Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 07:04 AM EDT

PDB ID	:	5W3N
BMRB ID	:	30304
Title	:	Molecular structure of FUS low sequence complexity domain protein fibrils
Authors	:	Murray, D.T.; Kato, M.; Lin, Y.; Thurber, K.; Hung, I.; McKnight, S.; Tycko, R.
Deposited on	:	2017-06-08

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 (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 (1)) were used in the production of this report:

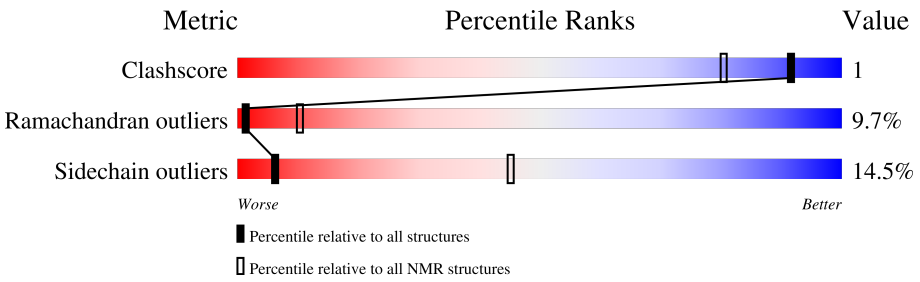
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 4%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	241	19% • • 75%
1	B	241	19% • • 75%
1	C	241	19% • • 75%
1	D	241	19% • • 75%
1	E	241	19% • • 75%
1	F	241	19% • • 75%
1	G	241	19% • • 75%
1	H	241	19% • • 75%
1	I	241	19% • • 75%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:43-A:97, B:43-B:97, C:43-C:97, D:43-D:97, E:43-E:97, F:43-F:97, G:43-G:97, H:43-H:97, I:43-I:97 (495)	1.72	3

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, 3, 4, 5, 6, 7, 8, 11, 12, 13, 15, 16, 19, 20
2	10, 17, 18
Single-model clusters	9; 14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7272 atoms, of which 3285 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	61	808	261	365	72	110	0
1	B	61	808	261	365	72	110	0
1	C	61	808	261	365	72	110	0
1	D	61	808	261	365	72	110	0
1	E	61	808	261	365	72	110	0
1	F	61	808	261	365	72	110	0
1	G	61	808	261	365	72	110	0
1	H	61	808	261	365	72	110	0
1	I	61	808	261	365	72	110	0

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP P35637
A	-25	SER	-	expression tag	UNP P35637
A	-24	TYR	-	expression tag	UNP P35637
A	-23	TYR	-	expression tag	UNP P35637
A	-22	HIS	-	expression tag	UNP P35637
A	-21	HIS	-	expression tag	UNP P35637
A	-20	HIS	-	expression tag	UNP P35637
A	-19	HIS	-	expression tag	UNP P35637
A	-18	HIS	-	expression tag	UNP P35637
A	-17	HIS	-	expression tag	UNP P35637
A	-16	ASP	-	expression tag	UNP P35637
A	-15	TYR	-	expression tag	UNP P35637
A	-14	ASP	-	expression tag	UNP P35637
A	-13	ILE	-	expression tag	UNP P35637
A	-12	PRO	-	expression tag	UNP P35637

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	THR	-	expression tag	UNP P35637
A	-10	THR	-	expression tag	UNP P35637
A	-9	GLU	-	expression tag	UNP P35637
A	-8	ASN	-	expression tag	UNP P35637
A	-7	LEU	-	expression tag	UNP P35637
A	-6	TYR	-	expression tag	UNP P35637
A	-5	PHE	-	expression tag	UNP P35637
A	-4	GLN	-	expression tag	UNP P35637
A	-3	GLY	-	expression tag	UNP P35637
A	-2	ALA	-	expression tag	UNP P35637
A	-1	MET	-	expression tag	UNP P35637
A	0	ASP	-	expression tag	UNP P35637
A	1	PRO	-	expression tag	UNP P35637
B	-26	MET	-	initiating methionine	UNP P35637
B	-25	SER	-	expression tag	UNP P35637
B	-24	TYR	-	expression tag	UNP P35637
B	-23	TYR	-	expression tag	UNP P35637
B	-22	HIS	-	expression tag	UNP P35637
B	-21	HIS	-	expression tag	UNP P35637
B	-20	HIS	-	expression tag	UNP P35637
B	-19	HIS	-	expression tag	UNP P35637
B	-18	HIS	-	expression tag	UNP P35637
B	-17	HIS	-	expression tag	UNP P35637
B	-16	ASP	-	expression tag	UNP P35637
B	-15	TYR	-	expression tag	UNP P35637
B	-14	ASP	-	expression tag	UNP P35637
B	-13	ILE	-	expression tag	UNP P35637
B	-12	PRO	-	expression tag	UNP P35637
B	-11	THR	-	expression tag	UNP P35637
B	-10	THR	-	expression tag	UNP P35637
B	-9	GLU	-	expression tag	UNP P35637
B	-8	ASN	-	expression tag	UNP P35637
B	-7	LEU	-	expression tag	UNP P35637
B	-6	TYR	-	expression tag	UNP P35637
B	-5	PHE	-	expression tag	UNP P35637
B	-4	GLN	-	expression tag	UNP P35637
B	-3	GLY	-	expression tag	UNP P35637
B	-2	ALA	-	expression tag	UNP P35637
B	-1	MET	-	expression tag	UNP P35637
B	0	ASP	-	expression tag	UNP P35637
B	1	PRO	-	expression tag	UNP P35637
C	-26	MET	-	initiating methionine	UNP P35637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-25	SER	-	expression tag	UNP P35637
C	-24	TYR	-	expression tag	UNP P35637
C	-23	TYR	-	expression tag	UNP P35637
C	-22	HIS	-	expression tag	UNP P35637
C	-21	HIS	-	expression tag	UNP P35637
C	-20	HIS	-	expression tag	UNP P35637
C	-19	HIS	-	expression tag	UNP P35637
C	-18	HIS	-	expression tag	UNP P35637
C	-17	HIS	-	expression tag	UNP P35637
C	-16	ASP	-	expression tag	UNP P35637
C	-15	TYR	-	expression tag	UNP P35637
C	-14	ASP	-	expression tag	UNP P35637
C	-13	ILE	-	expression tag	UNP P35637
C	-12	PRO	-	expression tag	UNP P35637
C	-11	THR	-	expression tag	UNP P35637
C	-10	THR	-	expression tag	UNP P35637
C	-9	GLU	-	expression tag	UNP P35637
C	-8	ASN	-	expression tag	UNP P35637
C	-7	LEU	-	expression tag	UNP P35637
C	-6	TYR	-	expression tag	UNP P35637
C	-5	PHE	-	expression tag	UNP P35637
C	-4	GLN	-	expression tag	UNP P35637
C	-3	GLY	-	expression tag	UNP P35637
C	-2	ALA	-	expression tag	UNP P35637
C	-1	MET	-	expression tag	UNP P35637
C	0	ASP	-	expression tag	UNP P35637
C	1	PRO	-	expression tag	UNP P35637
D	-26	MET	-	initiating methionine	UNP P35637
D	-25	SER	-	expression tag	UNP P35637
D	-24	TYR	-	expression tag	UNP P35637
D	-23	TYR	-	expression tag	UNP P35637
D	-22	HIS	-	expression tag	UNP P35637
D	-21	HIS	-	expression tag	UNP P35637
D	-20	HIS	-	expression tag	UNP P35637
D	-19	HIS	-	expression tag	UNP P35637
D	-18	HIS	-	expression tag	UNP P35637
D	-17	HIS	-	expression tag	UNP P35637
D	-16	ASP	-	expression tag	UNP P35637
D	-15	TYR	-	expression tag	UNP P35637
D	-14	ASP	-	expression tag	UNP P35637
D	-13	ILE	-	expression tag	UNP P35637
D	-12	PRO	-	expression tag	UNP P35637

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	THR	-	expression tag	UNP P35637
D	-10	THR	-	expression tag	UNP P35637
D	-9	GLU	-	expression tag	UNP P35637
D	-8	ASN	-	expression tag	UNP P35637
D	-7	LEU	-	expression tag	UNP P35637
D	-6	TYR	-	expression tag	UNP P35637
D	-5	PHE	-	expression tag	UNP P35637
D	-4	GLN	-	expression tag	UNP P35637
D	-3	GLY	-	expression tag	UNP P35637
D	-2	ALA	-	expression tag	UNP P35637
D	-1	MET	-	expression tag	UNP P35637
D	0	ASP	-	expression tag	UNP P35637
D	1	PRO	-	expression tag	UNP P35637
E	-26	MET	-	initiating methionine	UNP P35637
E	-25	SER	-	expression tag	UNP P35637
E	-24	TYR	-	expression tag	UNP P35637
E	-23	TYR	-	expression tag	UNP P35637
E	-22	HIS	-	expression tag	UNP P35637
E	-21	HIS	-	expression tag	UNP P35637
E	-20	HIS	-	expression tag	UNP P35637
E	-19	HIS	-	expression tag	UNP P35637
E	-18	HIS	-	expression tag	UNP P35637
E	-17	HIS	-	expression tag	UNP P35637
E	-16	ASP	-	expression tag	UNP P35637
E	-15	TYR	-	expression tag	UNP P35637
E	-14	ASP	-	expression tag	UNP P35637
E	-13	ILE	-	expression tag	UNP P35637
E	-12	PRO	-	expression tag	UNP P35637
E	-11	THR	-	expression tag	UNP P35637
E	-10	THR	-	expression tag	UNP P35637
E	-9	GLU	-	expression tag	UNP P35637
E	-8	ASN	-	expression tag	UNP P35637
E	-7	LEU	-	expression tag	UNP P35637
E	-6	TYR	-	expression tag	UNP P35637
E	-5	PHE	-	expression tag	UNP P35637
E	-4	GLN	-	expression tag	UNP P35637
E	-3	GLY	-	expression tag	UNP P35637
E	-2	ALA	-	expression tag	UNP P35637
E	-1	MET	-	expression tag	UNP P35637
E	0	ASP	-	expression tag	UNP P35637
E	1	PRO	-	expression tag	UNP P35637
F	-26	MET	-	initiating methionine	UNP P35637

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-25	SER	-	expression tag	UNP P35637
F	-24	TYR	-	expression tag	UNP P35637
F	-23	TYR	-	expression tag	UNP P35637
F	-22	HIS	-	expression tag	UNP P35637
F	-21	HIS	-	expression tag	UNP P35637
F	-20	HIS	-	expression tag	UNP P35637
F	-19	HIS	-	expression tag	UNP P35637
F	-18	HIS	-	expression tag	UNP P35637
F	-17	HIS	-	expression tag	UNP P35637
F	-16	ASP	-	expression tag	UNP P35637
F	-15	TYR	-	expression tag	UNP P35637
F	-14	ASP	-	expression tag	UNP P35637
F	-13	ILE	-	expression tag	UNP P35637
F	-12	PRO	-	expression tag	UNP P35637
F	-11	THR	-	expression tag	UNP P35637
F	-10	THR	-	expression tag	UNP P35637
F	-9	GLU	-	expression tag	UNP P35637
F	-8	ASN	-	expression tag	UNP P35637
F	-7	LEU	-	expression tag	UNP P35637
F	-6	TYR	-	expression tag	UNP P35637
F	-5	PHE	-	expression tag	UNP P35637
F	-4	GLN	-	expression tag	UNP P35637
F	-3	GLY	-	expression tag	UNP P35637
F	-2	ALA	-	expression tag	UNP P35637
F	-1	MET	-	expression tag	UNP P35637
F	0	ASP	-	expression tag	UNP P35637
F	1	PRO	-	expression tag	UNP P35637
G	-26	MET	-	initiating methionine	UNP P35637
G	-25	SER	-	expression tag	UNP P35637
G	-24	TYR	-	expression tag	UNP P35637
G	-23	TYR	-	expression tag	UNP P35637
G	-22	HIS	-	expression tag	UNP P35637
G	-21	HIS	-	expression tag	UNP P35637
G	-20	HIS	-	expression tag	UNP P35637
G	-19	HIS	-	expression tag	UNP P35637
G	-18	HIS	-	expression tag	UNP P35637
G	-17	HIS	-	expression tag	UNP P35637
G	-16	ASP	-	expression tag	UNP P35637
G	-15	TYR	-	expression tag	UNP P35637
G	-14	ASP	-	expression tag	UNP P35637
G	-13	ILE	-	expression tag	UNP P35637
G	-12	PRO	-	expression tag	UNP P35637

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	THR	-	expression tag	UNP P35637
G	-10	THR	-	expression tag	UNP P35637
G	-9	GLU	-	expression tag	UNP P35637
G	-8	ASN	-	expression tag	UNP P35637
G	-7	LEU	-	expression tag	UNP P35637
G	-6	TYR	-	expression tag	UNP P35637
G	-5	PHE	-	expression tag	UNP P35637
G	-4	GLN	-	expression tag	UNP P35637
G	-3	GLY	-	expression tag	UNP P35637
G	-2	ALA	-	expression tag	UNP P35637
G	-1	MET	-	expression tag	UNP P35637
G	0	ASP	-	expression tag	UNP P35637
G	1	PRO	-	expression tag	UNP P35637
H	-26	MET	-	initiating methionine	UNP P35637
H	-25	SER	-	expression tag	UNP P35637
H	-24	TYR	-	expression tag	UNP P35637
H	-23	TYR	-	expression tag	UNP P35637
H	-22	HIS	-	expression tag	UNP P35637
H	-21	HIS	-	expression tag	UNP P35637
H	-20	HIS	-	expression tag	UNP P35637
H	-19	HIS	-	expression tag	UNP P35637
H	-18	HIS	-	expression tag	UNP P35637
H	-17	HIS	-	expression tag	UNP P35637
H	-16	ASP	-	expression tag	UNP P35637
H	-15	TYR	-	expression tag	UNP P35637
H	-14	ASP	-	expression tag	UNP P35637
H	-13	ILE	-	expression tag	UNP P35637
H	-12	PRO	-	expression tag	UNP P35637
H	-11	THR	-	expression tag	UNP P35637
H	-10	THR	-	expression tag	UNP P35637
H	-9	GLU	-	expression tag	UNP P35637
H	-8	ASN	-	expression tag	UNP P35637
H	-7	LEU	-	expression tag	UNP P35637
H	-6	TYR	-	expression tag	UNP P35637
H	-5	PHE	-	expression tag	UNP P35637
H	-4	GLN	-	expression tag	UNP P35637
H	-3	GLY	-	expression tag	UNP P35637
H	-2	ALA	-	expression tag	UNP P35637
H	-1	MET	-	expression tag	UNP P35637
H	0	ASP	-	expression tag	UNP P35637
H	1	PRO	-	expression tag	UNP P35637
I	-26	MET	-	initiating methionine	UNP P35637

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-25	SER	-	expression tag	UNP P35637
I	-24	TYR	-	expression tag	UNP P35637
I	-23	TYR	-	expression tag	UNP P35637
I	-22	HIS	-	expression tag	UNP P35637
I	-21	HIS	-	expression tag	UNP P35637
I	-20	HIS	-	expression tag	UNP P35637
I	-19	HIS	-	expression tag	UNP P35637
I	-18	HIS	-	expression tag	UNP P35637
I	-17	HIS	-	expression tag	UNP P35637
I	-16	ASP	-	expression tag	UNP P35637
I	-15	TYR	-	expression tag	UNP P35637
I	-14	ASP	-	expression tag	UNP P35637
I	-13	ILE	-	expression tag	UNP P35637
I	-12	PRO	-	expression tag	UNP P35637
I	-11	THR	-	expression tag	UNP P35637
I	-10	THR	-	expression tag	UNP P35637
I	-9	GLU	-	expression tag	UNP P35637
I	-8	ASN	-	expression tag	UNP P35637
I	-7	LEU	-	expression tag	UNP P35637
I	-6	TYR	-	expression tag	UNP P35637
I	-5	PHE	-	expression tag	UNP P35637
I	-4	GLN	-	expression tag	UNP P35637
I	-3	GLY	-	expression tag	UNP P35637
I	-2	ALA	-	expression tag	UNP P35637
I	-1	MET	-	expression tag	UNP P35637
I	0	ASP	-	expression tag	UNP P35637
I	1	PRO	-	expression tag	UNP P35637

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: RNA-binding protein FUS

Chain A: 19% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y50 Y66 T71 P72 Y75 G76 S77 S83 Q88 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER

GLN GLN PRO SER TYR GLY GLY GLN GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLY SER GLY

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

• Molecule 1: RNA-binding protein FUS

Chain B: 19% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y50 Y66 T71 P72 Y75 G76 S77 S83 Q88 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER

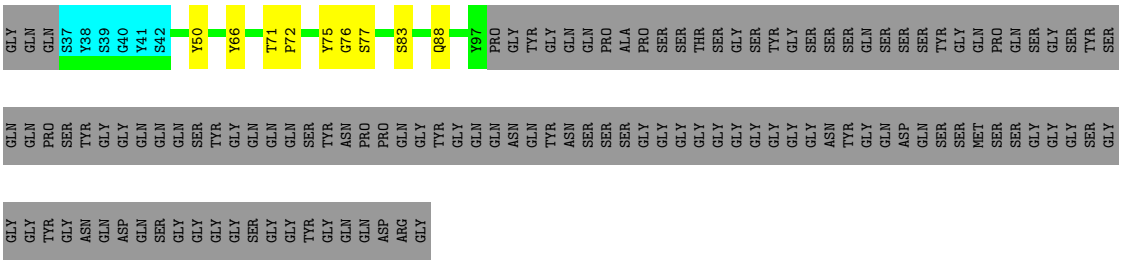
GLN GLN PRO SER TYR GLY GLY GLN GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY GLY GLY GLY SER GLY

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

• Molecule 1: RNA-binding protein FUS

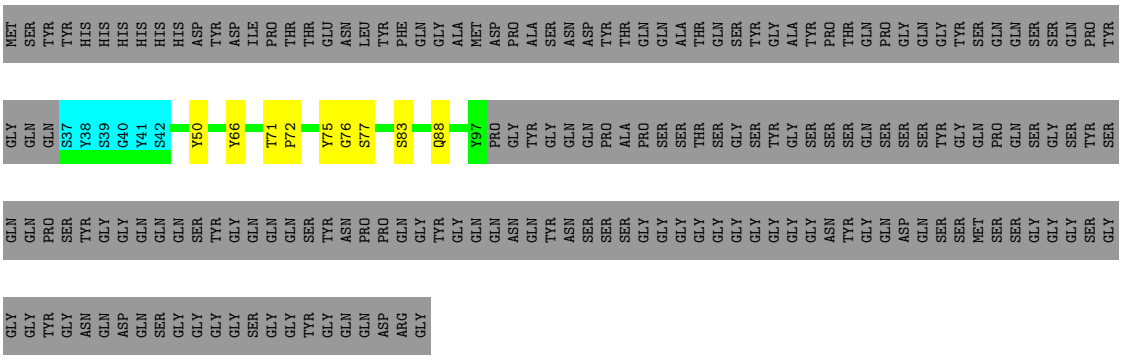
Chain C: 19% • • 75%

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



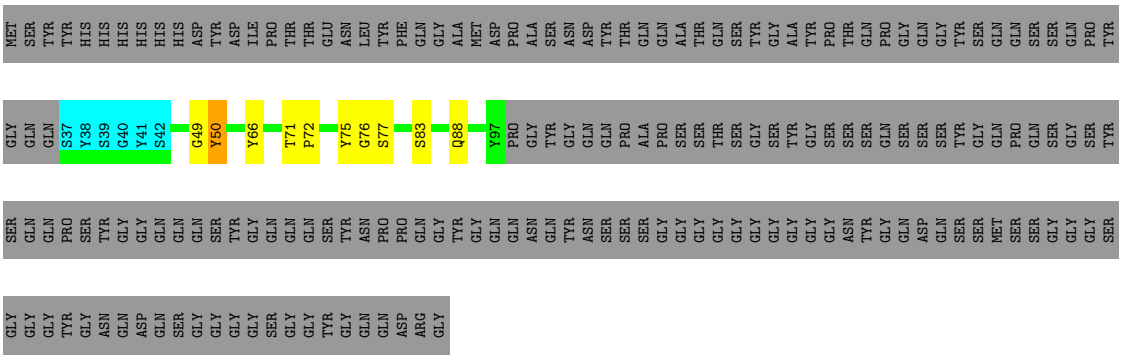
• Molecule 1: RNA-binding protein FUS

Chain D:



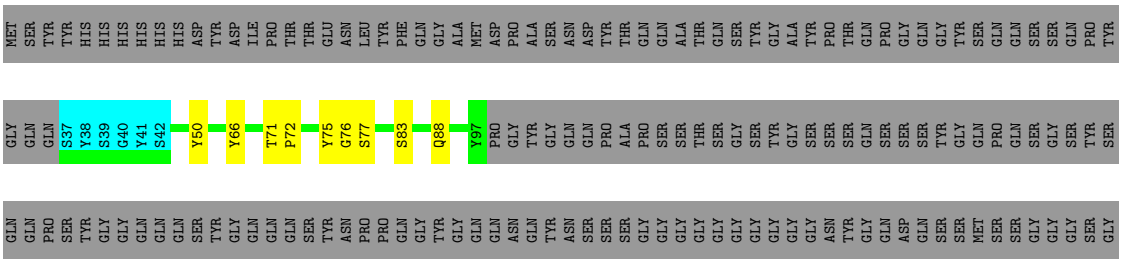
• Molecule 1: RNA-binding protein FUS

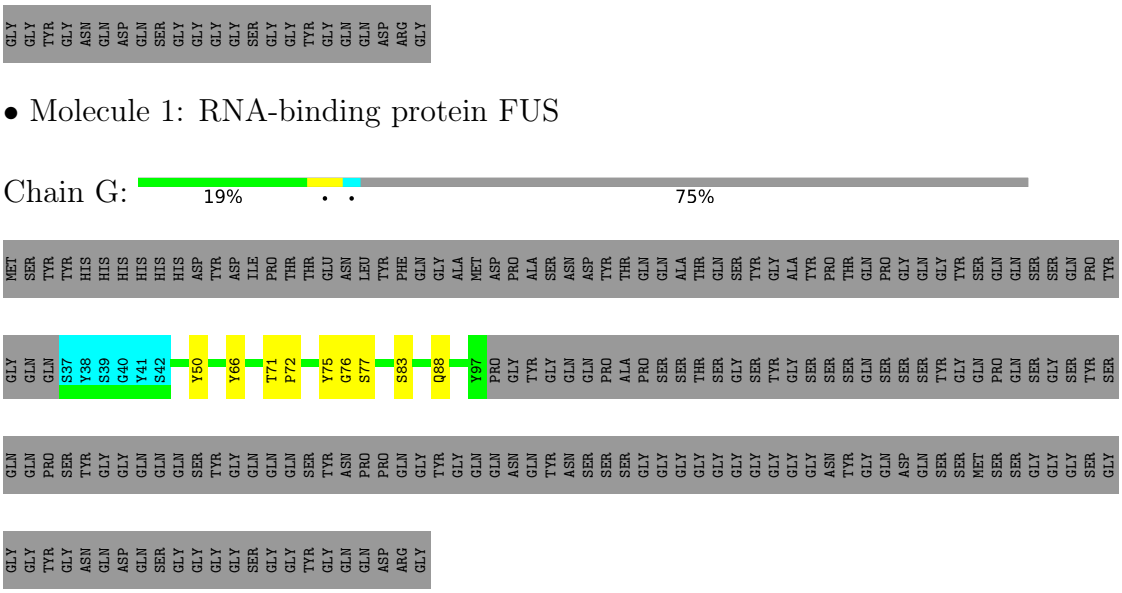
Chain E:



• Molecule 1: RNA-binding protein FUS

Chain F:




GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY SER GLY GLY TYR GLY GLN GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain G:
19%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y50 Y66 T71 P72 Y75 G76 S77 S83 Q88 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER
GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLY SER GLY
GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY SER GLY GLY TYR GLY GLN GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain H:
19%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y50 Y66 T71 P72 Y75 G76 S77 S83 Q88 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER
GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLY SER GLY
GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY SER GLY GLY TYR GLY GLN GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain I:
19%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y50 Y66 T71 P72 Y75 G76 S77 S83 Q88 G92 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER
TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

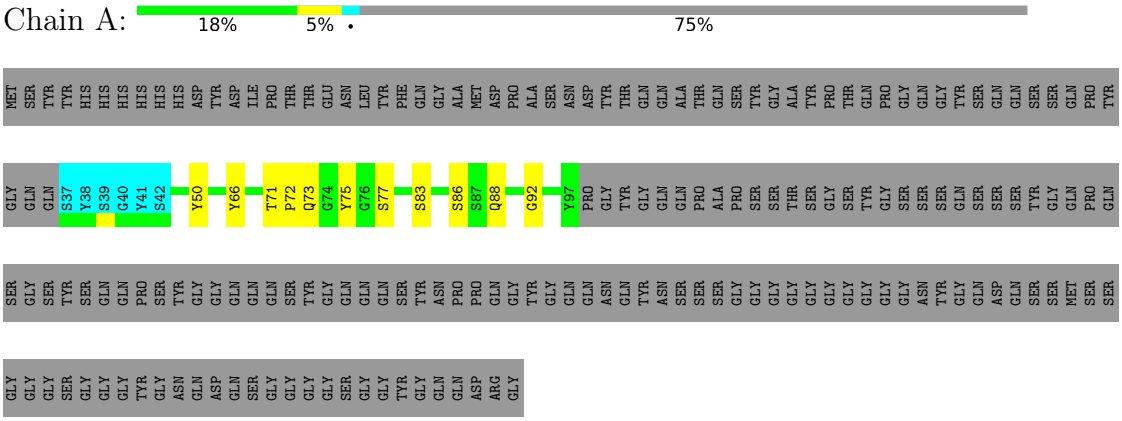
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

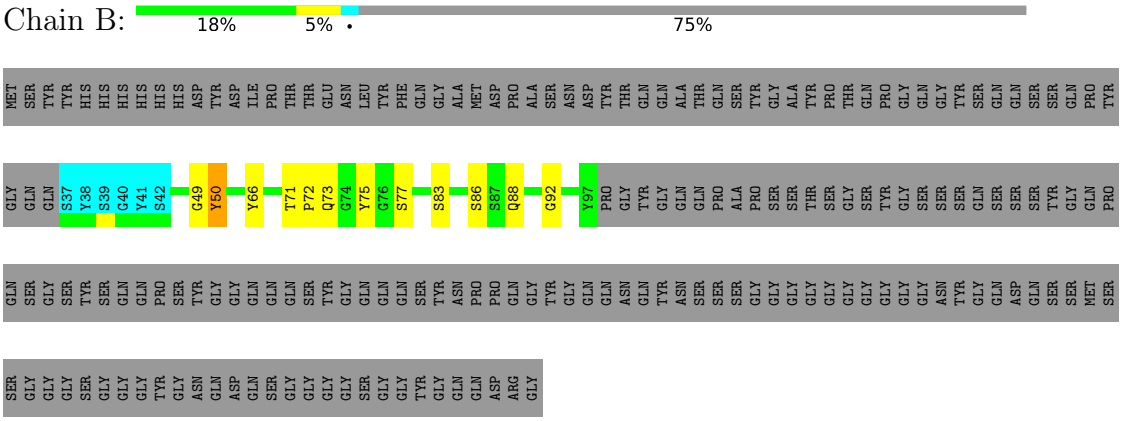
• Molecule 1: RNA-binding protein FUS

Chain A:



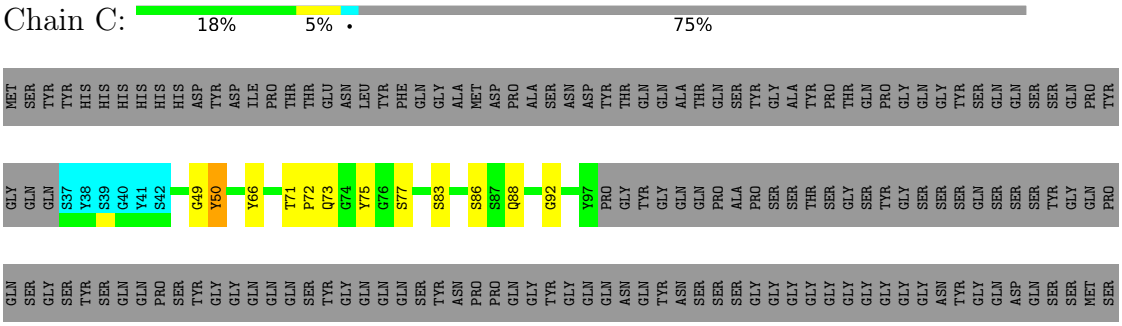
• Molecule 1: RNA-binding protein FUS

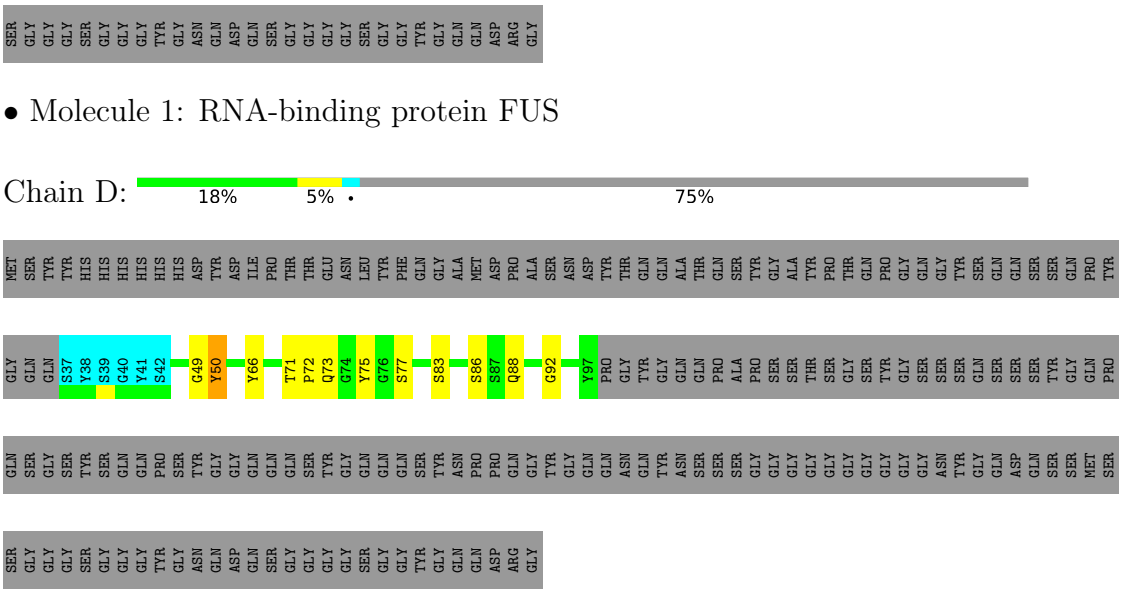
Chain B:

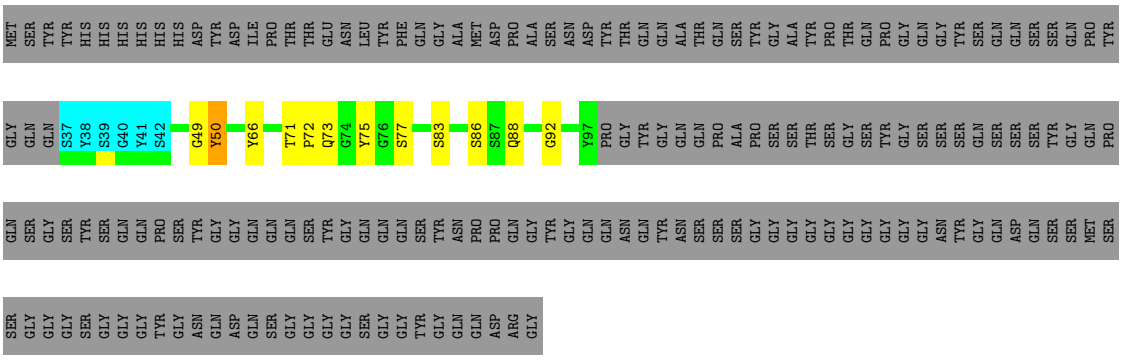


• Molecule 1: RNA-binding protein FUS

Chain C:

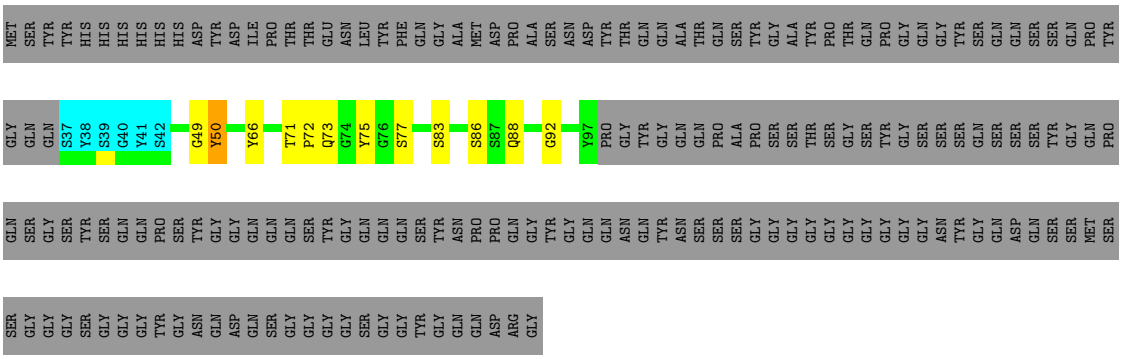



SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY GLY TYR GLY GLN GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain D:
18%
5%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 Q73 G74 Y75 G76 S77 S83 S86 S87 Q88 G92 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO
GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN SER SER TYR ASN 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 GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain E:
18%
5%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 Q73 G74 Y75 G76 S77 S83 S86 S87 Q88 G92 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO
GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN SER SER TYR ASN 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 GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain F:
18%
5%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 Q73 G74 Y75 G76 S77 S83 S86 S87 Q88 G92 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO
GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN SER SER TYR ASN 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 GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain G:
18%
5%
75%



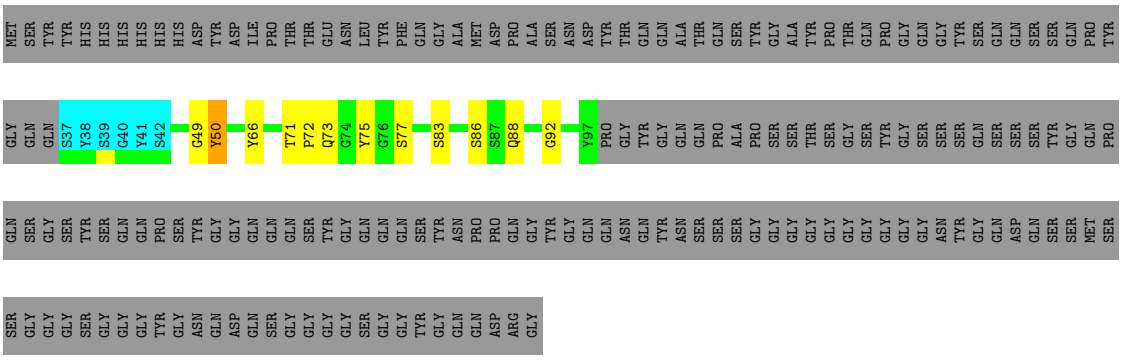
• Molecule 1: RNA-binding protein FUS

Chain H: 18% 5% • 75%



• Molecule 1: RNA-binding protein FUS

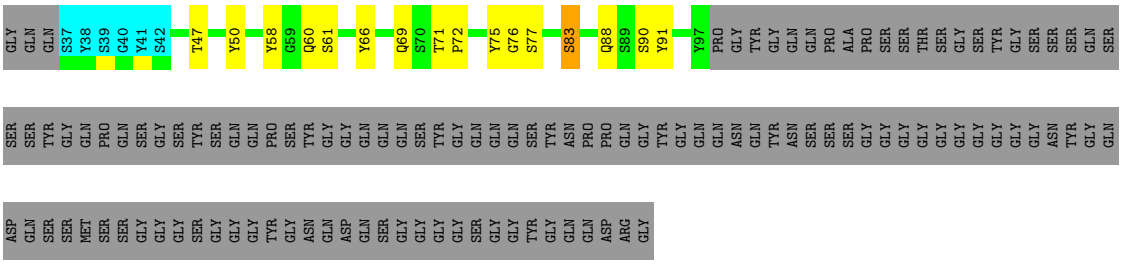
Chain I: 18% 5% • 75%



4.2.2 Score per residue for model 2

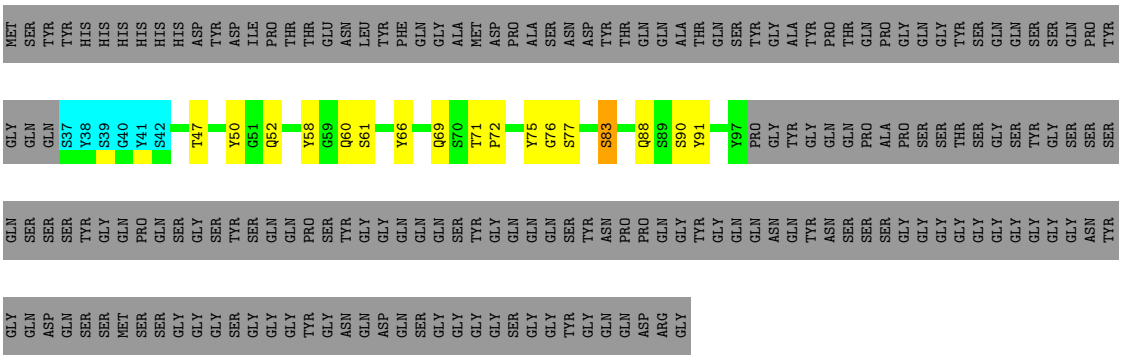
• Molecule 1: RNA-binding protein FUS

Chain A: 16% 6% • 75%



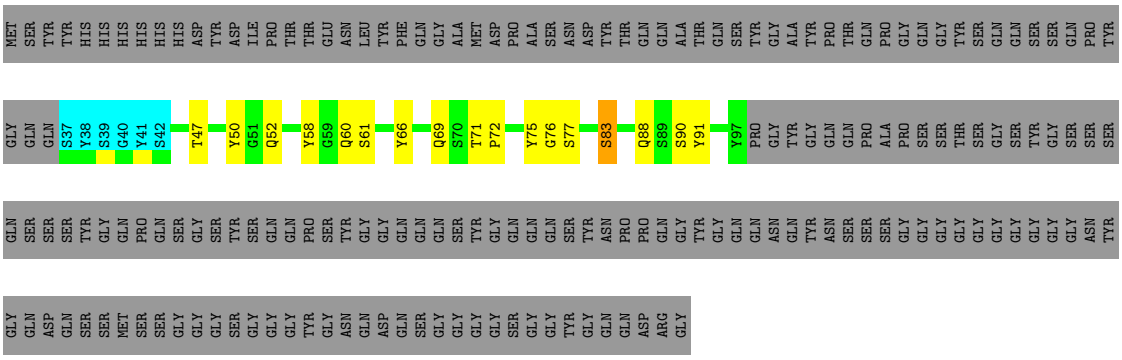
• Molecule 1: RNA-binding protein FUS

Chain B: 16% 7% • 75%



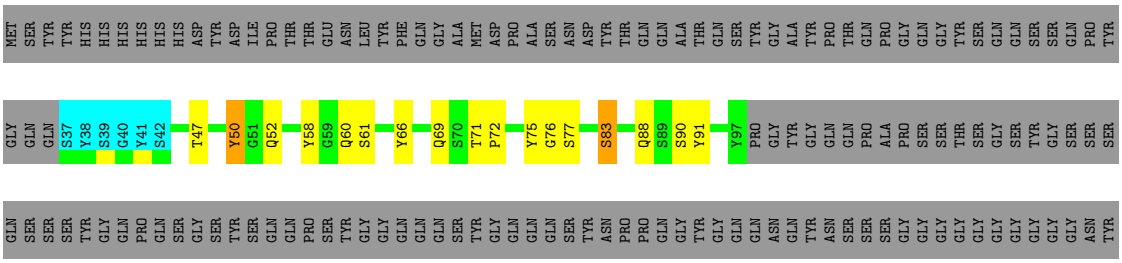
• Molecule 1: RNA-binding protein FUS

Chain C: 16% 7% • 75%



• Molecule 1: RNA-binding protein FUS

Chain D: 16% 6% • • 75%



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 GLN ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain E: 15% 7% • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 S48 G49 Y50 G51 Q52 Y58 G59 Q60 S61 Y66 Q69 S70 T71 P72 Y75 G76 S77 S83 Q88 S89 S90 Y91 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER

SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain F: 16% 6% • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 Y50 Y58 G59 Q60 S61 Y66 Q69 S70 T71 P72 Y75 G76 S77 S83 Q88 S89 S90 Y91 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER

SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 SER GLY GLY TYR GLY GLN GLN ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain G: 16% 7% • 75%

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

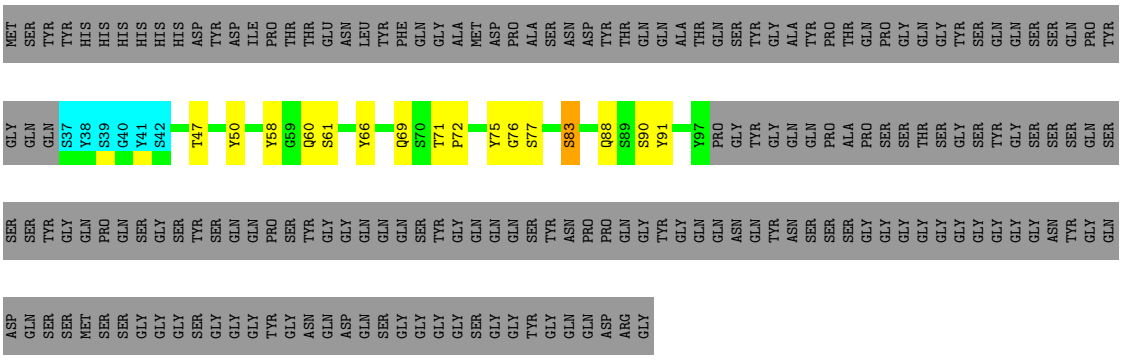
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 Y50 G51 Q52 Y58 G59 Q60 S61 Y66 Q69 S70 T71 P72 Y75 G76 S77 S83 Q88 S89 S90 Y91 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER

GLN SER SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

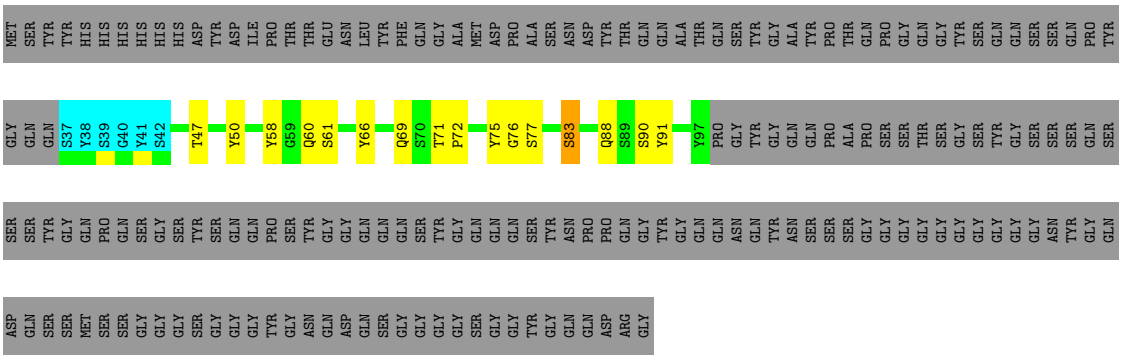
- Molecule 1: RNA-binding protein FUS

Chain H: 16% 6% • 75%



• Molecule 1: RNA-binding protein FUS

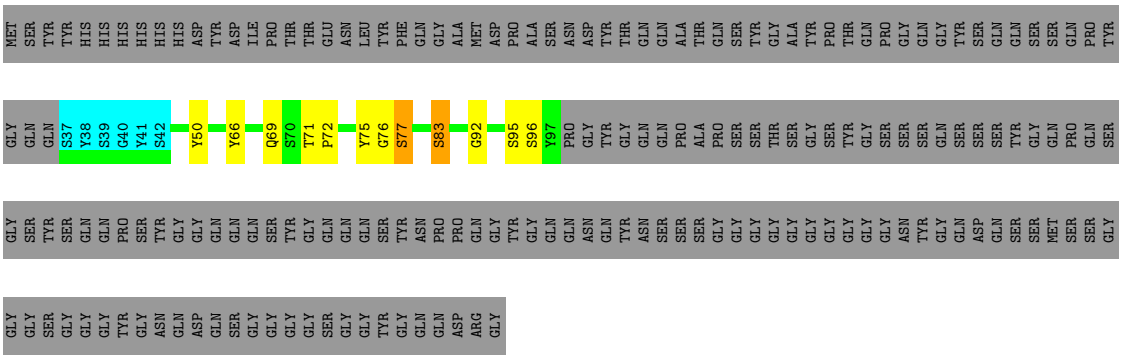
Chain I:



4.2.3 Score per residue for model 3 (medoid)

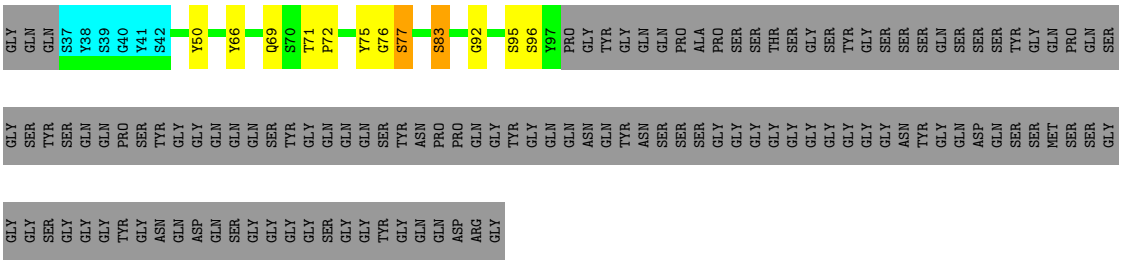
• Molecule 1: RNA-binding protein FUS

Chain A:



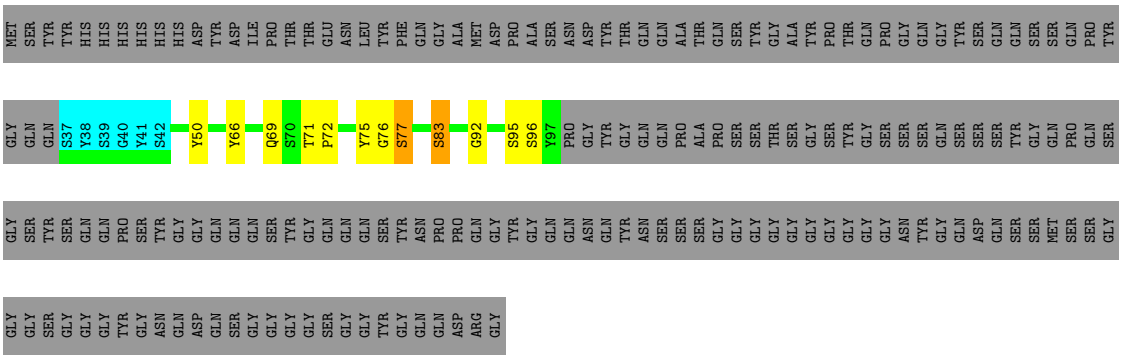
• Molecule 1: RNA-binding protein FUS

Chain B:



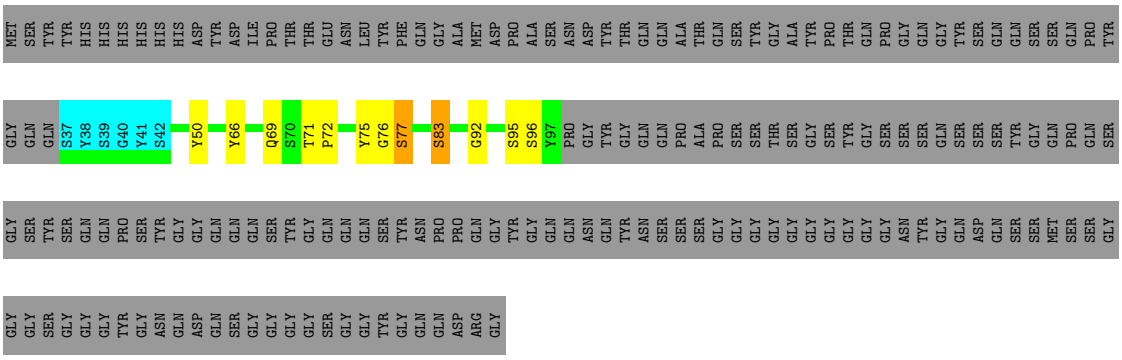
• Molecule 1: RNA-binding protein FUS

Chain C:



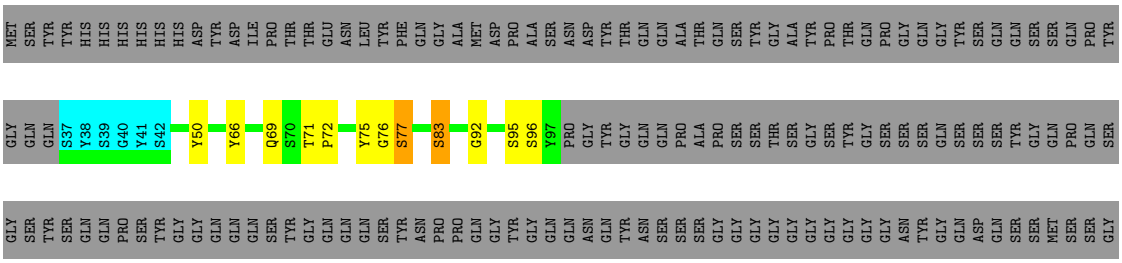
• Molecule 1: RNA-binding protein FUS

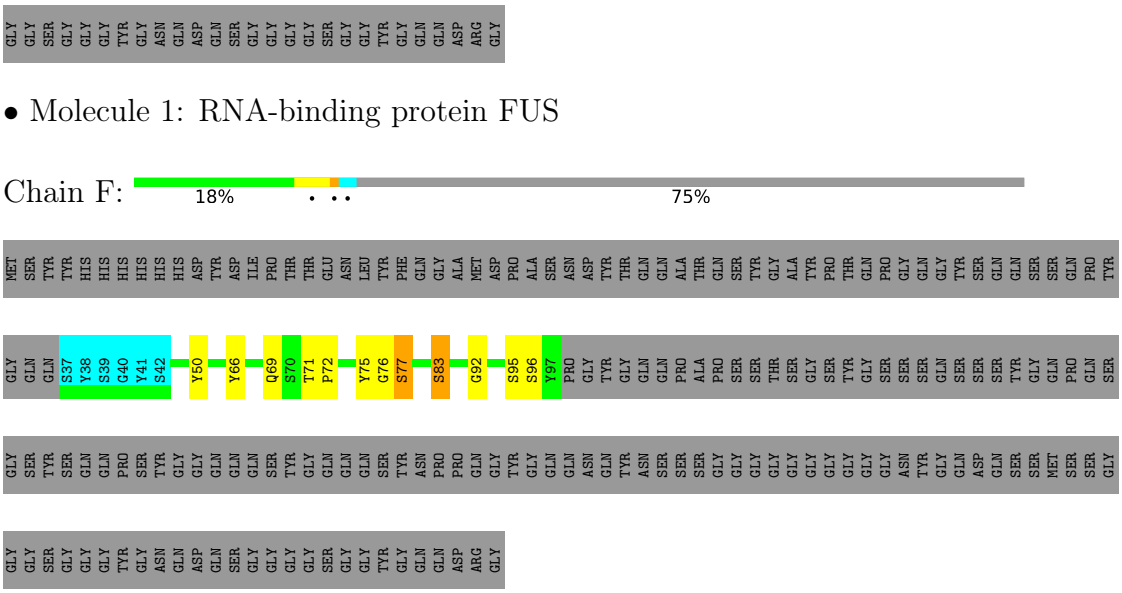
Chain D:



• Molecule 1: RNA-binding protein FUS

Chain E:



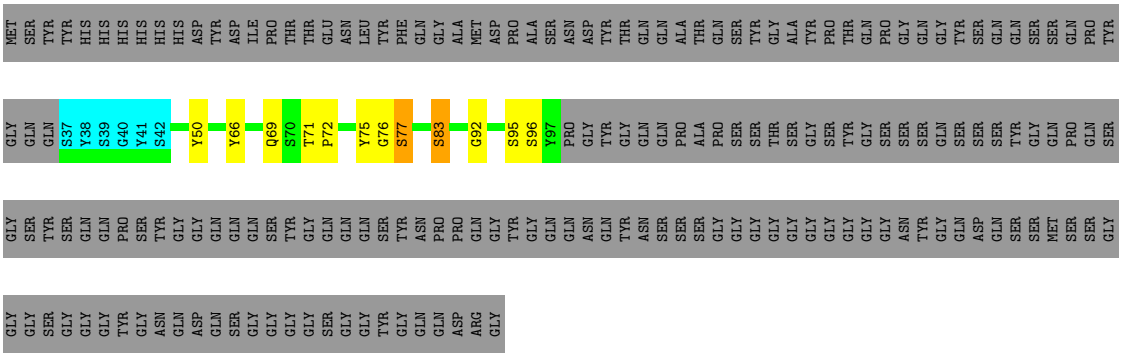


• Molecule 1: RNA-binding protein FUS

Chain F: 18% • •• 75%

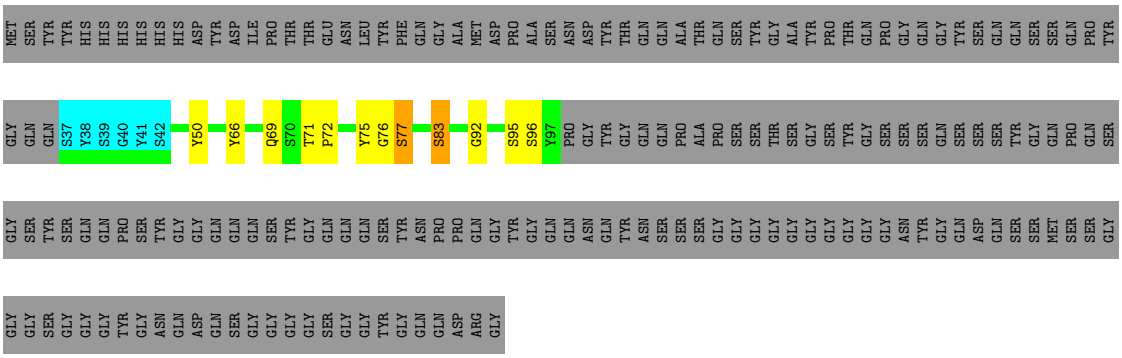
• Molecule 1: RNA-binding protein FUS

Chain G: 18% • •• 75%



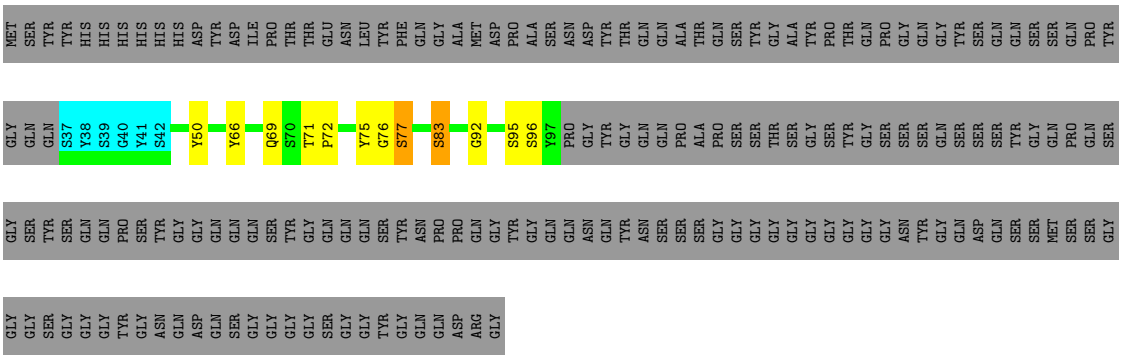
• Molecule 1: RNA-binding protein FUS

Chain H: 18% • •• 75%



• Molecule 1: RNA-binding protein FUS

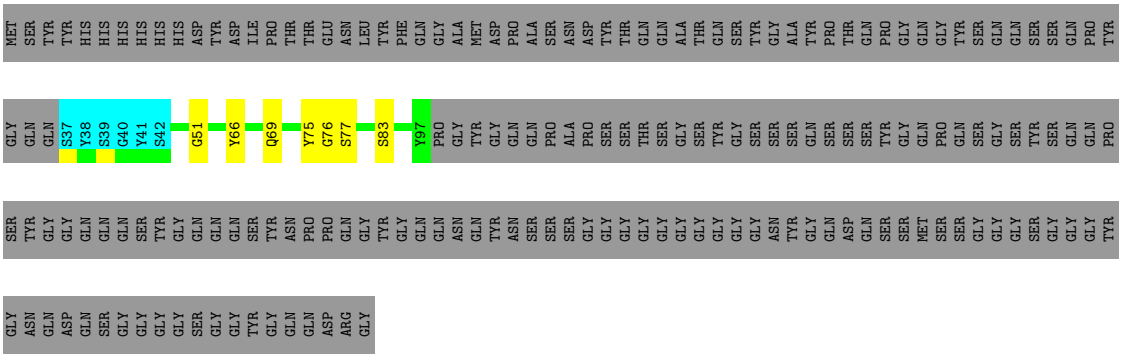
Chain I: 18% • •• 75%



4.2.4 Score per residue for model 4

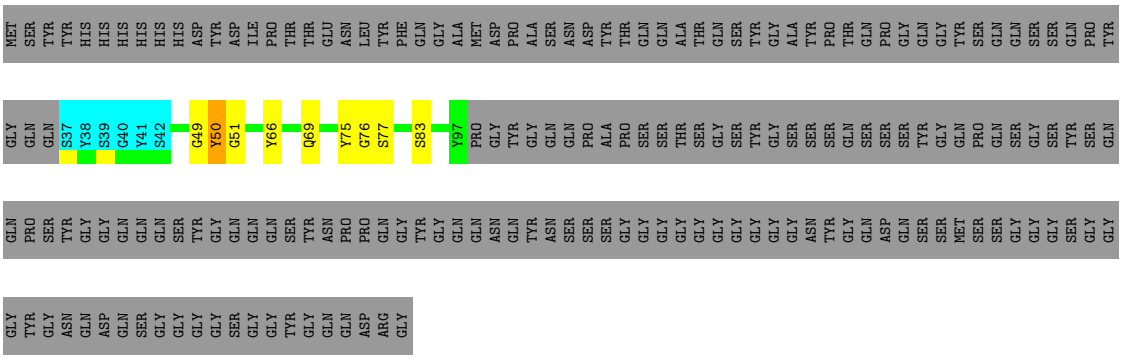
• Molecule 1: RNA-binding protein FUS

Chain A: 20% 75%



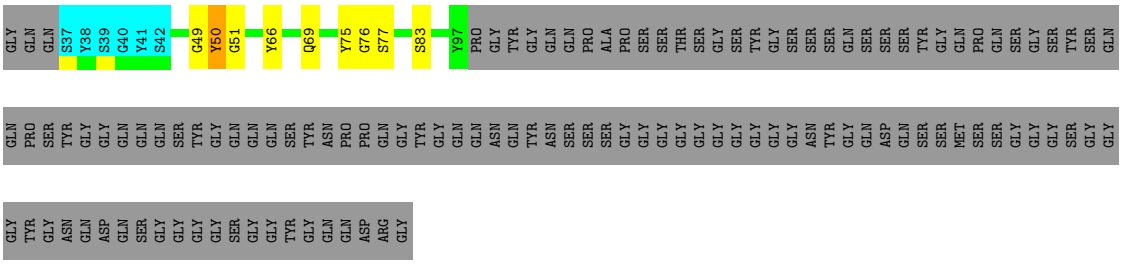
• Molecule 1: RNA-binding protein FUS

Chain B: 19% 75%



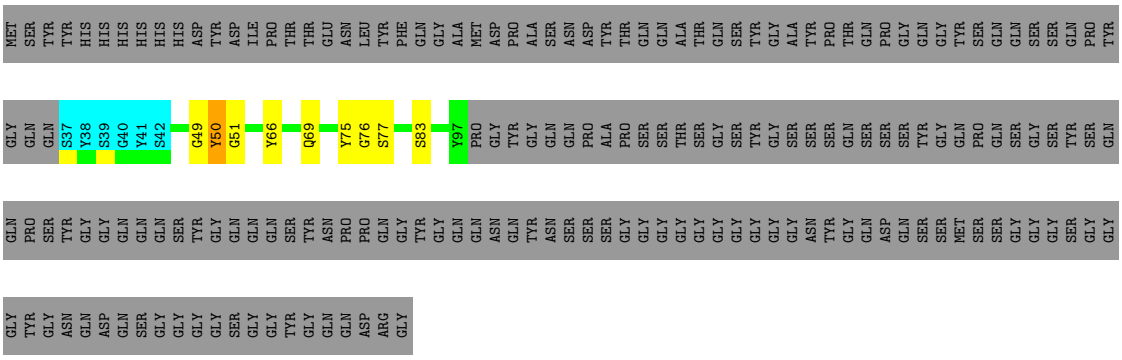
• Molecule 1: RNA-binding protein FUS

Chain C: 19% 75%



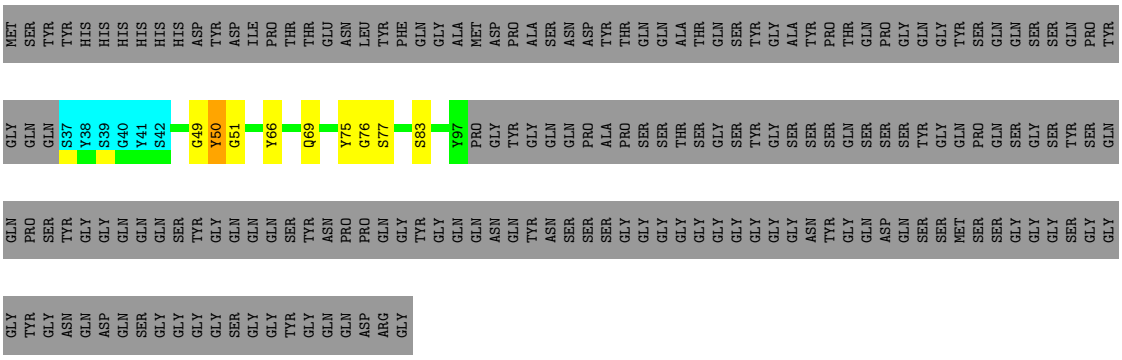
• Molecule 1: RNA-binding protein FUS

Chain D:



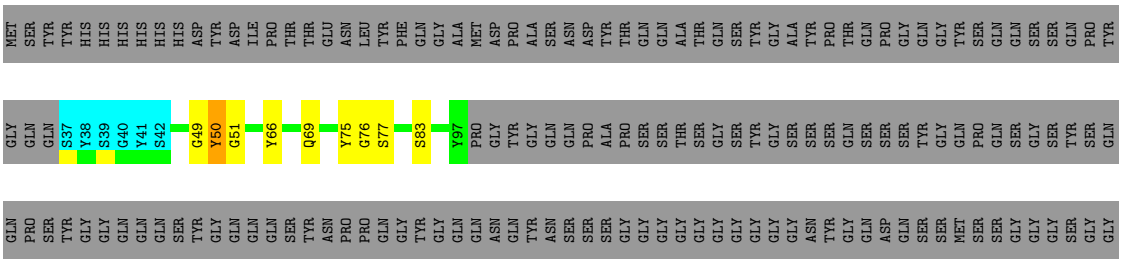
• Molecule 1: RNA-binding protein FUS

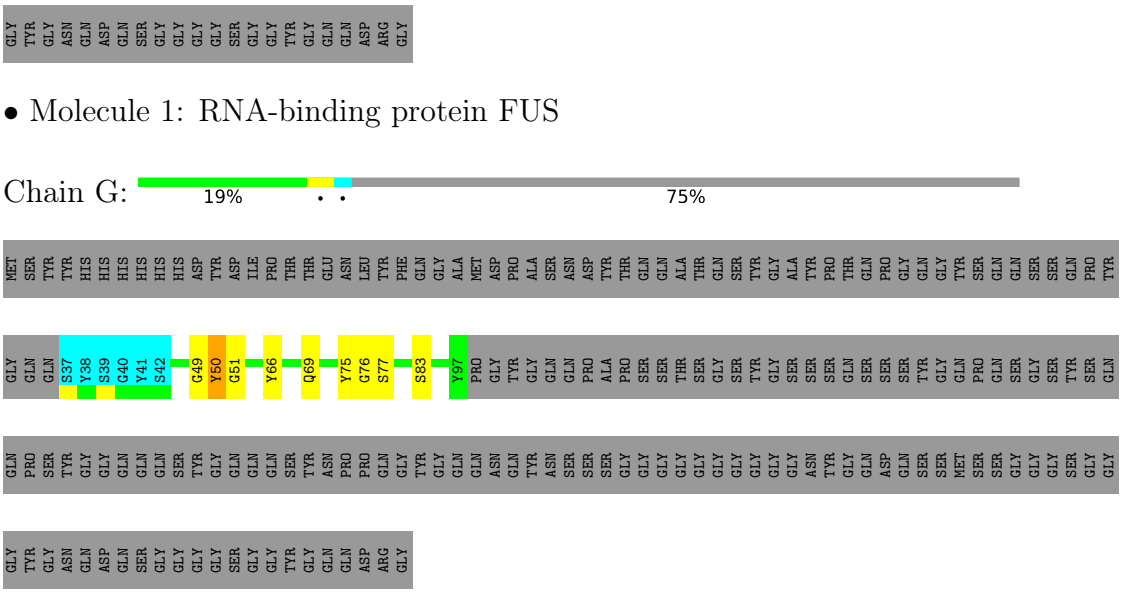
Chain E:



• Molecule 1: RNA-binding protein FUS

Chain F:



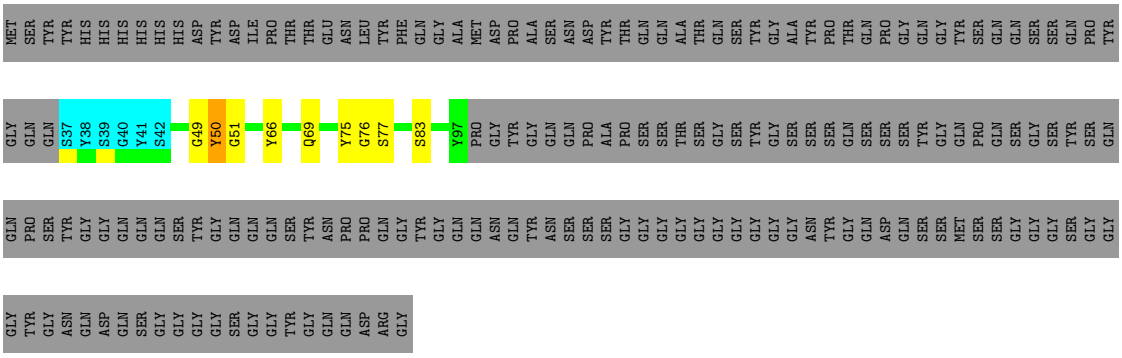


• Molecule 1: RNA-binding protein FUS

Chain G:

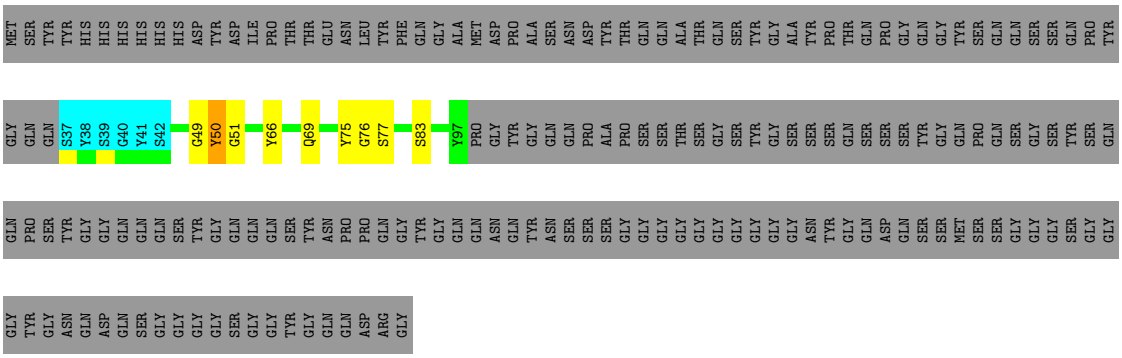
• Molecule 1: RNA-binding protein FUS

Chain H:



• Molecule 1: RNA-binding protein FUS

Chain I:



4.2.5 Score per residue for model 5

- Molecule 1: RNA-binding protein FUS

Chain A: 19% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 Y66 T71 P72 Y75 G76 Q88 Y91 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain B: 19% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 Y66 T71 P72 Y75 G76 Q88 Y91 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain C: 19% • • 75%

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

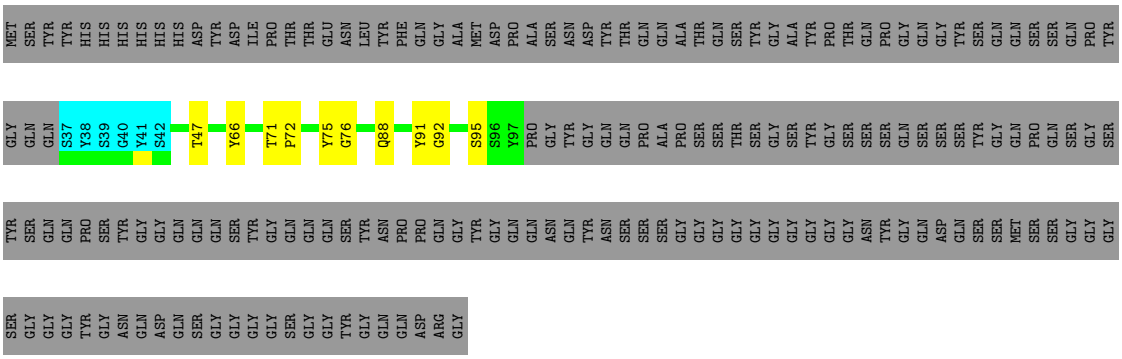
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y66 T71 P72 Y75 G76 Q88 Y91 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER

GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLY SER GLY

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

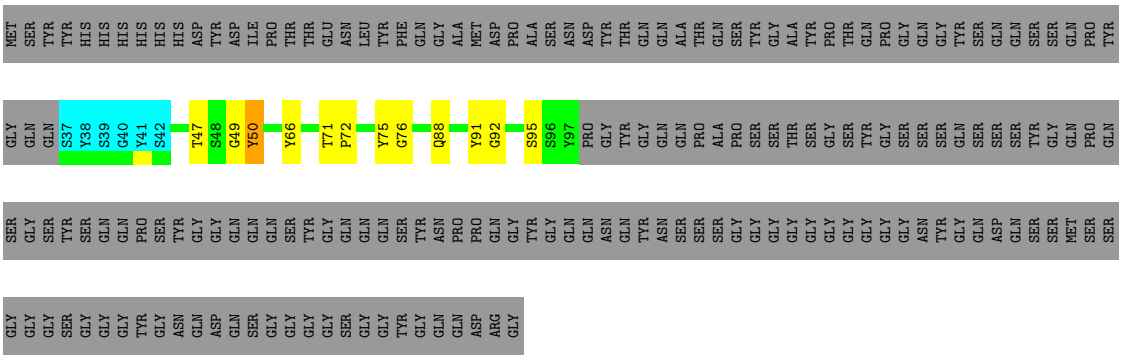
- Molecule 1: RNA-binding protein FUS

Chain D: 19% • • 75%



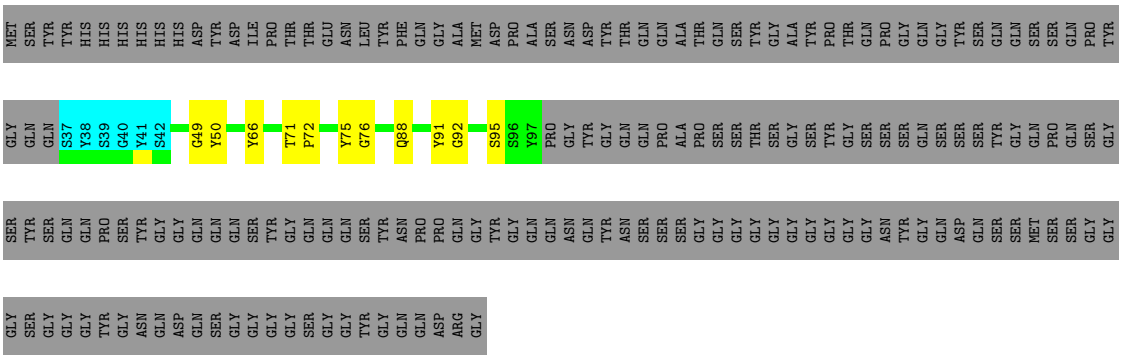
- Molecule 1: RNA-binding protein FUS

Chain E: 18% 5% • 75%



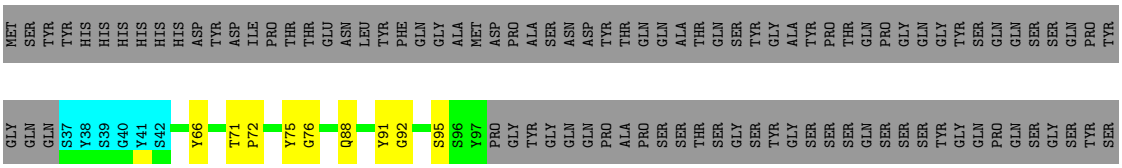
- Molecule 1: RNA-binding protein FUS

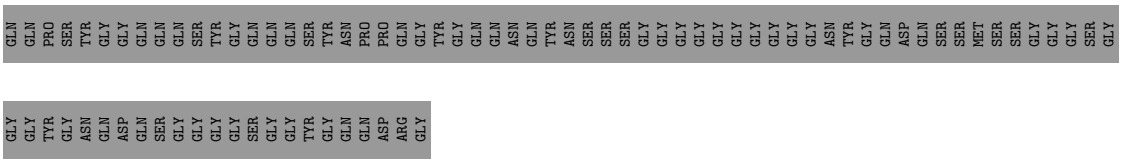
Chain F: 18% 5% • 75%



- Molecule 1: RNA-binding protein FUS

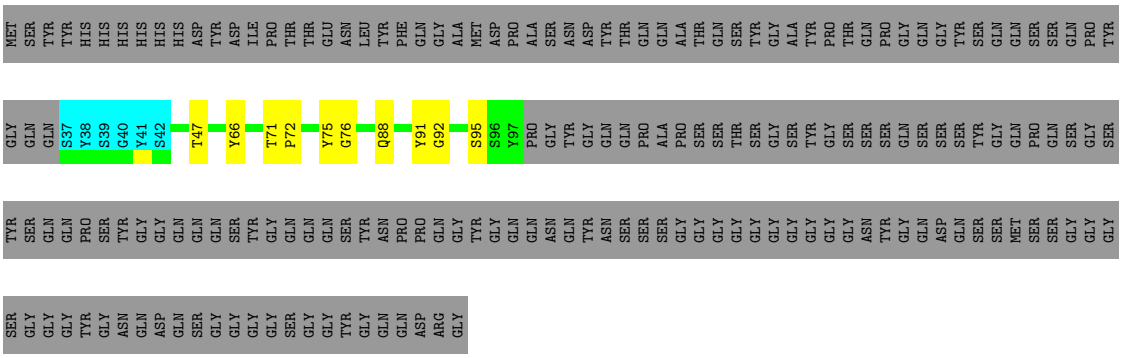
Chain G: 19% • • 75%





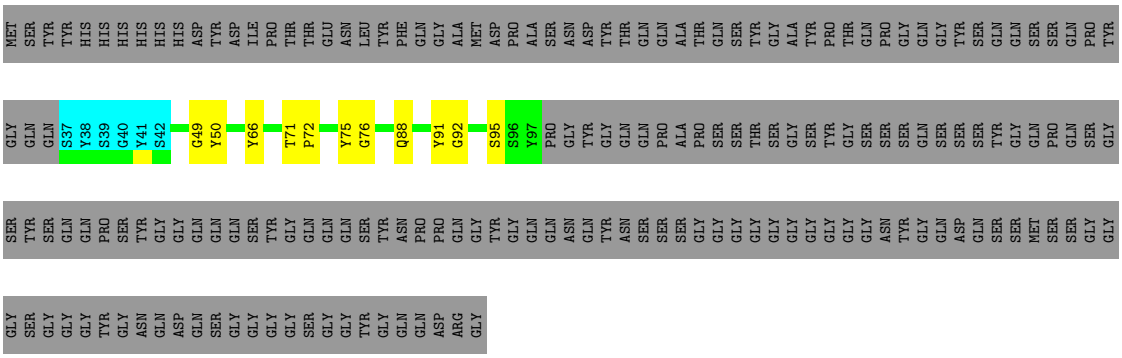
- Molecule 1: RNA-binding protein FUS

Chain H:



- Molecule 1: RNA-binding protein FUS

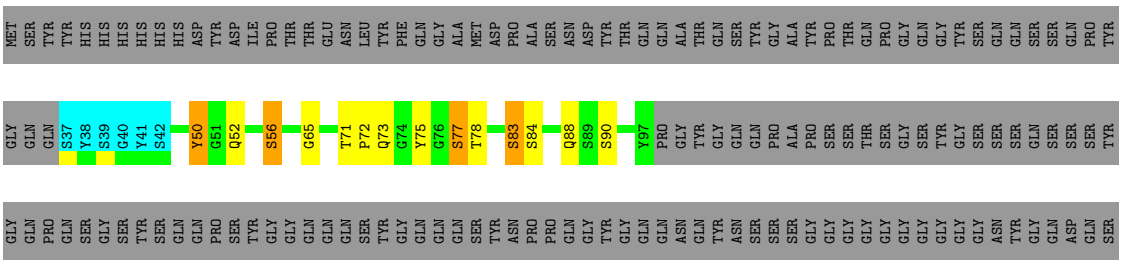
Chain I:



