



Full wwPDB NMR Structure Validation Report ⓘ

Dec 22, 2019 – 10:20 AM EST

PDB ID : 5W3N
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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.4
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

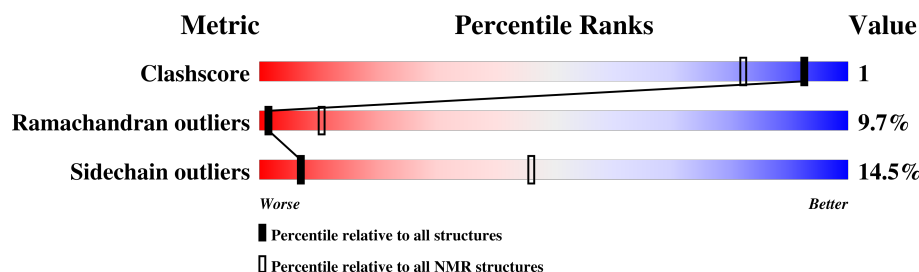
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	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

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)	0.99	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

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

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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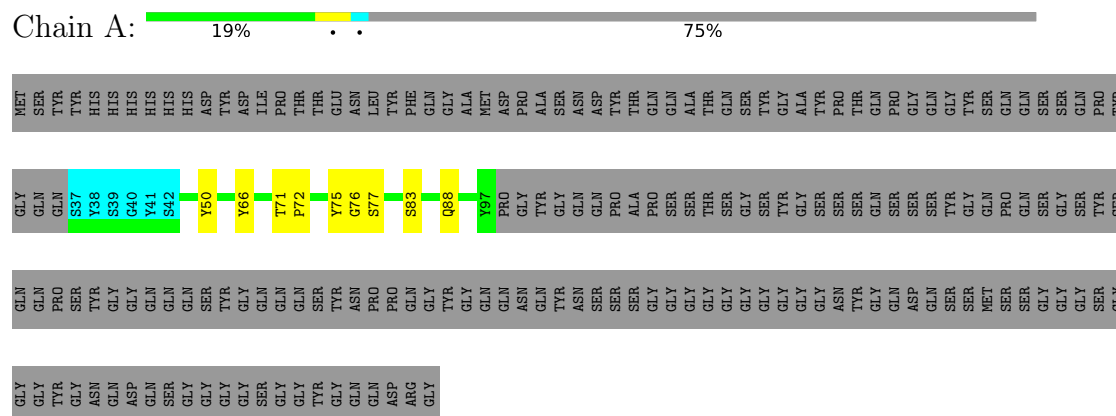
Chain	Residue	Modelled	Actual	Comment	Reference
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I	-24	TYR	-	expression tag	UNP P35637
I	-23	TYR	-	expression tag	UNP P35637
I	-22	HIS	-	expression tag	UNP P35637
I	-21	HIS	-	expression tag	UNP P35637
I	-20	HIS	-	expression tag	UNP P35637
I	-19	HIS	-	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
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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

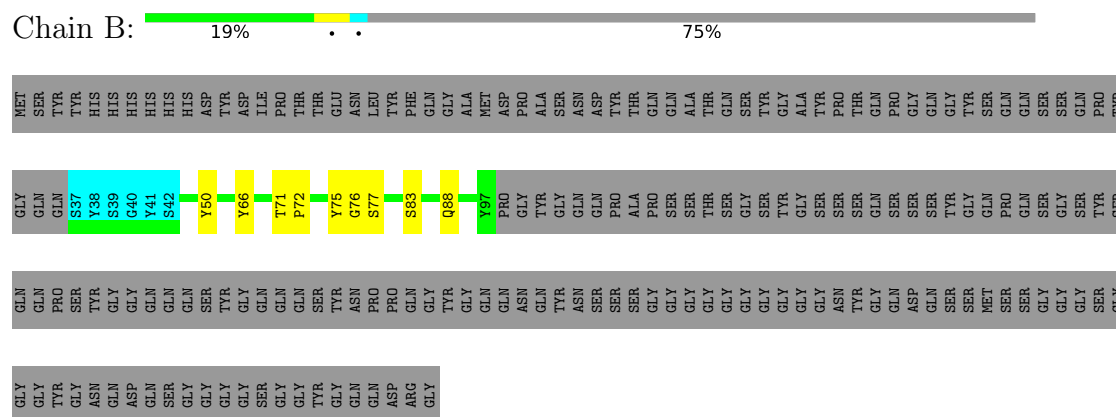
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

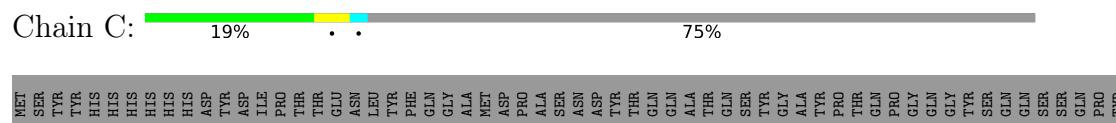
- Molecule 1: RNA-binding protein FUS

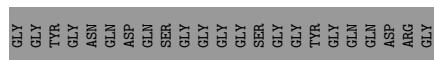
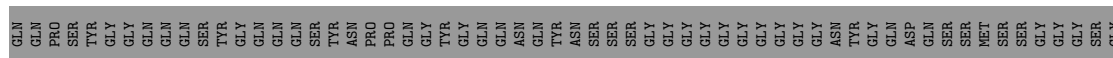
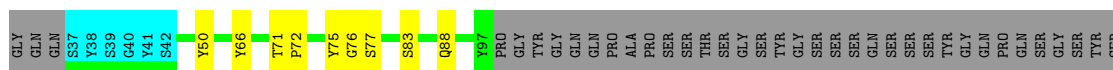


- Molecule 1: RNA-binding protein FUS



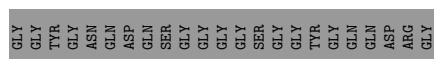
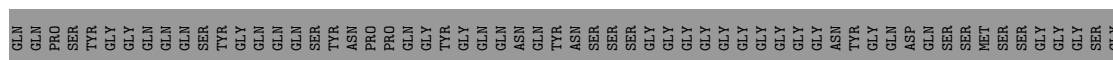
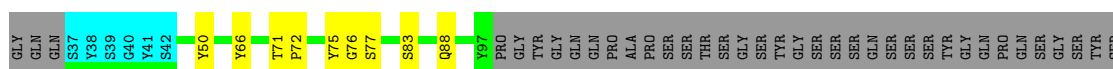
- Molecule 1: RNA-binding protein FUS





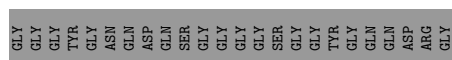
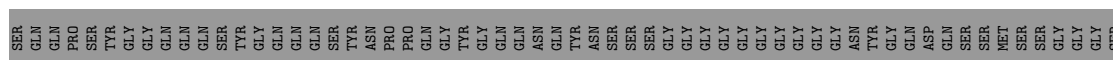
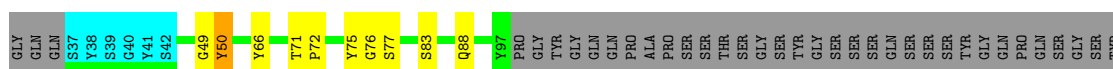
- Molecule 1: RNA-binding protein FUS

Chain D: 19% . . 75%



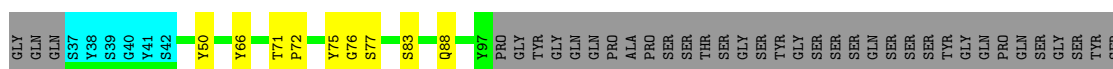
- Molecule 1: RNA-binding protein FUS

Chain E:  19% . . 75%



- Molecule 1: RNA-binding protein FUS

Chain F:  19% . . 75%



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:  19% . . 75%

NET	SER	TYR	THR	THR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	ASP	ASP	PRO	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	NET	ASP	PRO	ALA	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	GLN	SER	SER	TYR	GLY	ALA	TYR	PRO	PRO	THR	THR	GLN	PRO	GLY	GLN	GLY	GLY	TYR	SER	SER	SER	GLN	PRO
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GLY	GLN	GLN	S37	S38	S39	G40	Y41	S42	Y50	Y66	T71	P72	Y75	G76	S77	S83	Q88	Y97	PRO	GLY	TYR	GLY	GLN	GLN	PRO	PRO	ALA	PRO	PRO	SER	SER	SER	THR	SER	SER	GLY	SER	TYR	GLY	SER	SER	GLN	SER	SER	TYR	GLY	GLN	GLN	PRO	PRO	GLY	TYR
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[illegible]

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:  19% 75%

[illegible][illegible][illegible]

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% 2% 75%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ASP	PRO	PRO	THR	THR	GLU	ASN	LEU	PHE	THR	GLN	GLY	MET	ASP	ALA	PRO	ALA	SER	ASN	ASP	TYR	THR	GLN	GLN	THR	THR	ALA	TYR	THR	PRO	THR	GLN	GLY	GLY	GLY	TYR	SER	GLN	GLN	SER	SER	SER	SER	GLN	PRO
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[illegible][illegible]

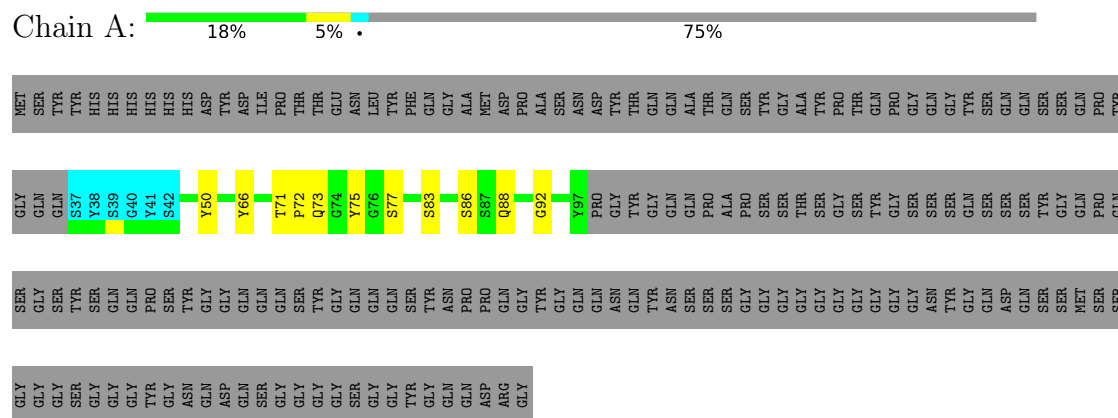
SER GLY GLY GLY TYR GLY ASN GLN ASP GLN SER GLY GLY GLY GLY SER GLY GLY TYR GLY GLN GLN ASP ARG GLY

4.2 Scores per residue for each member of the ensemble

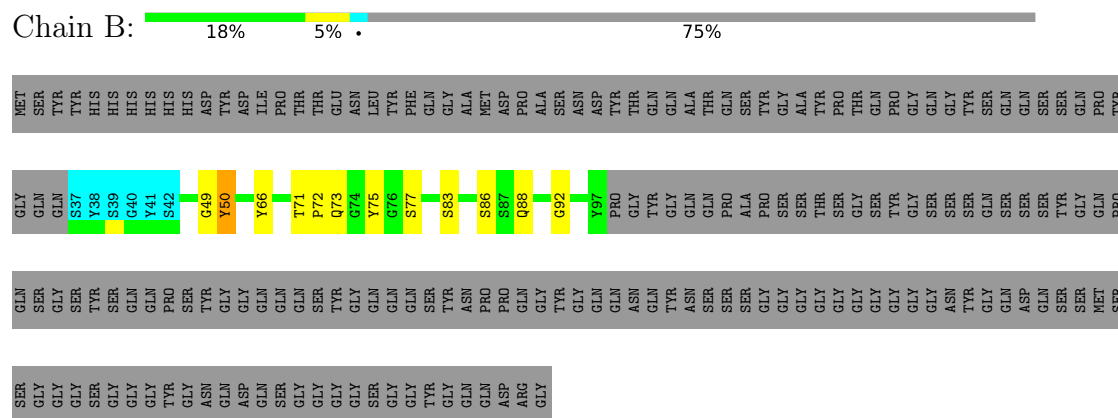
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

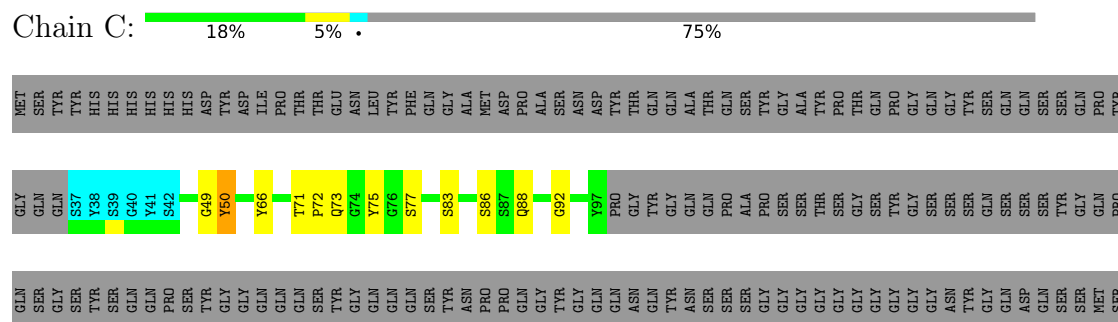
- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



SER GLY GLY GLY SER 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% 5% 75%

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

GLN	SER	GLY	SER	TYR	SER	GLN	GLN	PRO	SER	SER	TYR	GLY	GLY	GLN	GLN	GLN	GLN	ASN	TYR	TYR	ASN	PRO	PRO	GLN	GLY	TYR	GLY	GLY	GLN	GLN	ASN	GLN	TYR	GLN	ASN	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN	GLY	ASN	ASP	GLN	SER	SER	SER	MET
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SER	GLY	GLY	GLY	SER	GLY	GLY	TYR	GLY	ASN	GLN	ASP	GLN	SER	GLY	GLY	GLY	SER	GLY	TYR	GLY	GLN	GLN	ASP	ARG	GLY
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- Molecule 1: RNA-binding protein FUS

