	Type
1	2-2	40	ASN
1	2-3	23	GLN
1	2-3	31	GLN
1	2-3	36	GLN
1	2-3	40	ASN
1	2-4	23	GLN
1	2-4	31	GLN
1	2-4	36	GLN
1	2-4	40	ASN
1	2-5	22	GLN
1	2-5	23	GLN
1	2-5	31	GLN
1	2-5	36	GLN
1	2-5	40	ASN
1	2-6	22	GLN
1	2-6	23	GLN
1	2-6	31	GLN
1	2-6	36	GLN
1	2-6	40	ASN
1	2-7	23	GLN
1	2-7	31	GLN
1	2-7	36	GLN
1	2-7	40	ASN
1	2-8	23	GLN
1	2-8	31	GLN
1	2-8	36	GLN
1	2-8	40	ASN
1	3-1	31	GLN
1	3-2	31	GLN
1	3-3	31	GLN
1	3-4	31	GLN
1	3-5	31	GLN
1	3-6	31	GLN
1	3-7	31	GLN
1	3-8	31	GLN
1	4-1	14	GLN
1	4-1	22	GLN
1	4-1	31	GLN
1	4-1	36	GLN
1	4-2	14	GLN
1	4-2	22	GLN
1	4-2	31	GLN

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Mol	Chain	Res	Type
1	4-2	36	GLN
1	4-3	14	GLN
1	4-3	31	GLN
1	4-3	36	GLN
1	4-4	14	GLN
1	4-4	31	GLN
1	4-4	36	GLN
1	4-5	14	GLN
1	4-5	22	GLN
1	4-5	31	GLN
1	4-5	36	GLN
1	4-6	14	GLN
1	4-6	22	GLN
1	4-6	31	GLN
1	4-6	36	GLN
1	4-7	14	GLN
1	4-7	22	GLN
1	4-7	31	GLN
1	4-7	36	GLN
1	4-8	14	GLN
1	4-8	31	GLN
1	4-8	36	GLN
1	6-1	22	GLN
1	6-1	36	GLN
1	6-2	22	GLN
1	6-2	36	GLN
1	6-3	22	GLN
1	6-3	36	GLN
1	6-4	36	GLN
1	6-5	22	GLN
1	6-5	36	GLN
1	6-6	22	GLN
1	6-6	36	GLN
1	6-7	22	GLN
1	6-7	36	GLN
1	6-8	22	GLN
1	6-8	36	GLN
1	7-1	14	GLN
1	7-1	31	GLN
1	7-2	14	GLN
1	7-2	31	GLN
1	7-3	14	GLN

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Mol	Chain	Res	Type
1	7-3	31	GLN
1	7-4	14	GLN
1	7-4	31	GLN
1	7-5	14	GLN
1	7-5	31	GLN
1	7-6	14	GLN
1	7-6	31	GLN
1	7-7	14	GLN
1	7-7	31	GLN
1	7-8	14	GLN
1	7-8	31	GLN
1	8-1	22	GLN
1	8-1	31	GLN
1	8-1	40	ASN
1	8-2	22	GLN
1	8-2	31	GLN
1	8-2	40	ASN
1	8-3	22	GLN
1	8-3	31	GLN
1	8-3	40	ASN
1	8-4	31	GLN
1	8-4	40	ASN
1	8-5	22	GLN
1	8-5	31	GLN
1	8-5	40	ASN
1	8-6	22	GLN
1	8-6	31	GLN
1	8-6	40	ASN
1	8-7	22	GLN
1	8-7	31	GLN
1	8-7	40	ASN
1	8-8	22	GLN
1	8-8	31	GLN
1	8-8	40	ASN
1	9-1	31	GLN
1	9-1	37	GLN
1	9-2	31	GLN
1	9-2	37	GLN
1	9-3	31	GLN
1	9-3	37	GLN
1	9-4	16	GLN
1	9-4	31	GLN