4.2.6 Score per residue for model 6

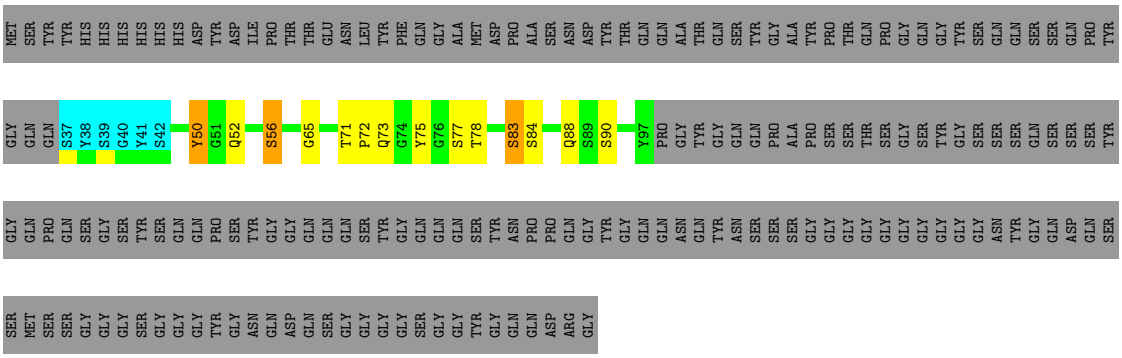
- Molecule 1: RNA-binding protein FUS

Chain A:



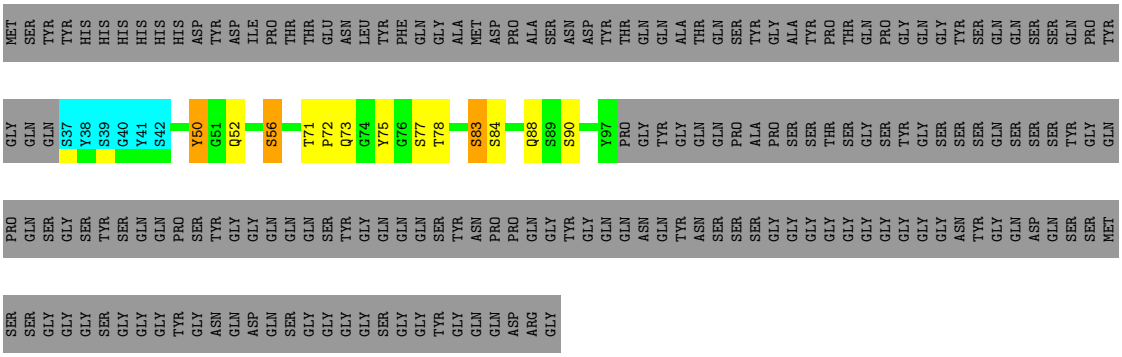
• Molecule 1: RNA-binding protein FUS

Chain B:



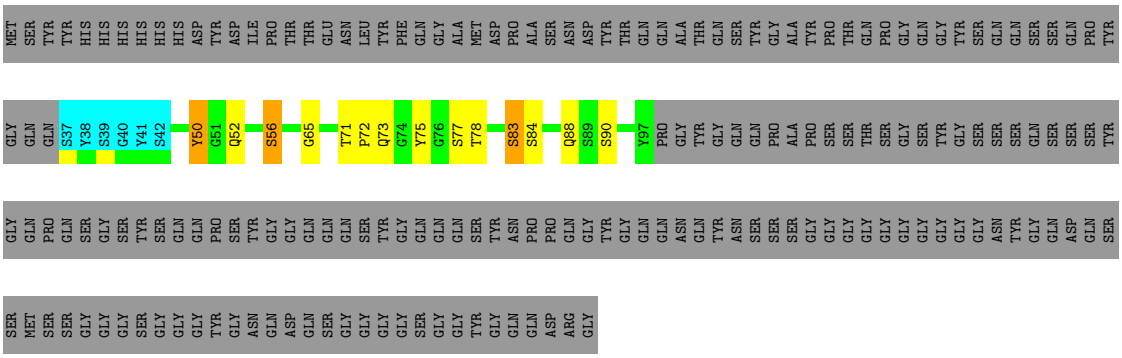
• Molecule 1: RNA-binding protein FUS

Chain C:



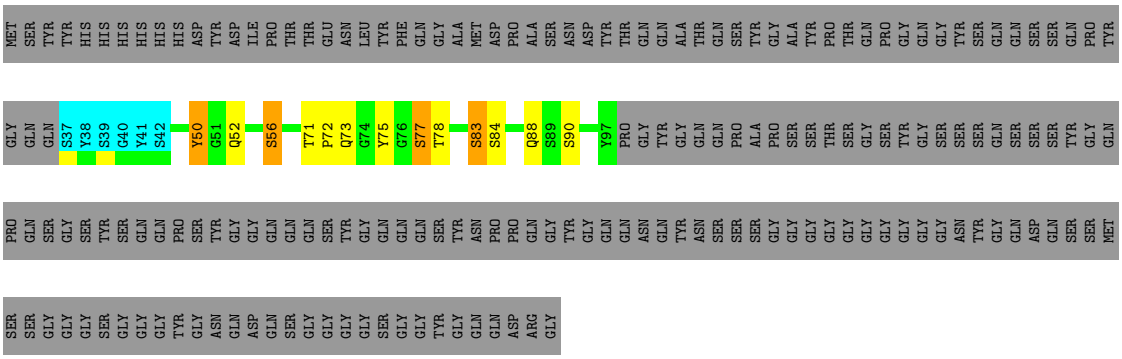
• Molecule 1: RNA-binding protein FUS

Chain D:



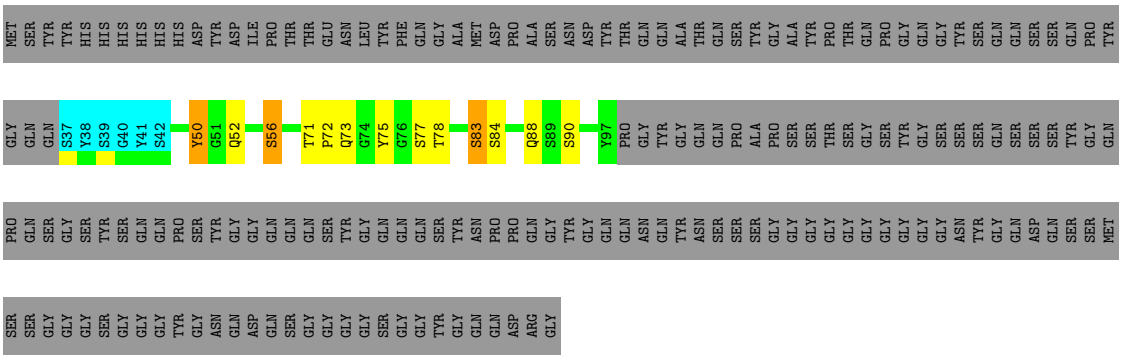
• Molecule 1: RNA-binding protein FUS

Chain E:



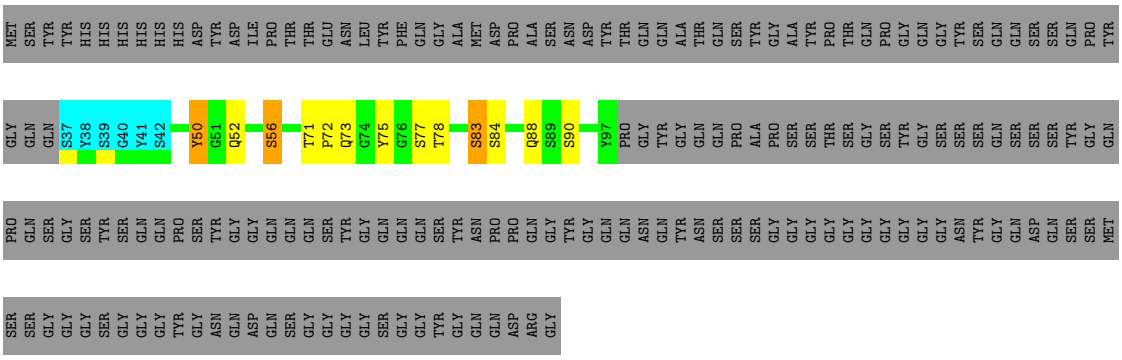
- Molecule 1: RNA-binding protein FUS

Chain F: 17% • •• 75%



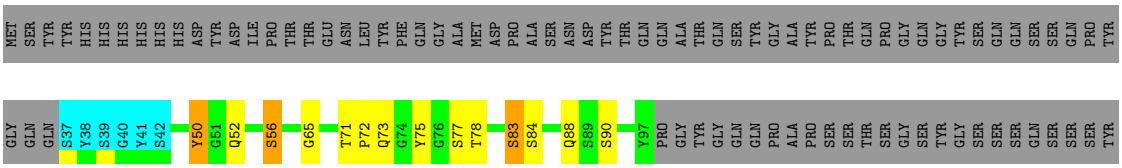
- Molecule 1: RNA-binding protein FUS

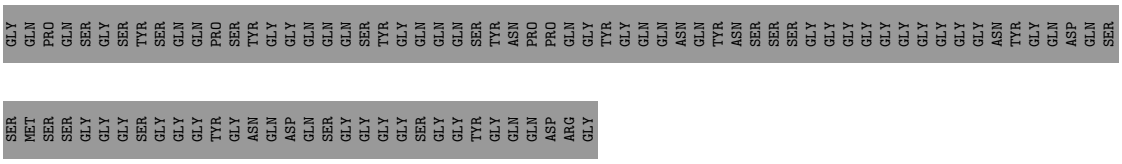
Chain G: 17% • •• 75%



- Molecule 1: RNA-binding protein FUS

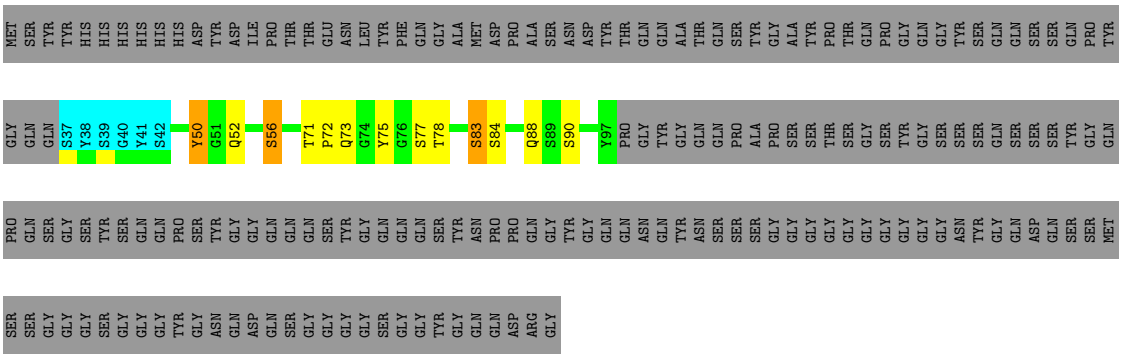
Chain H: 17% 5% •• 75%





• Molecule 1: RNA-binding protein FUS

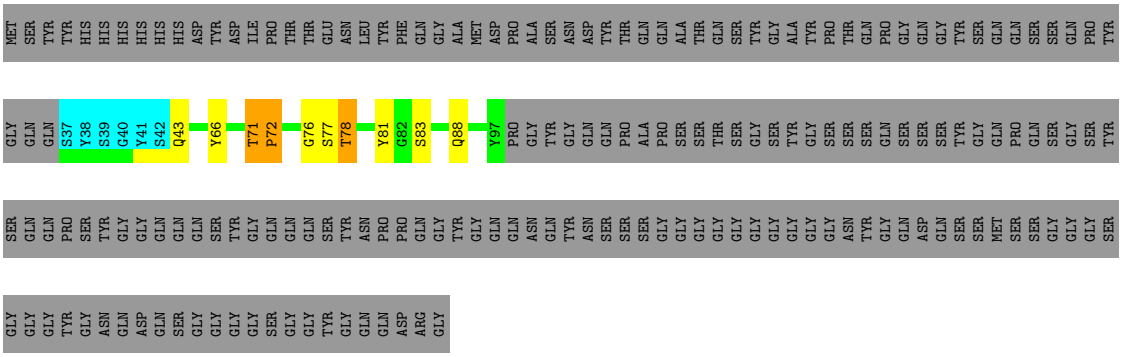
Chain I: 17% 75%



4.2.7 Score per residue for model 7

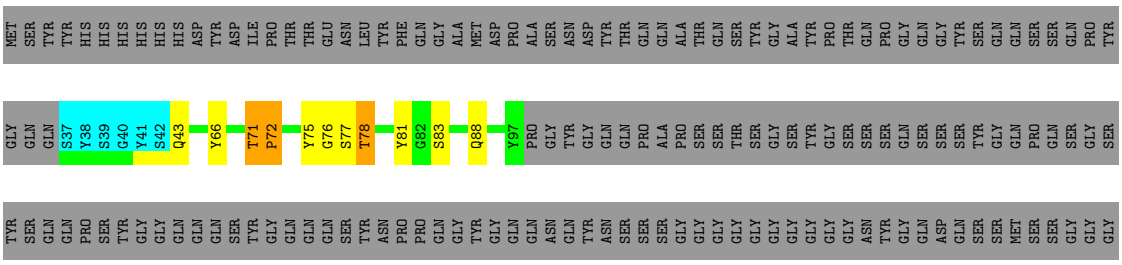
• Molecule 1: RNA-binding protein FUS

Chain A: 19% 75%



• Molecule 1: RNA-binding protein FUS

Chain B: 18% 75%



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

• Molecule 1: RNA-binding protein FUS

Chain C: 18% • • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 Y66 T71 P72 Y75 G76 S77 T78 Y81 G82 S83 Q88 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain D: 18% • • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 Y66 T71 P72 Y75 G76 S77 T78 Y81 G82 S83 Q88 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain E: 17% • • • 75%

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

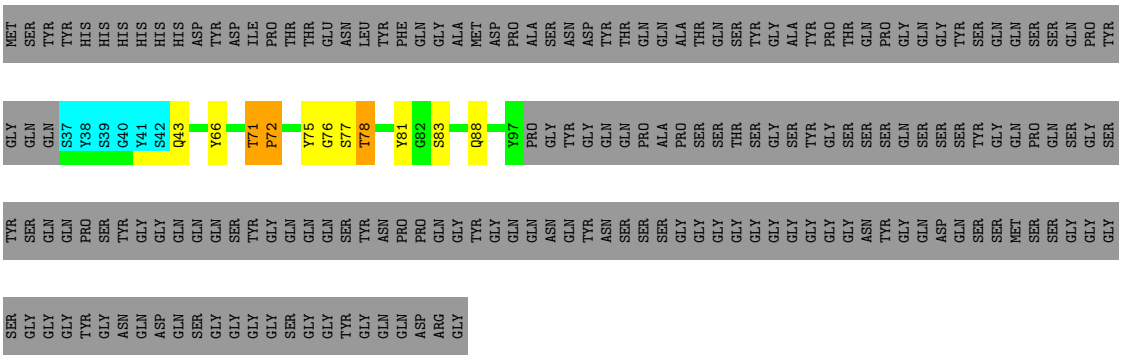
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 G49 Y50 Y66 T71 P72 Y75 G76 S77 T78 Y81 G82 S83 Q88 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN

SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

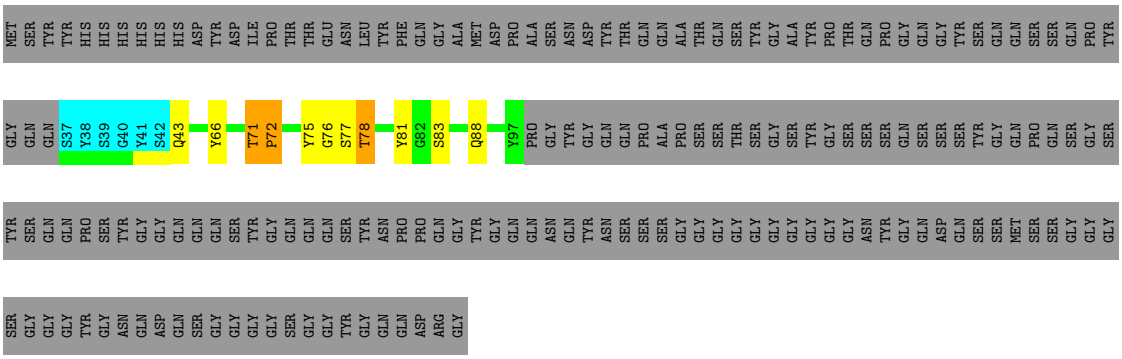
• Molecule 1: RNA-binding protein FUS

Chain F: 18% • • • 75%



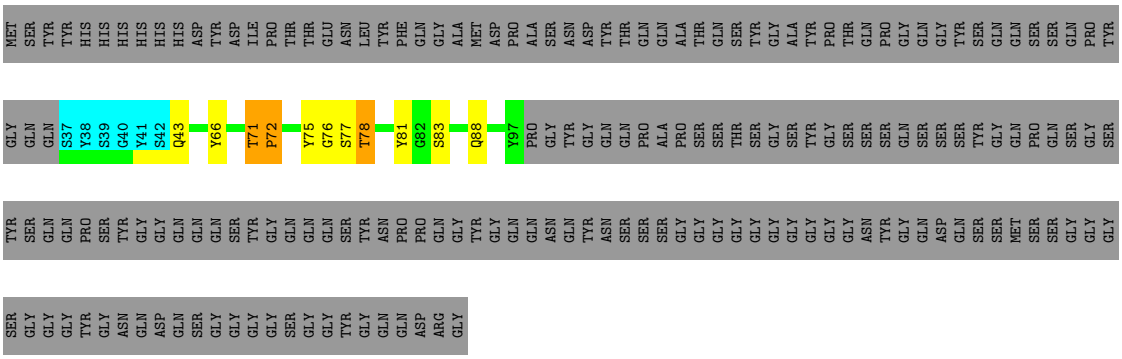
• Molecule 1: RNA-binding protein FUS

Chain G: 18% • • • 75%



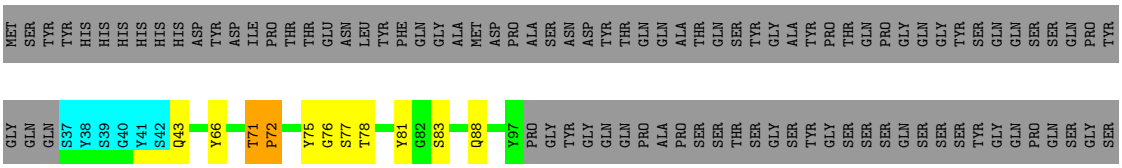
• Molecule 1: RNA-binding protein FUS

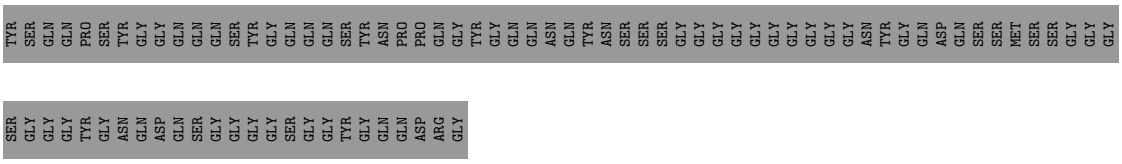
Chain H: 18% • • • 75%



• Molecule 1: RNA-binding protein FUS

Chain I: 18% • • • 75%

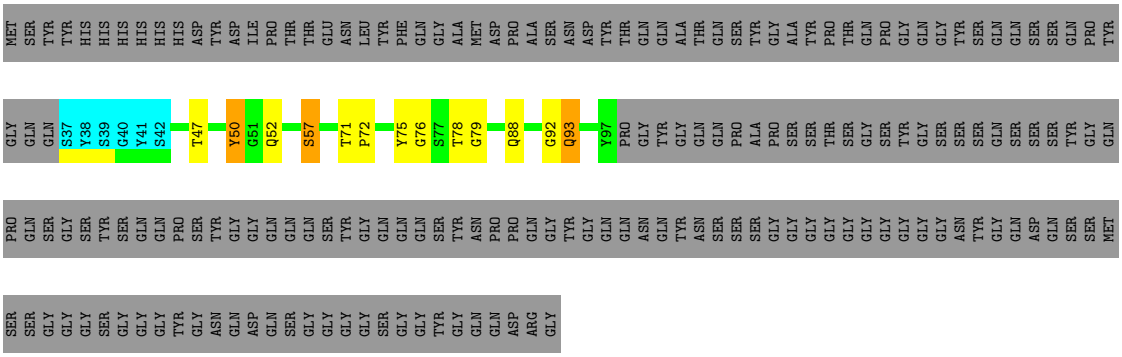




4.2.8 Score per residue for model 8

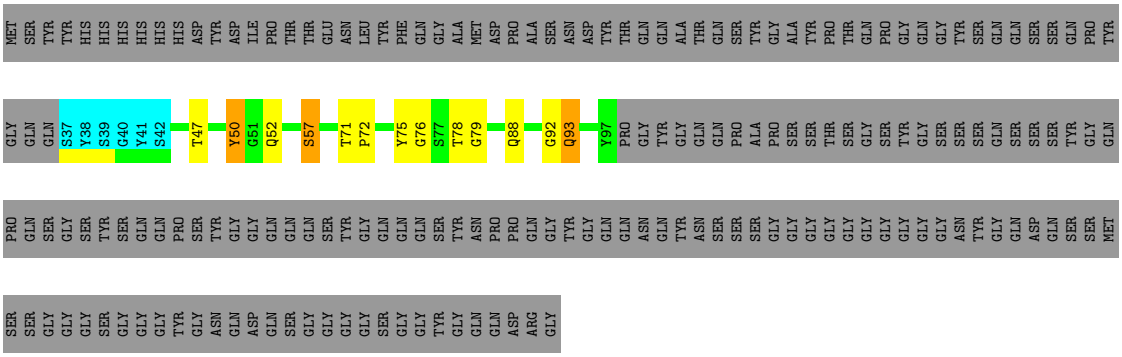
- Molecule 1: RNA-binding protein FUS

Chain A: 17% 75%



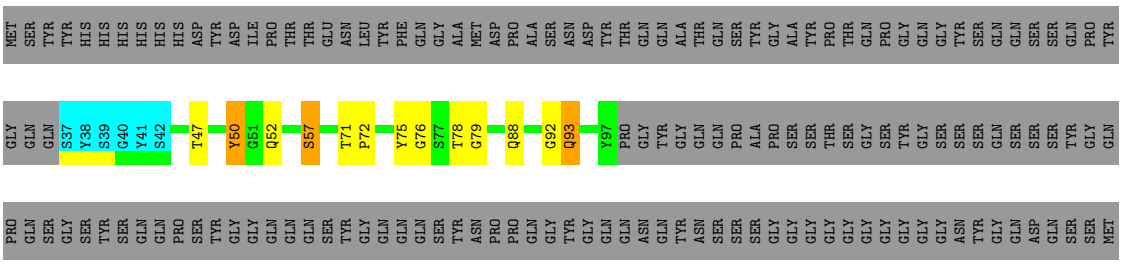
- Molecule 1: RNA-binding protein FUS

Chain B: 17% 75%



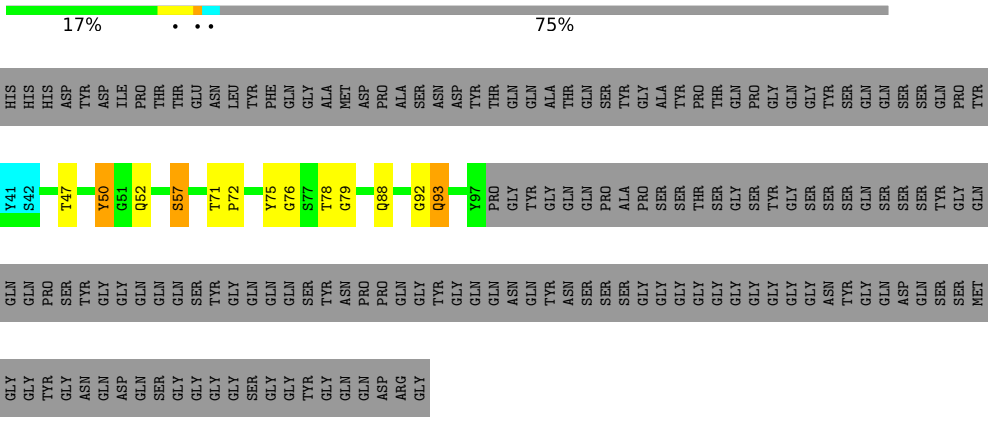
- Molecule 1: RNA-binding protein FUS

Chain C: 17% 75%



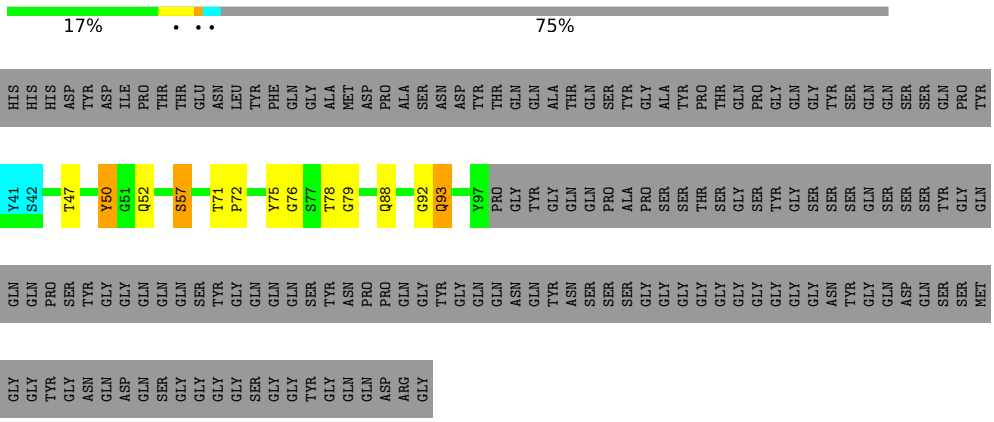
• Molecule 1: RNA-binding protein FUS

Chain D:



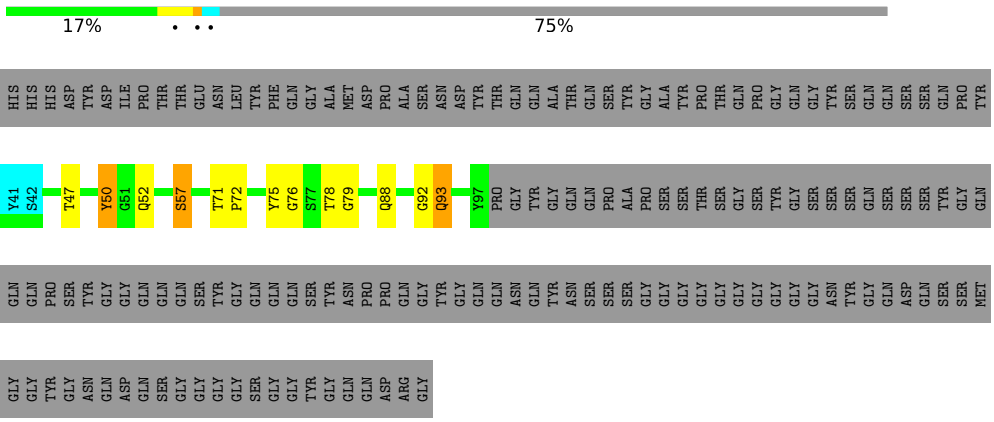
• Molecule 1: RNA-binding protein FUS

Chain E:



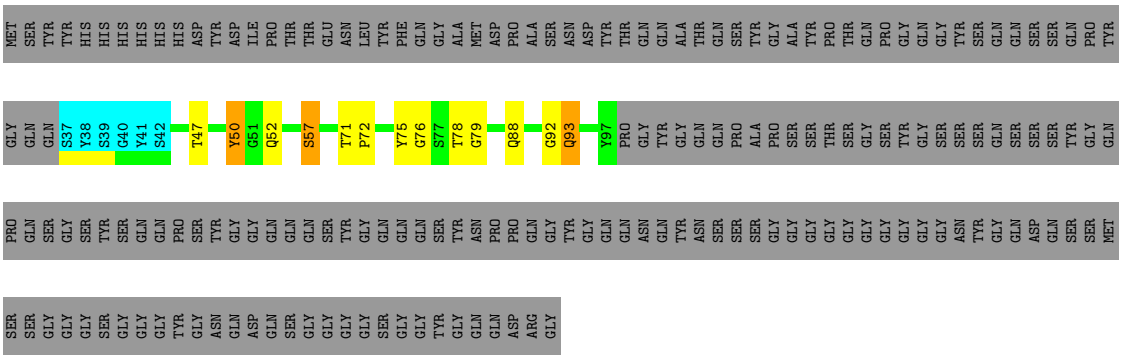
• Molecule 1: RNA-binding protein FUS

Chain F:



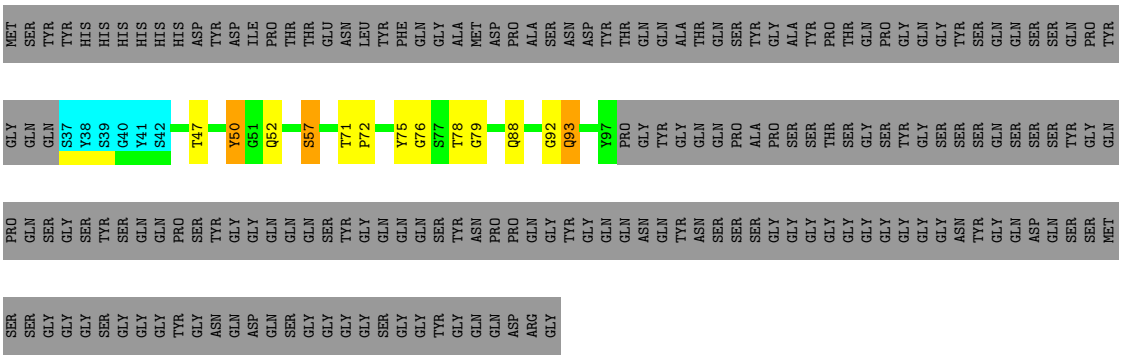
• Molecule 1: RNA-binding protein FUS

Chain G:



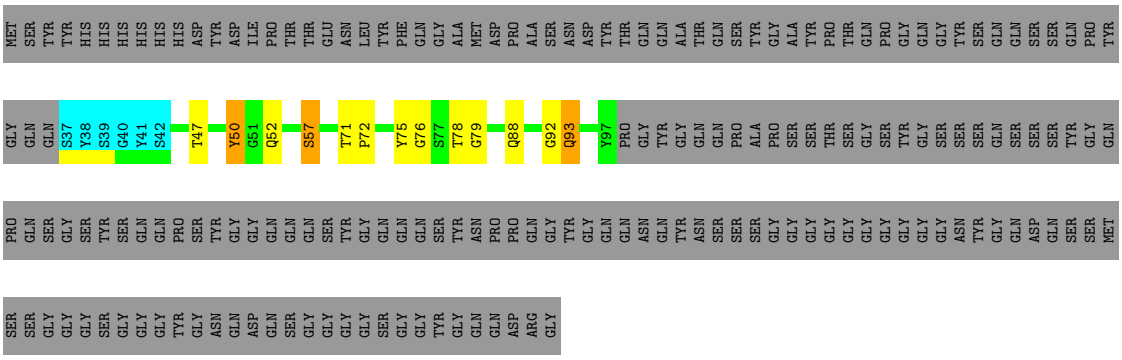
• Molecule 1: RNA-binding protein FUS

Chain H: 17% 75%



• Molecule 1: RNA-binding protein FUS

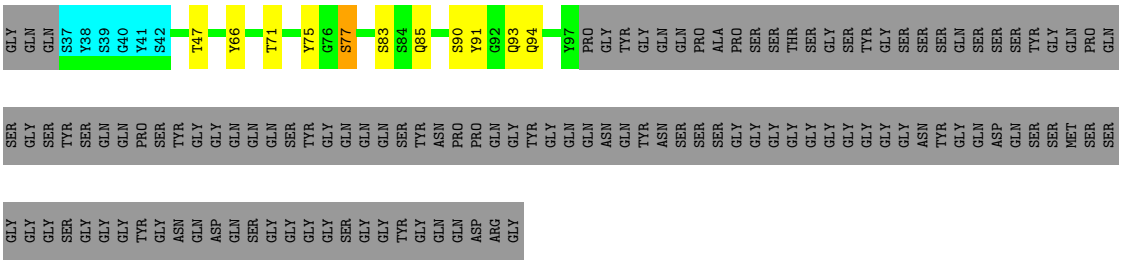
Chain I: 17% 75%



4.2.9 Score per residue for model 9

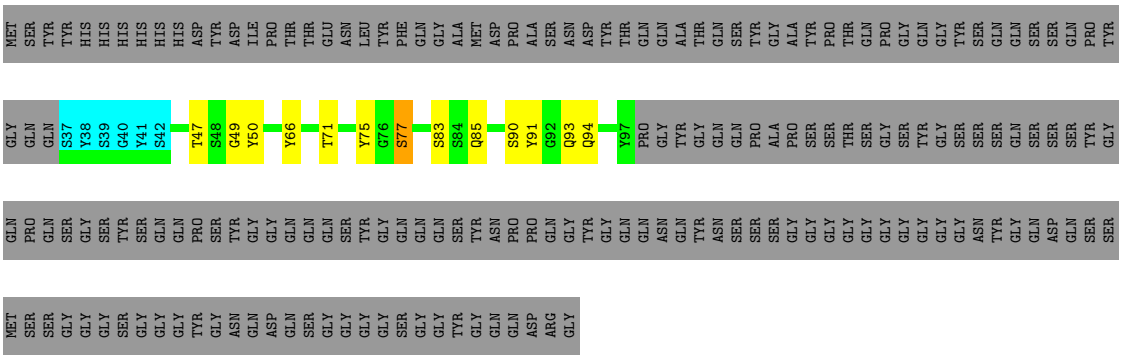
• Molecule 1: RNA-binding protein FUS

Chain A: 18% 75%



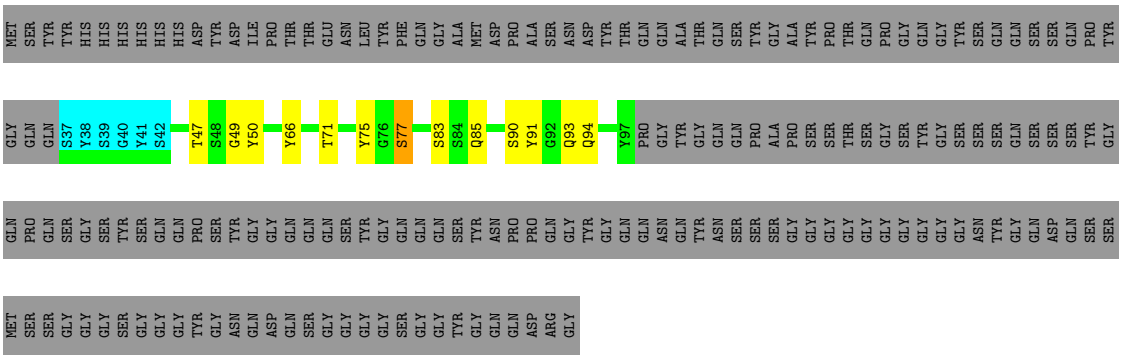
- Molecule 1: RNA-binding protein FUS

Chain B: 17% 5% • 75%



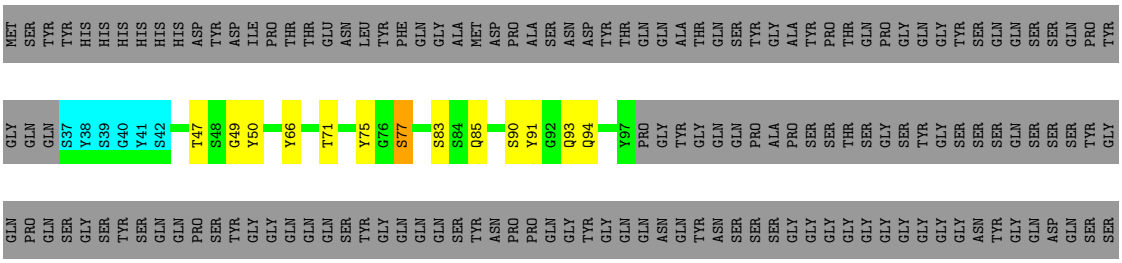
- Molecule 1: RNA-binding protein FUS

Chain C: 17% 5% • 75%



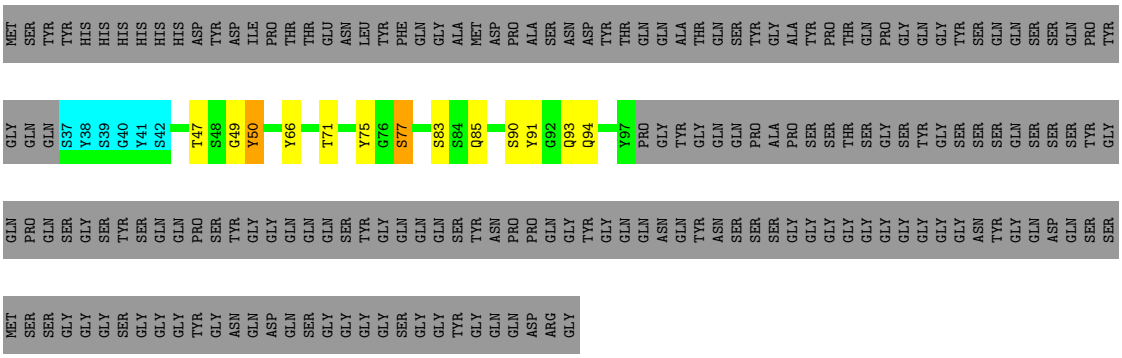
- Molecule 1: RNA-binding protein FUS

Chain D: 17% 5% • 75%



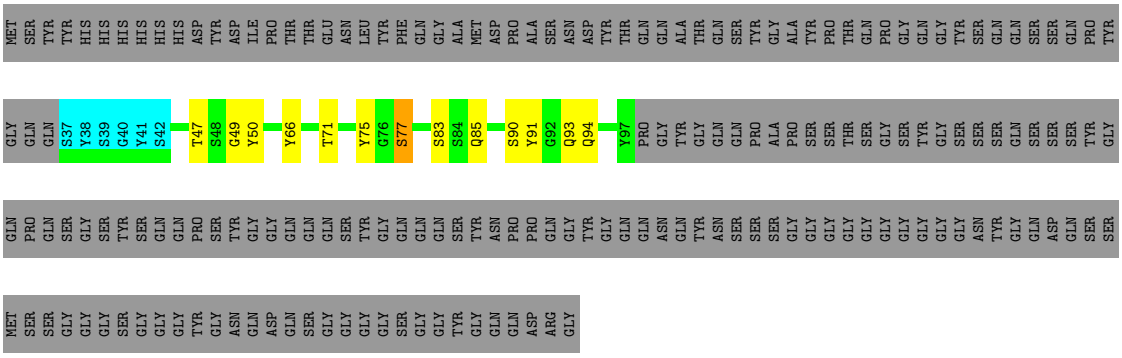
• Molecule 1: RNA-binding protein FUS

Chain E:



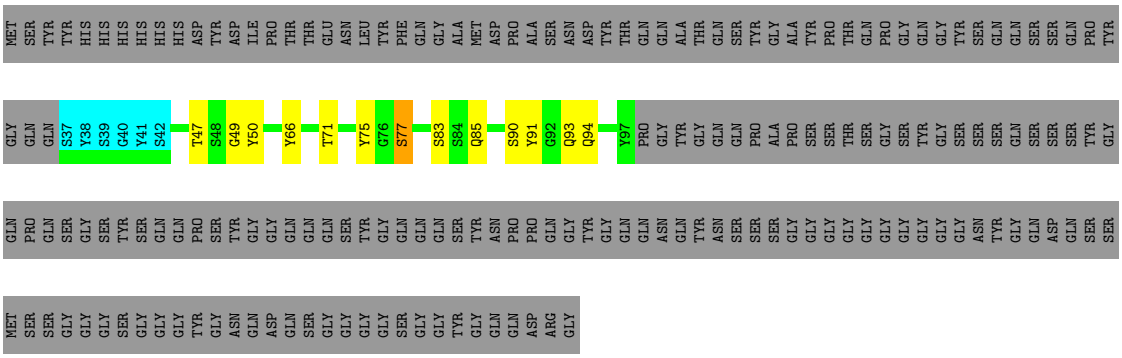
• Molecule 1: RNA-binding protein FUS

Chain F:



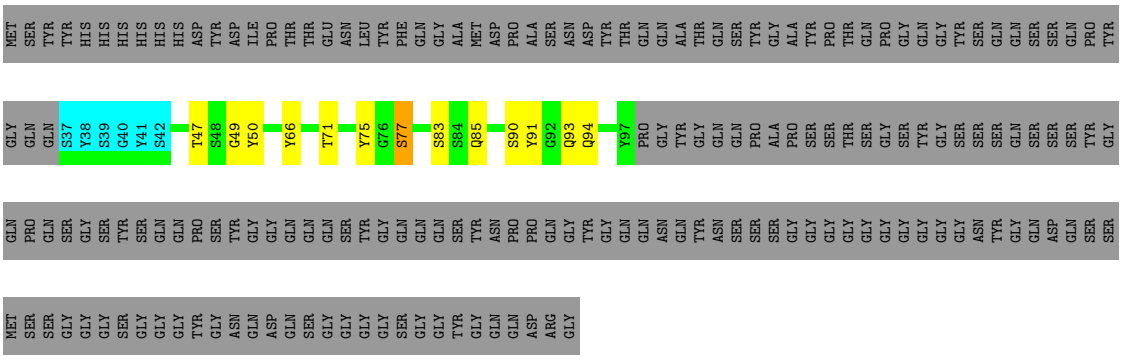
• Molecule 1: RNA-binding protein FUS

Chain G:



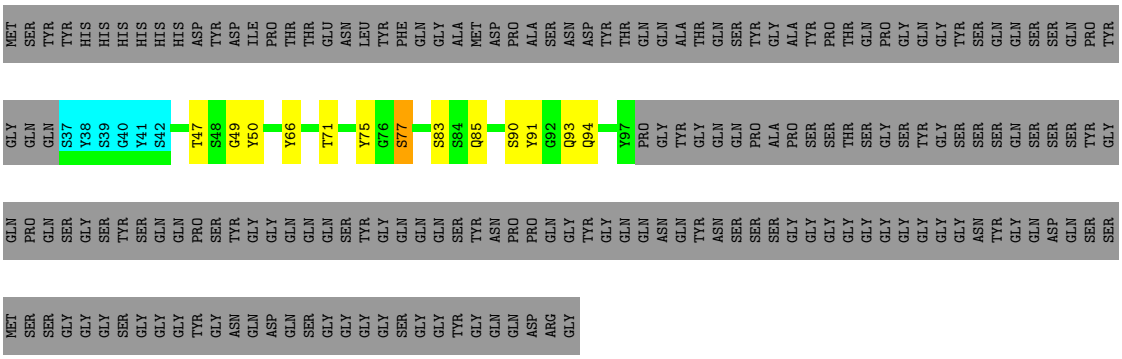
• Molecule 1: RNA-binding protein FUS

Chain H:



• Molecule 1: RNA-binding protein FUS

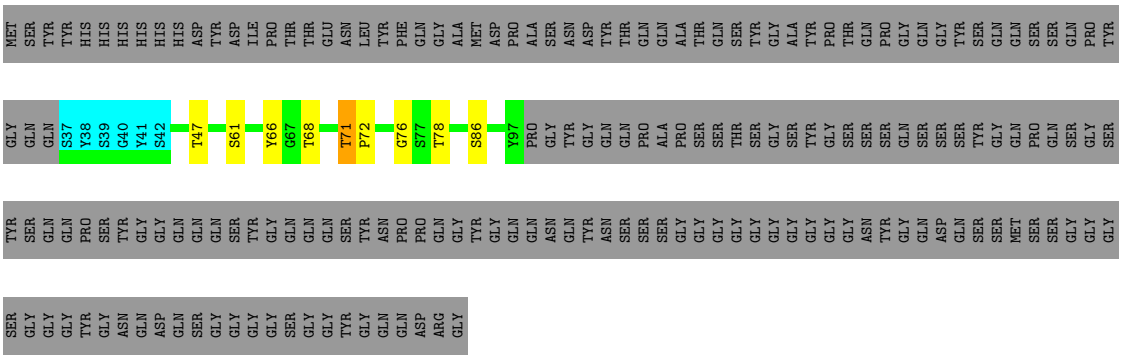
Chain I:



4.2.10 Score per residue for model 10

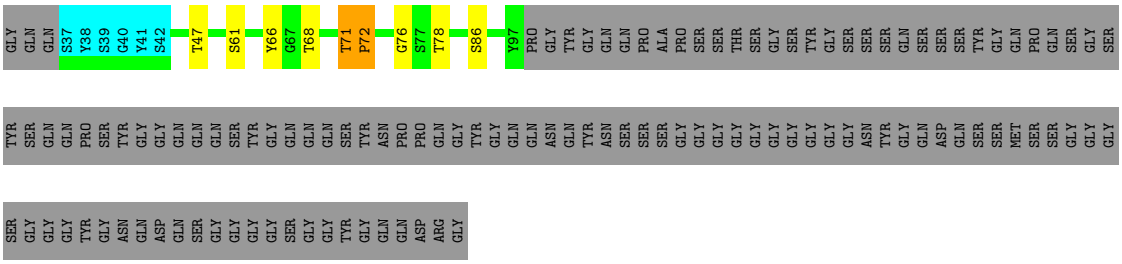
• Molecule 1: RNA-binding protein FUS

Chain A:



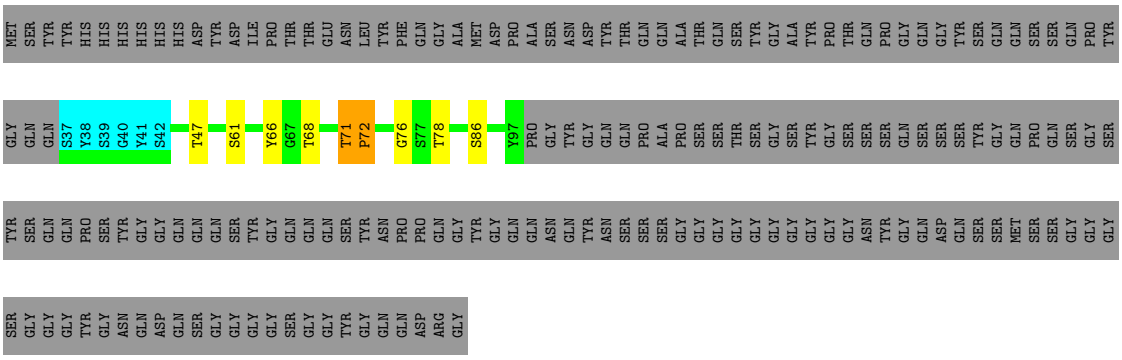
• Molecule 1: RNA-binding protein FUS

Chain B:



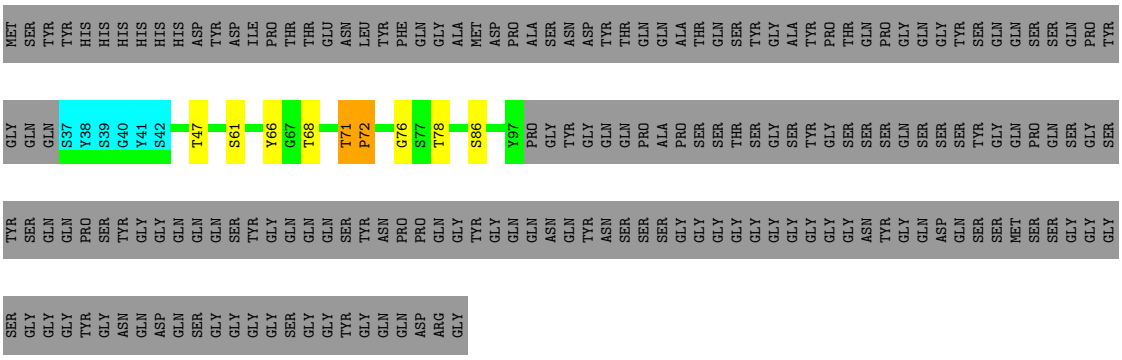
• Molecule 1: RNA-binding protein FUS

Chain C:



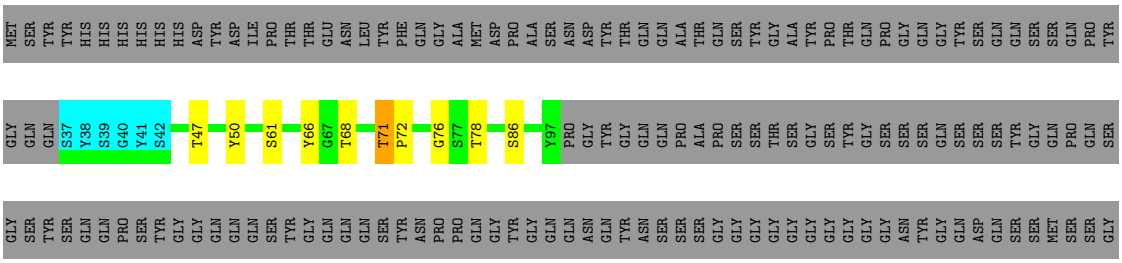
• Molecule 1: RNA-binding protein FUS

Chain D:



• Molecule 1: RNA-binding protein FUS

Chain E:



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

• Molecule 1: RNA-binding protein FUS

Chain F: 19% ... 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 S61 Y66 G67 T68 T71 P72 G76 S77 T78 S86 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain G: 19% ... 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 S61 Y66 G67 T68 T71 P72 G76 S77 T78 S86 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain H: 19% ... 75%

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

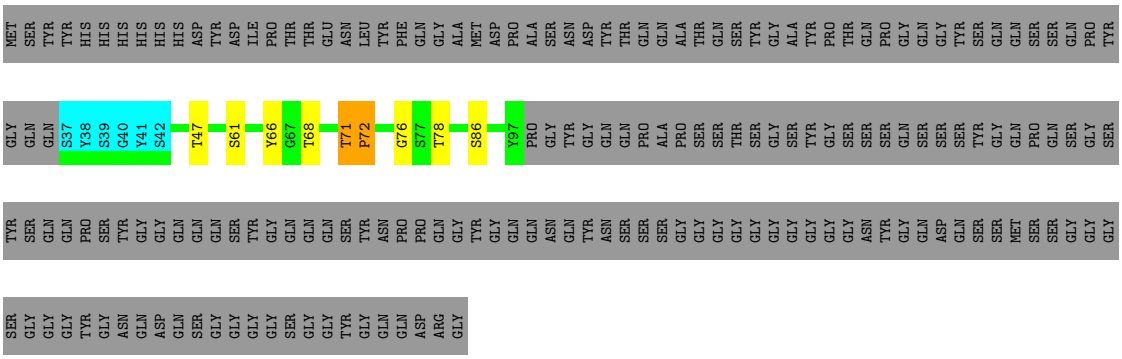
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 S61 Y66 G67 T68 T71 P72 G76 S77 T78 S86 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

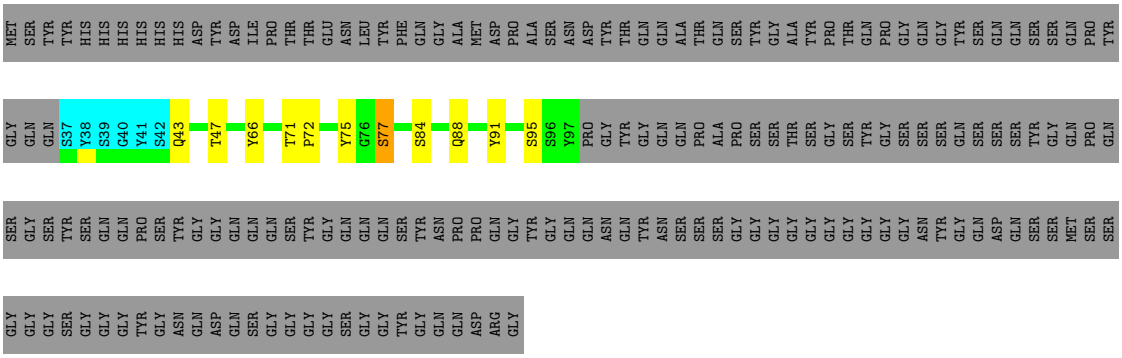
Chain I: 19% ... 75%



4.2.11 Score per residue for model 11

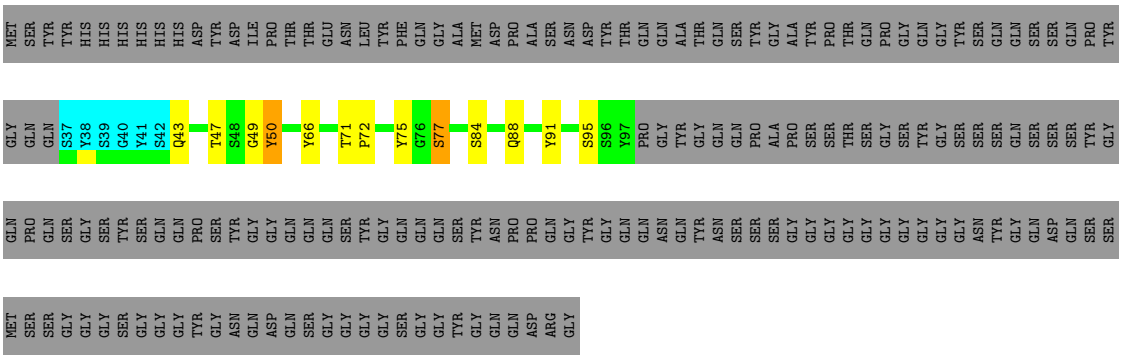
- Molecule 1: RNA-binding protein FUS

Chain A:



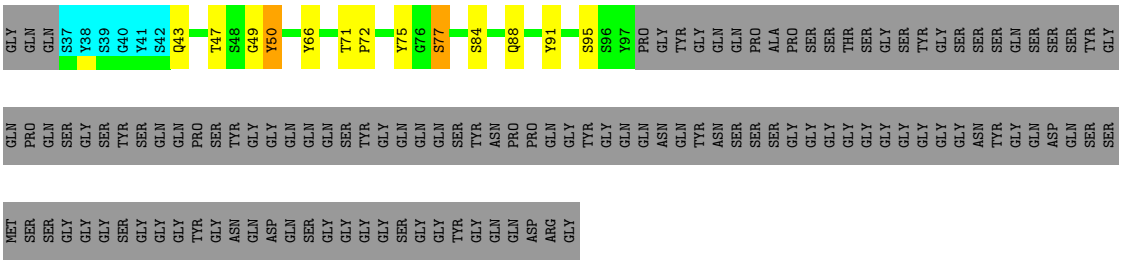
- Molecule 1: RNA-binding protein FUS

Chain B:



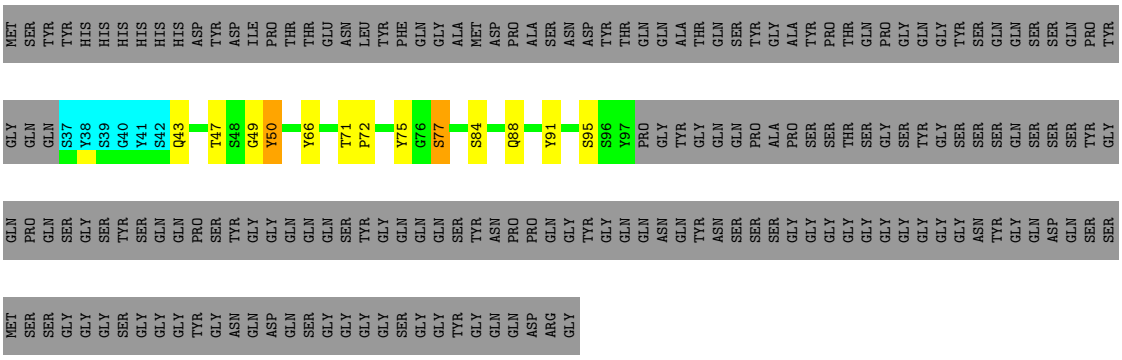
- Molecule 1: RNA-binding protein FUS

Chain C:



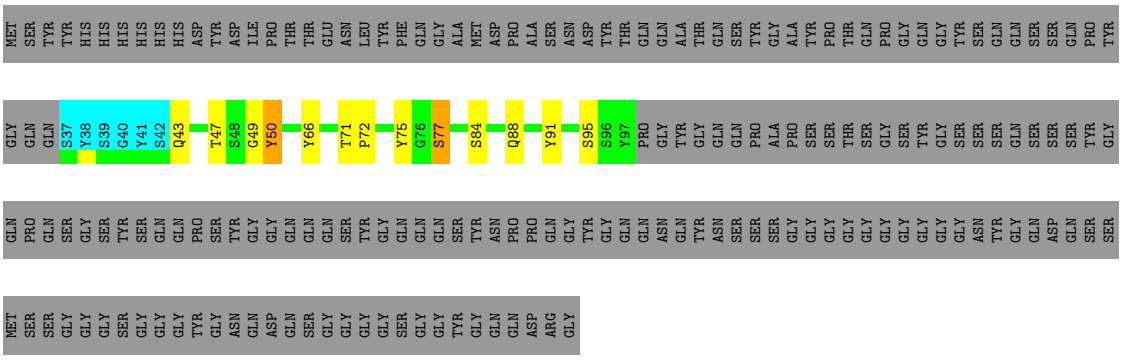
• Molecule 1: RNA-binding protein FUS

Chain D: 17% 5% • • 75%



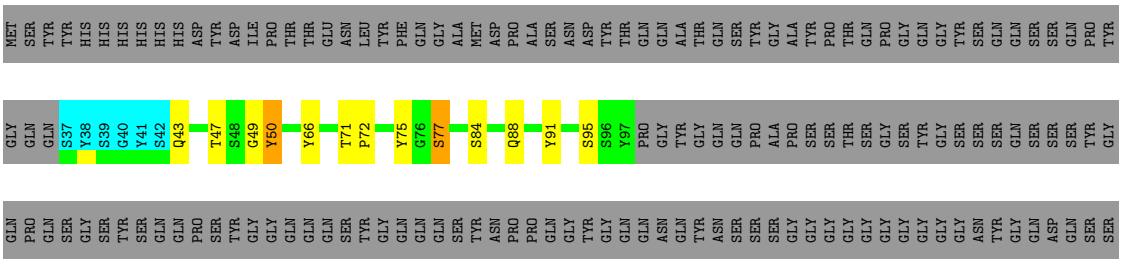
• Molecule 1: RNA-binding protein FUS

Chain E: 17% 5% • • 75%



• Molecule 1: RNA-binding protein FUS

Chain F: 17% 5% • • 75%



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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain G: 17% 5% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 T47 S48 G49 Y50 Y66 T71 P72 Y75 G76 S77 S84 Q88 Y91 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY

GLN PRO GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain H: 18% • • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 T47 S48 G49 Y50 Y66 T71 Y75 G76 S77 S84 Q88 Y91 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN

PRO GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain I: 17% 5% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 T47 S48 G49 Y50 Y66 T71 Y75 G76 S77 S84 Q88 Y91 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY

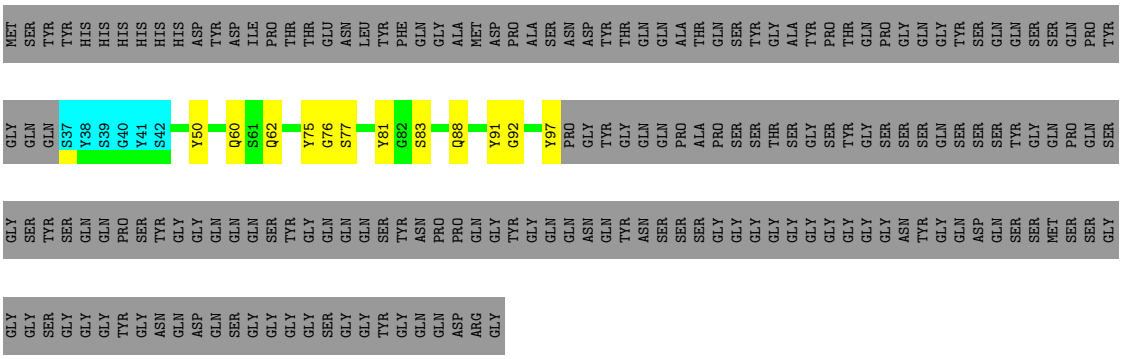
GLN PRO GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER

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 GLN ASP ARG GLY

4.2.12 Score per residue for model 12

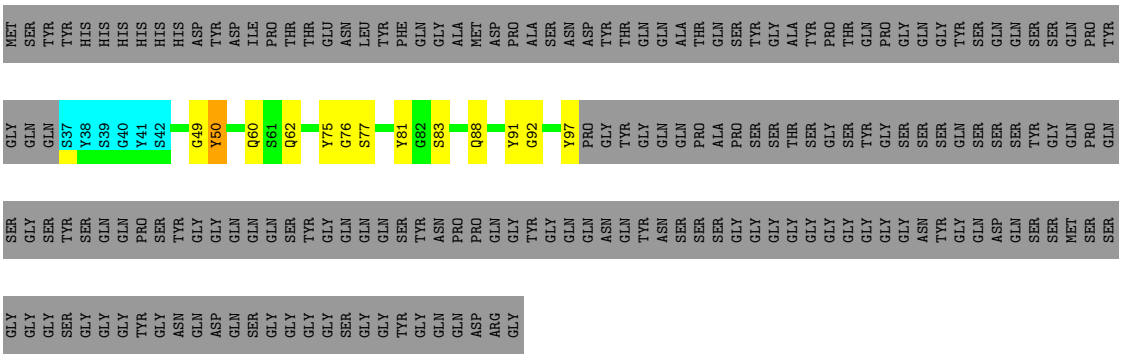
- Molecule 1: RNA-binding protein FUS

Chain A: 18% 5% • 75%



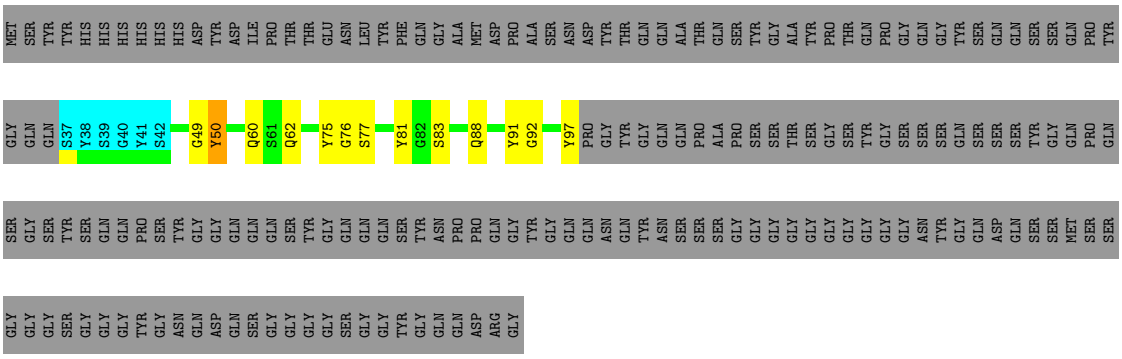
- Molecule 1: RNA-binding protein FUS

Chain B: 17% 5% • 75%



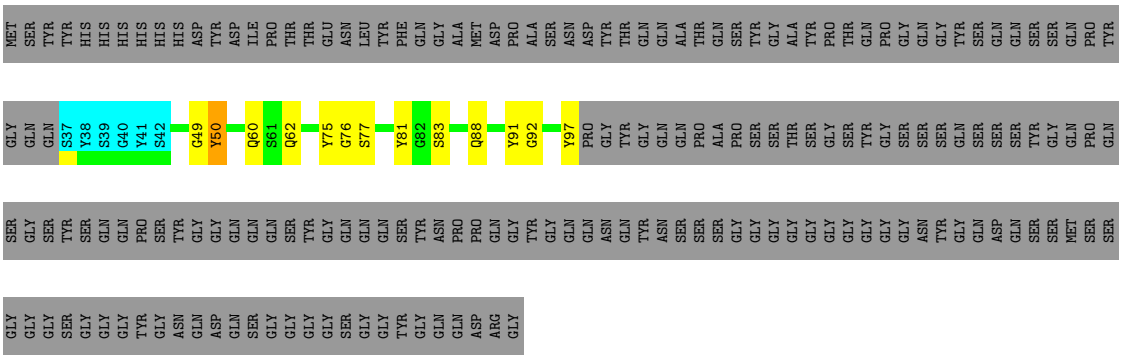
- Molecule 1: RNA-binding protein FUS

Chain C: 17% 5% • 75%



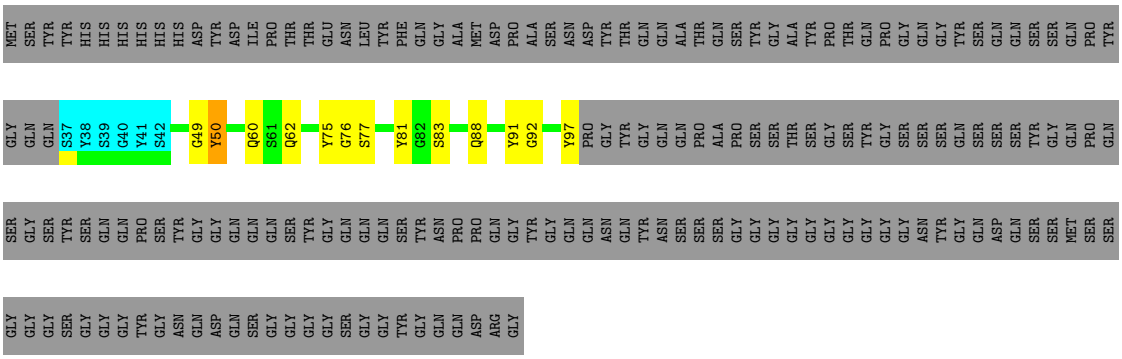
- Molecule 1: RNA-binding protein FUS

Chain D: 17% 5% • 75%



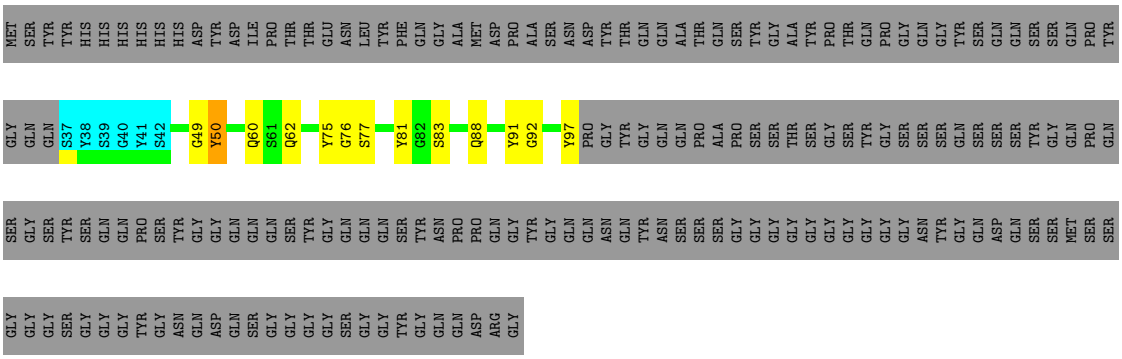
• Molecule 1: RNA-binding protein FUS

Chain E: 17% 5% • 75%



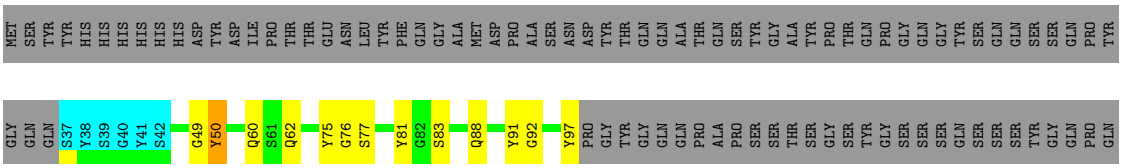
• Molecule 1: RNA-binding protein FUS

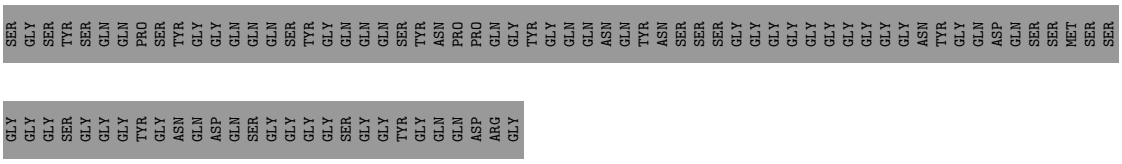
Chain F: 17% 5% • 75%



• Molecule 1: RNA-binding protein FUS

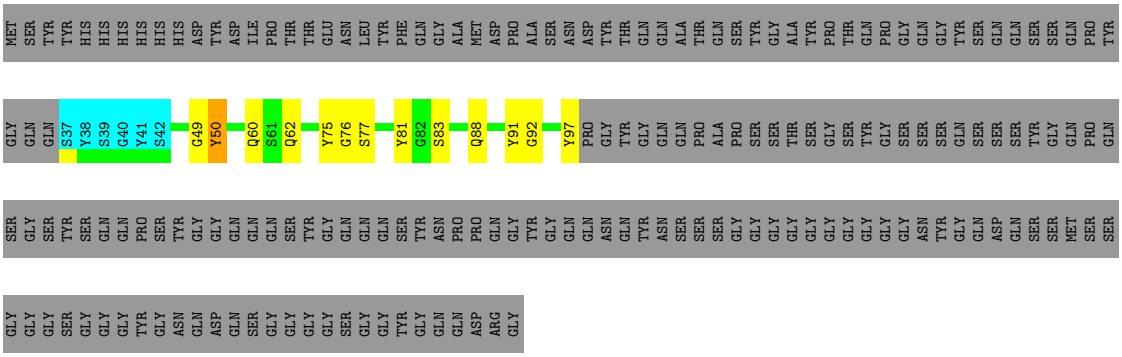
Chain G: 17% 5% • 75%





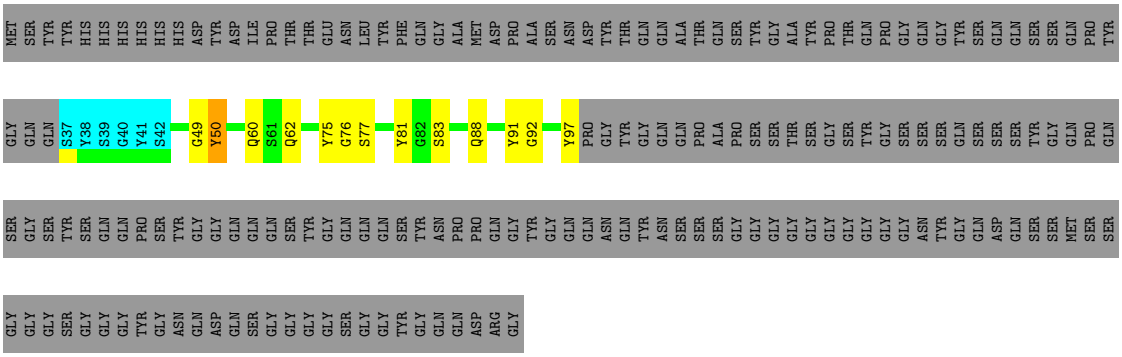
• Molecule 1: RNA-binding protein FUS

Chain H:



• Molecule 1: RNA-binding protein FUS

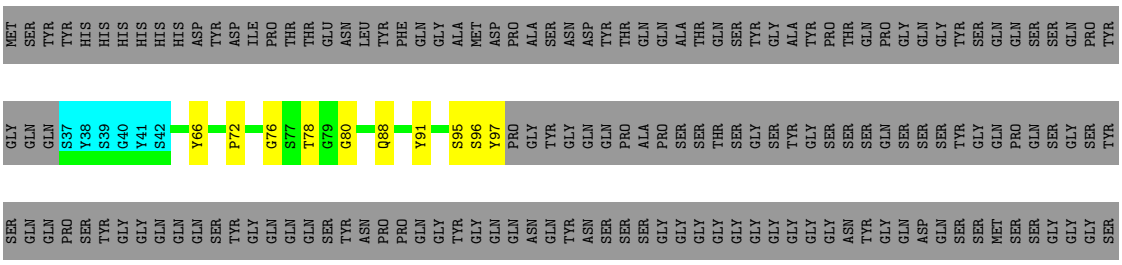
Chain I:

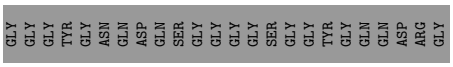


4.2.13 Score per residue for model 13

• Molecule 1: RNA-binding protein FUS

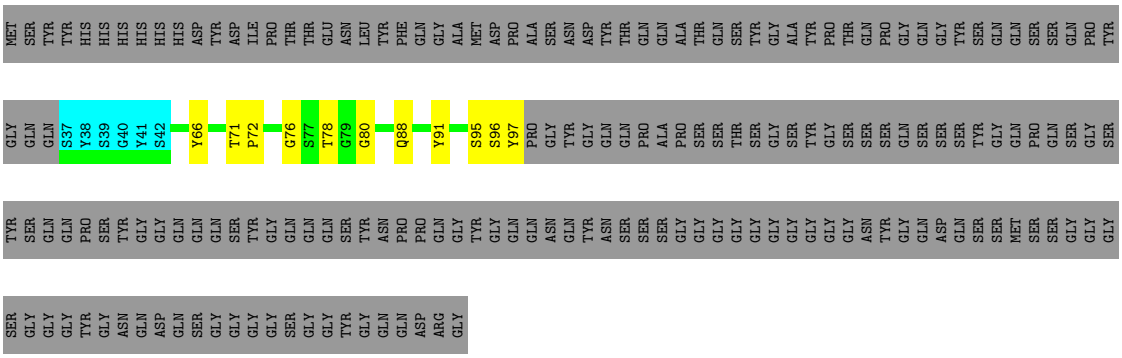
Chain A:





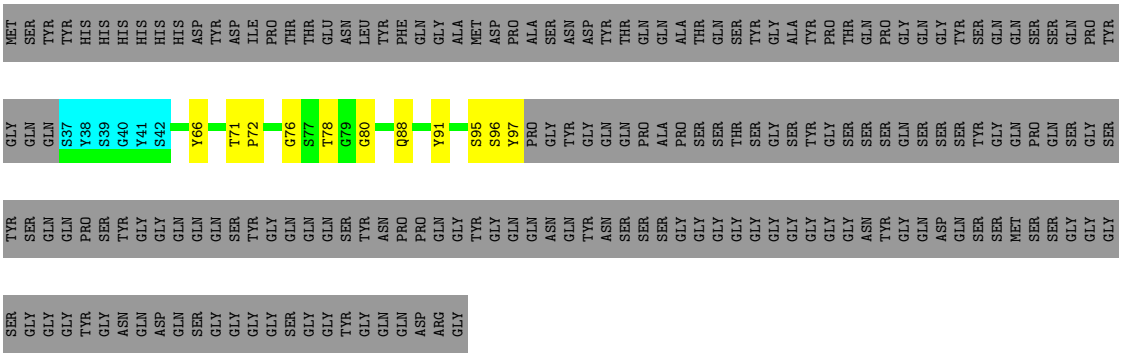
• Molecule 1: RNA-binding protein FUS

Chain B:



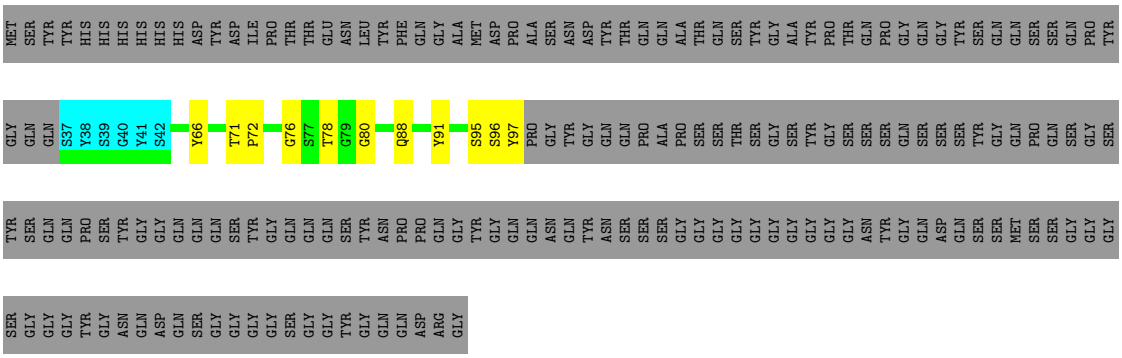
• Molecule 1: RNA-binding protein FUS

Chain C:



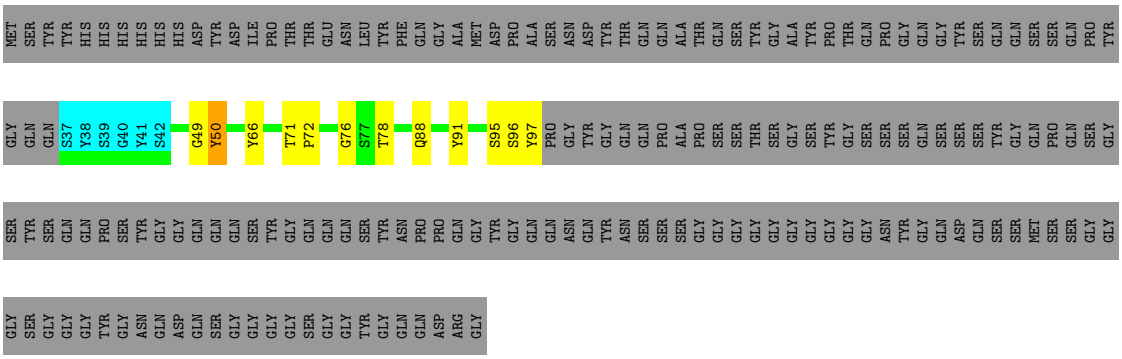
• Molecule 1: RNA-binding protein FUS

Chain D:



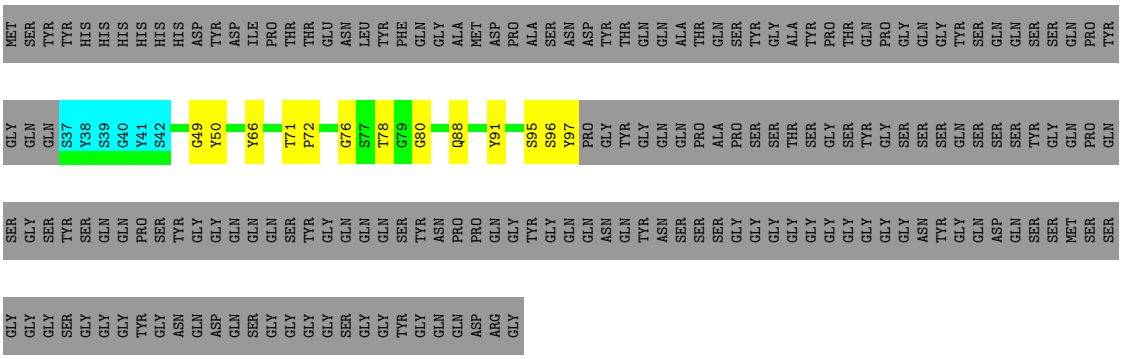
• Molecule 1: RNA-binding protein FUS

Chain E:



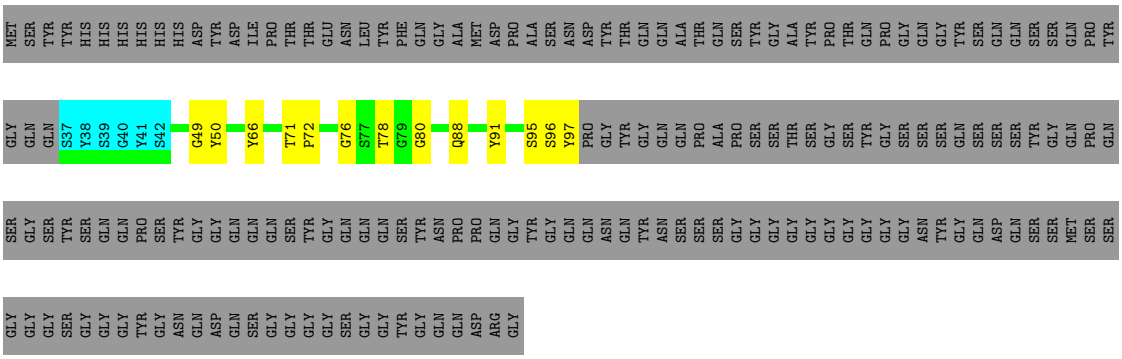
• Molecule 1: RNA-binding protein FUS

Chain F: 17% 5% • 75%



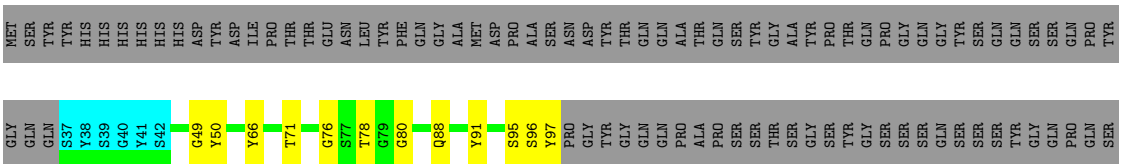
• Molecule 1: RNA-binding protein FUS

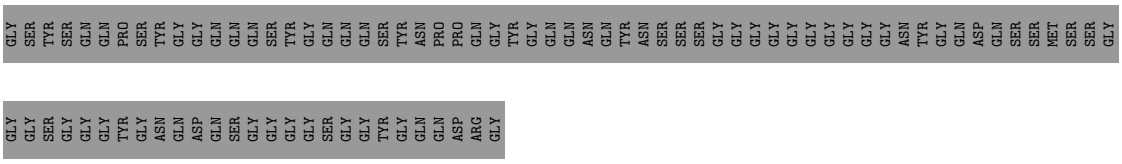
Chain G: 17% 5% • 75%



• Molecule 1: RNA-binding protein FUS

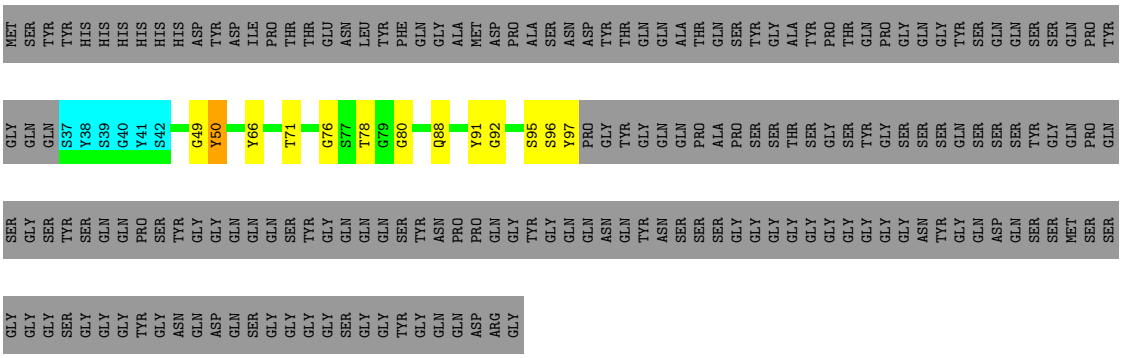
Chain H: 18% 5% • 75%





• Molecule 1: RNA-binding protein FUS

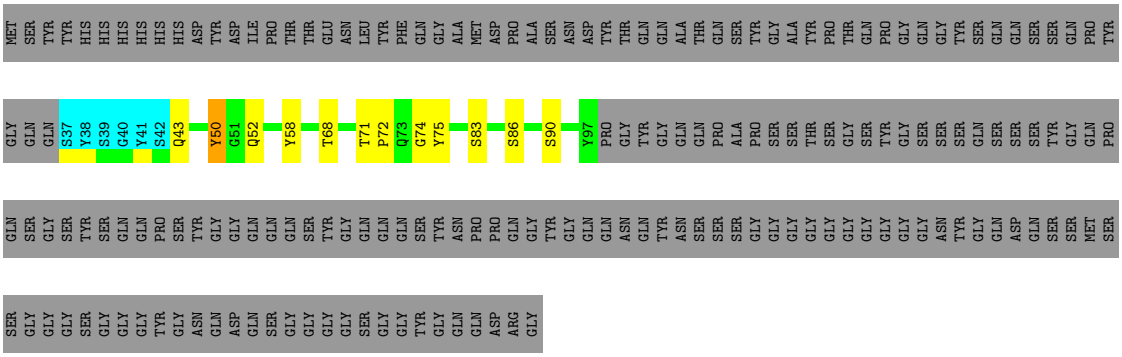
Chain I: 17% 5% • 75%



4.2.14 Score per residue for model 14

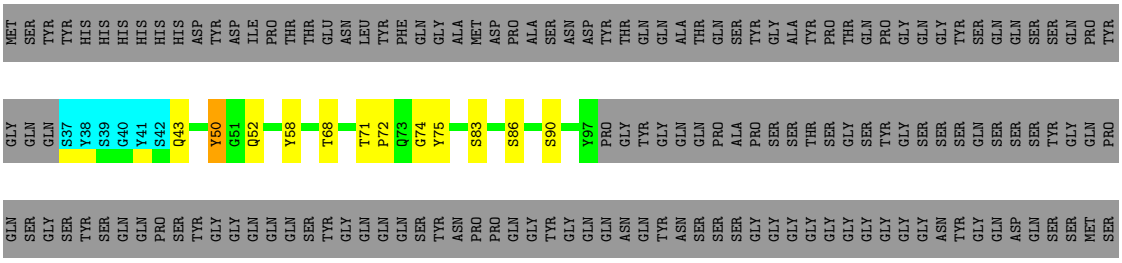
• Molecule 1: RNA-binding protein FUS

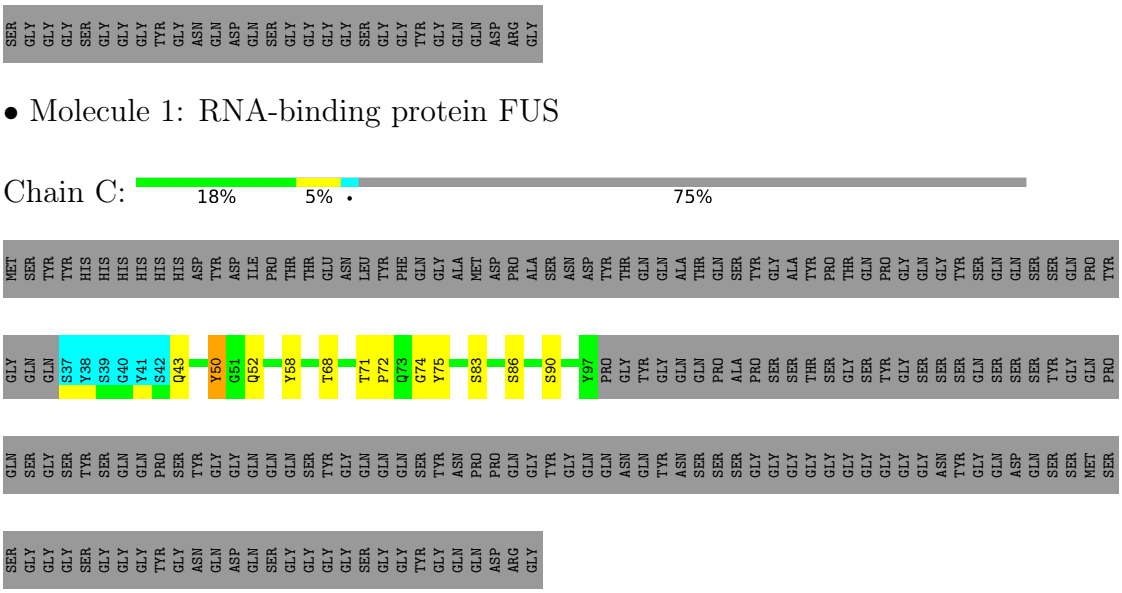
Chain A: 18% 5% • 75%

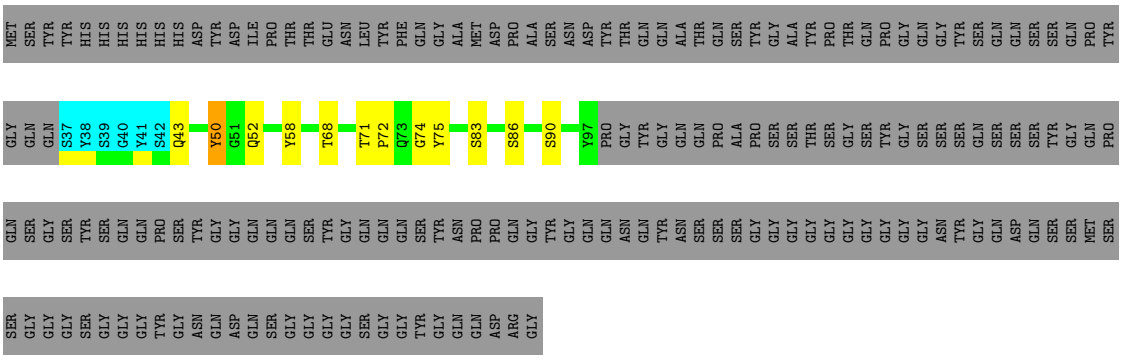


• Molecule 1: RNA-binding protein FUS

Chain B: 18% 5% • 75%

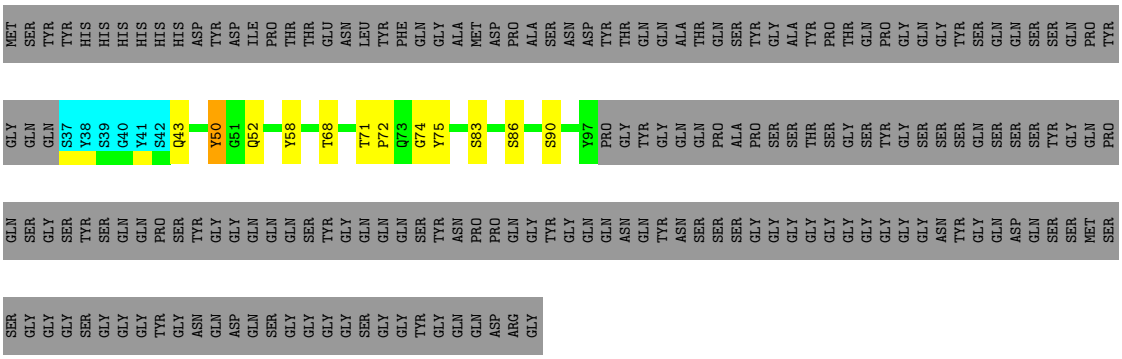



SER GLY GLY GLY SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY GLY TYR GLY GLN GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain C:
18%
5%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 Y50 G51 Q52 Y58 T68 T71 P72 Q73 G74 Y75 S83 S86 S90 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER GLN SER SER SER TYR GLY GLN PRO
GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER GLY GLY 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 GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain D:
18%
5%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 Y50 G51 Q52 Y58 T68 T71 P72 Q73 G74 Y75 S83 S86 S90 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER GLN SER SER SER TYR GLY GLN PRO
GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER GLY GLY 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 GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain E:
18%
5%
75%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO ALA SER ASN ASP TYR THR GLN GLN ALA THR GLN SER TYR GLY ALA TYR PRO THR GLN PRO GLY GLN GLY TYR SER GLN GLN SER SER GLN PRO TYR
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Q43 Y50 G51 Q52 Y58 T68 T71 P72 Q73 G74 Y75 S83 S86 S90 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER GLN SER SER SER TYR GLY GLN PRO
GLN SER GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER GLY GLY 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 GLN ASP ARG GLY
• Molecule 1: RNA-binding protein FUS
Chain F:
18%
5%
75%