Chain E:  18% 5% 77%

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

- Molecule 1: RNA-binding protein FUS

Chain F:  18% 5% 77%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	ASP	PRO	THR	THR	GLU	ASN	LEU	PHE	TYR	GLN	GLY	ALA	MET	ASP	PRO	ALA	SER	ASN	ASP	TYR	THR	GLN	GLN	THR	ALA	GLN	GLN	TYR	GLY	ALA	TYR	PRO	THR	GLN	PRO	GLY	GLN	GLY	GLY	TYR	SER	GLN	GLN	SER	SER	GLN	PRO
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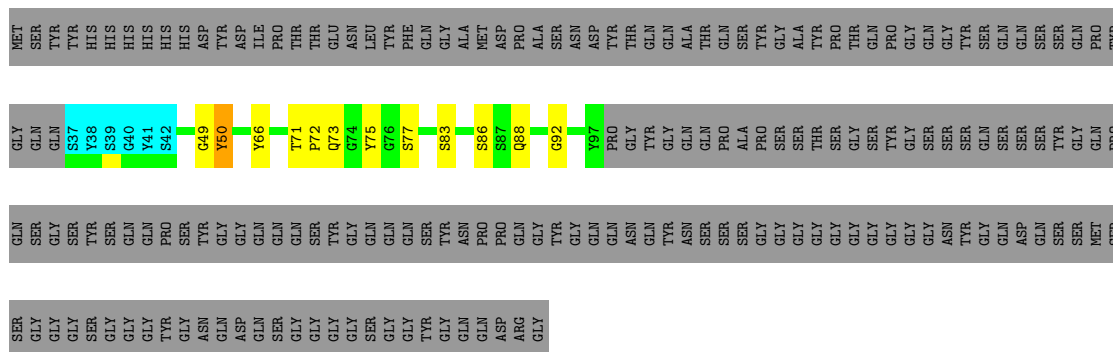
GLY	GLN	GLM	S37	Y38	S39	G40	Y41	S42	G49	Y50	Y66	T71	P72	Q73	G74	Y75	G76	S77	S83	S86	S87	Q88	G92	Y97	PRO	GLY	TYR	GLY	GLM	GLN	PRO	PRO	ALA	PRO	SER	SER	SER	THR	SER	GLY	GLY	SER	TYR	GLY	SER	SER	SER	GLN	SER	SER	SER	TYR	GLY	GLN
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[illegible]

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

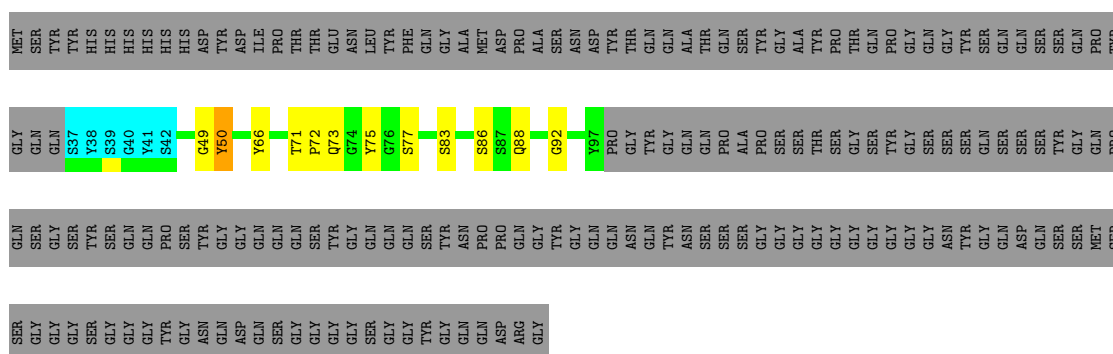
- Molecule 1: RNA-binding protein FUS

Chain G: 18% 5% 77%



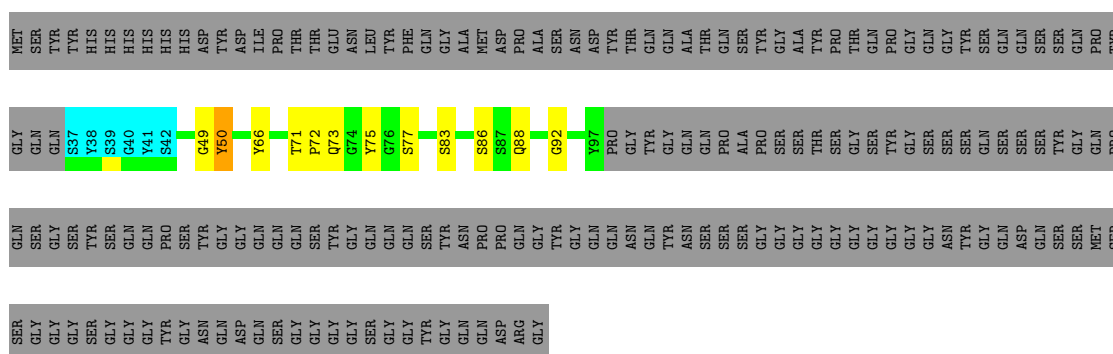
• Molecule 1: RNA-binding protein FUS

Chain H: 18% 5% 75%



• Molecule 1: RNA-binding protein FUS

Chain I: 18% 5% 75%

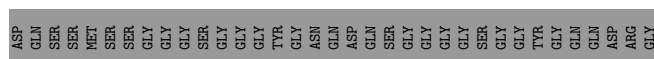
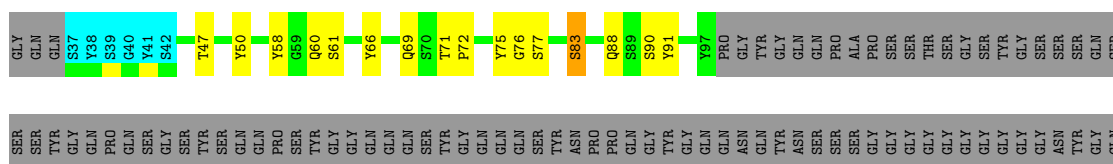


4.2.2 Score per residue for model 2

• Molecule 1: RNA-binding protein FUS

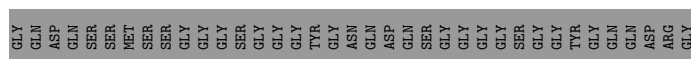
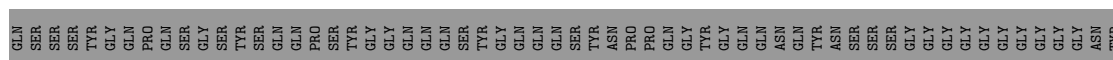
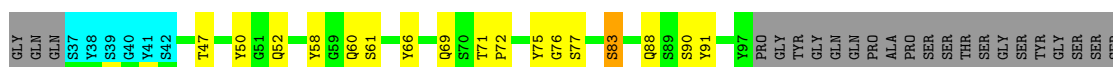
Chain A: 16% 6% 75%





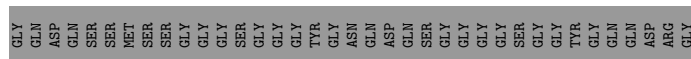
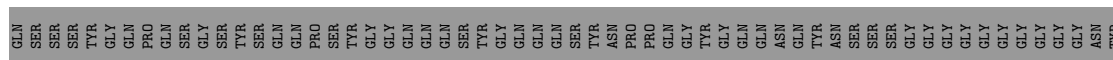
- Molecule 1: RNA-binding protein FUS