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Mol	Chain	Res	Type
1	9-5	31	GLN
1	9-5	37	GLN
1	9-6	31	GLN
1	9-6	37	GLN
1	9-7	31	GLN
1	9-7	37	GLN
1	9-8	16	GLN
1	9-8	31	GLN
1	10-1	29	GLN
1	10-2	29	GLN
1	10-3	29	GLN
1	10-4	16	GLN
1	10-4	29	GLN
1	10-6	29	GLN
1	10-7	29	GLN
1	10-8	16	GLN
1	10-8	29	GLN
1	11-1	14	GLN
1	11-1	31	GLN
1	11-1	36	GLN
1	11-2	14	GLN
1	11-2	31	GLN
1	11-2	36	GLN
1	11-3	14	GLN
1	11-3	31	GLN
1	11-3	36	GLN
1	11-4	14	GLN
1	11-4	31	GLN
1	11-4	36	GLN
1	11-5	14	GLN
1	11-5	31	GLN
1	11-5	36	GLN
1	11-6	14	GLN
1	11-6	31	GLN
1	11-6	36	GLN
1	11-7	14	GLN
1	11-7	31	GLN
1	11-7	36	GLN
1	11-8	14	GLN
1	11-8	31	GLN
1	11-8	36	GLN
1	12-1	31	GLN

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Mol	Chain	Res	Type
1	12-2	31	GLN
1	12-3	31	GLN
1	12-4	16	GLN
1	12-4	31	GLN
1	12-5	31	GLN
1	12-6	31	GLN
1	12-7	31	GLN
1	12-8	16	GLN
1	12-8	31	GLN
1	13-1	22	GLN
1	13-1	23	GLN
1	13-1	31	GLN
1	13-2	22	GLN
1	13-2	23	GLN
1	13-2	31	GLN
1	13-3	22	GLN
1	13-3	23	GLN
1	13-3	31	GLN
1	13-4	23	GLN
1	13-4	31	GLN
1	13-5	22	GLN
1	13-5	23	GLN
1	13-5	31	GLN
1	13-6	22	GLN
1	13-6	23	GLN
1	13-6	31	GLN
1	13-7	22	GLN
1	13-7	23	GLN
1	13-7	31	GLN
1	13-8	23	GLN
1	13-8	31	GLN
1	14-4	16	GLN
1	14-8	16	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

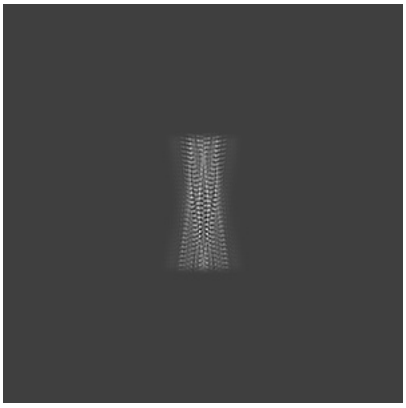
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22169. These allow visual inspection of the internal detail of the map and identification of artifacts.

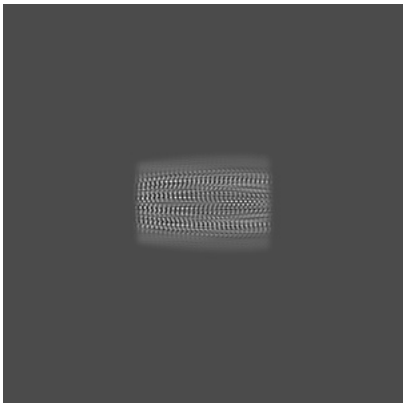
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

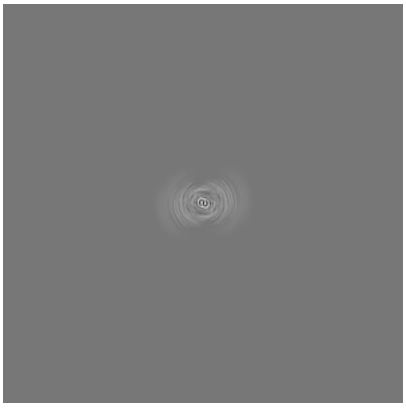
6.1.1 Primary map



X



Y

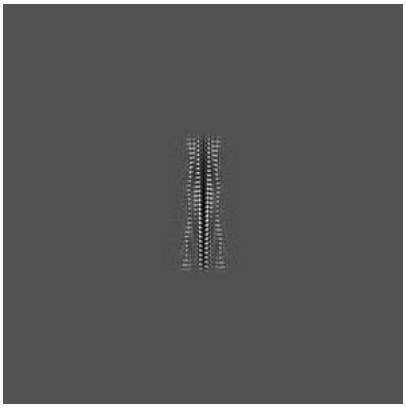


Z

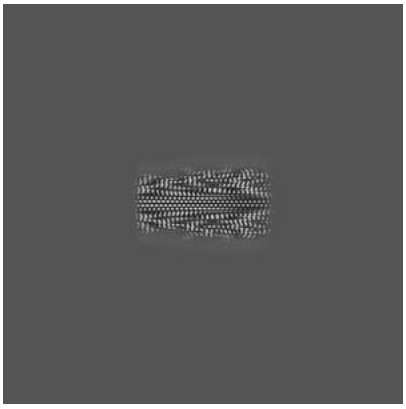
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