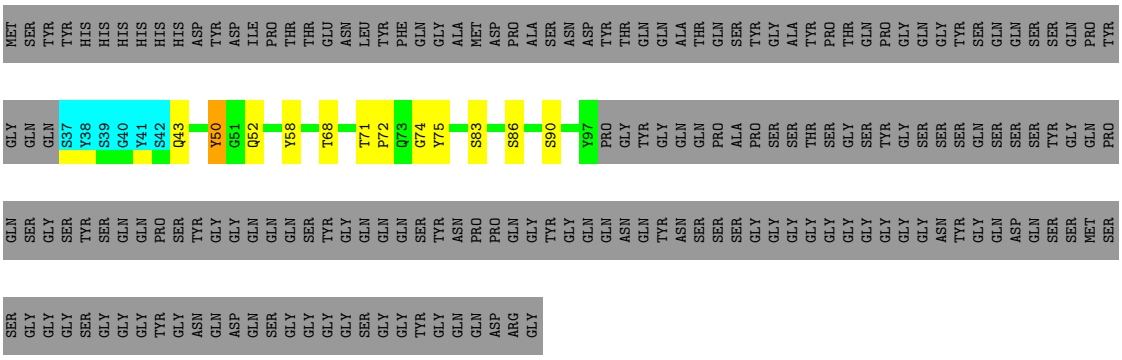
• Molecule 1: RNA-binding protein FUS

Chain G: 18% 5% • 75%



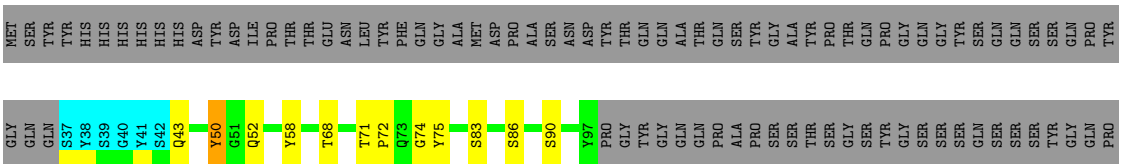
• Molecule 1: RNA-binding protein FUS

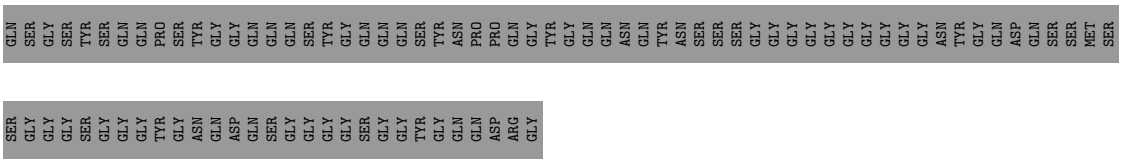
Chain H: 18% 5% • 75%



• Molecule 1: RNA-binding protein FUS

Chain I: 18% 5% • 75%

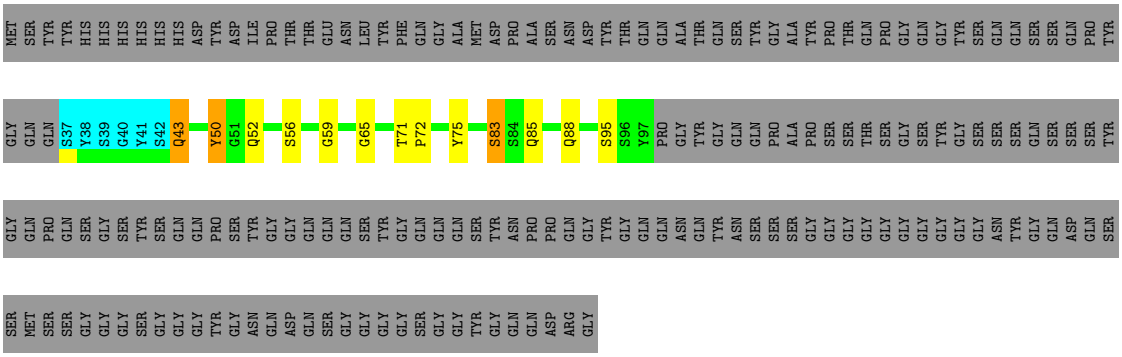




4.2.15 Score per residue for model 15

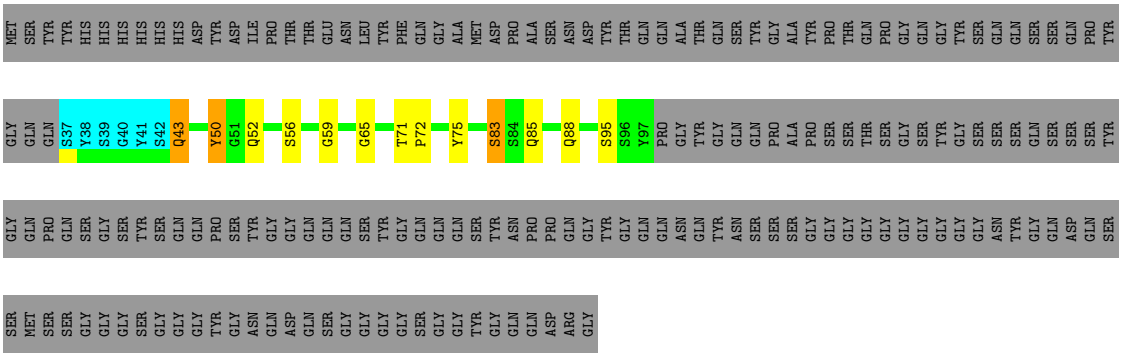
- Molecule 1: RNA-binding protein FUS

Chain A: 17% 75%



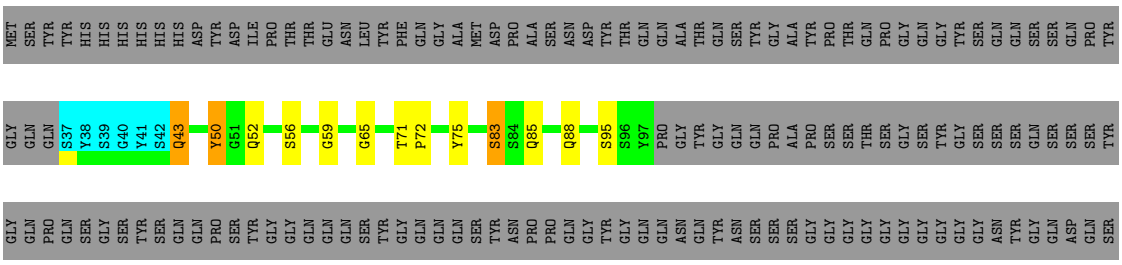
- Molecule 1: RNA-binding protein FUS

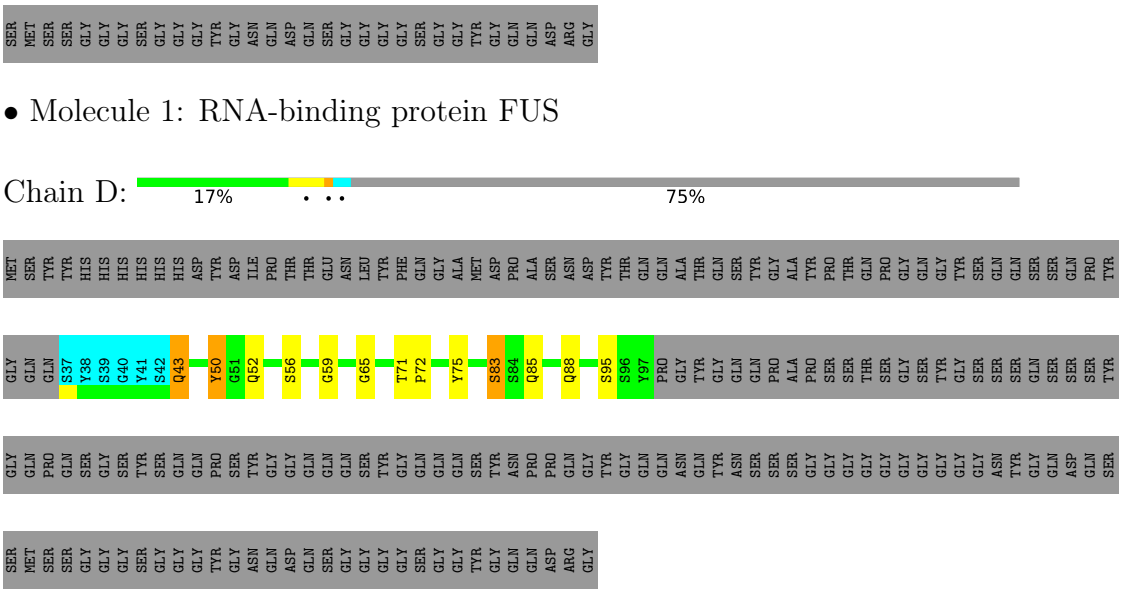
Chain B: 17% 75%



- Molecule 1: RNA-binding protein FUS

Chain C: 17% 75%



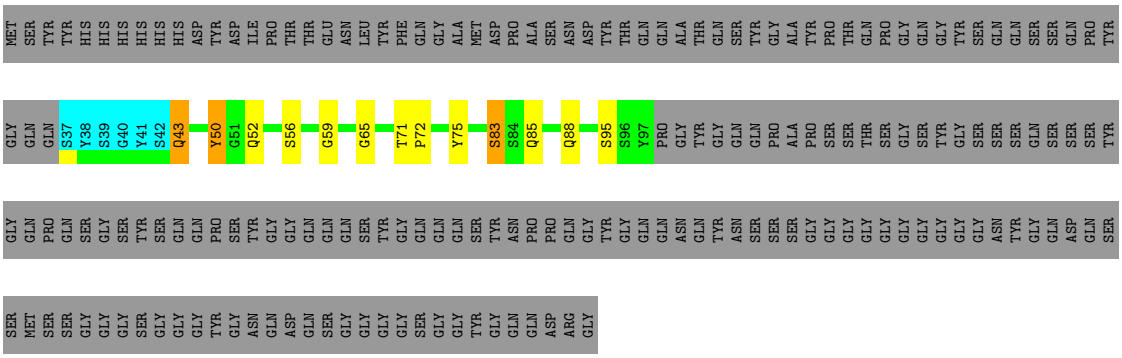


• Molecule 1: RNA-binding protein FUS

Chain D: 17% 75%

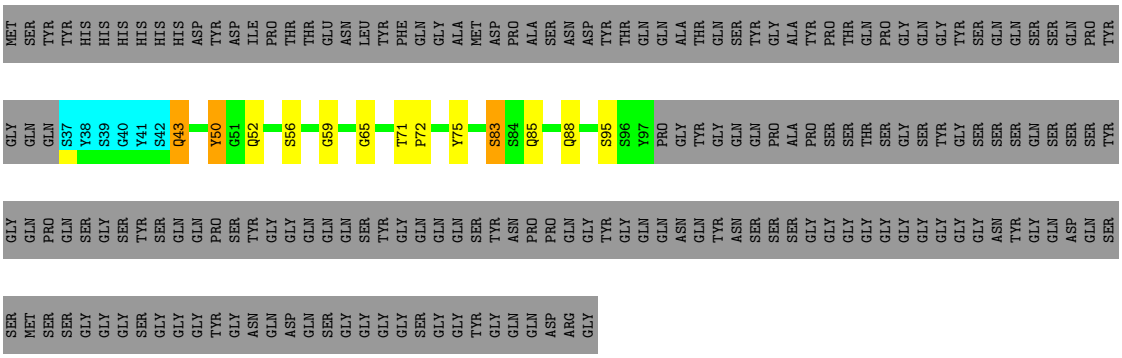
• Molecule 1: RNA-binding protein FUS

Chain E: 17% 75%



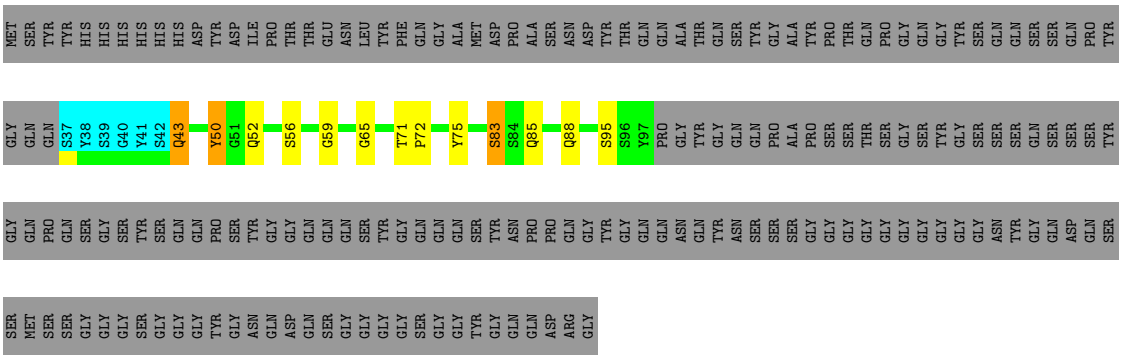
• Molecule 1: RNA-binding protein FUS

Chain F: 17% 75%



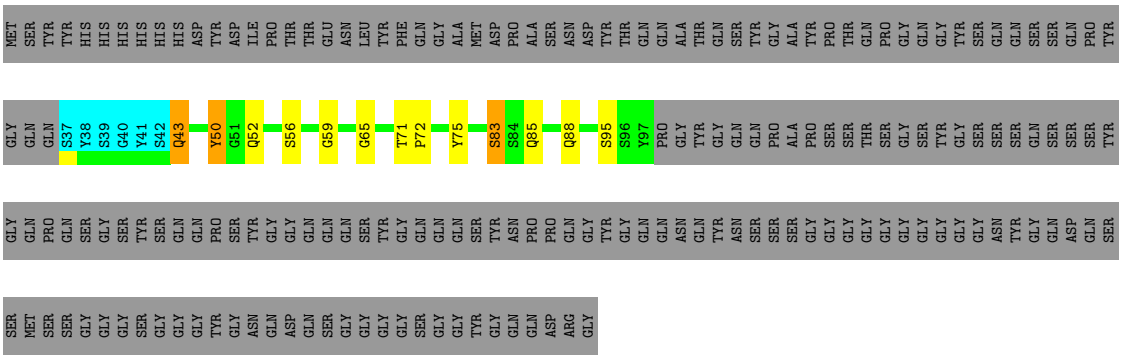
• Molecule 1: RNA-binding protein FUS

Chain G: 17% 75%



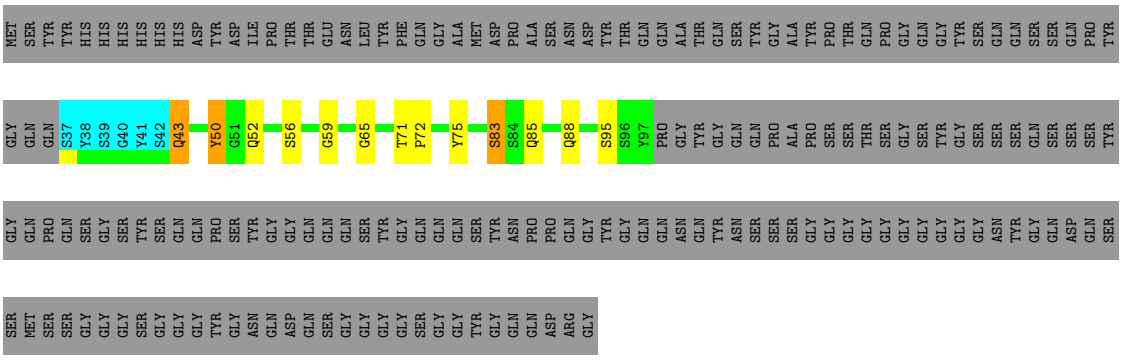
• Molecule 1: RNA-binding protein FUS

Chain H: 17% • •• 75%



• Molecule 1: RNA-binding protein FUS

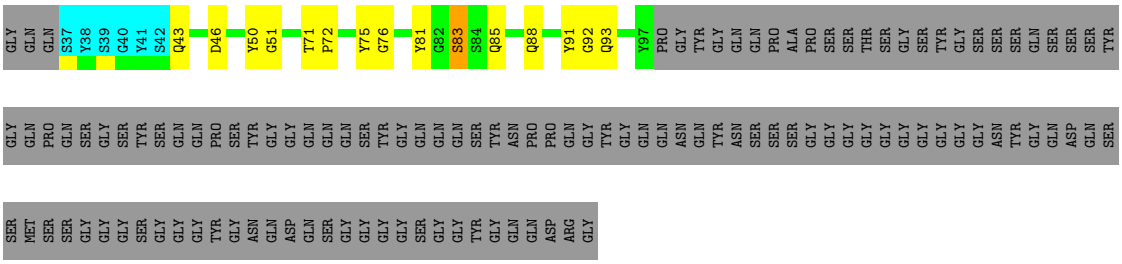
Chain I: 17% • •• 75%



4.2.16 Score per residue for model 16

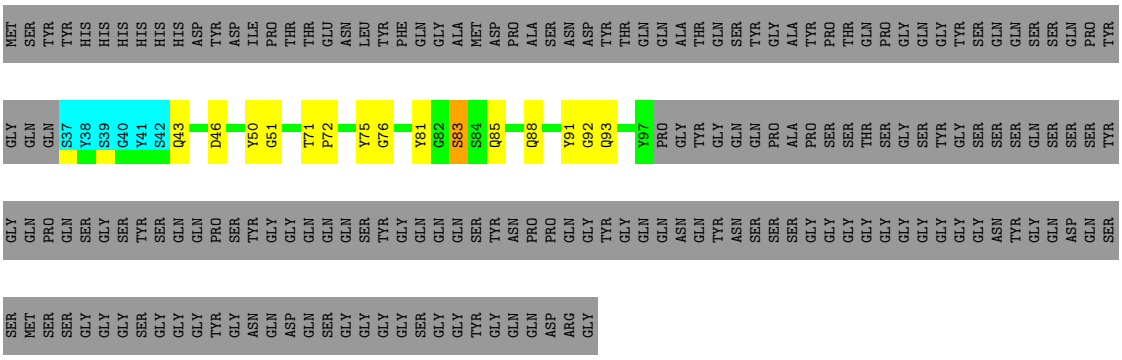
• Molecule 1: RNA-binding protein FUS

Chain A: 17% 6% • 75%



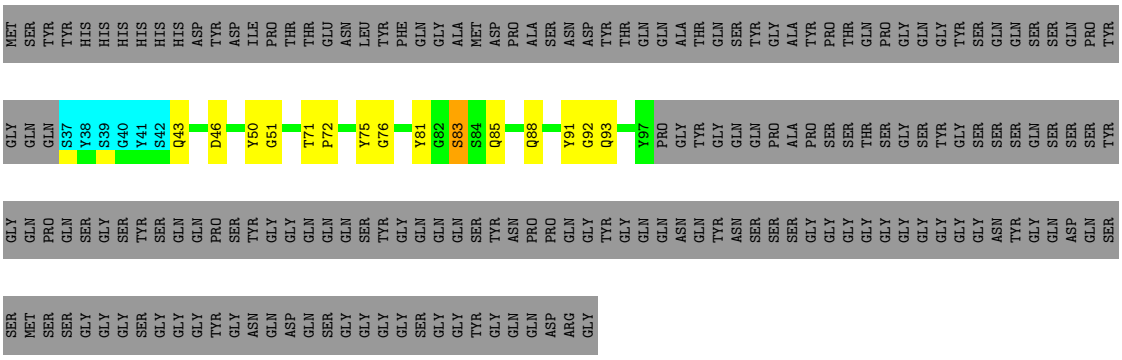
• Molecule 1: RNA-binding protein FUS

Chain B: 17% 6% • 75%



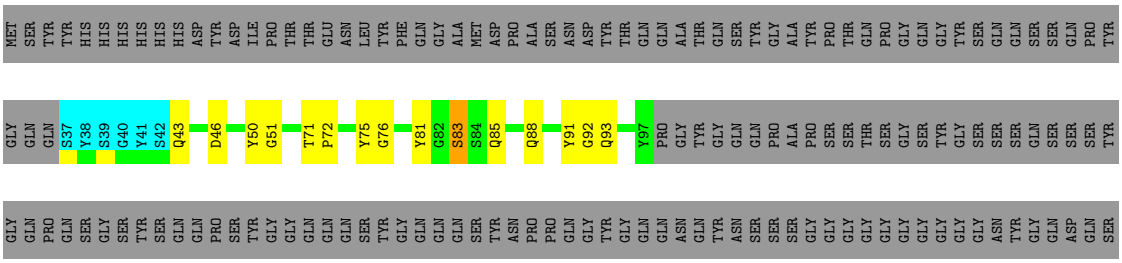
• Molecule 1: RNA-binding protein FUS

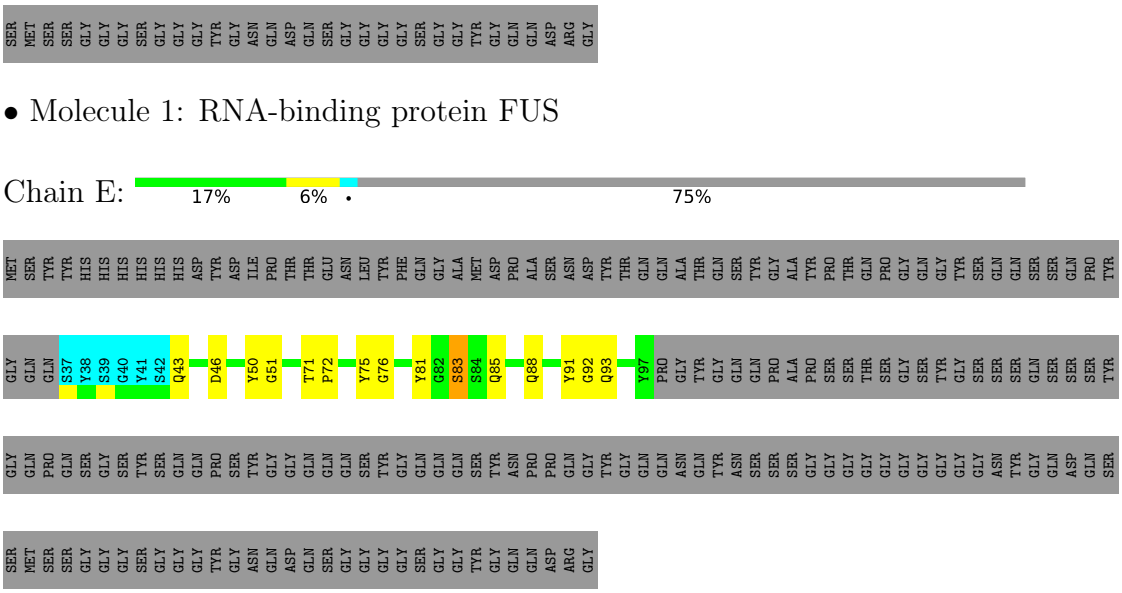
Chain C: 17% 6% • 75%



• Molecule 1: RNA-binding protein FUS

Chain D: 17% 6% • 75%



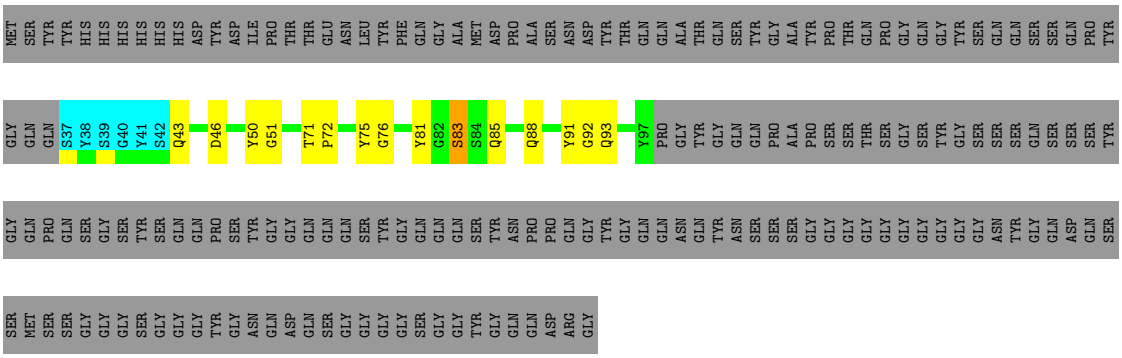


• Molecule 1: RNA-binding protein FUS

Chain E: 17% 6% • 75%

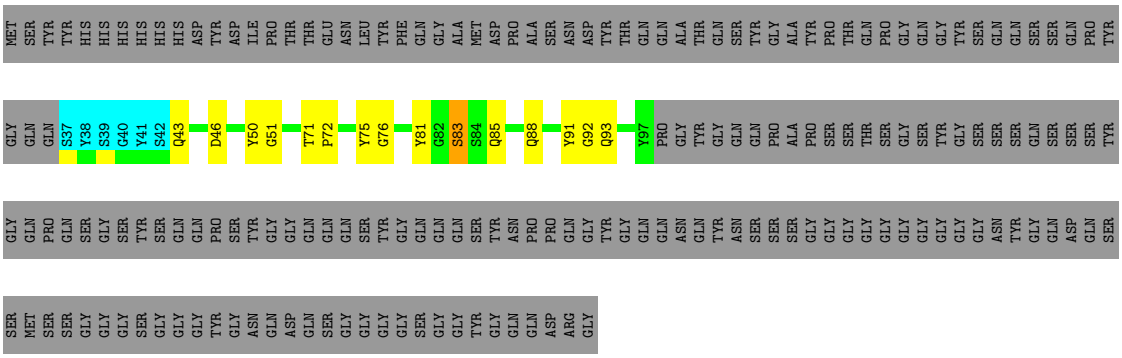
• Molecule 1: RNA-binding protein FUS

Chain F: 17% 6% • 75%



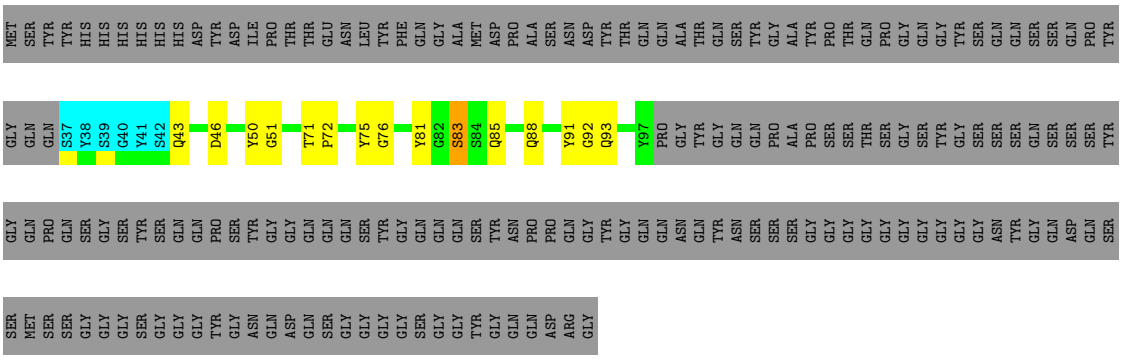
• Molecule 1: RNA-binding protein FUS

Chain G: 17% 6% • 75%



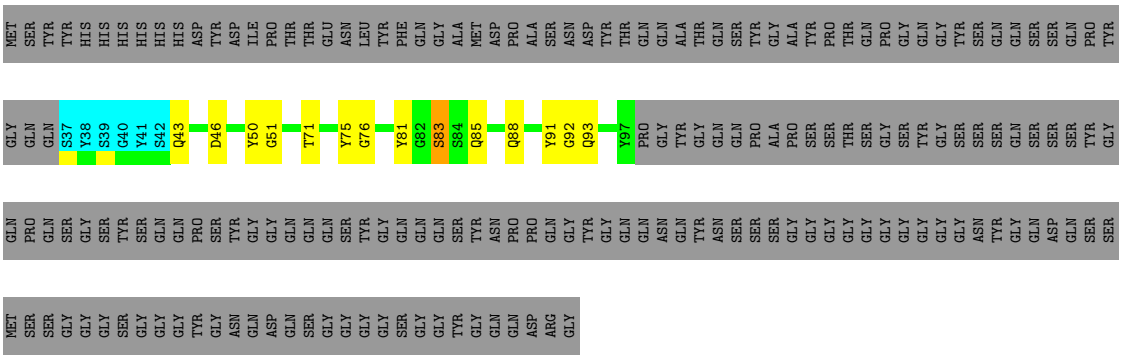
• Molecule 1: RNA-binding protein FUS

Chain H: 17% 6% • 75%



• Molecule 1: RNA-binding protein FUS

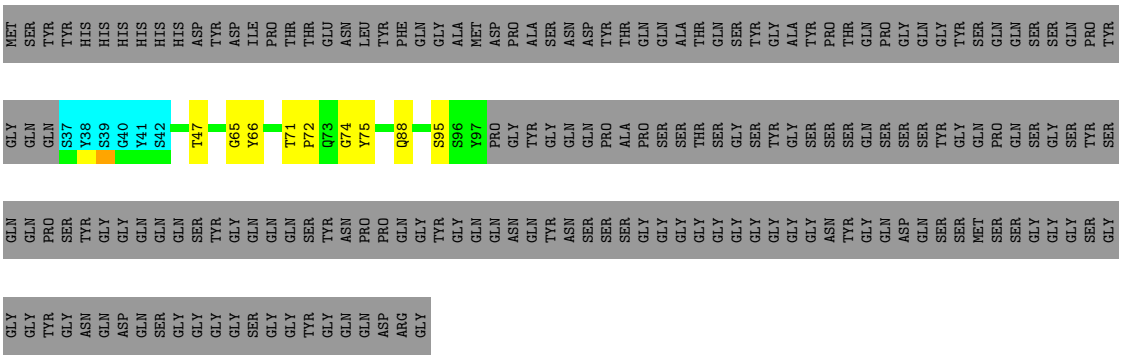
Chain I: 17% 5% • 75%



4.2.17 Score per residue for model 17

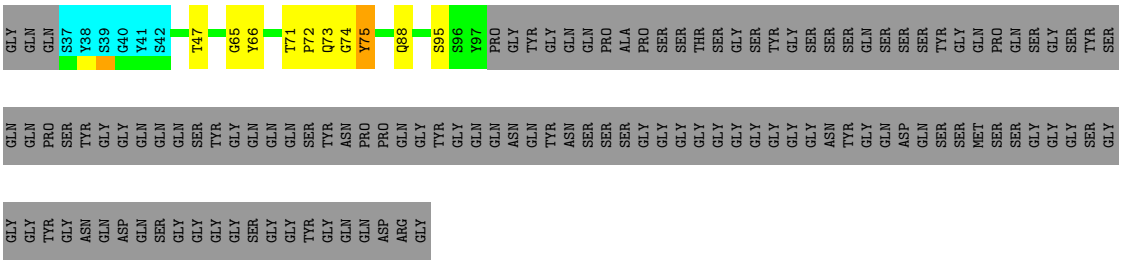
• Molecule 1: RNA-binding protein FUS

Chain A: 19% • • 75%



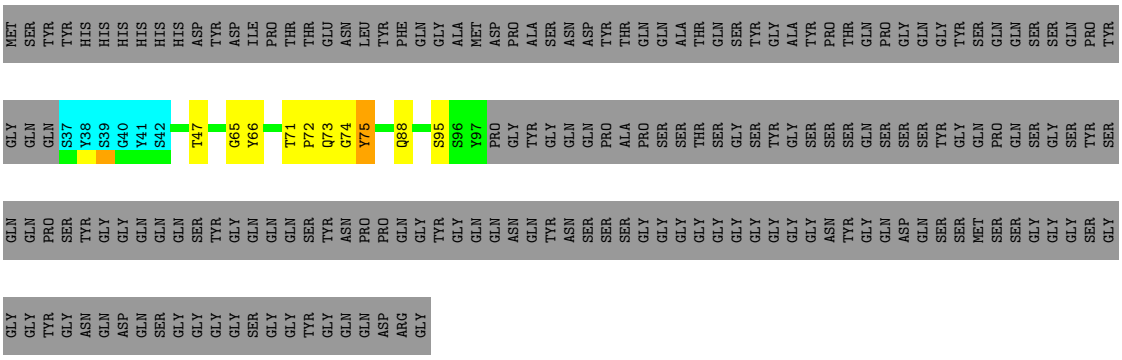
• Molecule 1: RNA-binding protein FUS

Chain B: 19% • • 75%



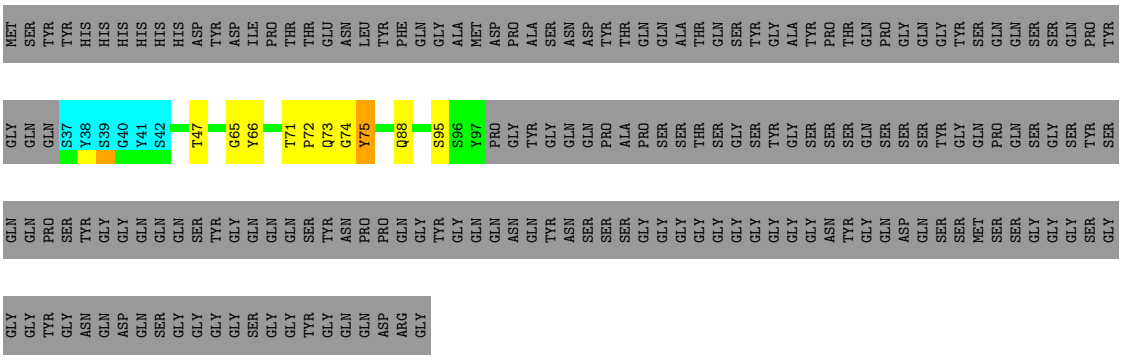
• Molecule 1: RNA-binding protein FUS

Chain C:



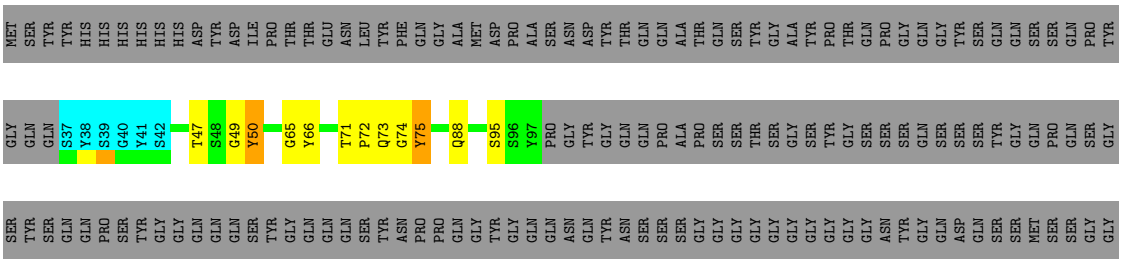
• Molecule 1: RNA-binding protein FUS

Chain D:



• Molecule 1: RNA-binding protein FUS

Chain E:



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

• Molecule 1: RNA-binding protein FUS

Chain F: 19% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 G65 Y66 T71 P72 Q73 G74 Y75 Q88 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER

GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLY SER GLY

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

• Molecule 1: RNA-binding protein FUS

Chain G: 19% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 G65 Y66 T71 P72 Q73 G74 Y75 Q88 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER

GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLY SER GLY

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

• Molecule 1: RNA-binding protein FUS

Chain H: 19% • • 75%

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

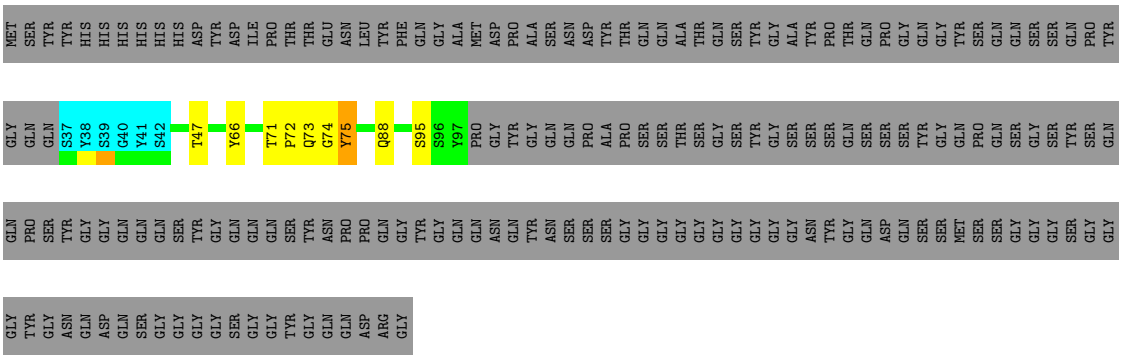
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 T47 G65 Y66 T71 P72 Q73 G74 Y75 Q88 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER

GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLY SER GLY

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

• Molecule 1: RNA-binding protein FUS

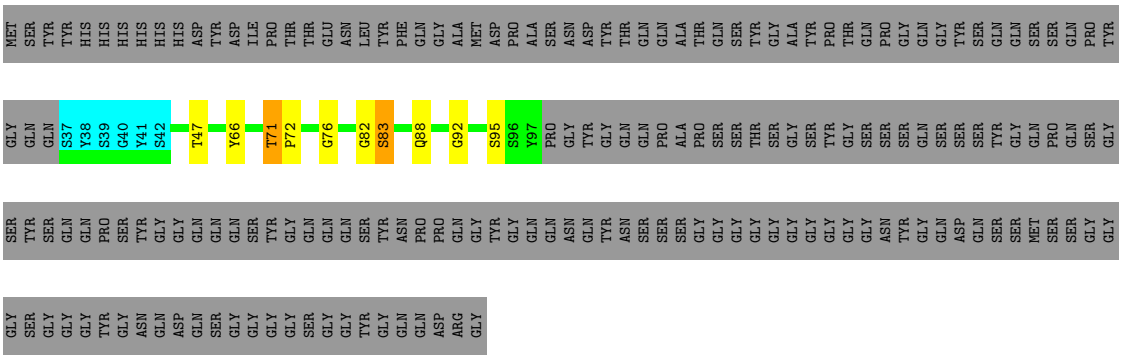
Chain I: 19% • • 75%



4.2.18 Score per residue for model 18

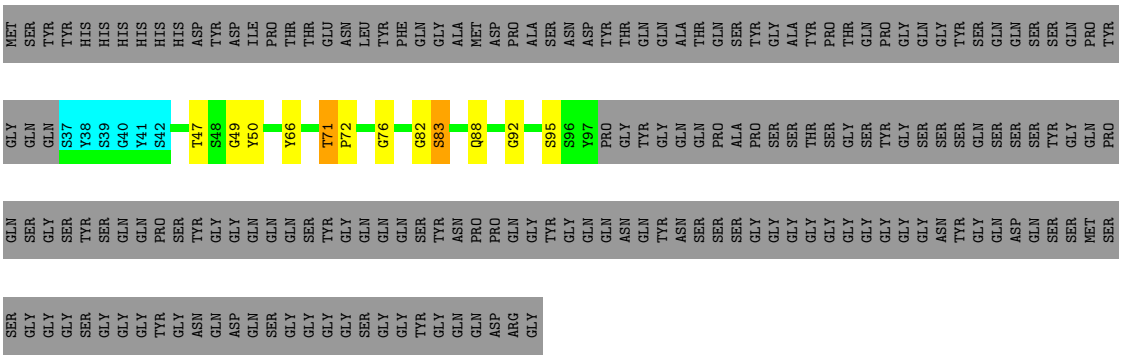
• Molecule 1: RNA-binding protein FUS

Chain A: 19% • • • 75%



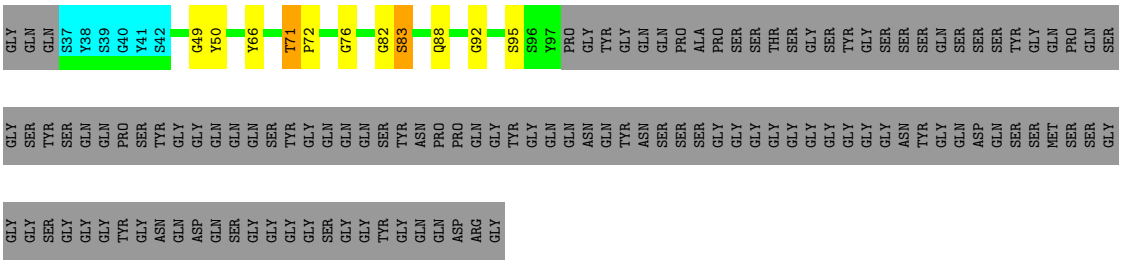
• Molecule 1: RNA-binding protein FUS

Chain B: 18% • • • 75%



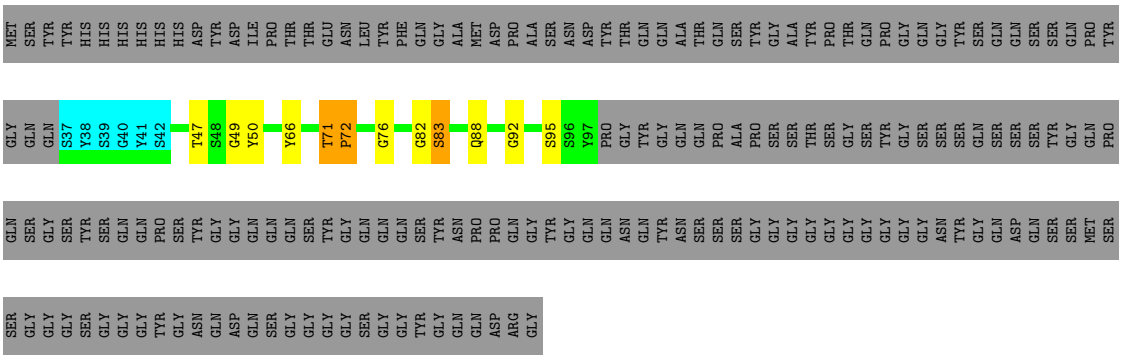
• Molecule 1: RNA-binding protein FUS

Chain C: 18% • • • 75%



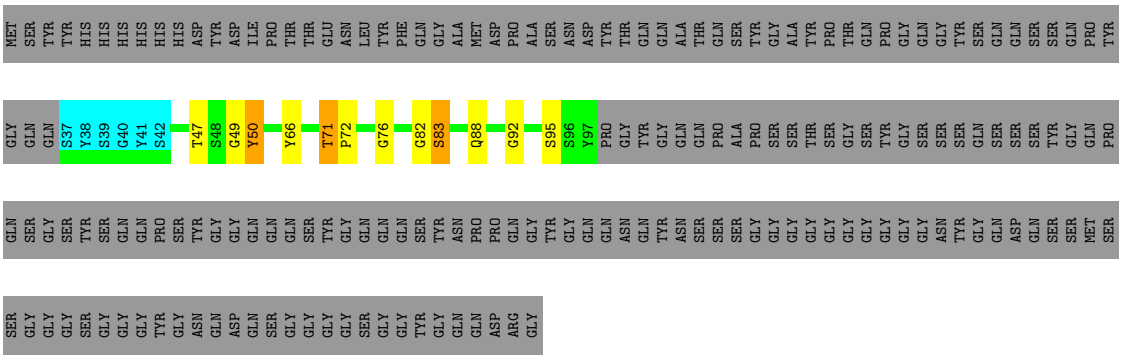
• Molecule 1: RNA-binding protein FUS

Chain D:



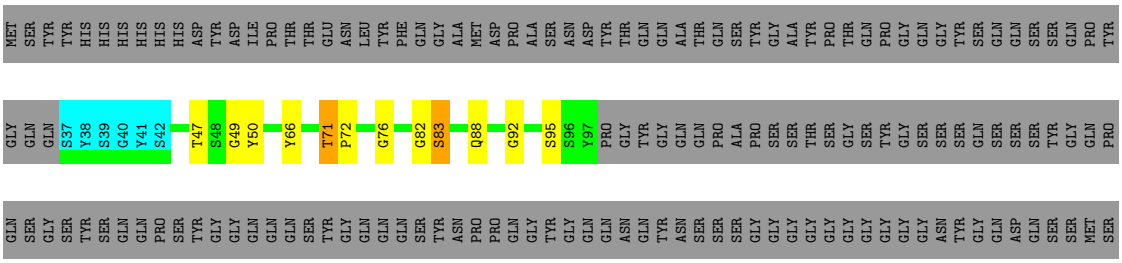
• Molecule 1: RNA-binding protein FUS

Chain E:



• Molecule 1: RNA-binding protein FUS

Chain F:



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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain G: 18% ... 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 G76 G82 S83 Q88 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER

GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain H: 18% ... 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 G76 G82 S83 Q88 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER

GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain I: 18% ... 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 G76 G82 S83 Q88 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER

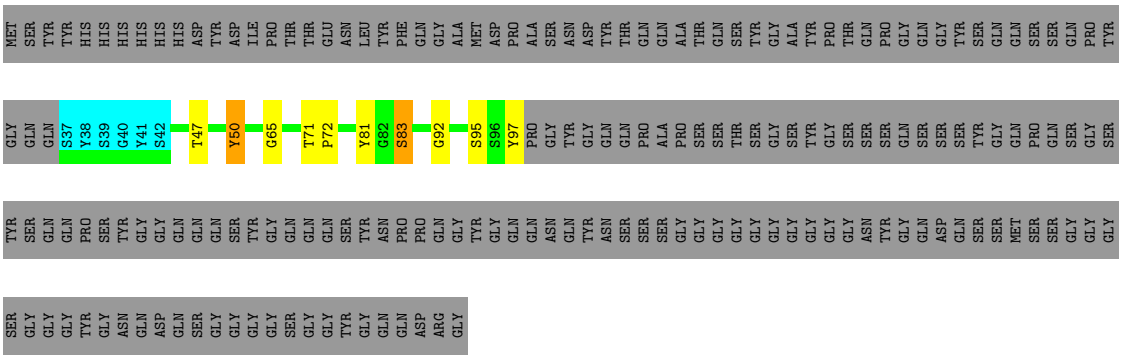
GLY SER TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN PRO PRO GLN GLY TYR GLY GLN GLN ASN GLN TYR ASN SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY ASN TYR GLY GLN ASP GLN SER SER MET SER SER GLY

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

4.2.19 Score per residue for model 19

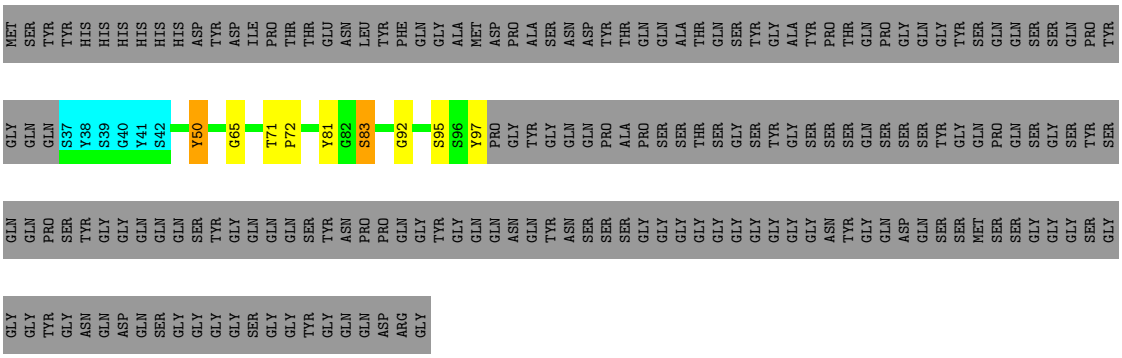
• Molecule 1: RNA-binding protein FUS

Chain A: 19% ... 75%



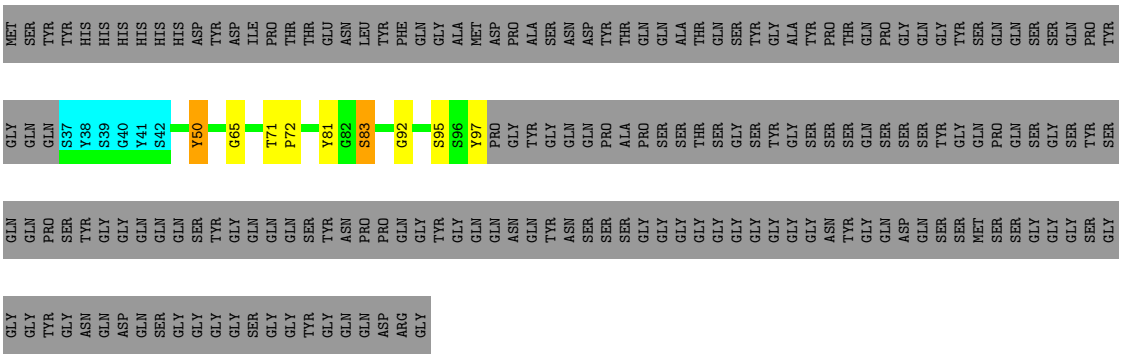
• Molecule 1: RNA-binding protein FUS

Chain B: 19% ... 75%



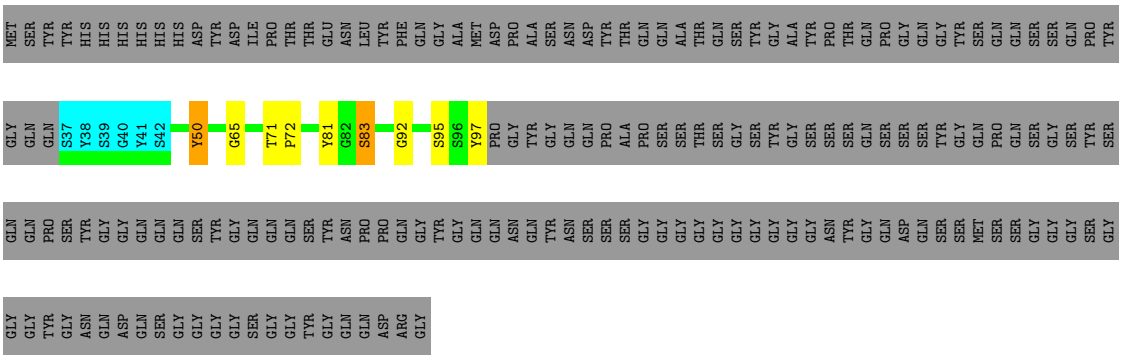
• Molecule 1: RNA-binding protein FUS

Chain C: 19% ... 75%



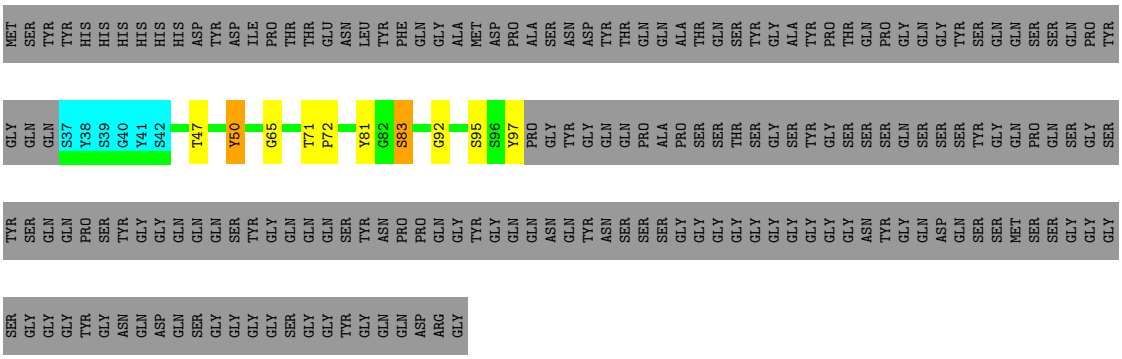
• Molecule 1: RNA-binding protein FUS

Chain D: 19% ... 75%



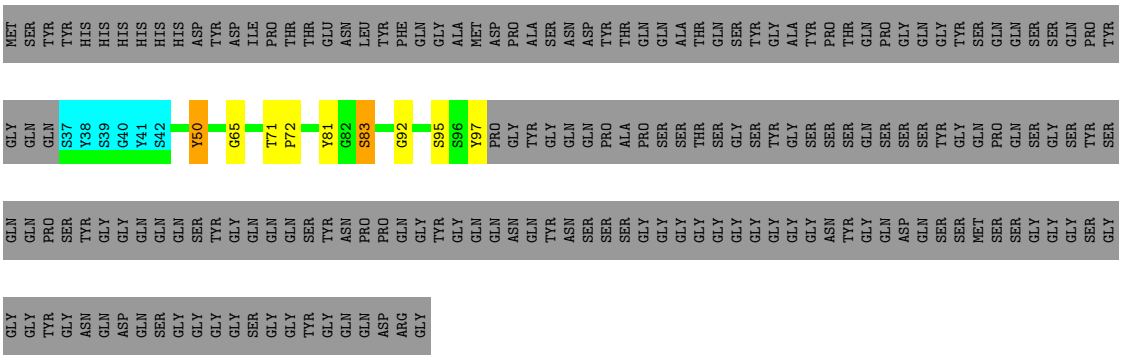
• Molecule 1: RNA-binding protein FUS

Chain E: 19% • • • 75%



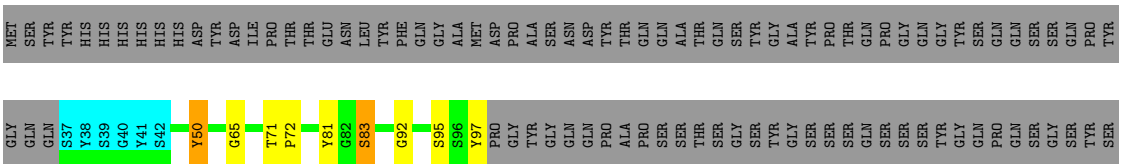
• Molecule 1: RNA-binding protein FUS

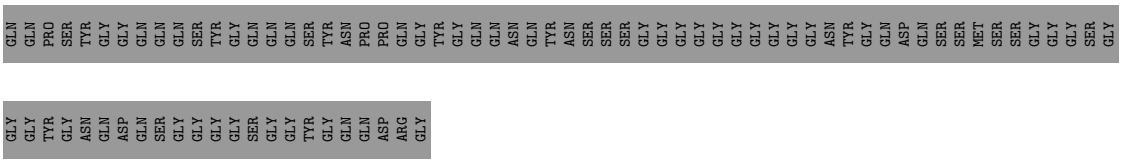
Chain F: 19% • • • 75%



• Molecule 1: RNA-binding protein FUS

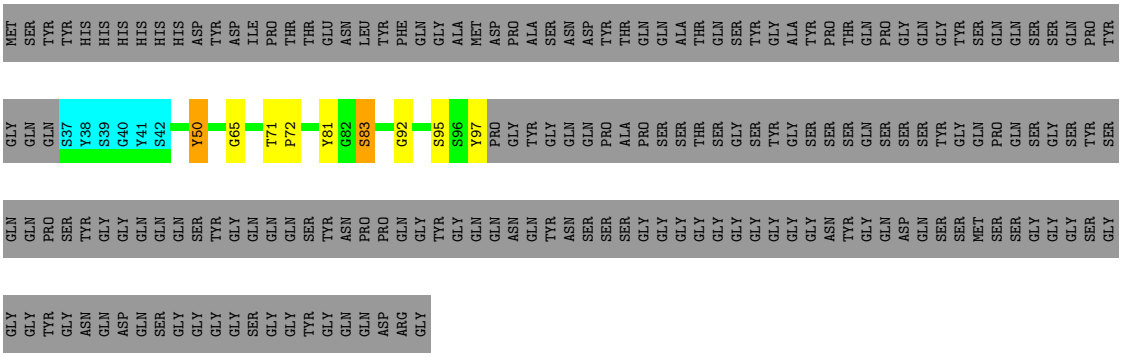
Chain G: 19% • • • 75%





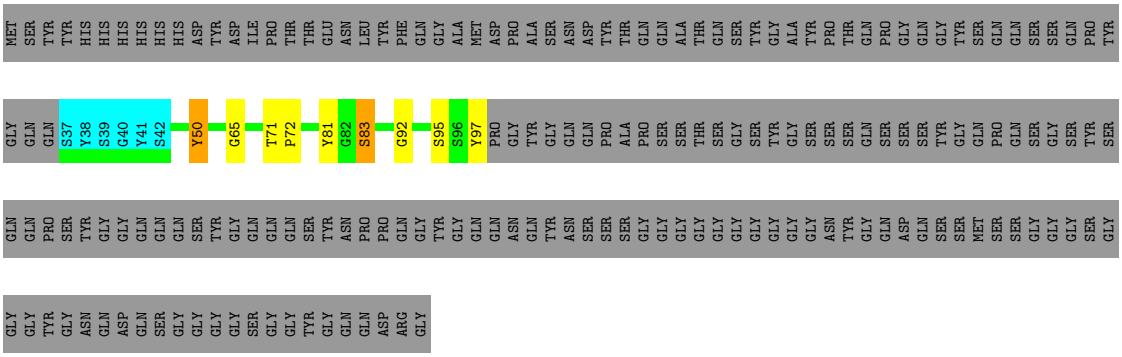
• Molecule 1: RNA-binding protein FUS

Chain H:



• Molecule 1: RNA-binding protein FUS

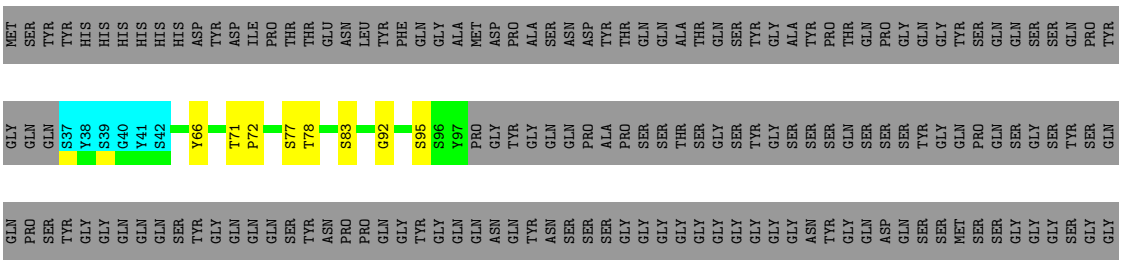
Chain I:



4.2.20 Score per residue for model 20

• Molecule 1: RNA-binding protein FUS

Chain A:



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

• Molecule 1: RNA-binding protein FUS

Chain B: 20% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y66 T71 P72 S77 T78 S83 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER GLN

GLN PRO SER TYR GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain C: 20% • • 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 Y66 T71 P72 S77 T78 S83 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER TYR SER GLN

GLN PRO SER TYR GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

• Molecule 1: RNA-binding protein FUS

Chain D: 19% • • 75%

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

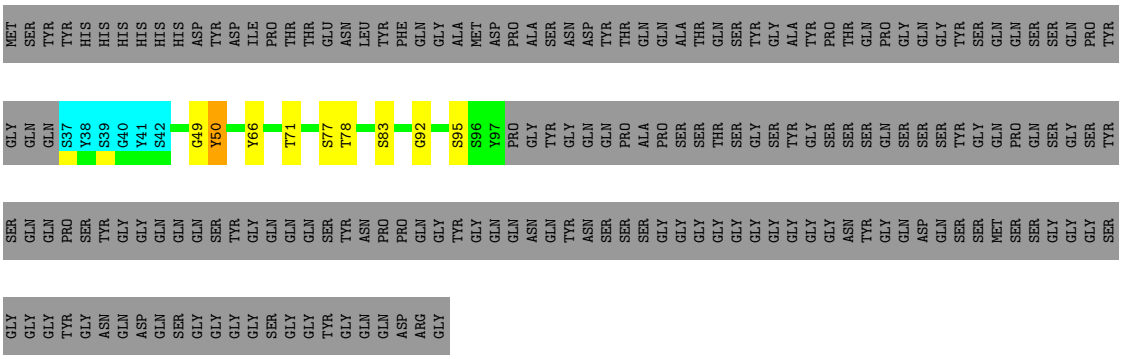
GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 S77 T78 S83 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

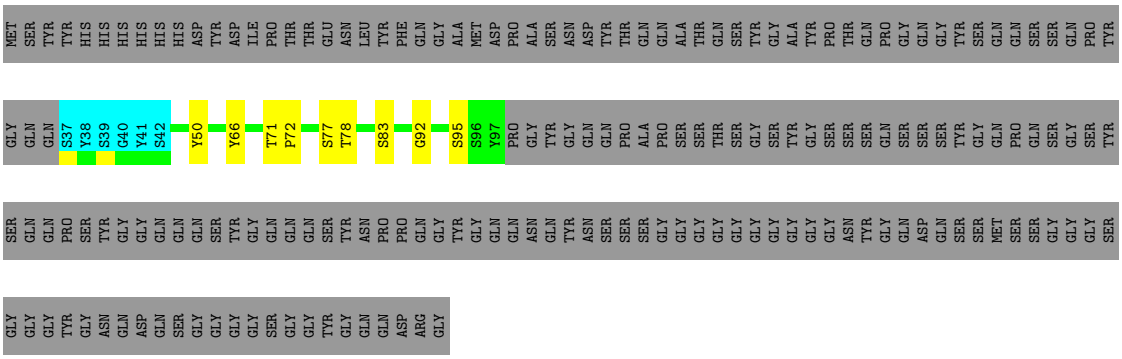
• Molecule 1: RNA-binding protein FUS

Chain E: 19% • • 75%



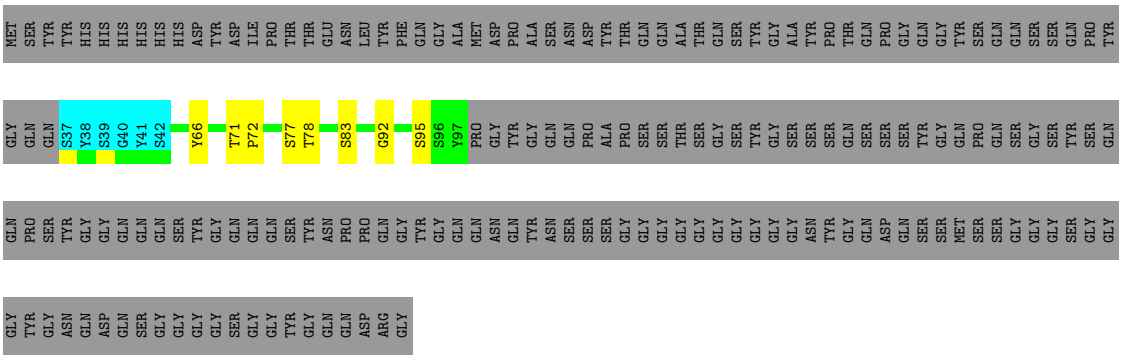
• Molecule 1: RNA-binding protein FUS

Chain F: 19% • • 75%



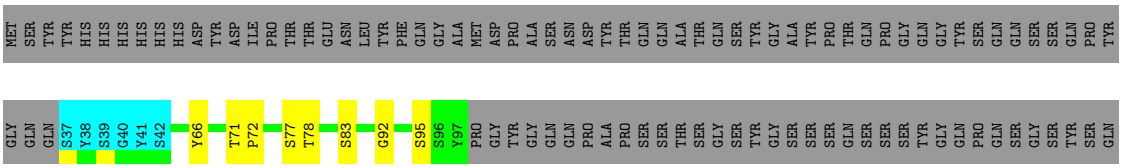
• Molecule 1: RNA-binding protein FUS

Chain G: 20% • • 75%



• Molecule 1: RNA-binding protein FUS

Chain H: 20% • • 75%



GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

- Molecule 1: RNA-binding protein FUS

Chain I: 19% 75%

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

GLY GLN GLN S37 Y38 S39 G40 Y41 S42 G49 Y50 Y66 T71 P72 S77 T78 S83 G92 S95 S96 Y97 PRO GLY TYR GLY GLN GLN PRO ALA PRO SER SER THR SER GLY SER TYR GLY SER SER SER GLN SER SER SER TYR GLY GLN PRO GLN SER GLY SER