Chain B: 16% 7% 75%



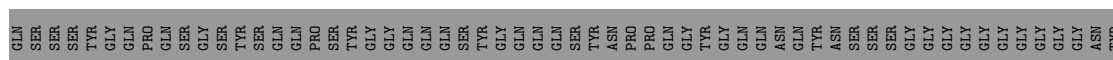
- Molecule 1: RNA-binding protein FUS

Chain C: 16% 7% 75%



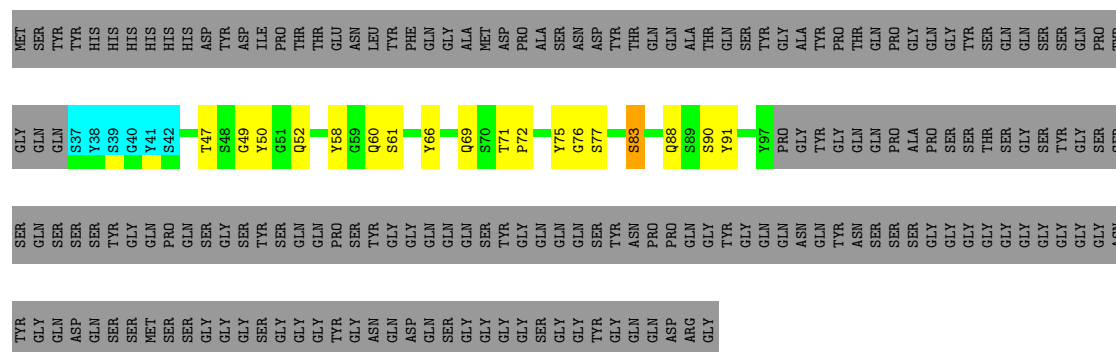
- Molecule 1: RNA-binding protein FUS

Chain D:  16% 6% 2% 2% 75%



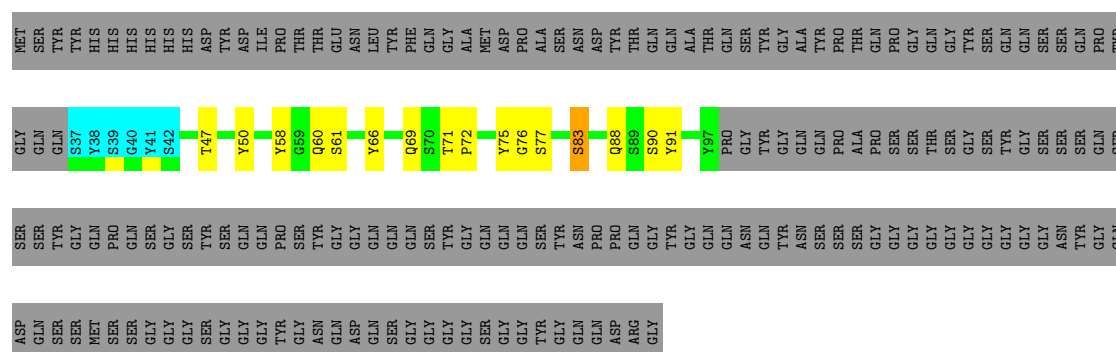
- Molecule 1: RNA-binding protein FUS

Chain E:  15% 7% 78%



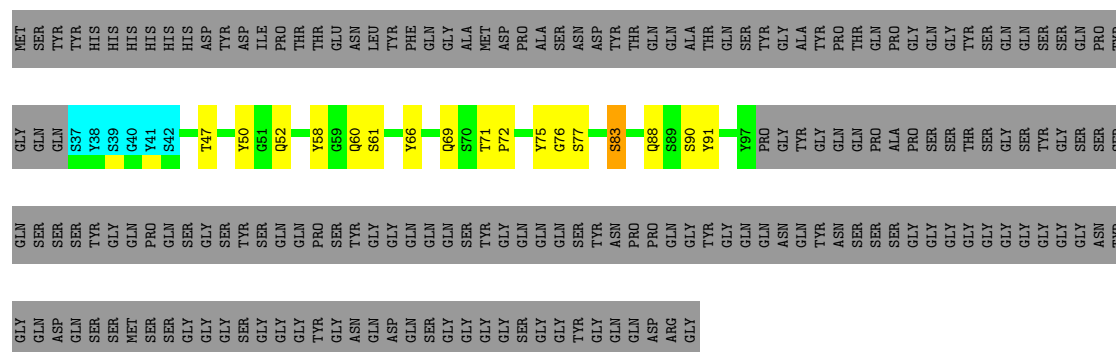
- Molecule 1: RNA-binding protein FUS

Chain F: 16% 6% • 75%



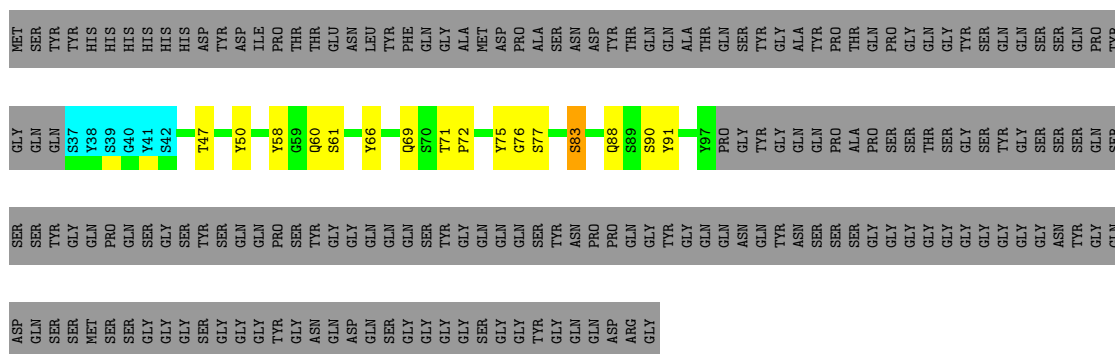
- Molecule 1: RNA-binding protein FUS

Chain G: 16% 7% • 75%



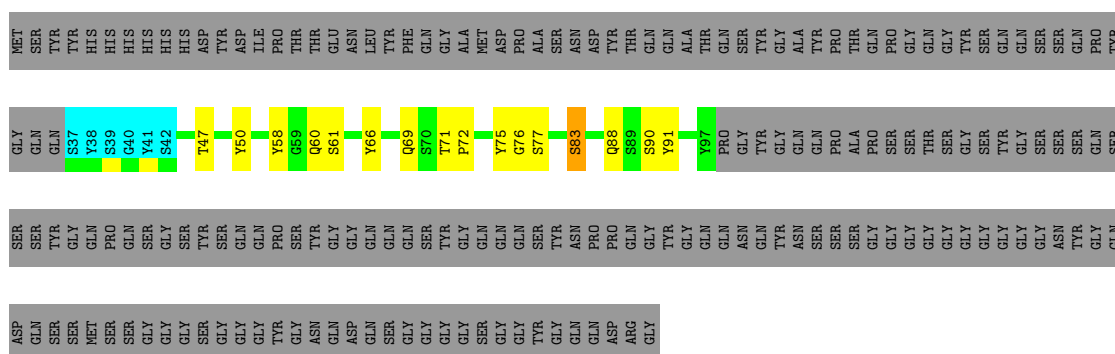
- Molecule 1: RNA-binding protein FUS

Chain H:  16% 6% • 75%



• Molecule 1: RNA-binding protein FUS

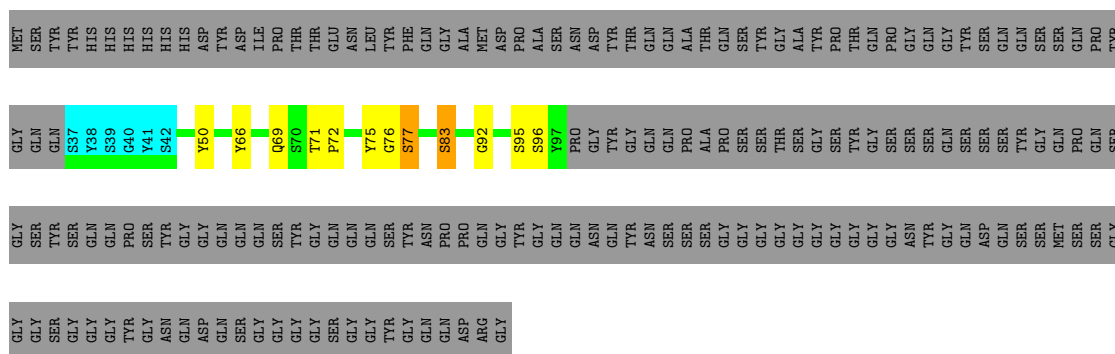
Chain I: 16% 6% 75%



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: RNA-binding protein FUS

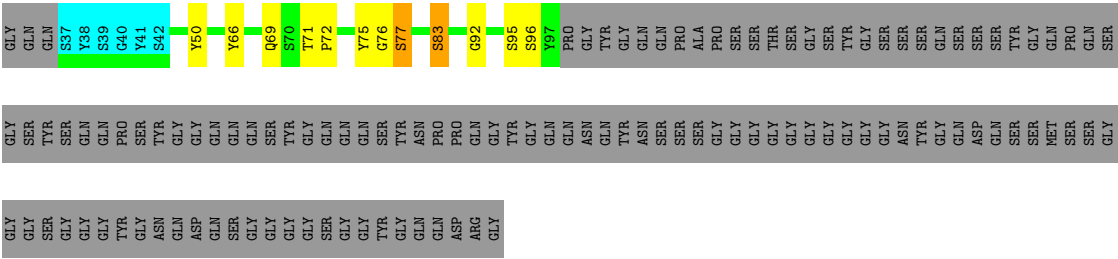
Chain A: 18% 6% 75%



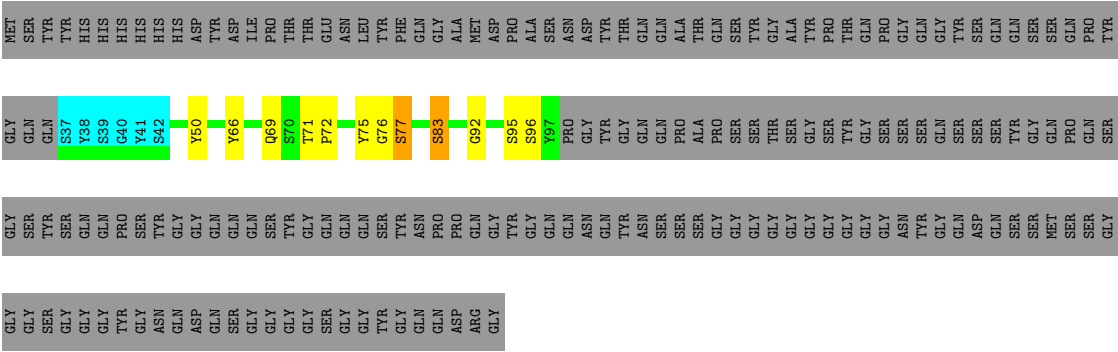
• Molecule 1: RNA-binding protein FUS

Chain B: 18% 6% 75%

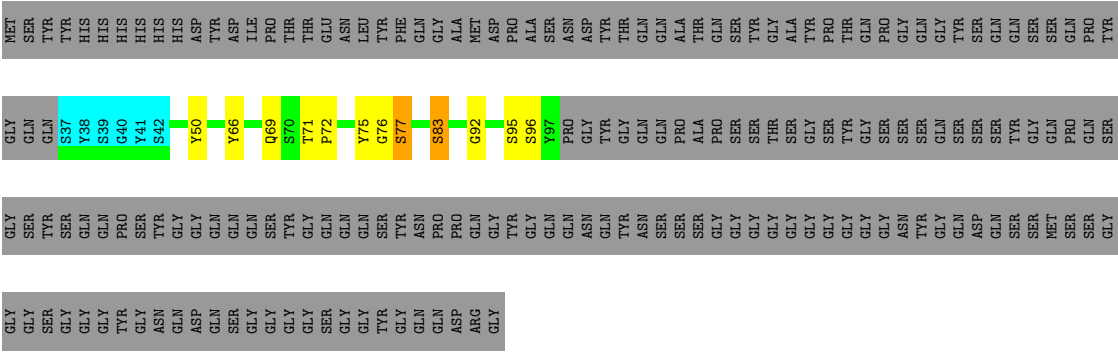




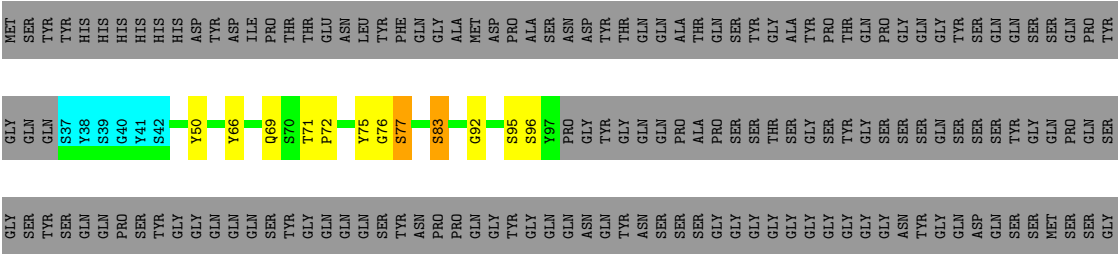
• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



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

- Molecule 1: RNA-binding protein FUS

Chain F: 18% . . . 75%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ASP	ILE	PRO	THR	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	MET	ASP	ASP	PRO	PRO	ALA	SER	ASN	ASP	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	GLN	GLN	PRO	PRO	GLY	GLY	GLY	TYR	SER	SER	SER	SER	GLN	GLN	PRO
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GLY	GLN	GLN	S37	Y38	S39	G40	Y41	S42		Y50		Y66		Q69	S70	T71	P72		Y75	G76	S77		S83		G92		S95	S96	Y97	PRO	PRO	GLY	GLY	TYR	GLY	GLN	GLN	PRO	PRO	ALA	PRO	PRO	PRO	SER	SER	SER	THR	SER	GLY	TYR	GLY	SER	SER	SER	GLN	PRO	GLN
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[illegible]

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

- Molecule 1: RNA-binding protein FUS

Chain G: 18% ... 75%

[illegible]

GLY	GLN	GLM	GLN	S37	Y38	S39	G40	Y41	S42	Y50	Y66	Q69	S70	T71	P72	Y75	G76	S77	S83	G92	S95	S96	Y97	PRO	PRO	GLY	GLY	GLY	GLN	GLN	PRO	PRO	ALA	PRO	PRO	SER	SER	THR	SER	SER	SER	SER	SER	SER	TYR	GLN	GLN	PRO	GLN
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[illegible]

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%

[illegible]

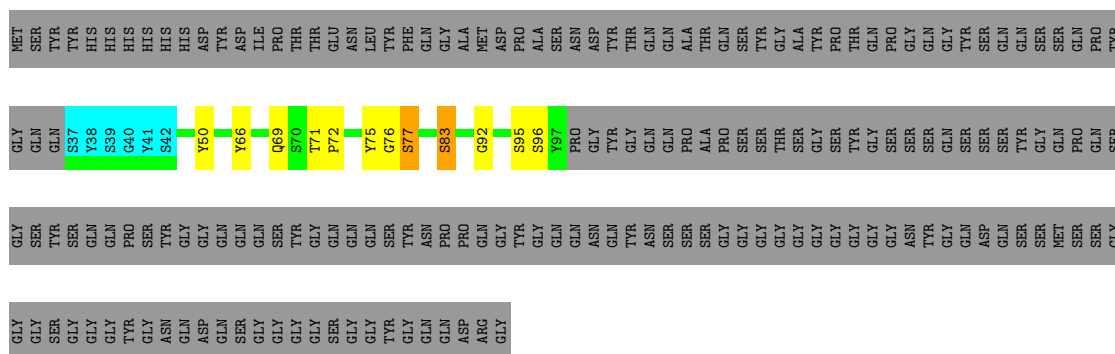
GLY	GLN	GLN	S37	Y38	S39	G40	Y41	S42	Y50	Y66	Q69	S70	T71	P72	Y75	G76	S77	S83	G92	S95	S96	S97	PRO	PRO	GLY	GLY	GLY	GLN	GLN	PRO	ALA	ALA	PRO	PRO	SER	SER	SER	THR	SER	GLY	SER	SER	SER	SER	SER	TYR	GLN	GLN	PRO	GLN
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GLY	SER	Tyr	SER	GLN	GLN	PRO	PRO	Tyr	GLY	GLY	GLN	GLN	GLN	GLN	GLN	Tyr	Tyr	SER	ASN	ASN	PRO	PRO	GLN	GLN	GLY	GLY	Tyr	GLY	GLN	GLN	ASN	ASN	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLN	GLN	ASP	GLN	GLN	SER	SER	SER	MET	MET	SER	SER
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ASP
ARG
GLY

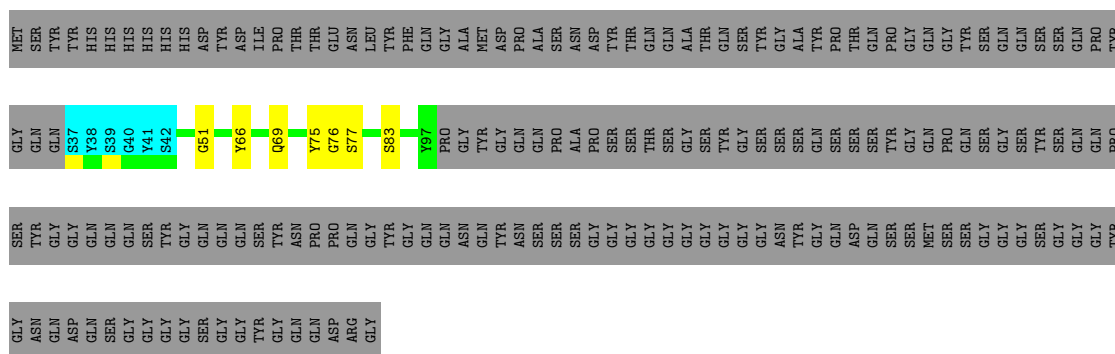
- Molecule 1: RNA-binding protein FUS

Chain I: 18% 2% 2% 75%

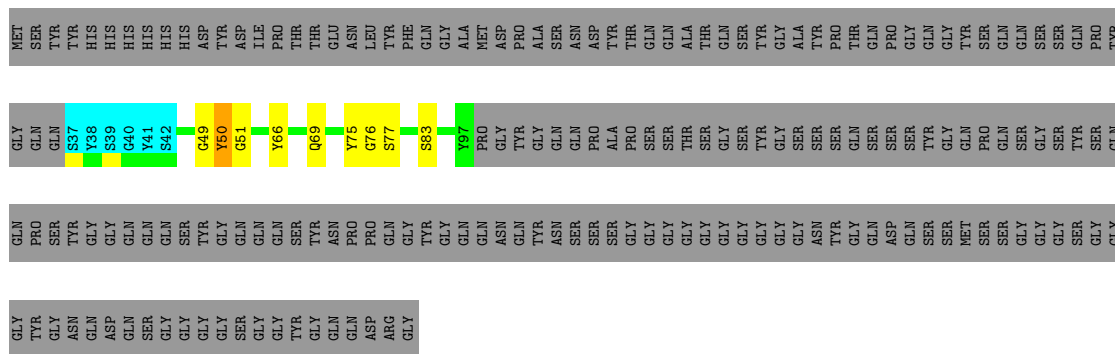


4.2.4 Score per residue for model 4

- Molecule 1: RNA-binding protein FUS

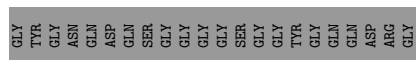
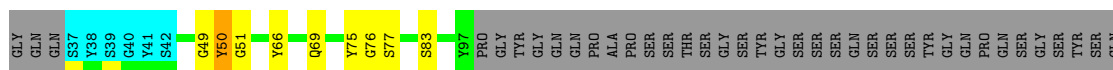