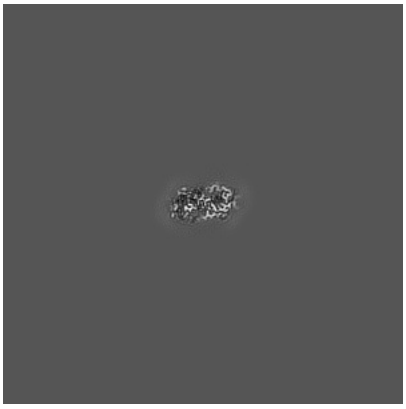
6.2.1 Primary map



X Index: 200



Y Index: 200

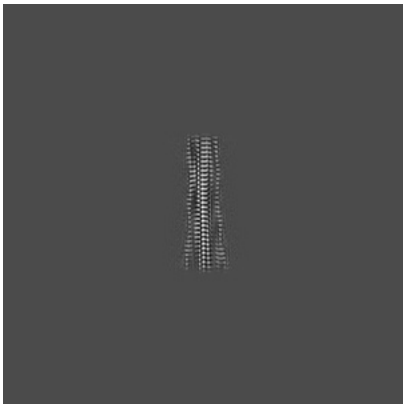


Z Index: 200

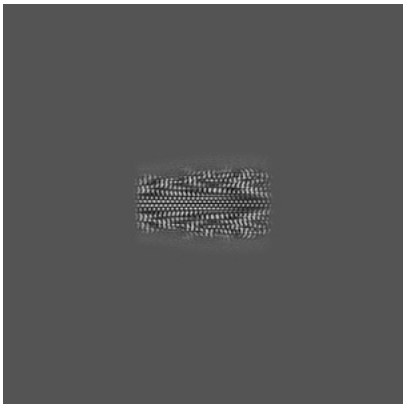
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

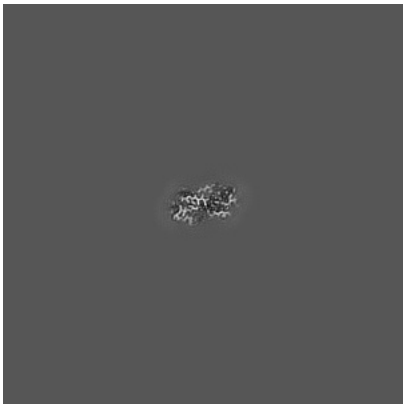
6.3.1 Primary map



X Index: 202



Y Index: 200

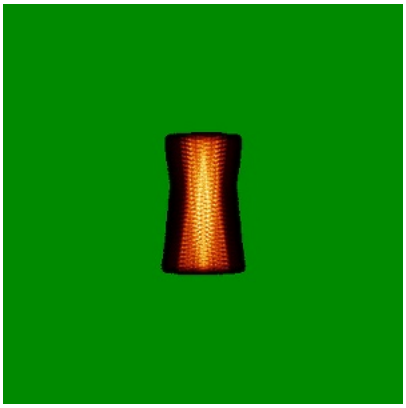


Z Index: 192

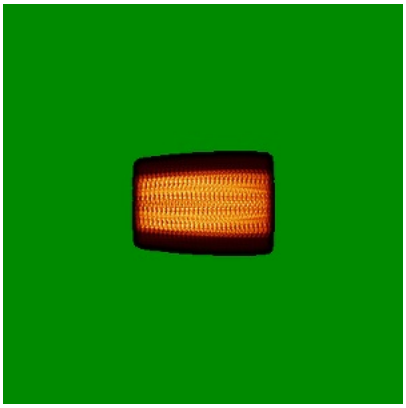
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