TYR SER GLN GLN PRO SER TYR GLY GLY GLN GLN GLN SER TYR GLY GLN GLN GLN SER TYR ASN 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 GLN ASP ARG GLY

5 Refinement protocol and experimental data overview (i)

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

Of the 4928 calculated structures, 20 were deposited, based on the following criterion: *structures with no violations, lowest energy, and derived from one of 44 independent calculations*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.45

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	218
Number of shifts mapped to atoms	218
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

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 (i)

6.1 Standard geometry (i)

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 (i)

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	B	397	329	329	1±2
1	C	397	329	329	2±2
1	D	397	329	329	2±2
1	E	397	329	329	2±2
1	F	397	329	329	2±2
1	G	397	329	329	2±2
1	H	397	329	329	1±2
1	I	397	329	329	1±1
1	A	397	329	329	1±1
All	All	71460	59220	59220	194

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:71:THR:HG22	1:D:72:PRO:CD	0.46	2.39	10	3
1:G:71:THR:HG22	1:G:72:PRO:CD	0.46	2.40	10	3
1:H:71:THR:HG22	1:H:72:PRO:CD	0.46	2.40	10	3
1:F:71:THR:HG22	1:F:72:PRO:CD	0.46	2.40	10	3
1:C:71:THR:HG22	1:C:72:PRO:CD	0.46	2.39	10	3
1:B:71:THR:HG22	1:B:72:PRO:CD	0.46	2.40	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:71:THR:HG22	1:E:72:PRO:CD	0.46	2.40	10	3
1:I:71:THR:HG22	1:I:72:PRO:CD	0.46	2.40	10	3
1:A:71:THR:HG22	1:A:72:PRO:CD	0.46	2.40	10	3
1:E:49:GLY:O	1:E:50:TYR:C	0.45	2.55	11	11
1:B:71:THR:HG22	1:B:72:PRO:HD2	0.45	1.89	10	2
1:C:71:THR:HG22	1:C:72:PRO:HD2	0.45	1.89	10	2
1:D:71:THR:HG22	1:D:72:PRO:HD2	0.45	1.89	10	2
1:C:71:THR:C	1:D:71:THR:OG1	0.45	2.55	9	4
1:D:71:THR:C	1:E:71:THR:OG1	0.45	2.55	9	4
1:E:71:THR:C	1:F:71:THR:OG1	0.45	2.55	9	4
1:F:71:THR:HG22	1:F:72:PRO:HD2	0.45	1.89	10	2
1:G:71:THR:HG22	1:G:72:PRO:HD2	0.45	1.89	10	2
1:H:71:THR:HG22	1:H:72:PRO:HD2	0.45	1.89	10	2
1:B:71:THR:C	1:C:71:THR:OG1	0.45	2.55	9	4
1:I:71:THR:HG22	1:I:72:PRO:HD2	0.45	1.89	10	2
1:A:71:THR:HG22	1:A:72:PRO:HD2	0.45	1.89	10	2
1:F:71:THR:C	1:G:71:THR:OG1	0.44	2.55	9	4
1:E:71:THR:HG22	1:E:72:PRO:HD2	0.44	1.89	10	2
1:G:71:THR:C	1:H:71:THR:OG1	0.44	2.55	9	4
1:E:82:GLY:O	1:E:83:SER:C	0.44	2.56	18	1
1:D:90:SER:HG	1:D:91:TYR:HD1	0.43	1.55	9	1
1:F:90:SER:HG	1:F:91:TYR:HD1	0.43	1.56	9	1
1:G:90:SER:HG	1:G:91:TYR:HD1	0.43	1.56	9	1
1:C:90:SER:HG	1:C:91:TYR:HD1	0.43	1.55	9	1
1:I:90:SER:HG	1:I:91:TYR:HD1	0.43	1.56	9	1
1:A:71:THR:C	1:B:71:THR:OG1	0.43	2.57	9	3
1:B:90:SER:HG	1:B:91:TYR:HD1	0.43	1.55	9	1
1:E:90:SER:HG	1:E:91:TYR:HD1	0.43	1.56	9	1
1:H:71:THR:C	1:I:71:THR:OG1	0.43	2.57	9	4
1:G:82:GLY:O	1:G:83:SER:C	0.43	2.57	18	1
1:H:90:SER:HG	1:H:91:TYR:HD1	0.43	1.57	9	1
1:H:82:GLY:O	1:H:83:SER:C	0.43	2.57	18	1
1:D:49:GLY:O	1:D:50:TYR:C	0.43	2.57	11	7
1:F:82:GLY:O	1:F:83:SER:C	0.43	2.57	18	1
1:C:49:GLY:O	1:C:50:TYR:C	0.42	2.57	11	6
1:B:49:GLY:O	1:B:50:TYR:C	0.42	2.58	11	6
1:A:90:SER:HG	1:A:91:TYR:HD1	0.42	1.55	9	1
1:D:72:PRO:N	1:E:71:THR:OG1	0.42	2.53	16	3
1:A:82:GLY:O	1:A:83:SER:C	0.42	2.57	18	1
1:D:82:GLY:O	1:D:83:SER:C	0.42	2.57	18	1
1:F:49:GLY:O	1:F:50:TYR:C	0.42	2.57	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:49:GLY:O	1:I:50:TYR:C	0.42	2.57	11	9
1:C:82:GLY:O	1:C:83:SER:C	0.42	2.57	18	1
1:F:72:PRO:N	1:G:71:THR:OG1	0.42	2.53	16	3
1:B:82:GLY:O	1:B:83:SER:C	0.42	2.57	18	1
1:I:82:GLY:O	1:I:83:SER:C	0.42	2.57	18	1
1:C:72:PRO:N	1:D:71:THR:OG1	0.42	2.53	16	3
1:E:72:PRO:N	1:F:71:THR:OG1	0.42	2.53	16	3
1:B:72:PRO:N	1:C:71:THR:OG1	0.42	2.53	16	3
1:G:72:PRO:N	1:H:71:THR:OG1	0.42	2.53	16	3
1:D:78:THR:HG21	1:E:75:TYR:CE2	0.42	2.49	7	1
1:G:49:GLY:O	1:G:50:TYR:C	0.42	2.57	11	7
1:B:78:THR:HG21	1:C:75:TYR:CE2	0.42	2.49	7	1
1:A:78:THR:HG21	1:B:75:TYR:CE2	0.42	2.49	7	1
1:G:78:THR:HG21	1:H:75:TYR:CE2	0.42	2.49	7	1
1:E:78:THR:HG21	1:F:75:TYR:CE2	0.41	2.49	7	1
1:F:78:THR:HG21	1:G:75:TYR:CE2	0.41	2.49	7	1
1:H:78:THR:HG21	1:I:75:TYR:CE2	0.41	2.49	7	1
1:A:72:PRO:N	1:B:71:THR:OG1	0.41	2.53	16	3
1:H:49:GLY:O	1:H:50:TYR:C	0.41	2.57	11	7
1:C:78:THR:HG21	1:D:75:TYR:CE2	0.41	2.49	7	1
1:E:73:GLN:O	1:E:75:TYR:N	0.41	2.53	17	1
1:H:73:GLN:O	1:H:75:TYR:N	0.41	2.54	17	1
1:H:72:PRO:N	1:I:71:THR:OG1	0.41	2.54	16	1
1:D:73:GLN:O	1:D:75:TYR:N	0.41	2.54	17	1
1:G:73:GLN:O	1:G:75:TYR:N	0.41	2.54	17	1
1:B:73:GLN:O	1:B:75:TYR:N	0.41	2.54	17	1
1:C:73:GLN:O	1:C:75:TYR:N	0.41	2.54	17	1
1:F:73:GLN:O	1:F:75:TYR:N	0.41	2.54	17	1
1:I:73:GLN:O	1:I:75:TYR:N	0.41	2.54	17	1
1:D:50:TYR:C	1:E:49:GLY:O	0.40	2.60	2	1

6.3 Torsion angles (i)

6.3.1 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 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	54/241 (22%)	35±2 (66±4%)	13±3 (25±5%)	5±2 (9±5%)	1 11
1	B	54/241 (22%)	35±2 (66±5%)	13±3 (25±5%)	5±2 (10±4%)	1 10
1	C	54/241 (22%)	35±2 (66±5%)	13±2 (25±5%)	5±2 (10±4%)	1 10
1	D	54/241 (22%)	35±2 (66±5%)	13±3 (25±5%)	5±2 (10±4%)	1 10
1	E	54/241 (22%)	36±2 (66±4%)	13±2 (24±5%)	6±2 (10±4%)	1 9
1	F	54/241 (22%)	35±2 (65±5%)	13±2 (25±5%)	5±2 (10±4%)	1 10
1	G	54/241 (22%)	35±2 (66±5%)	13±2 (25±5%)	5±2 (10±4%)	1 10
1	H	54/241 (22%)	35±2 (66±5%)	13±2 (25±5%)	5±2 (10±4%)	1 10
1	I	54/241 (22%)	36±2 (66±4%)	13±2 (24±4%)	5±2 (10±4%)	1 10
All	All	9720/43380 (22%)	6378 (66%)	2395 (25%)	947 (10%)	1 10

All 224 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	E	50	TYR	20
1	I	50	TYR	15
1	A	83	SER	14
1	B	83	SER	14
1	C	83	SER	14
1	D	72	PRO	14
1	D	83	SER	14
1	E	83	SER	14
1	F	83	SER	14
1	G	72	PRO	14
1	G	83	SER	14
1	H	83	SER	14
1	I	83	SER	14
1	B	72	PRO	13
1	C	72	PRO	13
1	F	50	TYR	13
1	F	72	PRO	13
1	H	72	PRO	13
1	I	72	PRO	13
1	A	72	PRO	12
1	B	50	TYR	12
1	C	50	TYR	12
1	D	50	TYR	12
1	G	50	TYR	12
1	H	50	TYR	12

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Mol	Chain	Res	Type	Models (Total)
1	E	72	PRO	11
1	I	92	GLY	11
1	A	76	GLY	11
1	B	76	GLY	11
1	C	76	GLY	11
1	D	76	GLY	11
1	E	76	GLY	11
1	F	76	GLY	11
1	G	76	GLY	11
1	H	76	GLY	11
1	I	76	GLY	11
1	A	50	TYR	10
1	A	77	SER	10
1	E	77	SER	10
1	A	92	GLY	9
1	B	77	SER	9
1	B	92	GLY	9
1	C	77	SER	9
1	C	92	GLY	9
1	D	77	SER	9
1	D	92	GLY	9
1	E	92	GLY	9
1	F	77	SER	9
1	F	92	GLY	9
1	G	77	SER	9
1	G	92	GLY	9
1	H	77	SER	9
1	H	92	GLY	9
1	I	77	SER	9
1	B	52	GLN	5
1	C	52	GLN	5
1	D	52	GLN	5
1	E	52	GLN	5
1	G	52	GLN	5
1	A	52	GLN	4
1	A	65	GLY	4
1	B	65	GLY	4
1	D	65	GLY	4
1	F	52	GLN	4
1	H	52	GLN	4
1	H	65	GLY	4
1	I	52	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	85	GLN	3
1	B	85	GLN	3
1	C	85	GLN	3
1	D	85	GLN	3
1	E	85	GLN	3
1	F	85	GLN	3
1	G	85	GLN	3
1	H	85	GLN	3
1	I	85	GLN	3
1	A	81	TYR	3
1	B	81	TYR	3
1	C	81	TYR	3
1	D	81	TYR	3
1	E	81	TYR	3
1	F	81	TYR	3
1	G	81	TYR	3
1	H	81	TYR	3
1	I	81	TYR	3
1	C	65	GLY	3
1	E	65	GLY	3
1	F	65	GLY	3
1	G	65	GLY	3
1	A	58	TYR	2
1	A	60	GLN	2
1	B	58	TYR	2
1	B	60	GLN	2
1	C	58	TYR	2
1	C	60	GLN	2
1	D	58	TYR	2
1	D	60	GLN	2
1	E	58	TYR	2
1	E	60	GLN	2
1	F	58	TYR	2
1	F	60	GLN	2
1	G	58	TYR	2
1	G	60	GLN	2
1	H	58	TYR	2
1	H	60	GLN	2
1	I	58	TYR	2
1	I	60	GLN	2
1	A	51	GLY	2
1	B	51	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	C	51	GLY	2
1	D	51	GLY	2
1	E	51	GLY	2
1	F	51	GLY	2
1	G	51	GLY	2
1	H	51	GLY	2
1	I	51	GLY	2
1	A	93	GLN	2
1	B	93	GLN	2
1	C	93	GLN	2
1	D	93	GLN	2
1	E	93	GLN	2
1	F	93	GLN	2
1	G	93	GLN	2
1	H	93	GLN	2
1	I	93	GLN	2
1	A	43	GLN	2
1	A	74	GLY	2
1	A	75	TYR	2
1	B	43	GLN	2
1	B	74	GLY	2
1	B	75	TYR	2
1	C	43	GLN	2
1	C	74	GLY	2
1	C	75	TYR	2
1	D	43	GLN	2
1	D	74	GLY	2
1	D	75	TYR	2
1	E	43	GLN	2
1	E	74	GLY	2
1	E	75	TYR	2
1	F	43	GLN	2
1	F	74	GLY	2
1	F	75	TYR	2
1	G	43	GLN	2
1	G	74	GLY	2
1	G	75	TYR	2
1	H	43	GLN	2
1	H	74	GLY	2
1	H	75	TYR	2
1	I	43	GLN	2
1	I	74	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	I	75	TYR	2
1	I	65	GLY	2
1	A	61	SER	1
1	B	61	SER	1
1	C	61	SER	1
1	D	61	SER	1
1	E	61	SER	1
1	F	61	SER	1
1	G	61	SER	1
1	H	61	SER	1
1	I	61	SER	1
1	A	56	SER	1
1	B	56	SER	1
1	C	56	SER	1
1	D	56	SER	1
1	E	56	SER	1
1	F	56	SER	1
1	G	56	SER	1
1	H	56	SER	1
1	I	56	SER	1
1	A	57	SER	1
1	A	79	GLY	1
1	B	57	SER	1
1	B	79	GLY	1
1	C	57	SER	1
1	C	79	GLY	1
1	D	57	SER	1
1	D	79	GLY	1
1	E	57	SER	1
1	E	79	GLY	1
1	F	57	SER	1
1	F	79	GLY	1
1	G	57	SER	1
1	G	79	GLY	1
1	H	57	SER	1
1	H	79	GLY	1
1	I	57	SER	1
1	I	79	GLY	1
1	A	62	GLN	1
1	B	62	GLN	1
1	C	62	GLN	1
1	D	62	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	E	62	GLN	1
1	F	62	GLN	1
1	G	62	GLN	1
1	H	62	GLN	1
1	I	62	GLN	1
1	A	80	GLY	1
1	B	80	GLY	1
1	C	80	GLY	1
1	D	80	GLY	1
1	F	80	GLY	1
1	G	80	GLY	1
1	H	80	GLY	1
1	I	80	GLY	1
1	A	59	GLY	1
1	B	59	GLY	1
1	C	59	GLY	1
1	D	59	GLY	1
1	E	59	GLY	1
1	F	59	GLY	1
1	G	59	GLY	1
1	H	59	GLY	1
1	I	59	GLY	1
1	A	91	TYR	1
1	B	91	TYR	1
1	C	91	TYR	1
1	D	91	TYR	1
1	E	91	TYR	1
1	F	91	TYR	1
1	G	91	TYR	1
1	H	91	TYR	1
1	I	91	TYR	1

6.3.2 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 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	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	6 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	6	45
1	C	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	6	46
1	D	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	6	45
1	E	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	6	45
1	F	44/182 (24%)	38±2 (86±4%)	6±2 (14±4%)	6	45
1	G	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	6	46
1	H	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	6	45
1	I	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	6	46
All	All	7920/32760 (24%)	6774 (86%)	1146 (14%)	6	45

All 243 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	71	THR	14
1	B	71	THR	14
1	C	71	THR	14
1	D	71	THR	14
1	E	71	THR	14
1	F	71	THR	14
1	G	71	THR	14
1	H	71	THR	14
1	I	71	THR	14
1	A	66	TYR	13
1	A	88	GLN	13
1	B	66	TYR	13
1	B	88	GLN	13
1	C	66	TYR	13
1	C	88	GLN	13
1	D	66	TYR	13
1	D	88	GLN	13
1	E	66	TYR	13
1	E	88	GLN	13
1	F	66	TYR	13
1	F	88	GLN	13
1	G	66	TYR	13
1	G	88	GLN	13
1	H	66	TYR	13
1	H	88	GLN	13

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Mol	Chain	Res	Type	Models (Total)
1	I	66	TYR	13
1	I	88	GLN	13
1	A	75	TYR	12
1	B	75	TYR	12
1	C	75	TYR	12
1	D	75	TYR	12
1	E	75	TYR	12
1	F	75	TYR	12
1	G	75	TYR	12
1	H	75	TYR	12
1	I	75	TYR	12
1	A	47	THR	9
1	E	47	THR	9
1	A	95	SER	9
1	B	95	SER	9
1	C	95	SER	9
1	D	95	SER	9
1	E	95	SER	9
1	F	95	SER	9
1	G	95	SER	9
1	H	95	SER	9
1	I	95	SER	9
1	B	47	THR	8
1	D	47	THR	8
1	F	47	THR	7
1	H	47	THR	7
1	A	83	SER	6
1	B	83	SER	6
1	C	47	THR	6
1	C	83	SER	6
1	D	83	SER	6
1	E	83	SER	6
1	F	83	SER	6
1	G	47	THR	6
1	G	83	SER	6
1	H	83	SER	6
1	I	47	THR	6
1	I	83	SER	6
1	A	78	THR	6
1	B	78	THR	6
1	C	78	THR	6
1	D	78	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	E	78	THR	6
1	F	78	THR	6
1	G	78	THR	6
1	H	78	THR	6
1	I	78	THR	6
1	A	91	TYR	5
1	B	91	TYR	5
1	C	91	TYR	5
1	D	91	TYR	5
1	E	91	TYR	5
1	F	91	TYR	5
1	G	91	TYR	5
1	H	91	TYR	5
1	I	91	TYR	5
1	A	50	TYR	5
1	B	50	TYR	5
1	C	50	TYR	5
1	D	50	TYR	5
1	E	50	TYR	5
1	F	50	TYR	5
1	G	50	TYR	5
1	H	50	TYR	5
1	I	50	TYR	5
1	A	77	SER	4
1	B	77	SER	4
1	C	77	SER	4
1	D	77	SER	4
1	E	77	SER	4
1	F	77	SER	4
1	G	77	SER	4
1	H	77	SER	4
1	I	77	SER	4
1	A	43	GLN	4
1	B	43	GLN	4
1	C	43	GLN	4
1	D	43	GLN	4
1	E	43	GLN	4
1	F	43	GLN	4
1	G	43	GLN	4
1	H	43	GLN	4
1	I	43	GLN	4
1	A	86	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	B	86	SER	3
1	C	86	SER	3
1	D	86	SER	3
1	E	86	SER	3
1	F	86	SER	3
1	G	86	SER	3
1	H	86	SER	3
1	I	86	SER	3
1	A	69	GLN	3
1	A	90	SER	3
1	B	69	GLN	3
1	B	90	SER	3
1	C	69	GLN	3
1	C	90	SER	3
1	D	69	GLN	3
1	D	90	SER	3
1	E	69	GLN	3
1	E	90	SER	3
1	F	69	GLN	3
1	F	90	SER	3
1	G	69	GLN	3
1	G	90	SER	3
1	H	69	GLN	3
1	H	90	SER	3
1	I	69	GLN	3
1	I	90	SER	3
1	A	97	TYR	3
1	B	97	TYR	3
1	C	97	TYR	3
1	D	97	TYR	3
1	E	97	TYR	3
1	F	97	TYR	3
1	G	97	TYR	3
1	H	97	TYR	3
1	I	97	TYR	3
1	A	73	GLN	2
1	B	73	GLN	2
1	C	73	GLN	2
1	D	73	GLN	2
1	E	73	GLN	2
1	F	73	GLN	2
1	G	73	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	H	73	GLN	2
1	I	73	GLN	2
1	A	96	SER	2
1	B	96	SER	2
1	C	96	SER	2
1	D	96	SER	2
1	E	96	SER	2
1	F	96	SER	2
1	G	96	SER	2
1	H	96	SER	2
1	I	96	SER	2
1	A	56	SER	2
1	A	84	SER	2
1	B	56	SER	2
1	B	84	SER	2
1	C	56	SER	2
1	C	84	SER	2
1	D	56	SER	2
1	D	84	SER	2
1	E	56	SER	2
1	E	84	SER	2
1	F	56	SER	2
1	F	84	SER	2
1	G	56	SER	2
1	G	84	SER	2
1	H	56	SER	2
1	H	84	SER	2
1	I	56	SER	2
1	I	84	SER	2
1	A	93	GLN	2
1	B	93	GLN	2
1	C	93	GLN	2
1	D	93	GLN	2
1	E	93	GLN	2
1	F	93	GLN	2
1	G	93	GLN	2
1	H	93	GLN	2
1	I	93	GLN	2
1	A	68	THR	2
1	B	68	THR	2
1	C	68	THR	2
1	D	68	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	E	68	THR	2
1	F	68	THR	2
1	G	68	THR	2
1	H	68	THR	2
1	I	68	THR	2
1	A	81	TYR	1
1	B	81	TYR	1
1	C	81	TYR	1
1	D	81	TYR	1
1	E	81	TYR	1
1	F	81	TYR	1
1	G	81	TYR	1
1	H	81	TYR	1
1	I	81	TYR	1
1	A	57	SER	1
1	B	57	SER	1
1	C	57	SER	1
1	D	57	SER	1
1	E	57	SER	1
1	F	57	SER	1
1	G	57	SER	1
1	H	57	SER	1
1	I	57	SER	1
1	A	94	GLN	1
1	B	94	GLN	1
1	C	94	GLN	1
1	D	94	GLN	1
1	E	94	GLN	1
1	F	94	GLN	1
1	G	94	GLN	1
1	H	94	GLN	1
1	I	94	GLN	1
1	A	61	SER	1
1	B	61	SER	1
1	C	61	SER	1
1	D	61	SER	1
1	E	61	SER	1
1	F	61	SER	1
1	G	61	SER	1
1	H	61	SER	1
1	I	61	SER	1
1	A	46	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	B	46	ASP	1
1	C	46	ASP	1
1	D	46	ASP	1
1	E	46	ASP	1
1	F	46	ASP	1
1	G	46	ASP	1
1	H	46	ASP	1
1	I	46	ASP	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *20170605a_fus_shifts.txt*

7.1.1 Bookkeeping (i)

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	218
Number of shifts mapped to atoms	218
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	46	-0.09 ± 0.37	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	35	-0.55 ± 0.30	None needed (imprecise)
$^{13}C'$	44	0.28 ± 0.30	None needed (< 0.5 ppm)
^{15}N	45	-1.66 ± 0.69	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 206 atoms were assigned a chemical shift out of a possible 5283. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	129/2556 (5%)	0/1080 (0%)	87/990 (9%)	42/486 (9%)
Sidechain	55/2079 (3%)	0/1314 (0%)	55/666 (8%)	0/99 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	22/648 (3%)	0/288 (0%)	22/360 (6%)	0/0 (—%)
Overall	206/5283 (4%)	0/2682 (0%)	164/2016 (8%)	42/585 (7%)

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

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 212 atoms were assigned a chemical shift out of a possible 5859. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	134/2835 (5%)	0/1197 (0%)	90/1098 (8%)	44/540 (8%)
Sidechain	56/2214 (3%)	0/1404 (0%)	56/711 (8%)	0/99 (0%)
Aromatic	22/810 (3%)	0/360 (0%)	22/450 (5%)	0/0 (—%)
Overall	212/5859 (4%)	0/2961 (0%)	168/2259 (7%)	44/639 (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.

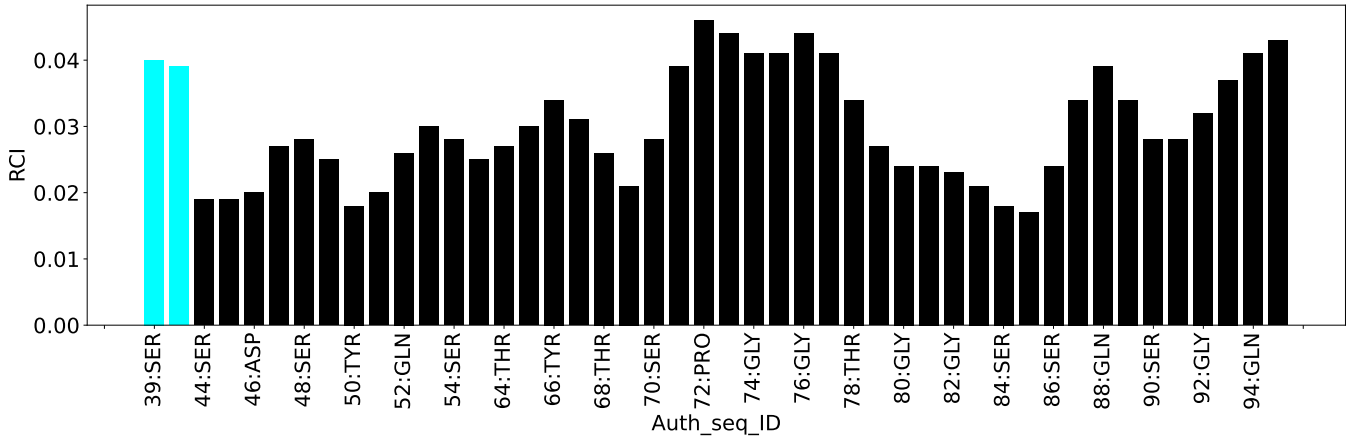
7.1.4 Statistically unusual chemical shifts (i)

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:


RCI
0.00
0.01
0.02
0.03
0.04
39:SER
44:SER
46:ASP
48:SER
50:TYR
52:GLN
54:SER
64:THR
66:TYR
68:THR
70:SER
72:PRO
74:GLY
76:GLY
78:THR
80:GLY
82:GLY
84:SER
86:SER
88:GLN
90:SER
92:GLY
94:GLN
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	157
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	68
Medium range (|i-j|>1 and |i-j|<5)	26
Long range (|i-j|≥5)	63
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	51
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue[1]	0.0

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.2	0.2
0.2-0.5 (Medium)	5.5	0.5
>0.5 (Large)	0.1	0.58

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	4.9	10.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

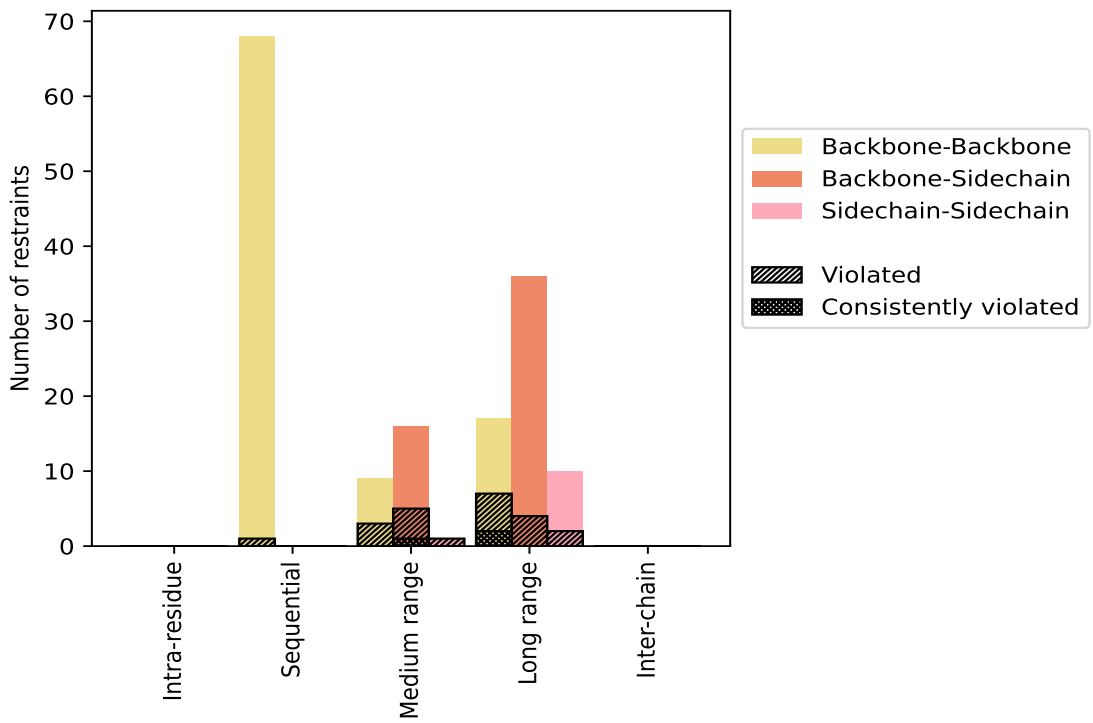
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	68	43.3	1	1.5	0.6	0	0.0	0.0
Backbone-Backbone	68	43.3	1	1.5	0.6	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	26	16.6	9	34.6	5.7	1	3.8	0.6
Backbone-Backbone	9	5.7	3	33.3	1.9	0	0.0	0.0
Backbone-Sidechain	16	10.2	5	31.2	3.2	1	6.2	0.6
Sidechain-Sidechain	1	0.6	1	100.0	0.6	0	0.0	0.0
Long range (|i-j|≥5)	63	40.1	13	20.6	8.3	2	3.2	1.3
Backbone-Backbone	17	10.8	7	41.2	4.5	2	11.8	1.3
Backbone-Sidechain	36	22.9	4	11.1	2.5	0	0.0	0.0
Sidechain-Sidechain	10	6.4	2	20.0	1.3	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	157	100.0	23	14.6	14.6	3	1.9	1.9
Backbone-Backbone	94	59.9	11	11.7	7.0	2	2.1	1.3
Backbone-Sidechain	52	33.1	9	17.3	5.7	1	1.9	0.6
Sidechain-Sidechain	11	7.0	3	27.3	1.9	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	5	5	0	10	0.25	0.38	0.08	0.24
2	0	0	5	6	0	11	0.23	0.36	0.09	0.2
3	0	0	5	7	0	12	0.24	0.43	0.1	0.2
4	0	0	3	7	0	10	0.24	0.42	0.09	0.22
5	0	1	2	7	0	10	0.2	0.42	0.09	0.16
6	0	0	4	8	0	12	0.26	0.37	0.06	0.26
7	0	0	4	7	0	11	0.2	0.27	0.05	0.19
8	0	0	5	5	0	10	0.3	0.54	0.15	0.25
9	0	0	3	8	0	11	0.21	0.35	0.07	0.2
10	0	1	4	4	0	9	0.24	0.44	0.1	0.19
11	0	0	3	4	0	7	0.21	0.27	0.04	0.19

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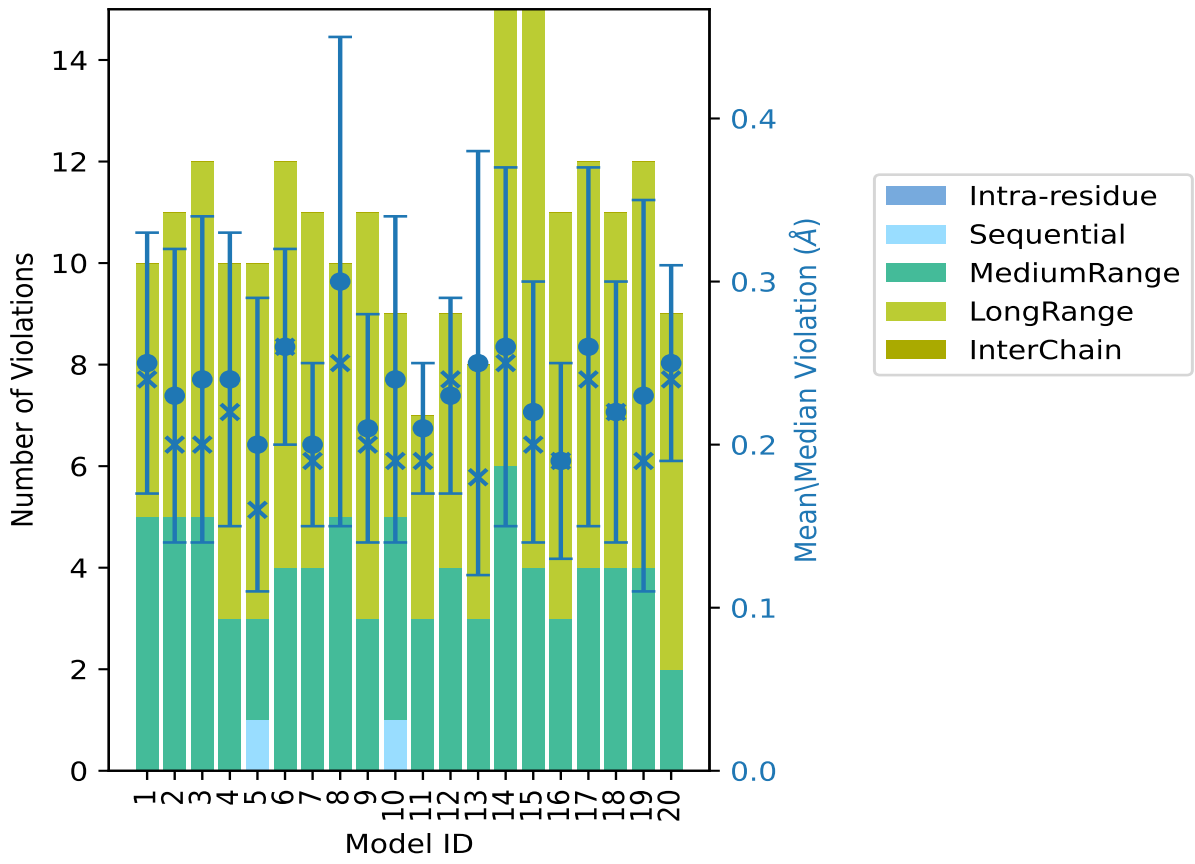
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	4	5	0	9	0.23	0.32	0.06	0.24
13	0	0	3	5	0	8	0.25	0.49	0.13	0.18
14	0	0	6	9	0	15	0.26	0.47	0.11	0.25
15	0	0	4	11	0	15	0.22	0.39	0.08	0.2
16	0	0	3	8	0	11	0.19	0.33	0.06	0.19
17	0	0	4	8	0	12	0.26	0.58	0.11	0.24
18	0	0	4	7	0	11	0.22	0.37	0.08	0.22
19	0	0	4	8	0	12	0.23	0.5	0.12	0.19
20	0	0	2	7	0	9	0.25	0.41	0.06	0.24

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

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



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

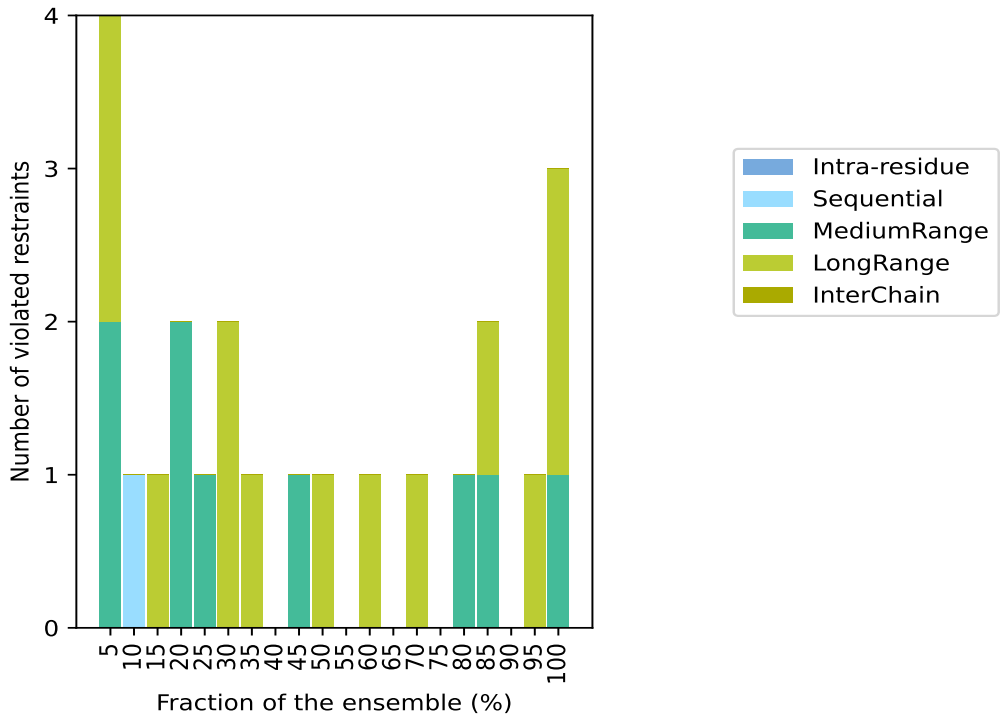
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 134(IR:0, SQ:67, MR:17, LR:50, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	2	2	0	4	1	5.0
0	1	0	0	0	1	2	10.0
0	0	0	1	0	1	3	15.0
0	0	2	0	0	2	4	20.0
0	0	1	0	0	1	5	25.0
0	0	0	2	0	2	6	30.0
0	0	0	1	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	1	0	0	1	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	1	0	0	1	16	80.0
0	0	1	1	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	0	1	2	0	3	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

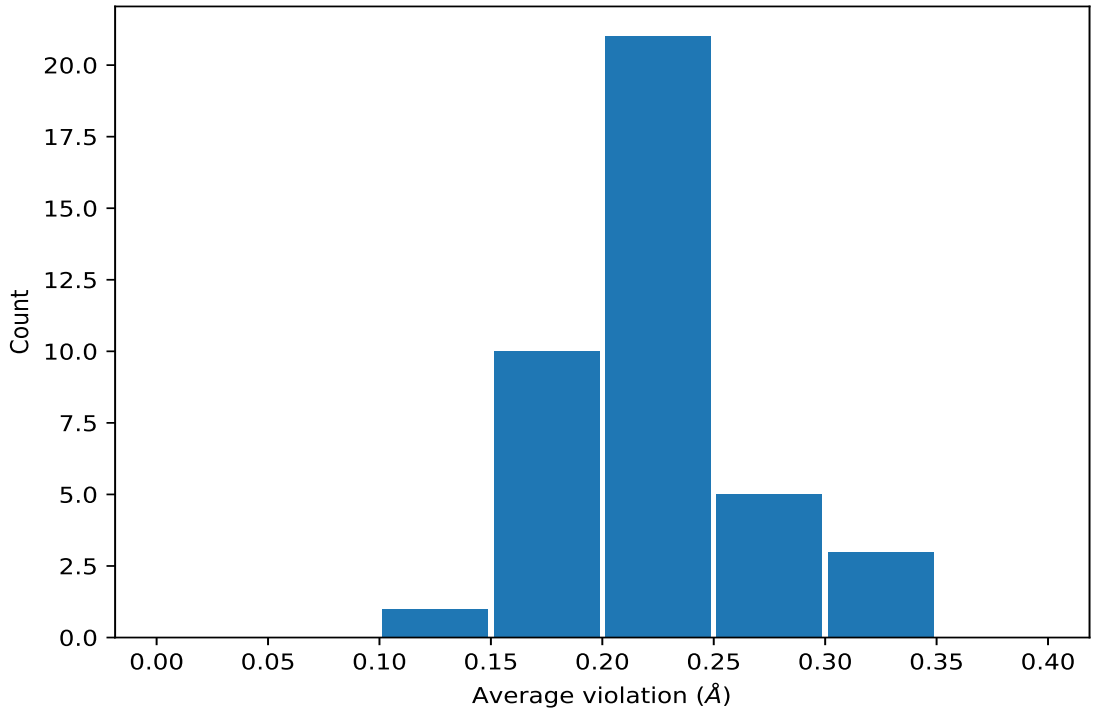
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	20	0.33	0.1	0.34
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	20	0.33	0.1	0.34
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	20	0.31	0.09	0.29
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	20	0.24	0.07	0.23
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	20	0.24	0.07	0.23
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	19	0.21	0.06	0.2
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	17	0.3	0.11	0.29
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	17	0.21	0.08	0.18
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	17	0.21	0.08	0.18
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	16	0.18	0.04	0.18
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	16	0.18	0.04	0.18
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	16	0.18	0.04	0.18
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	14	0.2	0.06	0.18
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	14	0.2	0.06	0.18
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	14	0.2	0.06	0.18
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	14	0.2	0.06	0.18