- Molecule 1: RNA-binding protein FUS

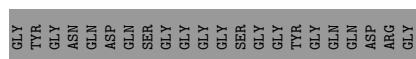
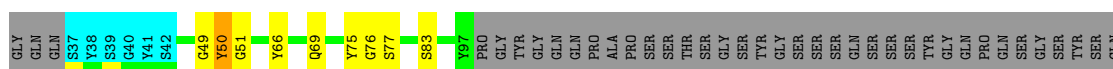


- Molecule 1: RNA-binding protein FUS

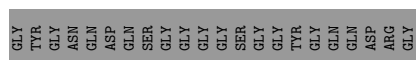
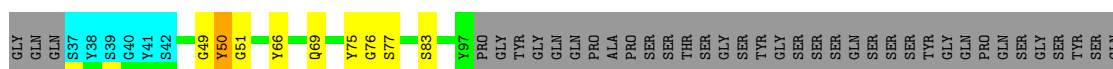




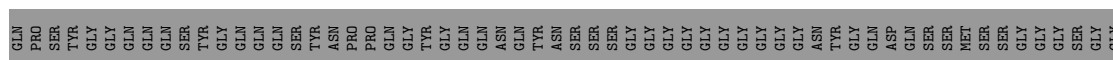
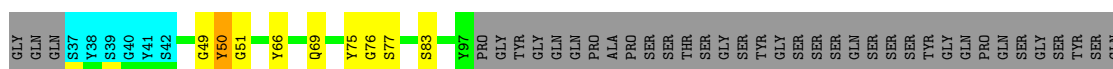
- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS

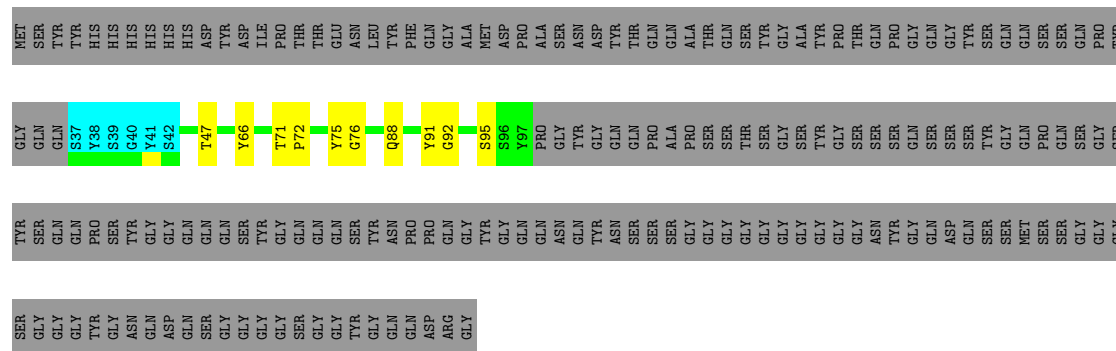


GLY
TYR
GLY
ASN
GLN
ASP
GLN
SER
GLY
GLY
GLY
GLY
SER
GLY
GLY
TYR
GLY
GLN
GLN
ASP
ARG
GLY

4.2.5 Score per residue for model 5

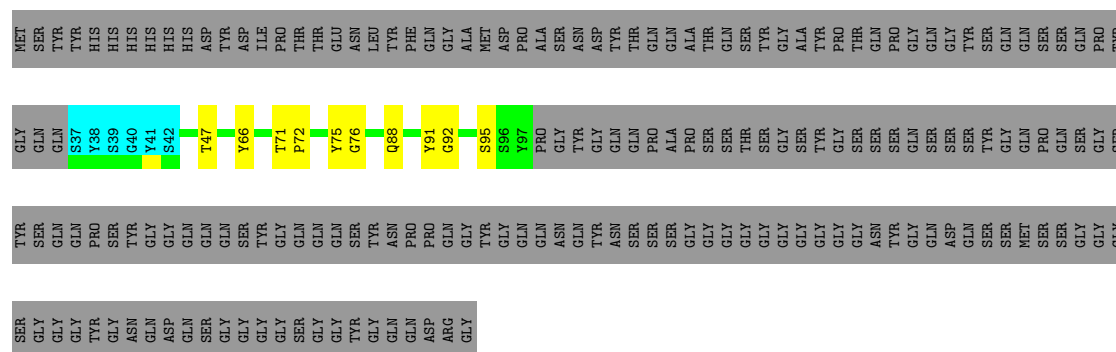
- Molecule 1: RNA-binding protein FUS

Chain A:



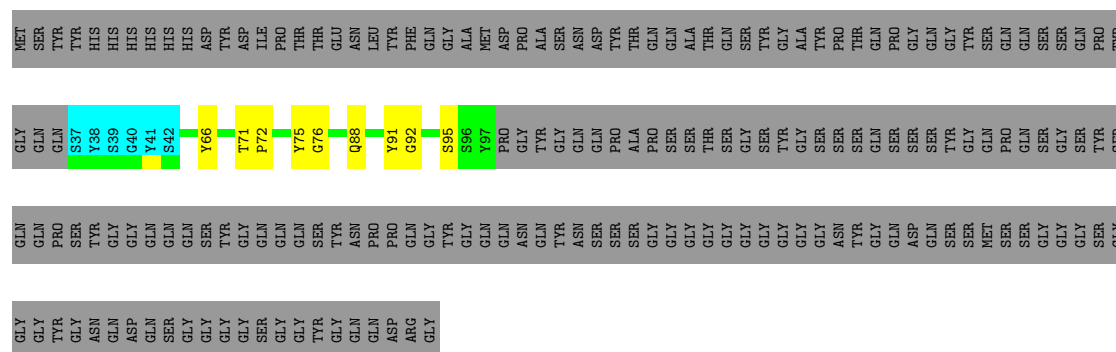
- Molecule 1: RNA-binding protein FUS

Chain B:  19% 22% 11% 75%



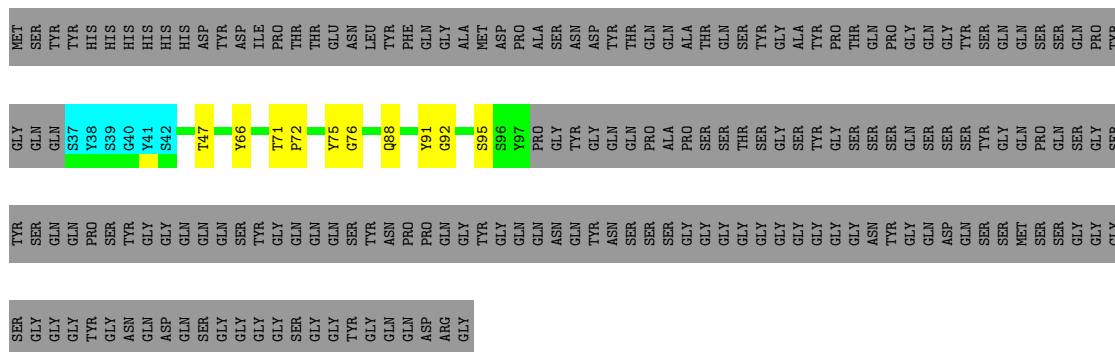
- Molecule 1: RNA-binding protein FUS

Chain C: 19% . . 75%

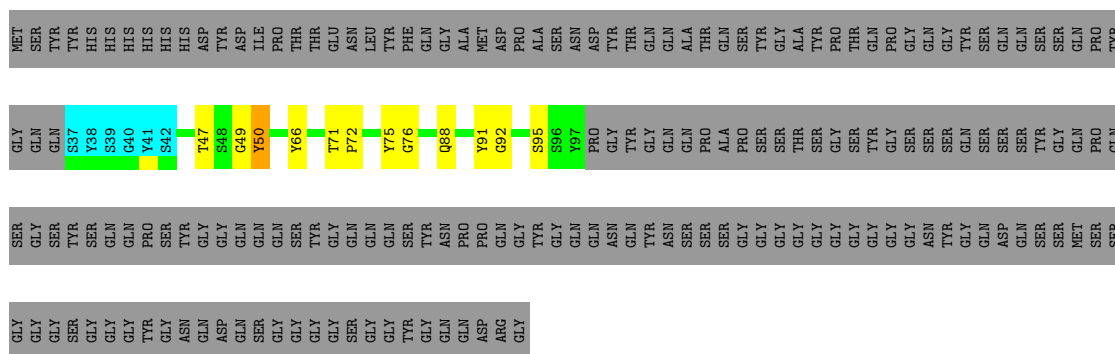


- Molecule 1: RNA-binding protein FUS

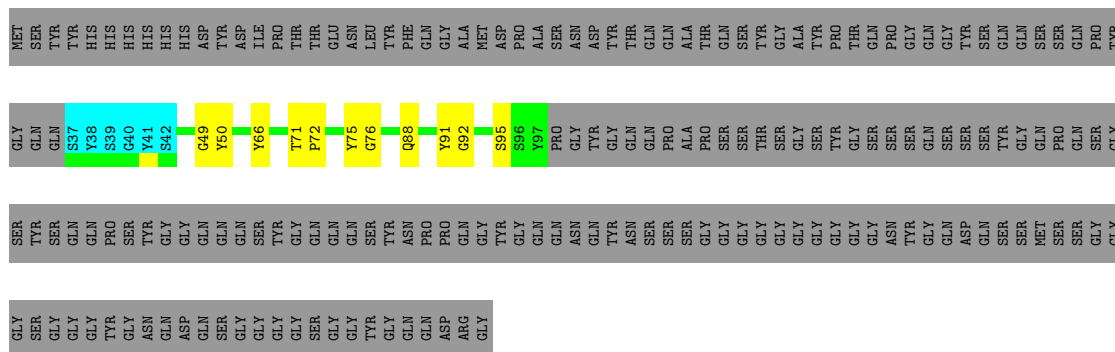
Chain D:  19% 1% 1% 75%



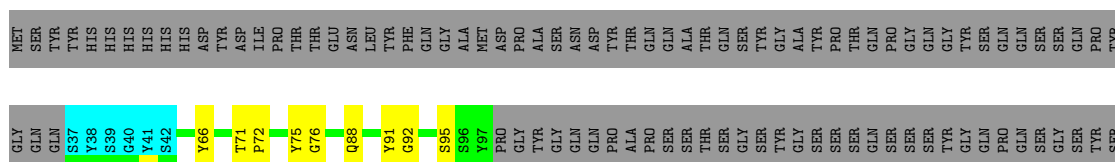
- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



[illegible]

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:  19% 75%

[illegible]

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	PRO	PRO	SER	SER	SER	THR	SER	SER	GLY	GLY	TYR	GLY	SER	SER	GLN	SER	SER	SER	SER	TYR	GLY	GLN	PRO	PRO	GLN	GLN	SER	SER	GLY
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[illegible]

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:  18% 5% 75%

MET	TYR	SER	THR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	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	THR	GLN	PRO	GLY	GLN	GLY	TYR	SER	GLN	PRO	TYR
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GLY	GLN	GLN	S37	Y38	S39	G40	Y41	S42	G49	Y50	Y66	T71	P72	Y75	O76	Q88	Y91	G92	S95	S96	Y97	PRO	GLY	TYR	GLY	GLN	GLN	PRO	ALA	ALA	PRO	PRO	SER	SER	SER	THR	SER	SER	GLY	SER	SER	SER	GLN	SER	SER	GLY	GLN	PRO	PRO	GLN	SER	SER
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SER	Tyr.	Ser.	Gln	Gln	Pro	Ser	Tyr	Gly	Gln	Gln	Gln	Gln	Asn	Asn	Pro	Pro	Gln	Gly	Tyr	Gln	Gln	Tyr	Asn	Ser	Ser	Ser	Gly	Gly	Gly	Gly	Gly	Gly	Gly	Gly	Gly	Gly	Asn	Gly	Tyr	Gln	Gln	Gln	ASP	Gln	Ser	Gln	Ser	MET	Ser	Ser	Ser	Ser	Gly
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GLY SER GLY GLY GLY TYR GLY GLN ASN GLN ASP GLN SER SER GLY GLY GLY GLY GLY TYR GLY GLN GLN ASP ARG GLY

4.2.6 Score per residue for model 6

- Molecule 1: RNA-binding protein FUS

Chain A:  17% . . . 75%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	ASP	ASP	PRO	THR	THR	GLU	ASN	LEU	PHE	TYR	GLY	GLN	GLY	ALA	ALA	MET	ASP	ASP	PRO	ALA	SER	ASN	ASN	GLN	GLN	THR	THR	GLN	ALA	ALA	THR	THR	GLN	GLN	SER	TYR	GLY	ALA	ALA	TYR	PRO	PRO	GLN	GLN	PRO	GLY	GLY	TYR	SER	SER	SER	SER	GLN	GLN	PRO
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[illegible][illegible]

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

- Molecule 1: RNA-binding protein FUS

Chain B: 17% 5% .. 75%

NET	SER	TYR	THR	THR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	ASP	ASP	PRO	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	NET	ASP	PRO	ALA	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	GLN	SER	SER	TYR	GLY	ALA	TYR	PRO	PRO	THR	THR	GLN	PRO	GLY	GLN	GLY	GLY	TYR	SER	SER	SER	GLN	PRO
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[illegible][illegible]

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
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- Molecule 1: RNA-binding protein FUS