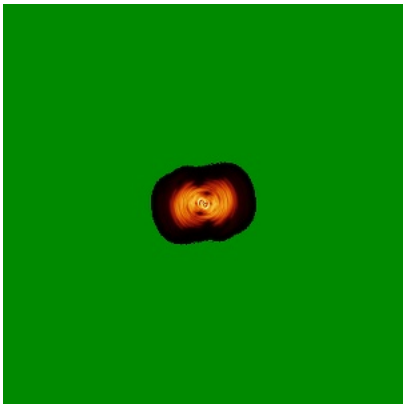
6.4.1 Primary map



X



Y

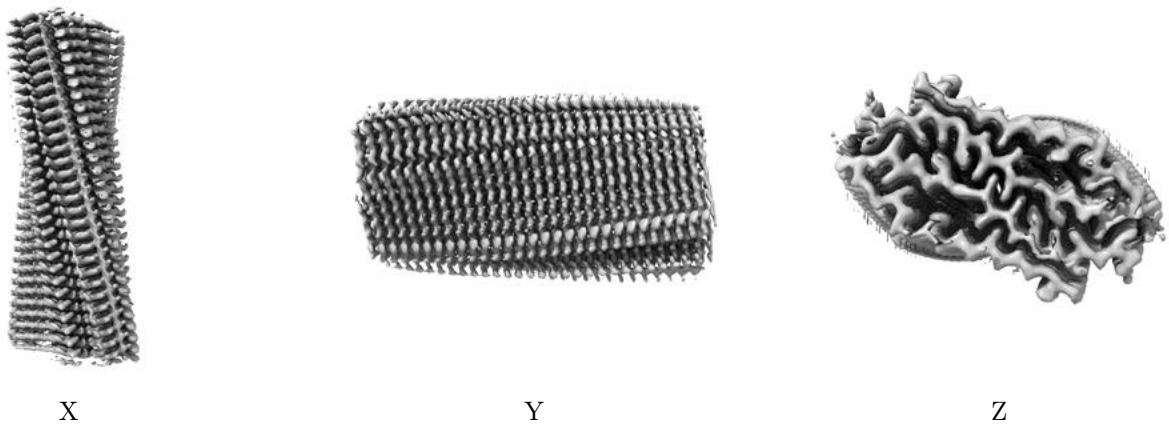


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

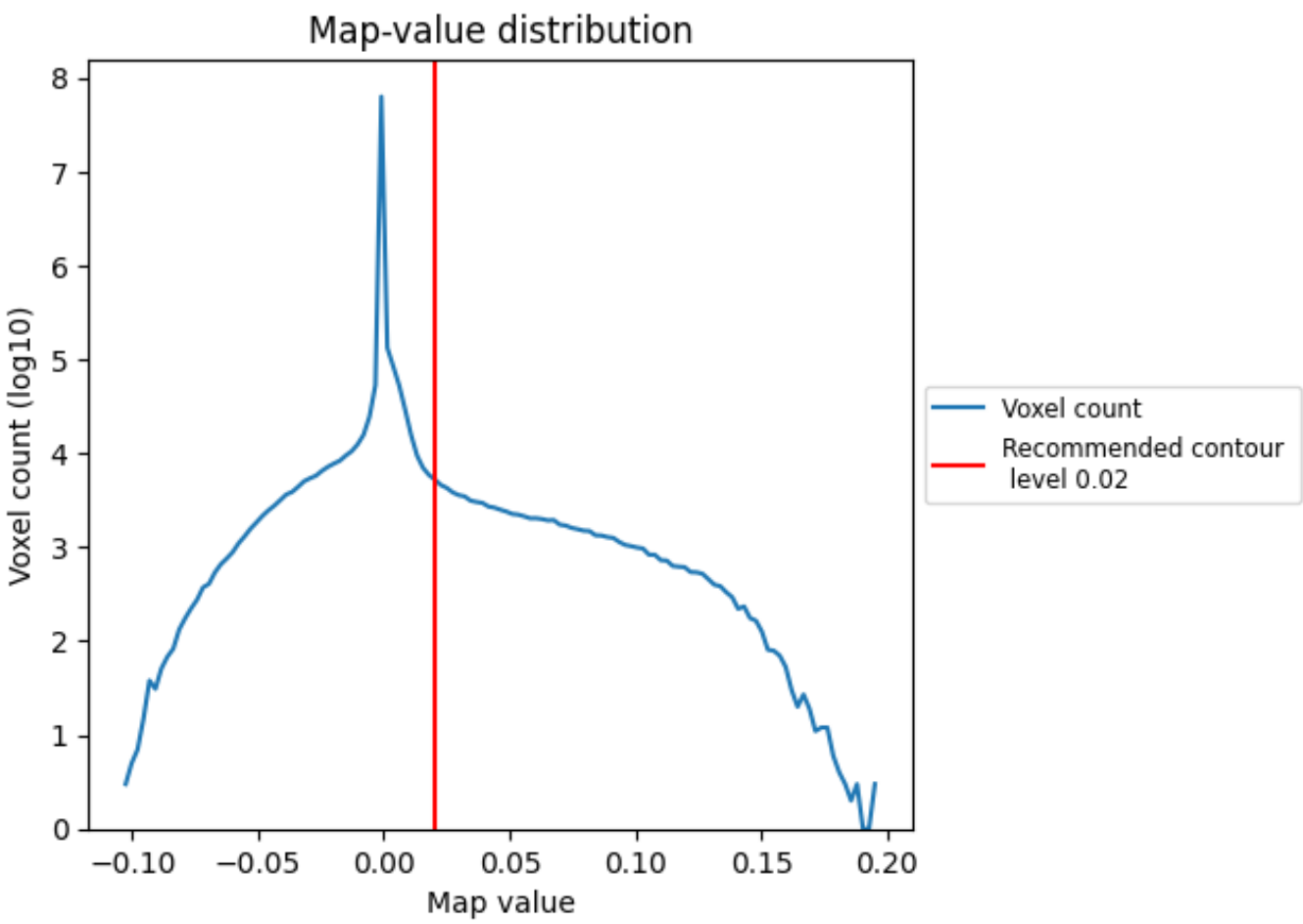
6.6 Mask visualisation (i)