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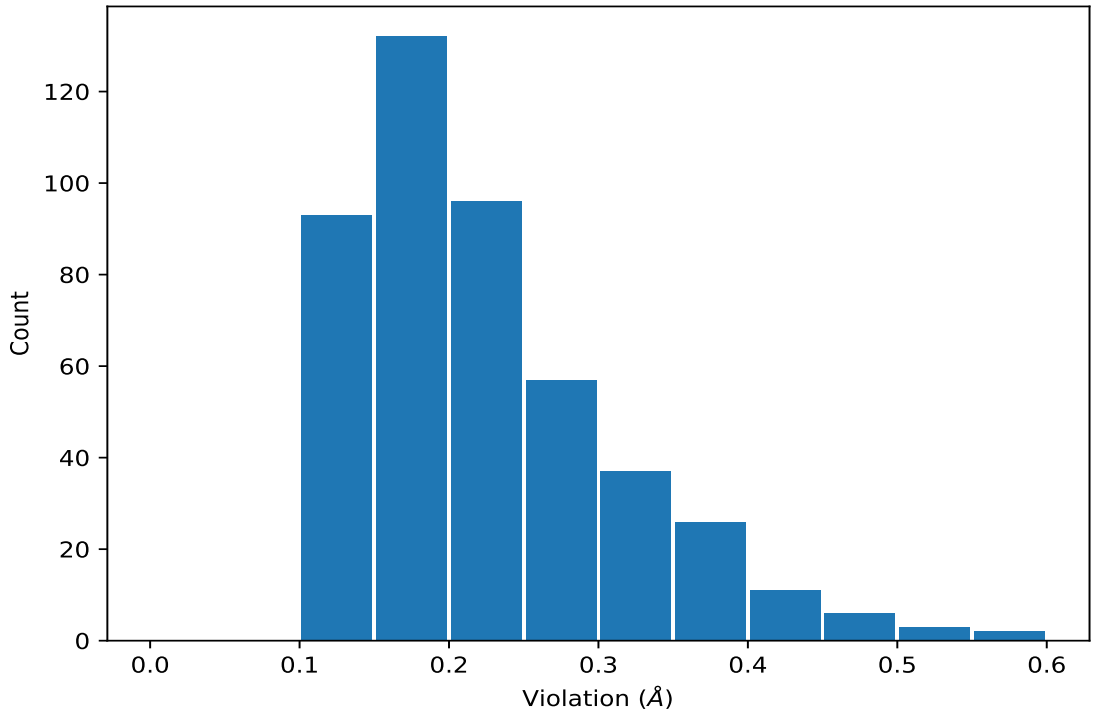
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	14	0.2	0.06	0.18
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	14	0.2	0.06	0.18
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	12	0.16	0.03	0.16
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	12	0.16	0.03	0.16
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	12	0.16	0.03	0.16
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	12	0.16	0.03	0.16
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	10	0.18	0.05	0.15
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	9	0.24	0.09	0.22
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	9	0.24	0.09	0.22
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	7	0.2	0.07	0.2
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	7	0.2	0.07	0.2
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	7	0.2	0.07	0.2
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	7	0.2	0.07	0.2
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	7	0.2	0.07	0.2
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	7	0.2	0.07	0.2
(2,12)	1:E:66:TYR:CA	1:E:49:GLY:CA	6	0.25	0.09	0.26
(2,15)	1:E:86:SER:CA	1:E:78:THR:CG2	6	0.16	0.04	0.16
(2,21)	1:E:72:PRO:CD	1:E:75:TYR:CA	5	0.17	0.07	0.15
(2,10)	1:E:46:ASP:CB	1:E:50:TYR:CB	4	0.3	0.1	0.32
(1,12)	1:A:80:GLY:CA	1:A:84:SER:CA	4	0.23	0.07	0.25
(1,12)	1:A:80:GLY:CA	1:A:86:SER:CA	4	0.23	0.07	0.25
(1,15)	1:A:50:TYR:C	1:A:45:THR:CA	3	0.25	0.06	0.26
(1,15)	1:A:50:TYR:C	1:A:47:THR:CA	3	0.25	0.06	0.26
(3,46)	1:A:79:GLY:N	1:A:80:GLY:N	2	0.13	0.02	0.13

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	17	0.58
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	17	0.58
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	8	0.54
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	8	0.52
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	19	0.5
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	13	0.49
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	14	0.47
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	19	0.47
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	19	0.47
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	8	0.46
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	8	0.46
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	10	0.44
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	3	0.43
(2,10)	1:E:46:ASP:CB	1:E:50:TYR:CB	14	0.42
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	4	0.42
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	5	0.42
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	5	0.42
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	3	0.41
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	3	0.41
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	20	0.41
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	20	0.41
(2,12)	1:E:66:TYR:CA	1:E:49:GLY:CA	15	0.39
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	13	0.39
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	13	0.39
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	1	0.38
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	18	0.37
(2,10)	1:E:46:ASP:CB	1:E:50:TYR:CB	6	0.37
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	14	0.37
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	14	0.37
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	2	0.36
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	2	0.36
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	2	0.36
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	1	0.36
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	1	0.36
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	4	0.36
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	4	0.36
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	2	0.35
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	9	0.35
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	9	0.35
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	9	0.35
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	9	0.35
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	9	0.35
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	9	0.35
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	6	0.35
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	6	0.35
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	15	0.35
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	15	0.35
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	15	0.34
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	14	0.34
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	14	0.34
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	14	0.34
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	14	0.34
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	14	0.34
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	14	0.34
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	8	0.34
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	8	0.34
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	3	0.33
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	16	0.33
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	16	0.33
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	17	0.33
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	17	0.33
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	10	0.32
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	13	0.32
(2,12)	1:E:66:TYR:CA	1:E:49:GLY:CA	14	0.32
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	12	0.32
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	12	0.32
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	9	0.31
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	17	0.31
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	17	0.31
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	6	0.31
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	6	0.31
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	10	0.31
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	10	0.31
(1,15)	1:A:50:TYR:C	1:A:45:THR:CA	14	0.31
(1,15)	1:A:50:TYR:C	1:A:47:THR:CA	14	0.31
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	5	0.3
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	1	0.3
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	4	0.3
(2,21)	1:E:72:PRO:CD	1:E:75:TYR:CA	6	0.3
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	18	0.3
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	18	0.3
(1,12)	1:A:80:GLY:CA	1:A:84:SER:CA	18	0.3
(1,12)	1:A:80:GLY:CA	1:A:86:SER:CA	18	0.3
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	1	0.29
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	9	0.29
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	17	0.29
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	6	0.29
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	6	0.29
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	6	0.29
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	6	0.29
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	6	0.29
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	6	0.29
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	3	0.29
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	3	0.29
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	3	0.29
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	14	0.28
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	18	0.28
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	12	0.28
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	7	0.27
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	11	0.27
(2,10)	1:E:46:ASP:CB	1:E:50:TYR:CB	15	0.27
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	19	0.27
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	19	0.27
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	20	0.27
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	20	0.27
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	12	0.26
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	17	0.26
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	3	0.26
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	7	0.26
(2,12)	1:E:66:TYR:CA	1:E:49:GLY:CA	6	0.26
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	1	0.26
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	1	0.26
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	1	0.26
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	1	0.26
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	1	0.26
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	1	0.26
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	12	0.26
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	12	0.26
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	8	0.26
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	8	0.26
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	8	0.26
(1,15)	1:A:50:TYR:C	1:A:45:THR:CA	6	0.26
(1,15)	1:A:50:TYR:C	1:A:47:THR:CA	6	0.26
(1,12)	1:A:80:GLY:CA	1:A:84:SER:CA	10	0.26
(1,12)	1:A:80:GLY:CA	1:A:86:SER:CA	10	0.26
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	6	0.25
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	4	0.25
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	16	0.25
(2,12)	1:E:66:TYR:CA	1:E:49:GLY:CA	2	0.25
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	6	0.25
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	6	0.25
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	7	0.25
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	7	0.25
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	14	0.25
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	14	0.25
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	20	0.25
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	20	0.25
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	15	0.25
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	8	0.24
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	11	0.24
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	20	0.24
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	12	0.24
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	15	0.24
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	17	0.24
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	8	0.24
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	8	0.24
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	20	0.24
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	20	0.24
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	7	0.24
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	7	0.24
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	7	0.24
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	7	0.24
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	7	0.24
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	7	0.24
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	17	0.24
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	17	0.24
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	17	0.24
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	17	0.24
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	17	0.24
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	17	0.24
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	4	0.24
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	4	0.24
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	5	0.24
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	5	0.24
(1,12)	1:A:80:GLY:CA	1:A:84:SER:CA	14	0.24
(1,12)	1:A:80:GLY:CA	1:A:86:SER:CA	14	0.24
(2,15)	1:E:86:SER:CA	1:E:78:THR:CG2	20	0.23
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	18	0.22
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	3	0.22
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	5	0.22
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	11	0.22
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	15	0.22
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	15	0.22
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	2	0.22
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	2	0.22
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	16	0.22
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	16	0.22
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	16	0.22
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	16	0.22
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	9	0.22
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	18	0.22
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	18	0.22
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	20	0.21
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	1	0.21
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	1	0.21
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	19	0.21
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	19	0.21
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	16	0.21
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	16	0.21
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	16	0.21
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	16	0.21
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	16	0.21
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	16	0.21
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	19	0.21
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	19	0.21
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	17	0.21
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	17	0.21
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	17	0.21
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	17	0.21
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	7	0.21
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	7	0.21
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	12	0.2
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	1	0.2
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	6	0.2
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	13	0.2
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	9	0.2
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	9	0.2
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	15	0.2
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	15	0.2
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	15	0.2
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	15	0.2
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	15	0.2
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	15	0.2
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	19	0.2
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	19	0.2
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	19	0.2
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	19	0.2
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	19	0.2
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	19	0.2
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	2	0.2
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	2	0.2
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	2	0.2
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	2	0.2
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	2	0.2
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	6	0.2
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	6	0.2
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	6	0.2
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	9	0.2
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	9	0.2
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	9	0.2
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	16	0.2
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	16	0.2
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	10	0.19
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	7	0.19
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	16	0.19
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	16	0.19
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	18	0.19
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	18	0.19
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	4	0.19
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	4	0.19
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	4	0.19
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	4	0.19
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	4	0.19
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	4	0.19
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	7	0.19
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	7	0.19
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	7	0.19
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	18	0.19
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	18	0.19
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	18	0.19
(1,35)	1:A:75:TYR:C	1:A:45:THR:CG2	14	0.19
(1,35)	1:A:75:TYR:C	1:A:47:THR:CG2	14	0.19
(1,35)	1:A:75:TYR:C	1:A:64:THR:CG2	14	0.19
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	3	0.19
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	3	0.19
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	3	0.19
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	3	0.19
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	11	0.19
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	11	0.19
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	4	0.18
(2,33)	1:E:49:GLY:C	1:E:52:GLN:CG	16	0.18
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	19	0.18
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	20	0.18
(2,15)	1:E:86:SER:CA	1:E:78:THR:CG2	14	0.18
(2,15)	1:E:86:SER:CA	1:E:78:THR:CG2	17	0.18
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	20	0.18
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	20	0.18
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	20	0.18
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	20	0.18
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	20	0.18
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	20	0.18
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	7	0.18
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	7	0.18
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	10	0.18
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	10	0.18
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	10	0.18
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	11	0.18
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	11	0.18
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	11	0.18
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	19	0.18
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	19	0.18
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	19	0.18
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	11	0.18
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	11	0.18
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	11	0.18
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	11	0.18
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	15	0.18
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	15	0.18
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	15	0.18
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	15	0.18
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	4	0.18
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	4	0.18
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	12	0.18
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	12	0.18
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	9	0.17
(2,23)	1:E:80:GLY:CA	1:E:83:SER:CA	12	0.17
(2,21)	1:E:72:PRO:CD	1:E:75:TYR:CA	3	0.17
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	17	0.17
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	17	0.17
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	17	0.17
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	17	0.17
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	17	0.17
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	17	0.17
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	17	0.17
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	1	0.17
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	1	0.17
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	1	0.17
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	2	0.17
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	2	0.17
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	2	0.17
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	13	0.17
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	13	0.17
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	13	0.17
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	15	0.17
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	15	0.17
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	15	0.17
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	13	0.17
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	13	0.17
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	13	0.17
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	13	0.17
(1,15)	1:A:50:TYR:C	1:A:45:THR:CA	15	0.17
(1,15)	1:A:50:TYR:C	1:A:47:THR:CA	15	0.17
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	16	0.16
(2,12)	1:E:66:TYR:CA	1:E:49:GLY:CA	19	0.16
(2,10)	1:E:46:ASP:CB	1:E:50:TYR:CB	2	0.16
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	10	0.16
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	10	0.16
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	11	0.16
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	11	0.16
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	8	0.16
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	8	0.16
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	8	0.16
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	8	0.16
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	8	0.16
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	8	0.16
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	5	0.16
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	5	0.16
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	5	0.16
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	5	0.16
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	5	0.16
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	5	0.16
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	9	0.16
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	9	0.16
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	9	0.16
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	9	0.16
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	9	0.16
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	2	0.16
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	2	0.16
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	7	0.16
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	7	0.16
(3,46)	1:A:79:GLY:N	1:A:80:GLY:N	10	0.15
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	3	0.15
(2,21)	1:E:72:PRO:CD	1:E:75:TYR:CA	1	0.15
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	5	0.15
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	5	0.15
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	19	0.15
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	19	0.15
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	19	0.15
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	19	0.15
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	9	0.15
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	9	0.15
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	5	0.14
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	19	0.14
(2,21)	1:E:72:PRO:CD	1:E:75:TYR:CA	8	0.14
(1,8)	1:A:46:ASP:CA	1:A:79:GLY:CA	13	0.14
(1,8)	1:A:46:ASP:CA	1:A:80:GLY:CA	13	0.14
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	3	0.14
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	3	0.14
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	3	0.14
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	3	0.14
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	3	0.14
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	3	0.14
(1,38)	1:A:49:GLY:C	1:A:45:THR:CB	1	0.14
(1,38)	1:A:49:GLY:C	1:A:47:THR:CB	1	0.14
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	5	0.14
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	5	0.14
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	5	0.14
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	17	0.14
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	17	0.14
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	17	0.14
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	5	0.14
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	5	0.14
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	5	0.14
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	5	0.14
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	6	0.14
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	6	0.14
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	6	0.14
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	7	0.14
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	7	0.14
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	7	0.14
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	7	0.14
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	3	0.14
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	3	0.14
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	8	0.14
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	8	0.14
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	4	0.13
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	15	0.13
(2,9)	1:E:66:TYR:CB	1:E:50:TYR:CB	18	0.13
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	2	0.13
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	14	0.13
(2,15)	1:E:86:SER:CA	1:E:78:THR:CG2	16	0.13
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	12	0.13
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	12	0.13
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	12	0.13
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	12	0.13
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	12	0.13
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	12	0.13
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	15	0.13
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	15	0.13
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	15	0.13
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	15	0.13
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	15	0.13
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	15	0.13
(1,43)	1:A:50:TYR:CB	1:A:39:SER:C	18	0.13
(1,43)	1:A:50:TYR:CB	1:A:40:GLY:C	18	0.13
(1,43)	1:A:50:TYR:CB	1:A:54:SER:C	18	0.13
(1,43)	1:A:50:TYR:CB	1:A:77:SER:C	18	0.13
(1,43)	1:A:50:TYR:CB	1:A:82:GLY:C	18	0.13
(1,43)	1:A:50:TYR:CB	1:A:92:GLY:C	18	0.13
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	4	0.13
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	4	0.13
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	4	0.13
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	4	0.13
(1,21)	1:A:67:GLY:CA	1:A:44:SER:CA	9	0.13
(1,21)	1:A:67:GLY:CA	1:A:95:SER:CA	9	0.13
(1,21)	1:A:40:GLY:CA	1:A:44:SER:CA	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:A:40:GLY:CA	1:A:95:SER:CA	9	0.13
(1,16)	1:A:89:SER:C	1:A:72:PRO:CA	2	0.13
(1,16)	1:A:89:SER:C	1:A:78:THR:CA	2	0.13
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	14	0.13
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	14	0.13
(2,30)	1:E:81:TYR:CA	1:E:78:THR:CB	19	0.12
(2,26)	1:E:70:SER:CA	1:E:93:GLN:CD	9	0.12
(2,16)	1:E:49:GLY:CA	1:E:46:ASP:CA	16	0.12
(2,15)	1:E:86:SER:CA	1:E:78:THR:CG2	7	0.12
(1,12)	1:A:80:GLY:CA	1:A:84:SER:CA	3	0.12
(1,12)	1:A:80:GLY:CA	1:A:86:SER:CA	3	0.12
(3,46)	1:A:79:GLY:N	1:A:80:GLY:N	5	0.11
(2,29)	1:E:95:SER:CA	1:E:67:GLY:CA	10	0.11
(2,21)	1:E:72:PRO:CD	1:E:75:TYR:CA	14	0.11
(2,15)	1:E:86:SER:CA	1:E:78:THR:CG2	15	0.11
(2,12)	1:E:66:TYR:CA	1:E:49:GLY:CA	16	0.11
(1,45)	1:A:45:THR:CG2	1:A:50:TYR:CZ	18	0.11
(1,45)	1:A:45:THR:CG2	1:A:75:TYR:CZ	18	0.11
(1,45)	1:A:47:THR:CG2	1:A:50:TYR:CZ	18	0.11
(1,45)	1:A:47:THR:CG2	1:A:75:TYR:CZ	18	0.11
(1,45)	1:A:64:THR:CG2	1:A:50:TYR:CZ	18	0.11
(1,45)	1:A:64:THR:CG2	1:A:75:TYR:CZ	18	0.11
(1,37)	1:A:49:GLY:C	1:A:45:THR:CG2	14	0.11
(1,37)	1:A:49:GLY:C	1:A:47:THR:CG2	14	0.11
(1,37)	1:A:49:GLY:C	1:A:64:THR:CG2	14	0.11
(1,13)	1:A:79:GLY:CA	1:A:84:SER:CA	13	0.11
(1,13)	1:A:79:GLY:CA	1:A:86:SER:CA	13	0.11

10 Dihedral-angle violation analysis (i)

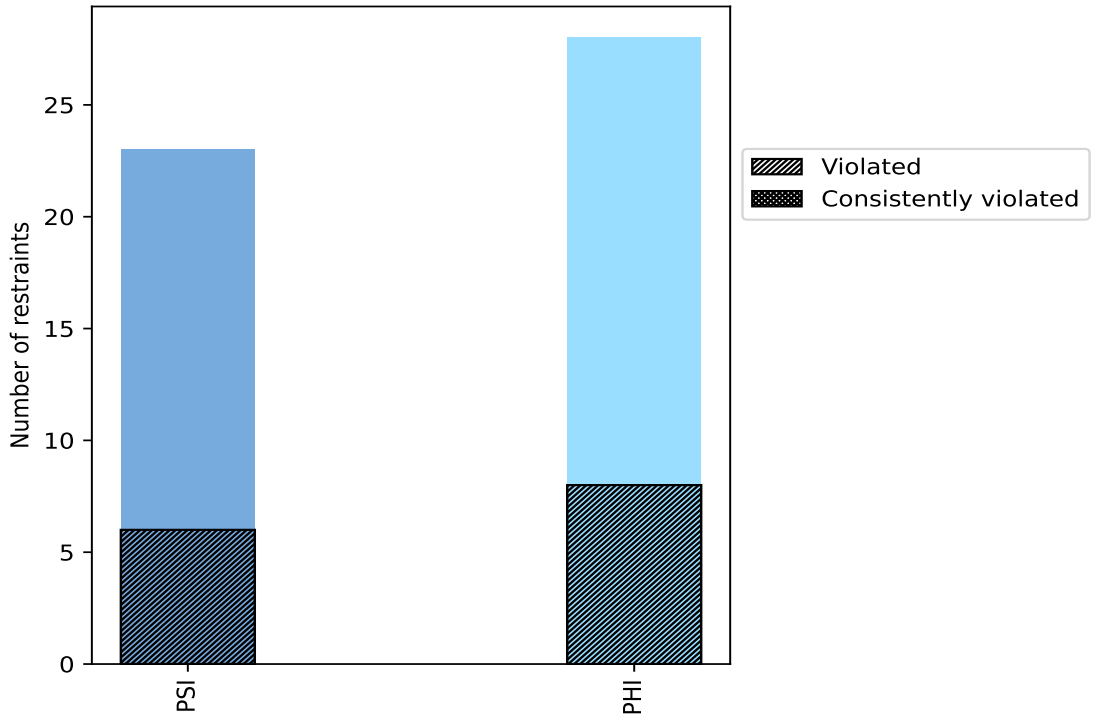
10.1 Summary of dihedral-angle violations (i)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	23	45.1	6	26.1	11.8	0	0.0	0.0
PHI	28	54.9	8	28.6	15.7	0	0.0	0.0
Total	51	100.0	14	27.5	27.5	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



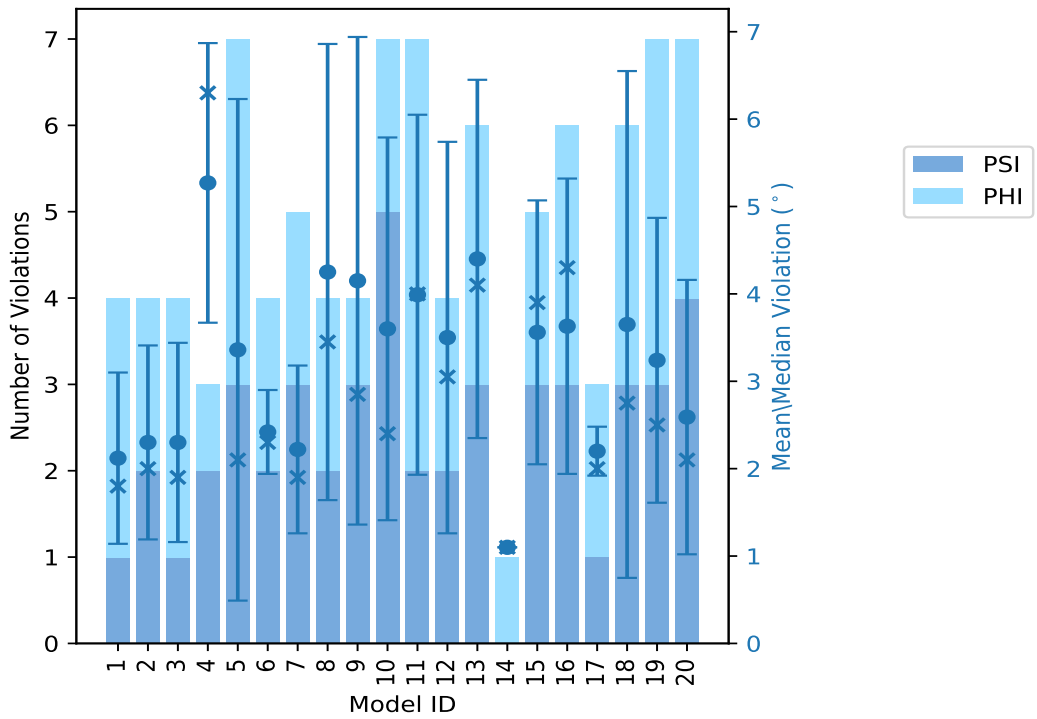
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	3	4	2.12	3.7	0.98	1.8
2	2	2	4	2.3	4.1	1.11	2.0
3	1	3	4	2.3	4.2	1.14	1.9
4	2	1	3	5.27	6.5	1.6	6.3
5	3	4	7	3.36	10.0	2.87	2.1
6	2	2	4	2.42	3.2	0.48	2.3
7	3	2	5	2.22	4.1	0.96	1.9
8	2	2	4	4.25	8.5	2.61	3.45
9	3	1	4	4.15	8.9	2.79	2.85
10	5	2	7	3.6	6.8	2.19	2.4
11	2	5	7	3.99	7.7	2.06	4.0
12	2	2	4	3.5	6.7	2.24	3.05
13	3	3	6	4.4	8.4	2.05	4.1
14	0	1	1	1.1	1.1	0.0	1.1
15	3	2	5	3.56	6.0	1.51	3.9
16	3	3	6	3.63	5.7	1.69	4.3
17	1	2	3	2.2	2.6	0.28	2.0
18	3	3	6	3.65	9.3	2.9	2.75
19	3	4	7	3.24	6.4	1.63	2.5
20	4	3	7	2.59	6.1	1.57	2.1

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	1	2	1	5.0
1	1	2	2	10.0
0	1	1	3	15.0
0	3	3	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
1	0	1	11	55.0

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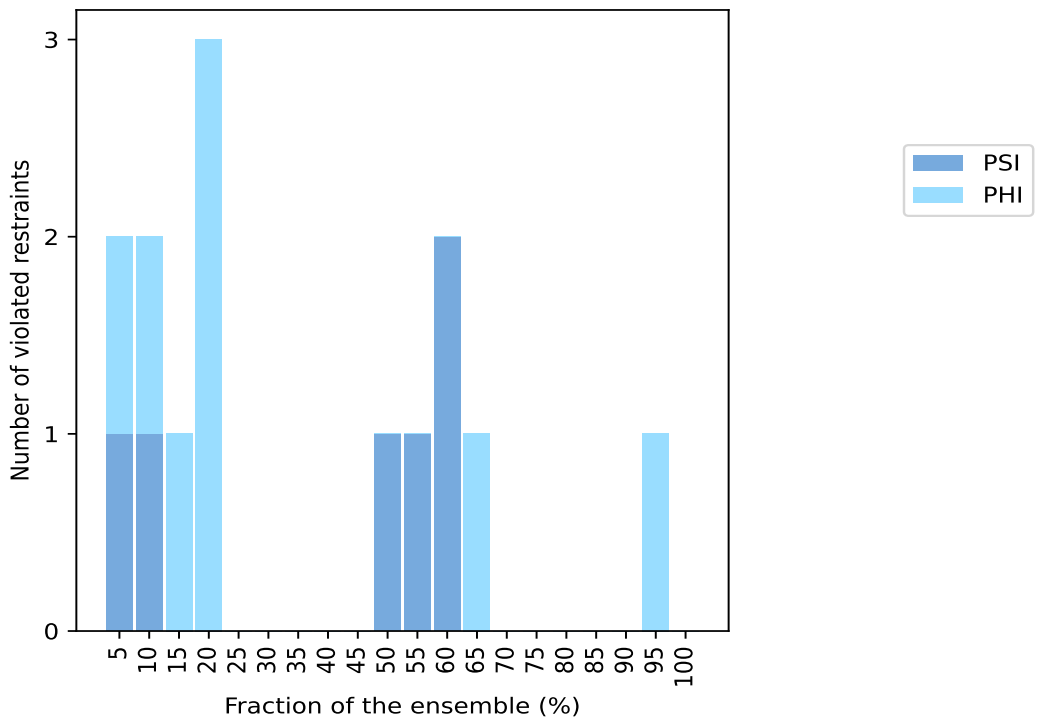
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
2	0	2	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)

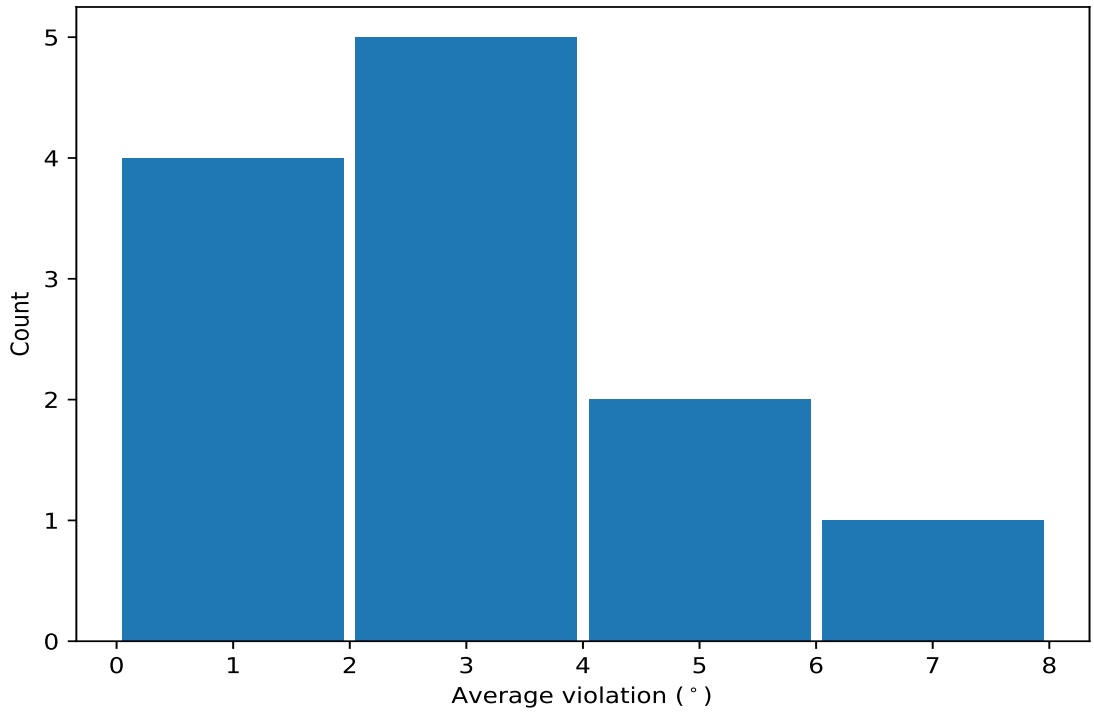


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

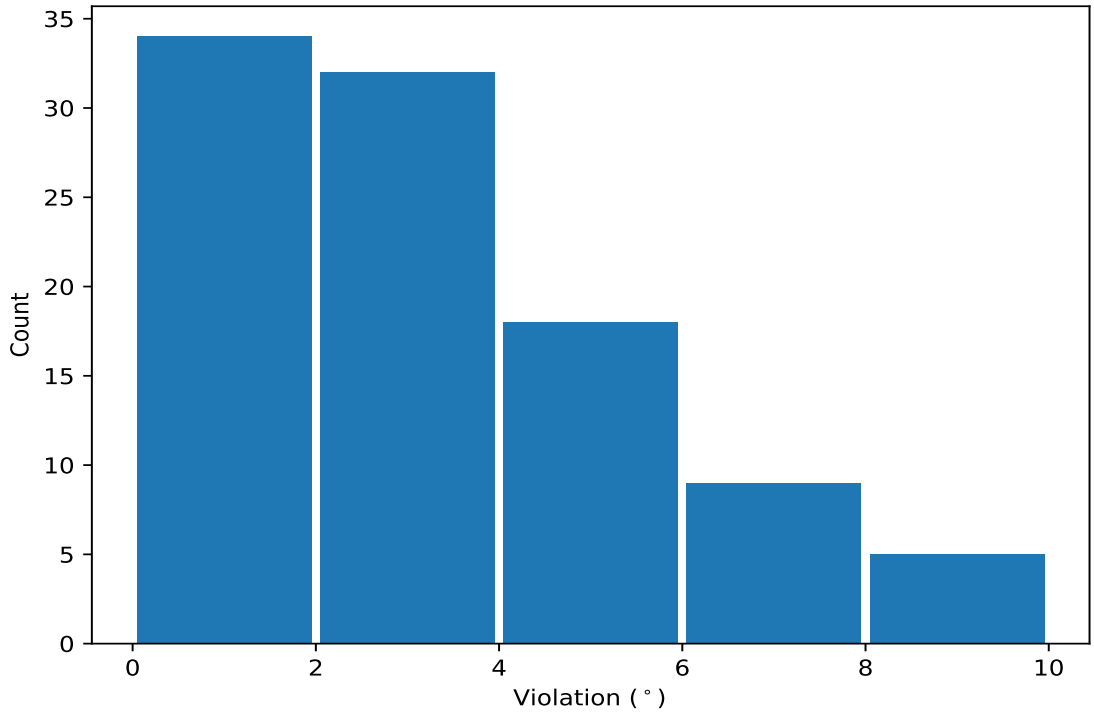
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	19	3.37	1.57	3.3
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	13	1.74	0.33	1.7
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	12	4.79	1.55	5.15
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	12	3.16	0.95	3.45
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	11	6.74	2.76	7.7
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	10	2.07	0.85	2.0
(1,36)	1:G:80:GLY:C	1:G:81:TYR:N	1:G:81:TYR:CA	1:G:81:TYR:C	4	2.3	1.05	1.95
(1,42)	1:G:88:GLN:C	1:G:89:SER:N	1:G:89:SER:CA	1:G:89:SER:C	4	1.7	0.5	1.65
(1,44)	1:G:89:SER:C	1:G:90:SER:N	1:G:90:SER:CA	1:G:90:SER:C	4	1.23	0.08	1.25
(1,32)	1:G:72:PRO:C	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	3	3.17	0.59	2.8
(1,30)	1:G:71:THR:C	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	2	4.4	0.5	4.4
(1,39)	1:G:86:SER:N	1:G:86:SER:CA	1:G:86:SER:C	1:G:87:SER:N	2	1.45	0.25	1.45

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	5	10.0
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	18	9.3
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	9	8.9
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	8	8.5
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	13	8.4
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	11	7.7
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	10	6.8
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	12	6.7
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	4	6.5
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	19	6.4
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	4	6.3
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	20	6.1
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	10	6.0
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	15	6.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	16	5.7
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	11	5.6
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	10	5.4
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	13	4.9
(1,30)	1:G:71:THR:C	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	19	4.9
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	16	4.8
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	13	4.8
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	18	4.7
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	11	4.6
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	16	4.6
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	12	4.5
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	3	4.2
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	18	4.1
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	2	4.1
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	7	4.1
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	8	4.1
(1,36)	1:G:80:GLY:C	1:G:81:TYR:N	1:G:81:TYR:CA	1:G:81:TYR:C	11	4.0
(1,32)	1:G:72:PRO:C	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	16	4.0
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	5	3.9
(1,30)	1:G:71:THR:C	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	15	3.9
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	15	3.9
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	1	3.7
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	9	3.4
(1,35)	1:G:78:THR:N	1:G:78:THR:CA	1:G:78:THR:C	1:G:79:GLY:N	13	3.4
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	5	3.3
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	20	3.3
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	6	3.2
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	19	3.1
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	4	3.0
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	8	2.8
(1,32)	1:G:72:PRO:C	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	11	2.8
(1,32)	1:G:72:PRO:C	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	13	2.7
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	17	2.6
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	19	2.5
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	10	2.4
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	15	2.4
(1,42)	1:G:88:GLN:C	1:G:89:SER:N	1:G:89:SER:CA	1:G:89:SER:C	19	2.3
(1,36)	1:G:80:GLY:C	1:G:81:TYR:N	1:G:81:TYR:CA	1:G:81:TYR:C	6	2.3
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	9	2.3
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	6	2.3
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	20	2.2
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	1	2.2
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	2	2.2
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	13	2.2
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	3	2.1
(1,42)	1:G:88:GLN:C	1:G:89:SER:N	1:G:89:SER:CA	1:G:89:SER:C	5	2.1
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	20	2.1
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	17	2.0
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	9	2.0
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	17	2.0
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	6	1.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	7	1.9
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	11	1.9
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	19	1.9
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	7	1.9
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	20	1.8
(1,31)	1:G:72:PRO:N	1:G:72:PRO:CA	1:G:72:PRO:C	1:G:73:GLN:N	7	1.8
(1,12)	1:G:53:SER:C	1:G:54:SER:N	1:G:54:SER:CA	1:G:54:SER:C	2	1.8
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	3	1.7
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	5	1.7
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	10	1.7
(1,39)	1:G:86:SER:N	1:G:86:SER:CA	1:G:86:SER:C	1:G:87:SER:N	10	1.7
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	19	1.6
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	12	1.6
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	15	1.6
(1,36)	1:G:80:GLY:C	1:G:81:TYR:N	1:G:81:TYR:CA	1:G:81:TYR:C	8	1.6
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	20	1.5
(1,33)	1:G:73:GLN:N	1:G:73:GLN:CA	1:G:73:GLN:C	1:G:74:GLY:N	16	1.5
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	1	1.4
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	7	1.4
(1,46)	1:G:92:GLY:C	1:G:93:GLN:N	1:G:93:GLN:CA	1:G:93:GLN:C	18	1.4
(1,44)	1:G:89:SER:C	1:G:90:SER:N	1:G:90:SER:CA	1:G:90:SER:C	11	1.3
(1,44)	1:G:89:SER:C	1:G:90:SER:N	1:G:90:SER:CA	1:G:90:SER:C	18	1.3
(1,36)	1:G:80:GLY:C	1:G:81:TYR:N	1:G:81:TYR:CA	1:G:81:TYR:C	5	1.3
(1,9)	1:G:49:GLY:N	1:G:49:GLY:CA	1:G:49:GLY:C	1:G:50:TYR:N	12	1.2
(1,44)	1:G:89:SER:C	1:G:90:SER:N	1:G:90:SER:CA	1:G:90:SER:C	3	1.2
(1,42)	1:G:88:GLN:C	1:G:89:SER:N	1:G:89:SER:CA	1:G:89:SER:C	1	1.2
(1,42)	1:G:88:GLN:C	1:G:89:SER:N	1:G:89:SER:CA	1:G:89:SER:C	16	1.2
(1,39)	1:G:86:SER:N	1:G:86:SER:CA	1:G:86:SER:C	1:G:87:SER:N	5	1.2
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	10	1.2
(1,7)	1:G:47:THR:C	1:G:48:SER:N	1:G:48:SER:CA	1:G:48:SER:C	14	1.1
(1,44)	1:G:89:SER:C	1:G:90:SER:N	1:G:90:SER:CA	1:G:90:SER:C	20	1.1
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	2	1.1
(1,19)	1:G:65:GLY:N	1:G:65:GLY:CA	1:G:65:GLY:C	1:G:66:TYR:N	18	1.1