Chain C:  17% . . . 75%

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

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

- Molecule 1: RNA-binding protein FUS

Chain D: 17% 5% .. 75%

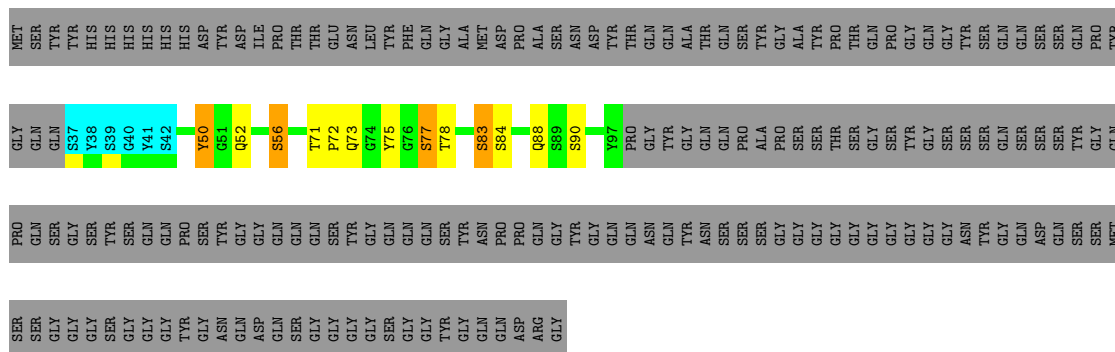
[illegible][illegible]

GLY	GLN	PRO	PRO	GLN	GLN	SER.	TYR	SER	SER	GLN	GLN	PRO	PRO	SER	TYR	GLY	GLY	GLN	GLN	GLN	GLN	GLN	ASN	ASN	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLN	GLN	ASP	GLP	GLN	GLN	
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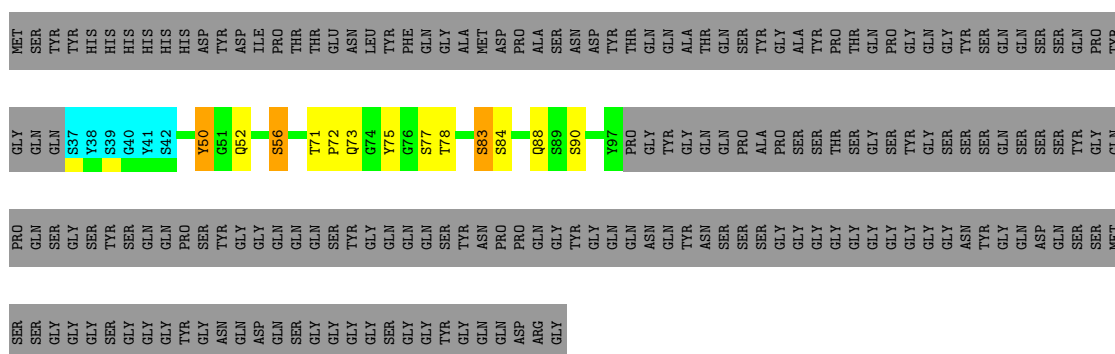
SER	MET	SER	SER	GLY	GLY	GLY	SER	GLY	GLY	GLY	TYR	GLY	ASN	GLN	ASP	GLN	SER	GLY	GLY	GLY	SER	GLY	GLY	TYR	GLY	GLN	ASP	GLN	ARG	GLY
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- Molecule 1: RNA-binding protein FUS

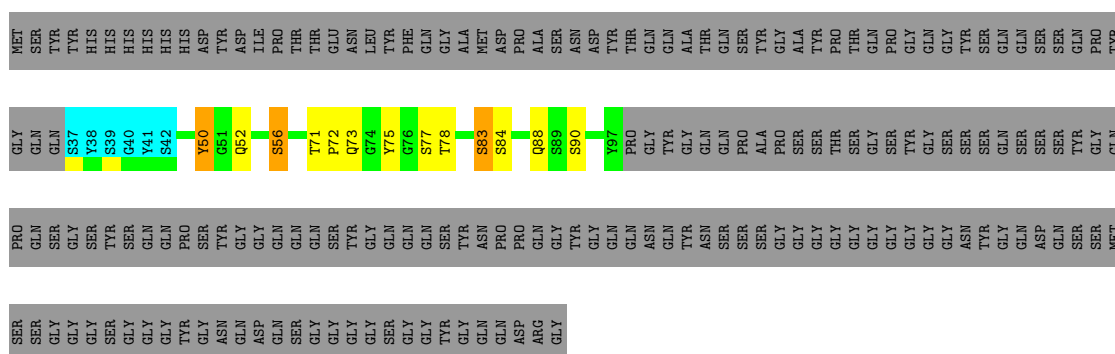
Chain E: 17% 75%



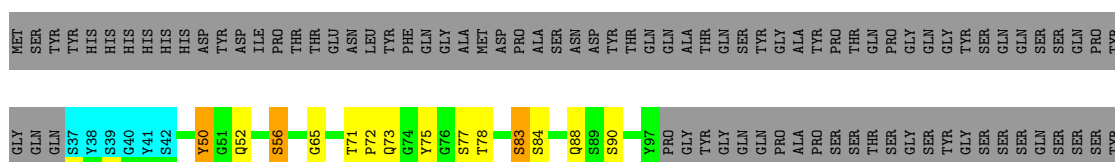
- Molecule 1: RNA-binding protein FUS

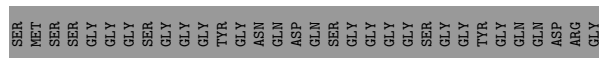
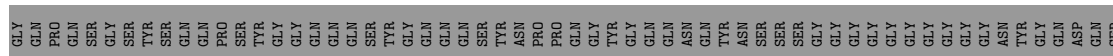


- Molecule 1: RNA-binding protein FUS

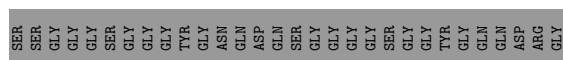
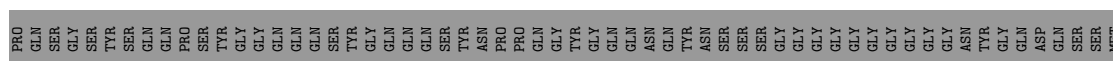
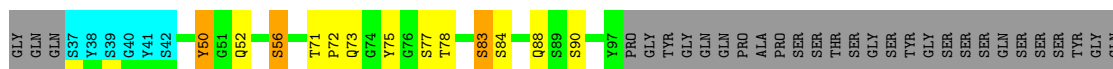


- Molecule 1: RNA-binding protein FUS



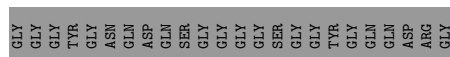
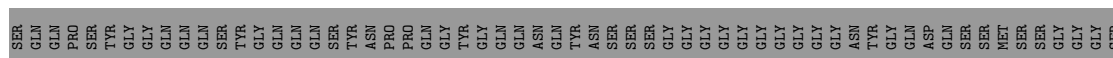
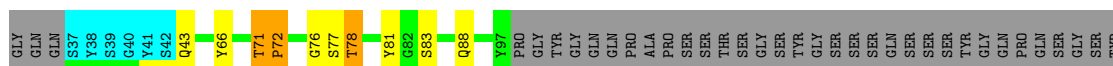


- Molecule 1: RNA-binding protein FUS

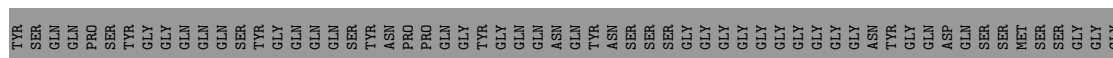
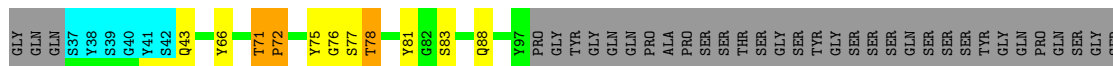
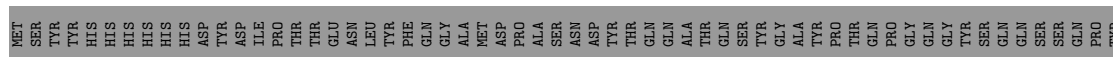


4.2.7 Score per residue for model 7

- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



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% ... 75%

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

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% ... 75%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	TYR	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	MET	ASP	PRO	ALA	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	THR	THR	GLN	GLN	PRO	GLY	GLN	GLY	TYR	SER	SER	GLN	PRO
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GLY	GLN	GLN	S37	Y38	S39	G40	Y41	S42	Q43		Y66		T71	P72		Y75	C76	S77	T78		Y81	G82	S83		Q88		Y97	PRO	GLY	TYR	GLY	GLN	GLN	PRO	ALA	PRO	SER	SER	THR	SER	SER	GLY	TYR	GLY	GLN	GLN	PRO	PRO	GLN	GLN	GLY	GLY
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[illegible]

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: 17% . . . 75%

NET	TYR	TYR	TYR	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	THR	GLN	GLN	ALA	ALA	THR	THR	THR	THR	GLN	GLN	PRO	GLY	GLY	GLY	TYR	SER	SER	GLN	GLN	PRO
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[illegible]

SER	GLY	SER	Tyr	SER	SER	GLN	GLN	PRO	PRO	SER	SER	Tyr	GLY	GLY	GLN	GLN	GLN	GLN	GLN	GLN	ASN	ASN	PRO	PRO	GLN	GLY	Tyr	Tyr	GLY	GLY	GLN	GLN	GLN	ASN	ASN	Tyr	Tyr	ASN	SER	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	ASP	GLN	SER	SER	SER	MET	SER
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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
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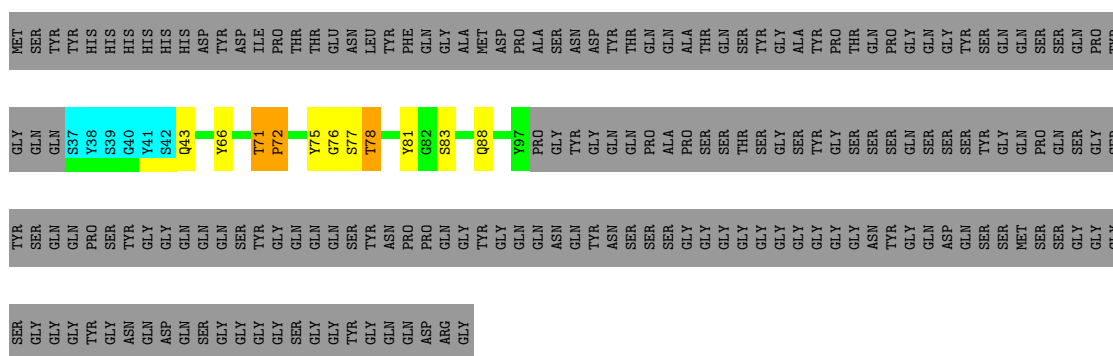
- Molecule 1: RNA-binding protein FUS

Chain F:  18% ... 75%



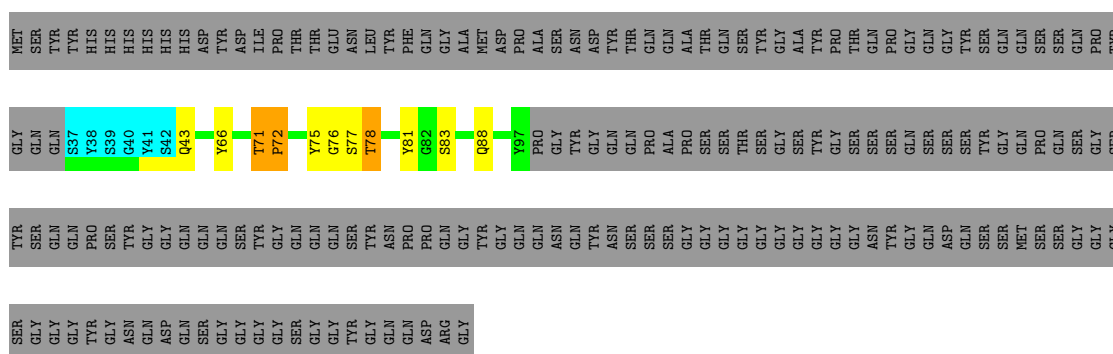
- Molecule 1: RNA-binding protein FUS

Chain G:  18% ... 75%



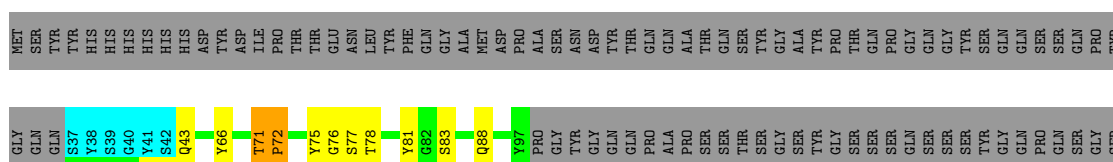
- Molecule 1: RNA-binding protein FUS

Chain H: 18% ... 75%



- Molecule 1: RNA-binding protein FUS

Chain I:  18% ... 75%



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

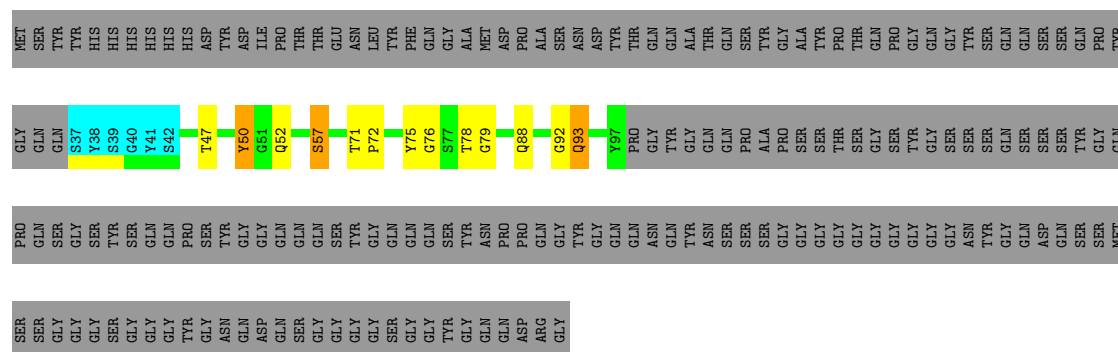
SER SER GLY GLY GLY SER SER GLY GLY TYR GLY ASN ASN GLN ASP GLN SER SER GLY GLY GLY SER GLY GLY TYR GLY GLN GLN ASP ARG GLY