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

7 Map analysis (i)

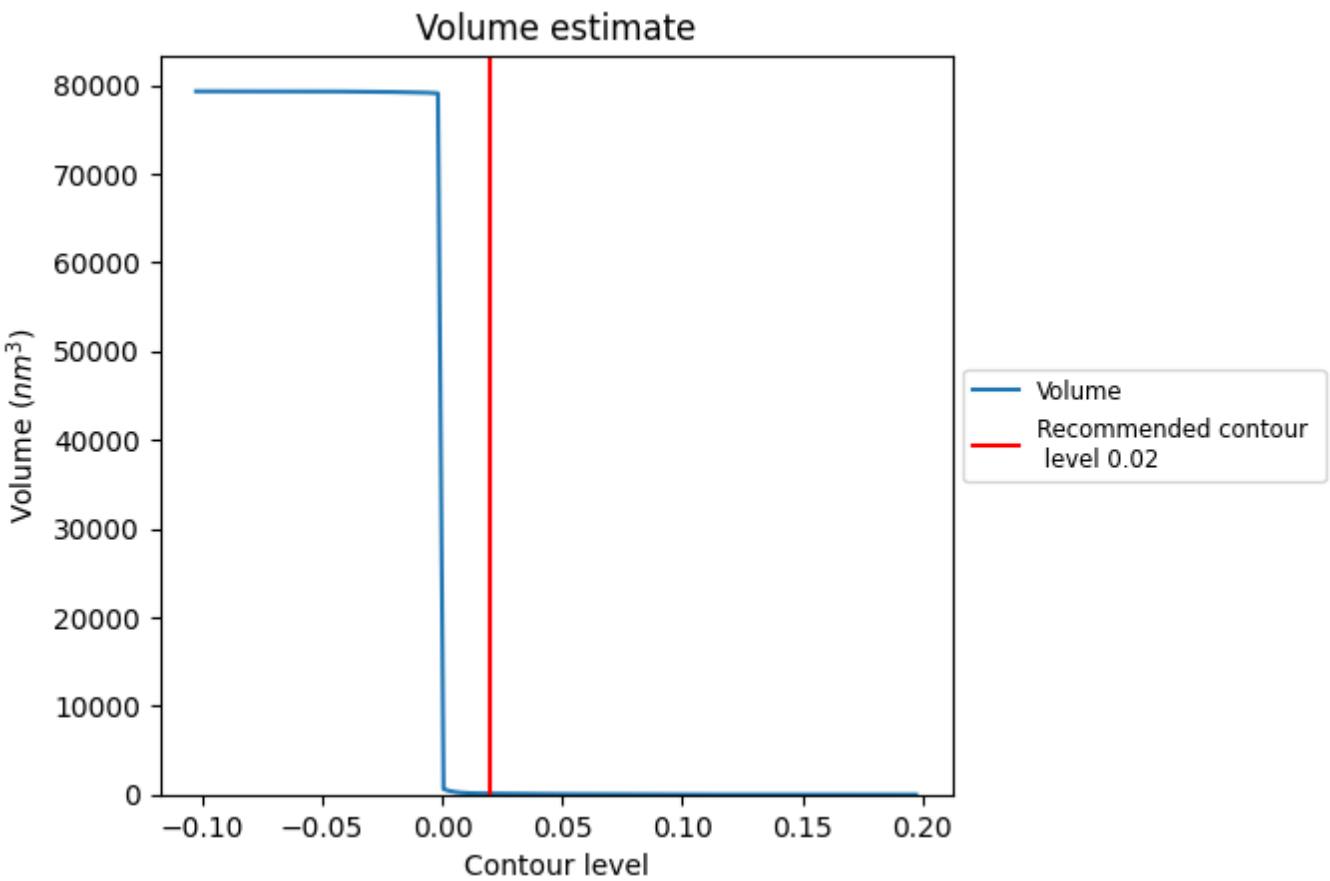
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