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

[illegible]

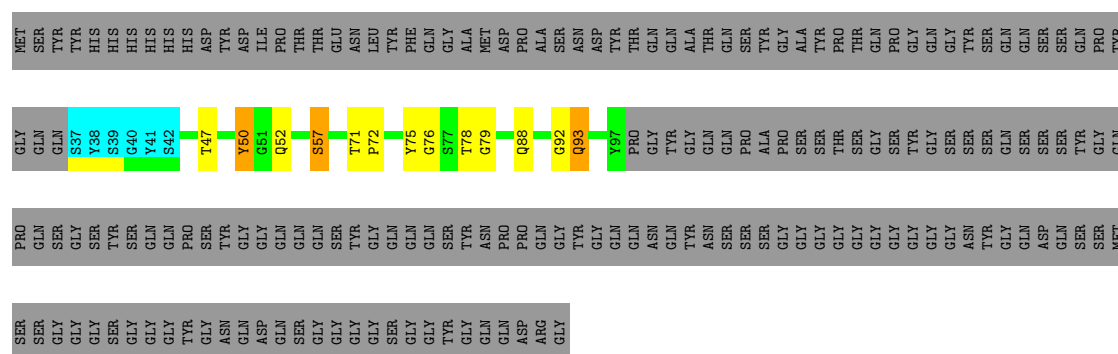
- Molecule 1: RNA-binding protein FUS

Chain D: 17% ... 75%



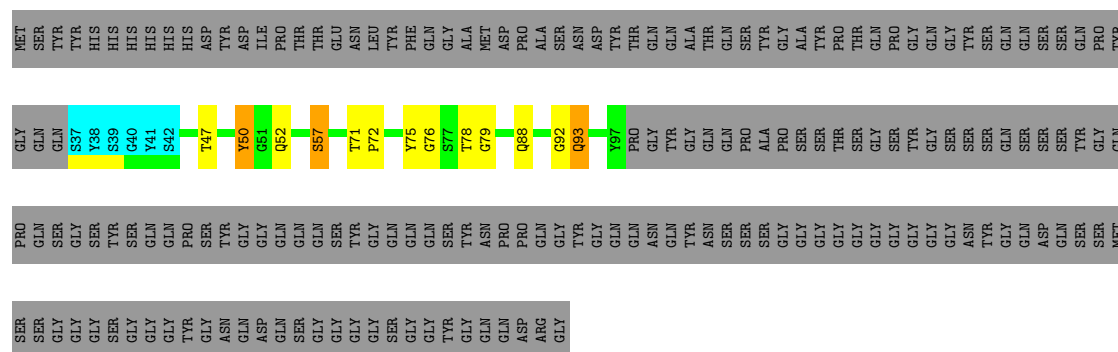
- Molecule 1: RNA-binding protein FUS

Chain E: 17% ... 75%



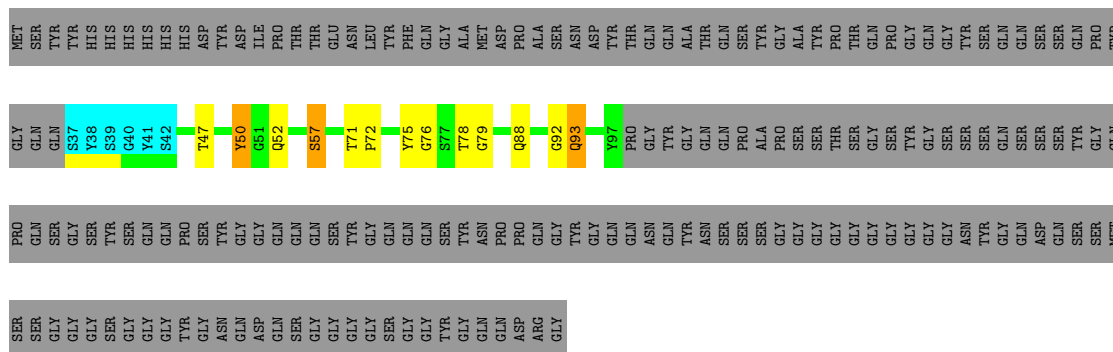
- Molecule 1: RNA-binding protein FUS

Chain F:  17% ... 75%

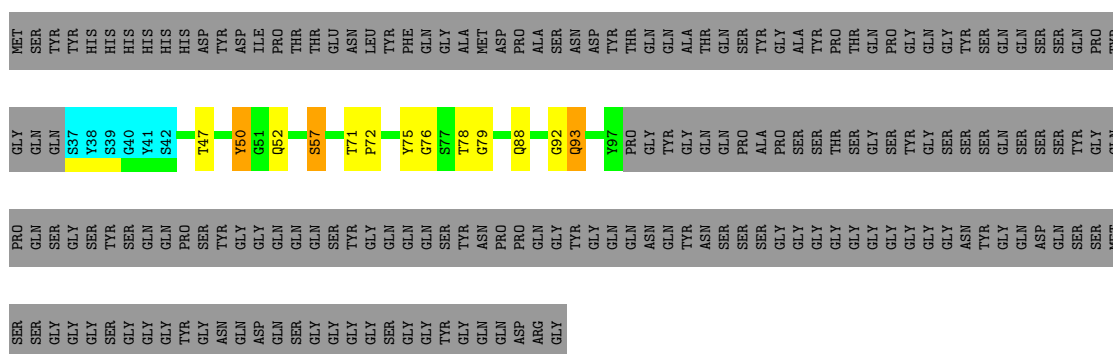


- Molecule 1: RNA-binding protein FUS

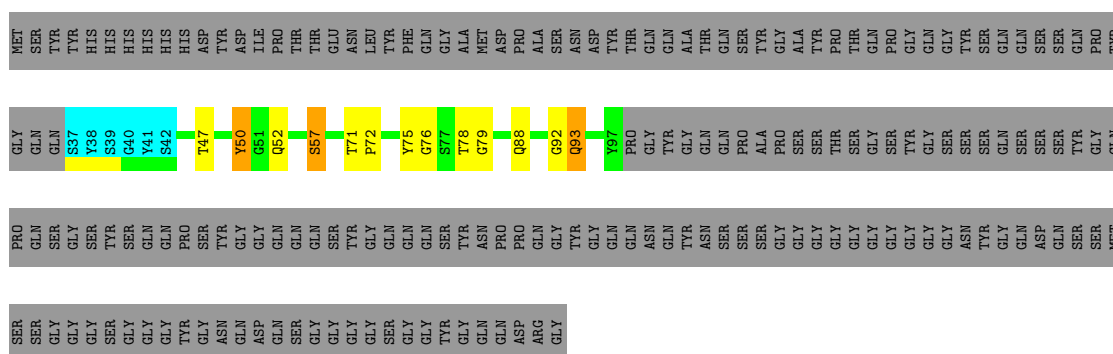
Chain G:  17% ... 75%



- Molecule 1: RNA-binding protein FUS



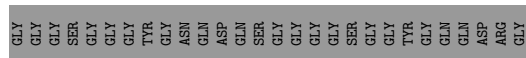
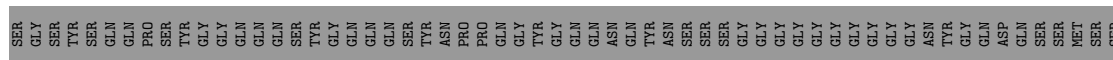
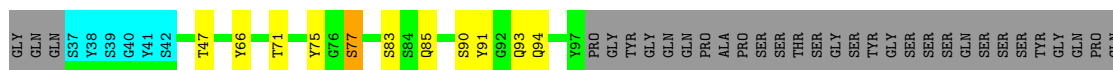
- Molecule 1: RNA-binding protein FUS



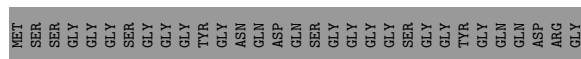
4.2.9 Score per residue for model 9

- Molecule 1: RNA-binding protein FUS

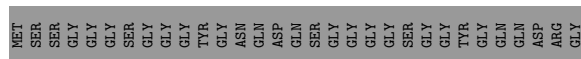
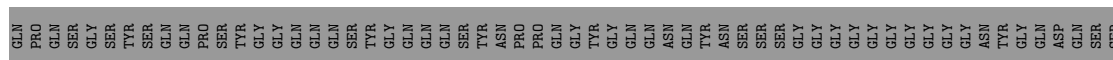




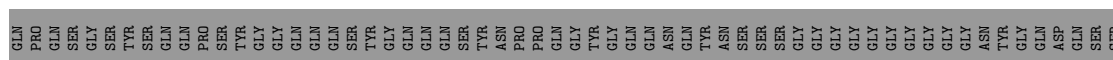
- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



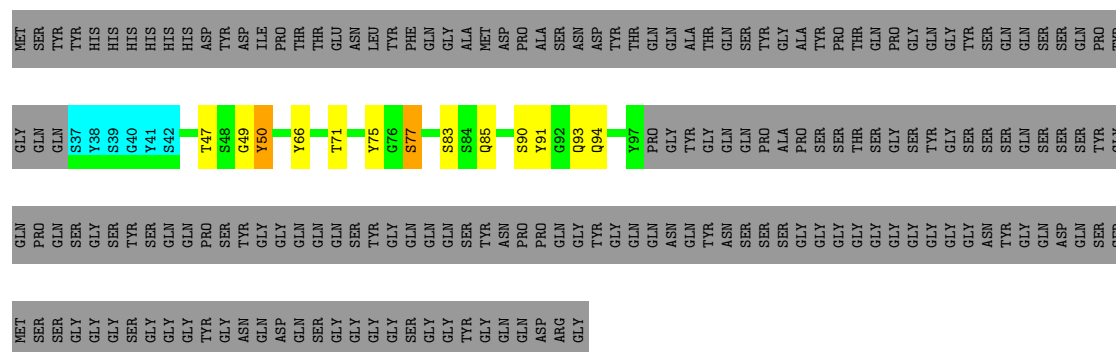
- Molecule 1: RNA-binding protein FUS



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

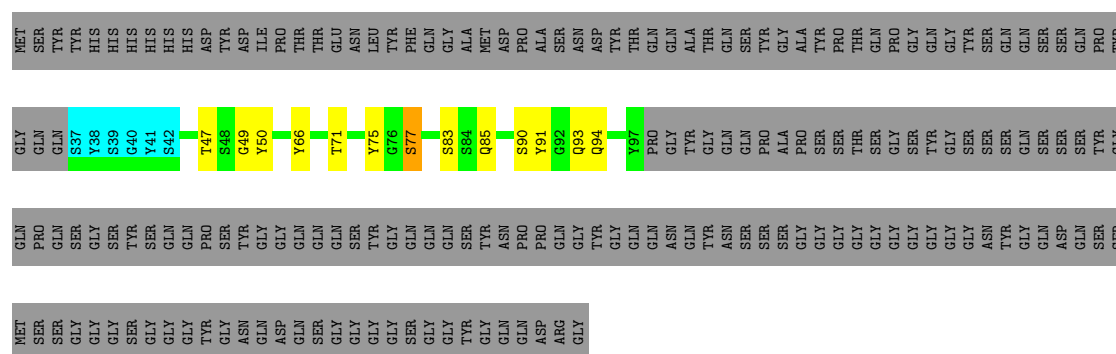
- Molecule 1: RNA-binding protein FUS

Chain E: 17% 5% .. 75%



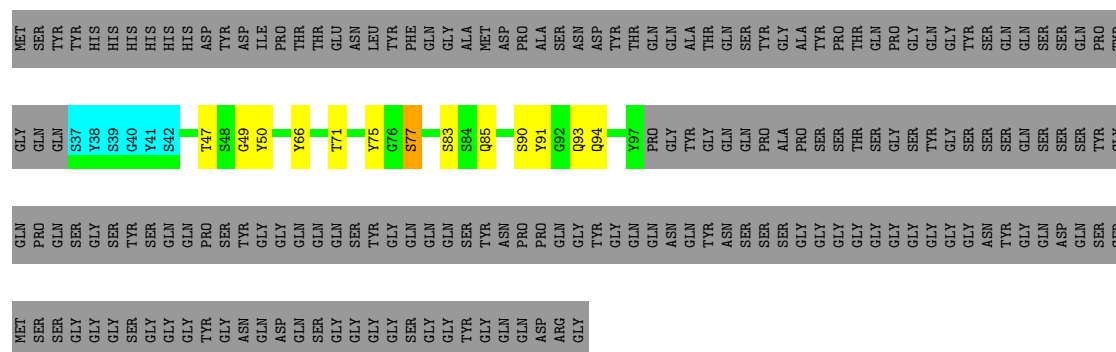
- Molecule 1: RNA-binding protein FUS

Chain F:  17% 5% 78%



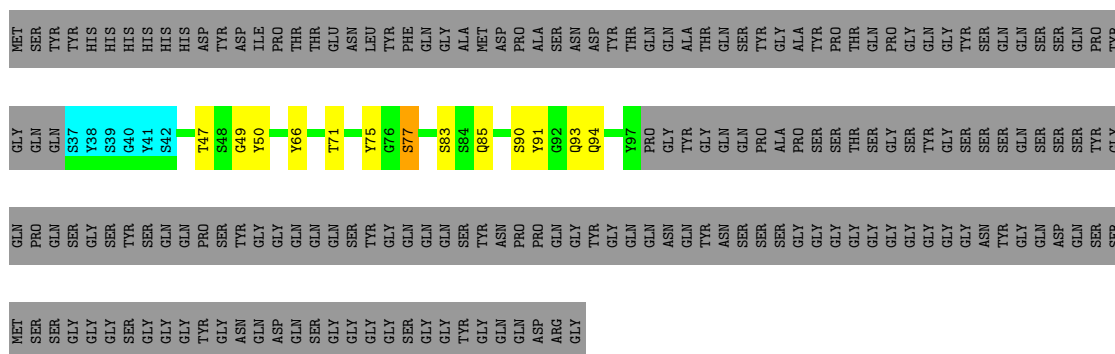
- Molecule 1: RNA-binding protein FUS

Chain G: 17% 5% 78%

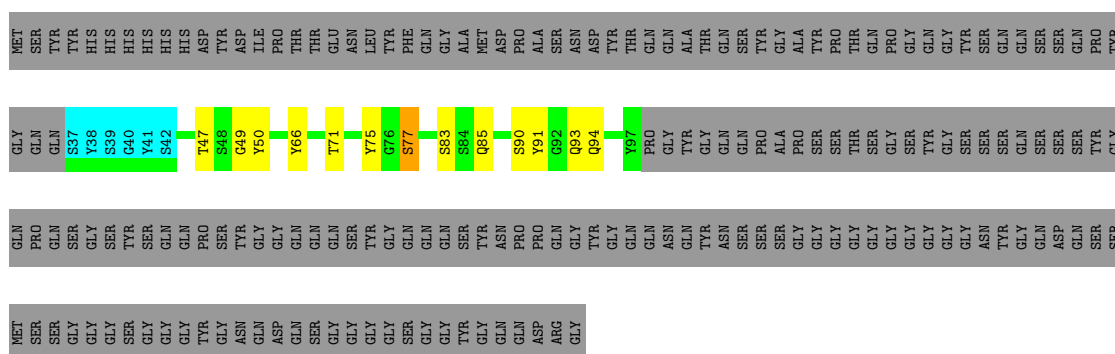


- Molecule 1: RNA-binding protein FUS

Chain H:  17% 5% 78%

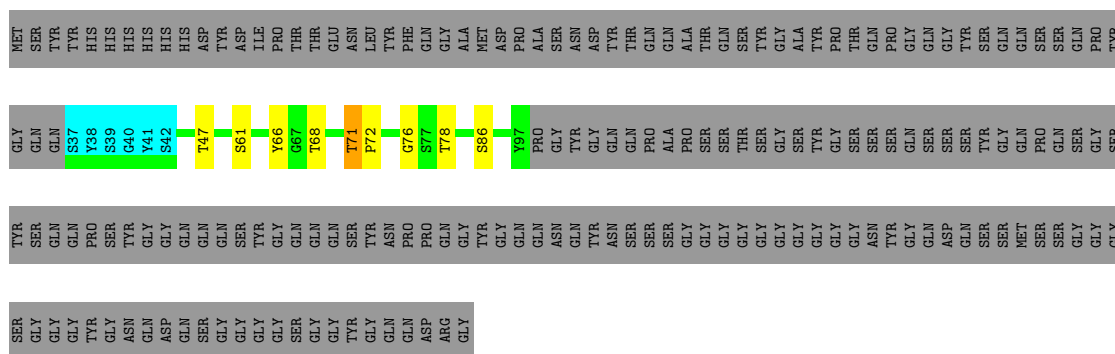


- Molecule 1: RNA-binding protein FUS



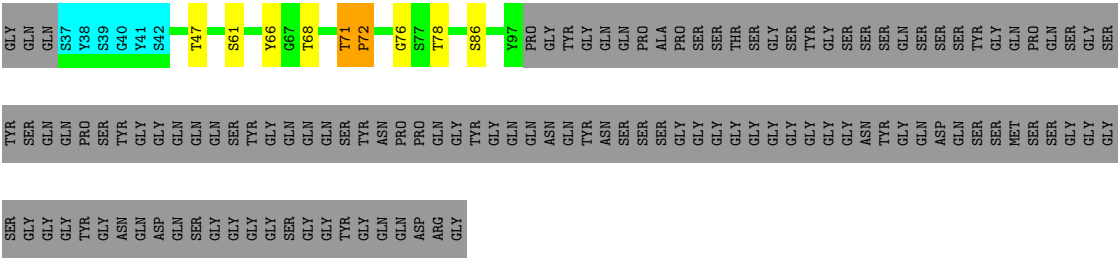
4.2.10 Score per residue for model 10

- Molecule 1: RNA-binding protein FUS

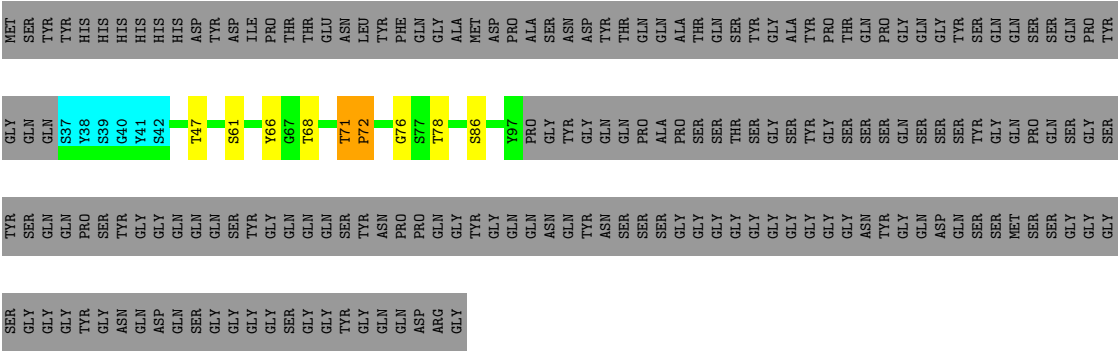


- Molecule 1: RNA-binding protein FUS

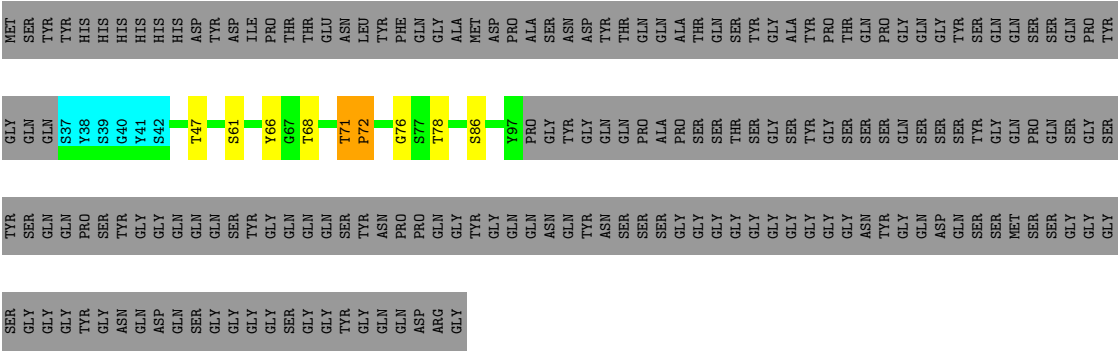




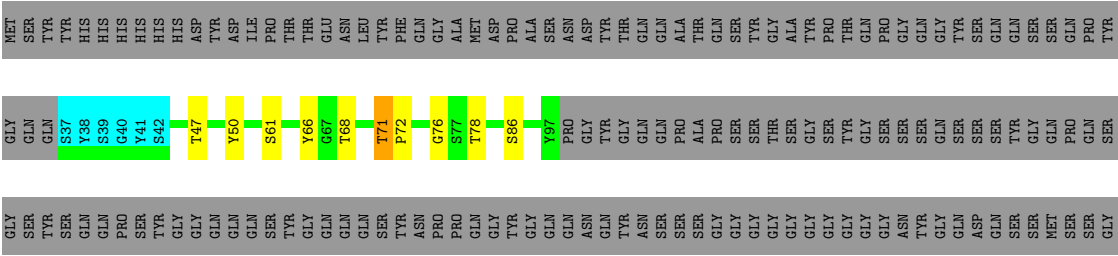
• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



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

- Molecule 1: RNA-binding protein FUS

Chain F:  19% ... 75%

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

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

- Molecule 1: RNA-binding protein FUS

Chain G:  19% ... 75%

[illegible]

GLY	GLN	GLM	GLM	S37	Y38	S39	G40	Y41	S42	T47	S61	Y66	G67	T68	T71	P72	G76	S77	T78	S86	Y97	P90	GLY	TYR	GLY	GLN	GLM	GLN	PRO	ALA	PRO	PRO	PRO	SER	SER	SER	THR	SER	GLY	GLY	TYR	GLY	SER	SER	GLM	GLN	PRO	GLM	GLN	GLY
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[illegible]

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:  19% ... 75%

[illegible]

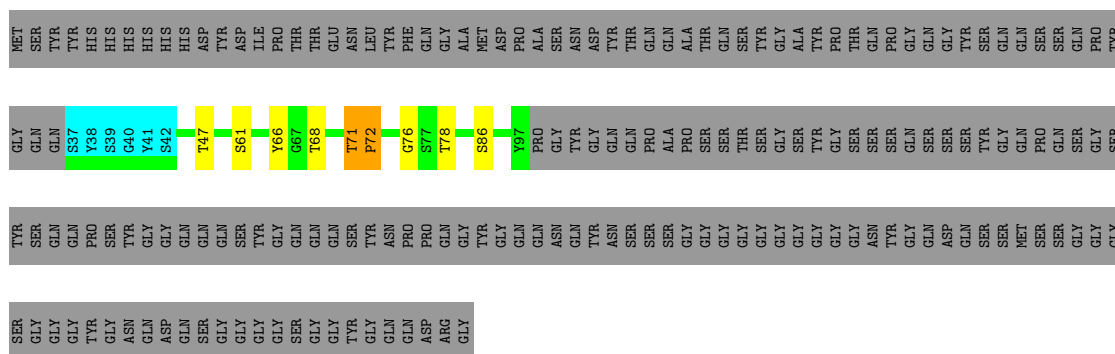
GLY	GLN	GLN	S37	Y38	S39	G40	Y41	S42	T47	S61	Y66	G67	T68	T71	P72	G76	S77	T78	S86	Y97	PRO	GLY	TYR	GLY	GLN	GLN	PRO	ALA	PRO	PRO	PRO	SER	SER	THR	SER	GLY	GLY	TYR	GLY	SER	SER	GLM	GLM	PRO	GLN	SER	GLY
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[illegible]