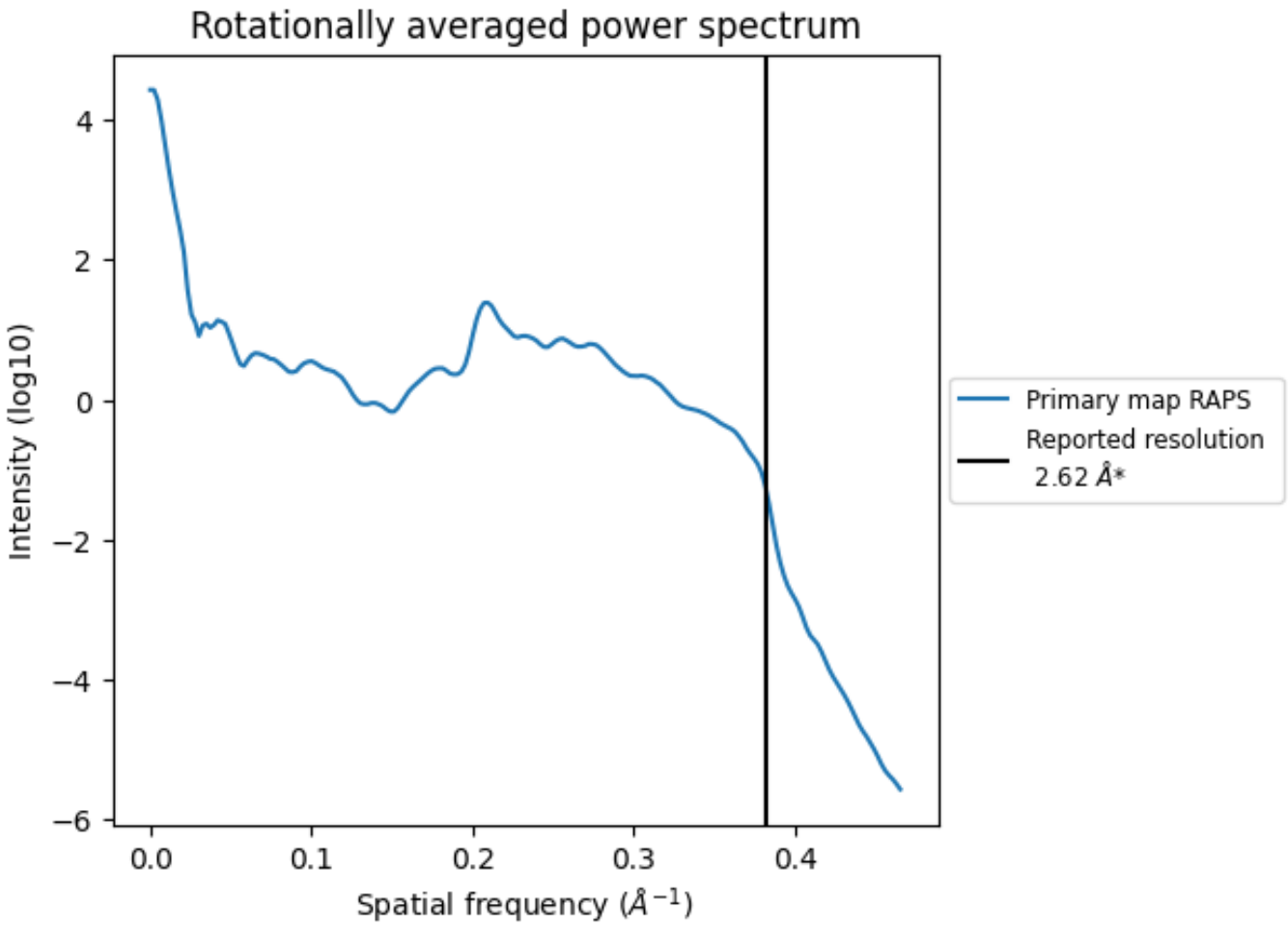
7.2 Volume estimate (i)



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.382 Å^{-1}

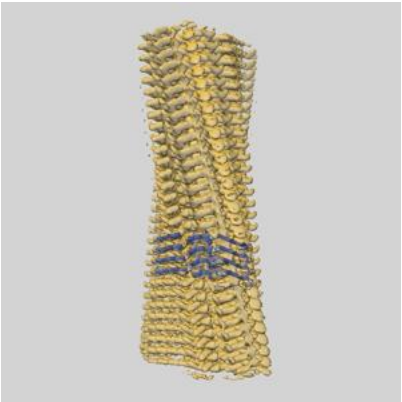
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

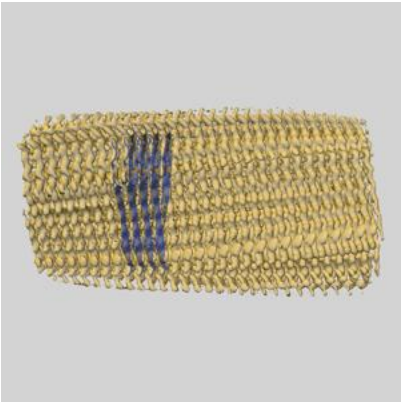
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22169 and PDB model 6XFM. Per-residue inclusion information can be found in section 3 on page 14.

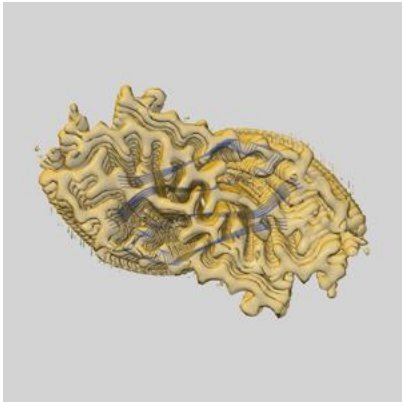
9.1 Map-model overlay (i)



X



Y



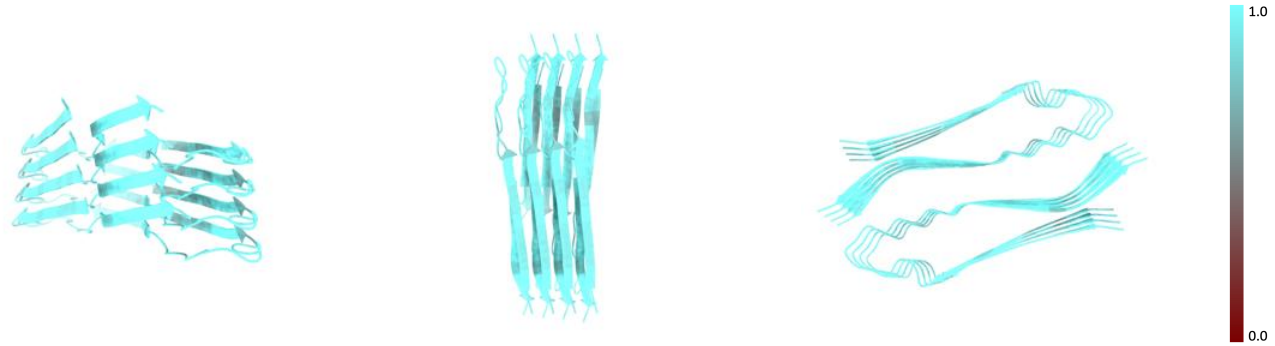
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

This section was not generated.

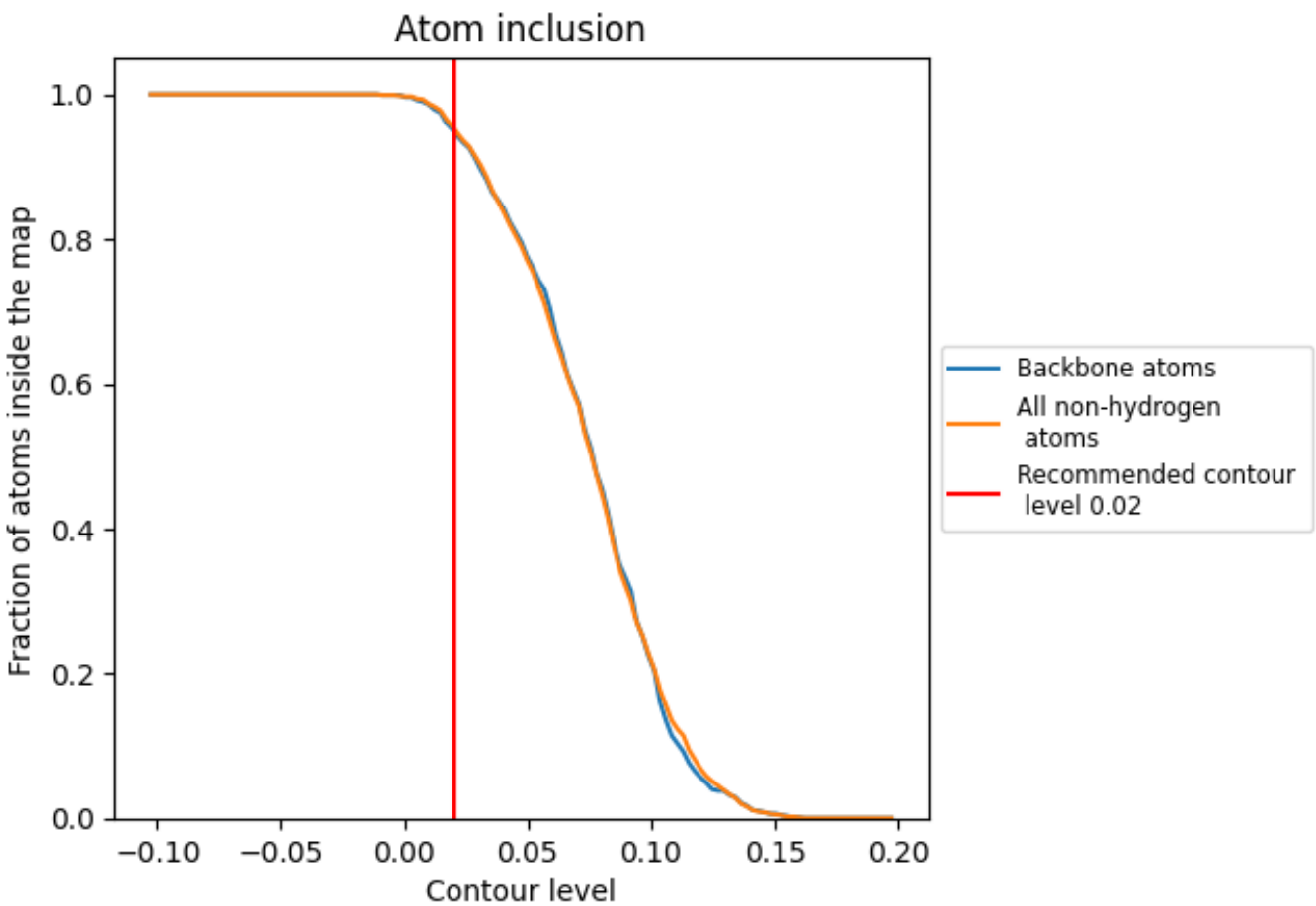
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.9540
1	0.9590
2	0.9650
3	0.9590
4	0.9450
5	0.9520
6	0.9590
7	0.9620
8	0.9590