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

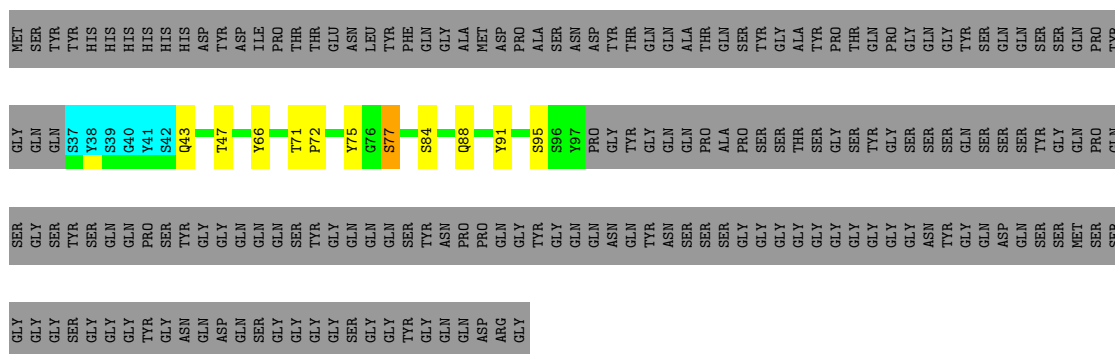
- Molecule 1: RNA-binding protein FUS

Chain I: 19% ... 75%

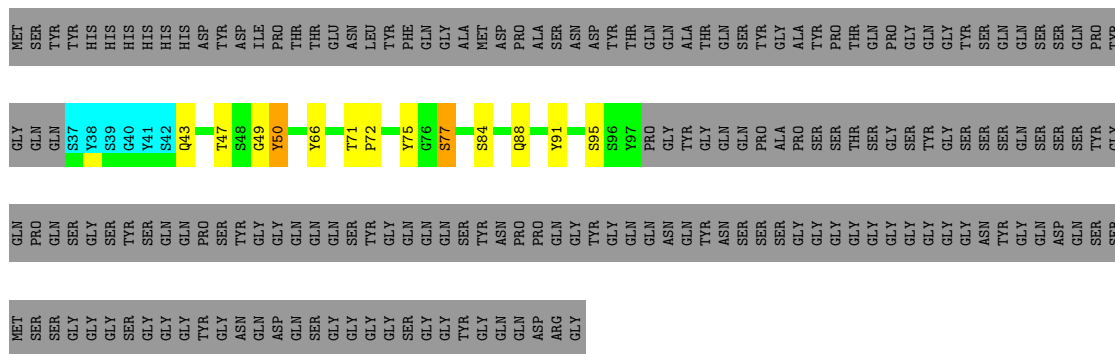


4.2.11 Score per residue for model 11

- Molecule 1: RNA-binding protein FUS

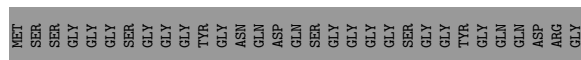


- Molecule 1: RNA-binding protein FUS

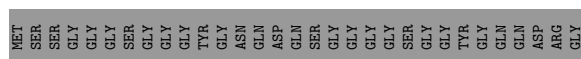


- Molecule 1: RNA-binding protein FUS

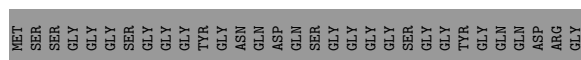




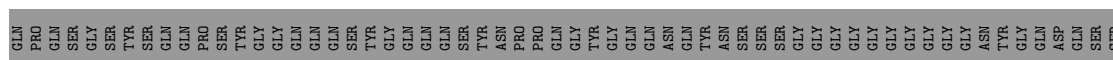
Chain D:  17% 5% .. 75%

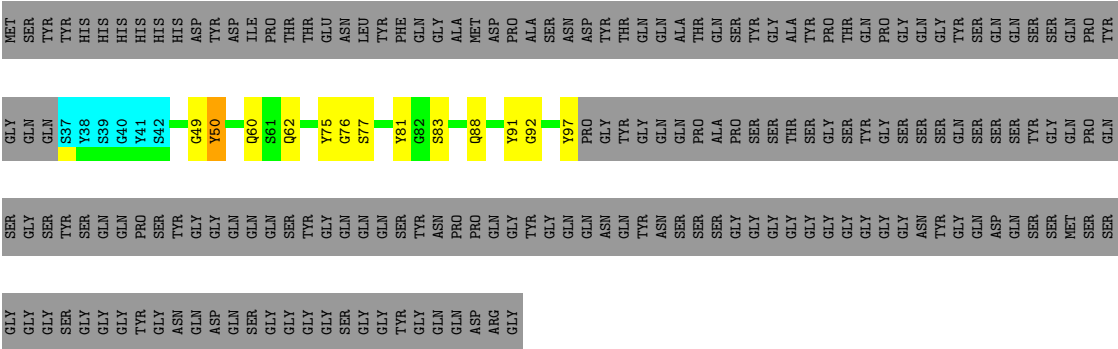


Chain E:  17% 5% 78%

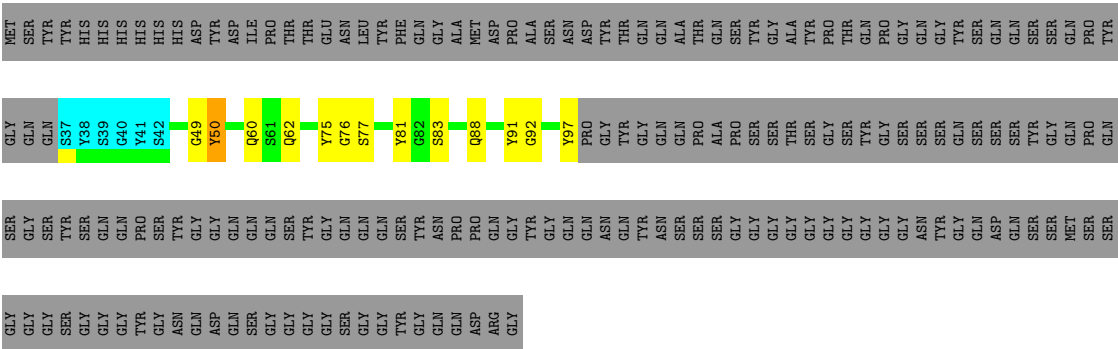


Chain F:  17% 5% .. 75%

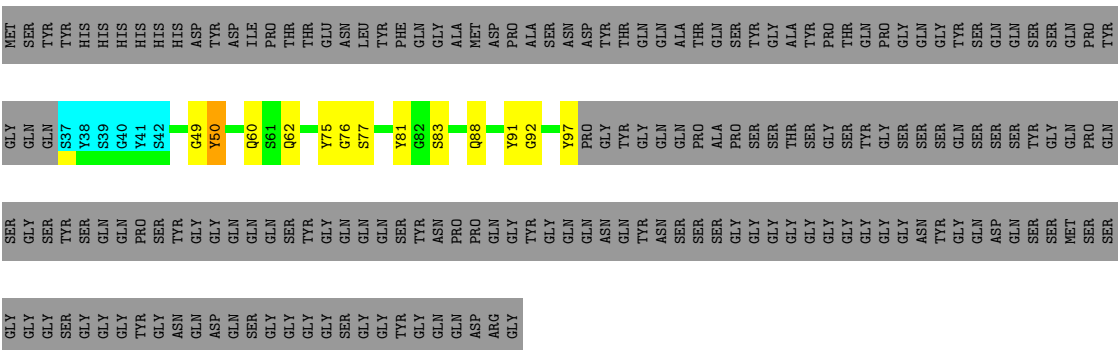




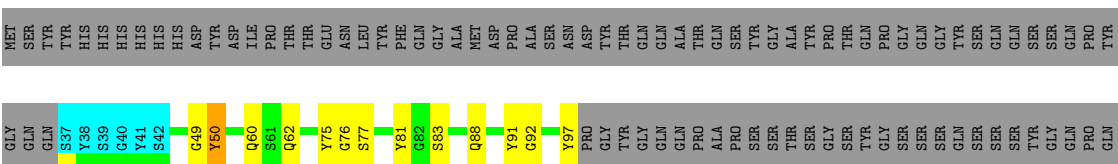
• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



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: 18% 5% • 75%

[illegible]

- Molecule 1: RNA-binding protein FUS

Chain C: 18% 5% 77%

[illegible]

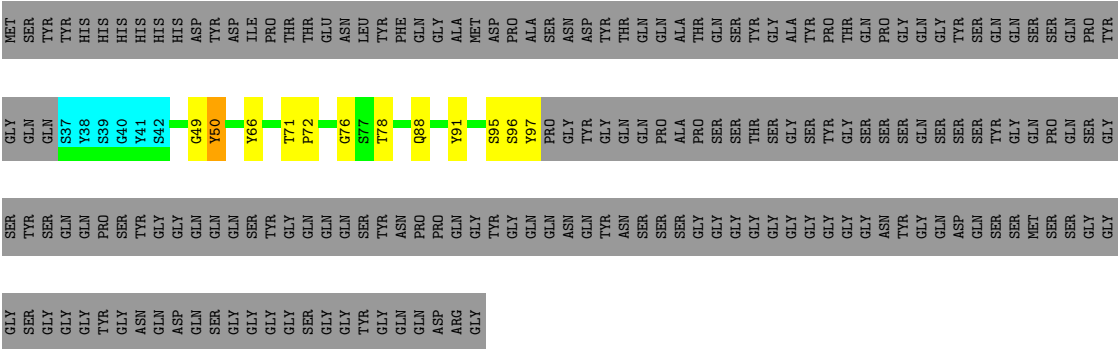
- Molecule 1: RNA-binding protein FUS

Chain D:  18% 5% 77%

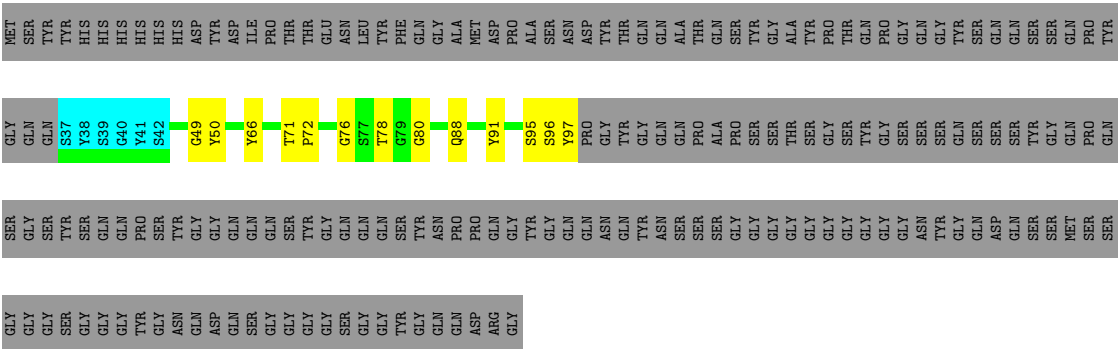
[illegible]

- Molecule 1: RNA-binding protein FUS

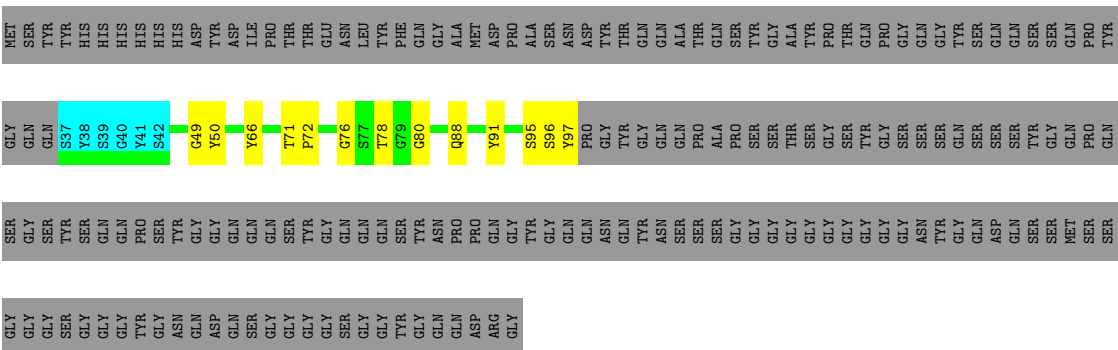
Chain E:  18% 5% 77%



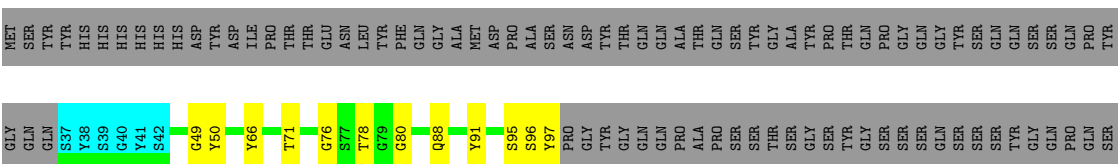
• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



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% 77%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	MET	ASP	ALA	PRO	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	GLN	SER	SER	GLY	ALA	TYR	PRO	PRO	GLN	GLY	GLY	GLY	TYR	SER	GLN	GLN	GLN	GLN	GLN	PRO
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GLY	GLN	GLN	S37	Y38	S39	S40	Y41	S42	Q43	Q44	Y50	G51	Q52		Y58	T68	T71	P72	Q73	G74	Y75	S83		S86		S90	Y97	PRO	GLY	GLY	TYR	GLY	GLN	GLN	GLN	PRO	PRO	ALA	ALA	PRO	PRO	PRO	SER	SER	SER	THR	SER	SER	GLY	SER	TYR	GLY	GLN	GLN	GLN	SER	SER	SER	SER	TYR	GLY	GLN	CLN
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[illegible]

SER	GLY	GLY	GLY	SER	GLY	GLY	TYR	GLY	ASN	GLN	ASP	GLN	SER	GLY	GLY	GLY	SER	GLY	TYR	GLY	GLN	GLN	ASP	ARG	GLY
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- Molecule 1: RNA-binding protein FUS

Chain D:  18% 5% 77%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	TYR	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	MET	ASP	PRO	ALA	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	THR	THR	GLN	GLN	PRO	GLY	GLN	GLY	TYR	SER	SER	GLN	PRO
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GLY	GLN	GLN	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	S48	S49	S50	S51	S52	S53	S54	S55	S56	S57	S58	S59	S60	S61	S62	S63	S64	S65	S66	S67	S68	S69	S70	S71	S72	S73	S74	S75	S76	S77	S78	S79	S80	S81	S82	S83	S84	S85	S86	S87	S88	S89	S90	S91	S92	S93	S94	S95	S96	S97	S98	S99	S100	S101	S102	S103	S104	S105	S106	S107	S108	S109	S110	S111	S112	S113	S114	S115	S116	S117	S118	S119	S120	S121	S122	S123	S124	S125	S126	S127	S128	S129	S130	S131	S132	S133	S134	S135	S136	S137	S138	S139	S140	S141	S142	S143	S144	S145	S146	S147	S148	S149	S150	S151	S152	S153	S154	S155	S156	S157	S158	S159	S160	S161	S162	S163	S164	S165	S166	S167	S168	S169	S170	S171	S172	S173	S174	S175	S176	S177	S178	S179	S180	S181	S182	S183	S184	S185	S186	S187	S188	S189	S190	S191	S192	S193	S194	S195	S196	S197	S198	S199	S200	S201	S202	S203	S204	S205	S206	S207	S208	S209	S210	S211	S212	S213	S214	S215	S216	S217	S218	S219	S220	S221	S222	S223	S224	S225	S226	S227	S228	S229	S230	S231	S232	S233	S234	S235	S236	S237	S238	S239	S240	S241	S242	S243	S244	S245	S246	S247	S248	S249	S250	S251	S252	S253	S254	S255	S256	S257	S258	S259	S260	S261	S262	S263	S264	S265	S266	S267	S268	S269	S270	S271	S272	S273	S274	S275	S276	S277	S278	S279	S280	S281	S282	S283	S284	S285	S286	S287	S288	S289	S290	S291	S292	S293	S294	S295	S296	S297	S298	S299	S300	S301	S302	S303	S304	S305	S306	S307	S308	S309	S310	S311	S312	S313	S314	S315	S316	S317	S318	S319	S320	S321	S322	S323	S324	S325	S326	S327	S328	S329	S330	S331	S332	S333	S334	S335	S336	S337	S338	S339	S340	S341	S342	S343	S344	S345	S346	S347	S348	S349	S350	S351	S352	S353	S354	S355	S356	S357	S358	S359	S360	S361	S362	S363	S364	S365	S366	S367	S368	S369	S370	S371	S372	S373	S374	S375	S376	S377	S378	S379	S380	S381	S382	S383	S384	S385	S386	S387	S388	S389	S390	S391	S392	S393	S394	S395	S396	S397	S398	S399	S400	S401	S402	S403	S404	S405	S406	S407	S408	S409	S410	S411	S412	S413	S414	S415	S416	S417	S418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552
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[illegible]

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SER
GLY
GLY
TYR
GLY
GLN
GLN
ASP
ARG
GLY

- Molecule 1: RNA-binding protein FUS

Chain E:  18% 5% 77%

MET	TYR	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	PHE	THR	GLN	GLY	ALA	MET	ASP	ALA	PRO	ASP	ASN	TYR	THR	GLN	GLN	ALA	ALA	THR	GLN	GLN	GLN	GLN	GLY	GLY	GLY	TYR	TYR	GLY	GLY	GLN	GLN	GLN	PRO
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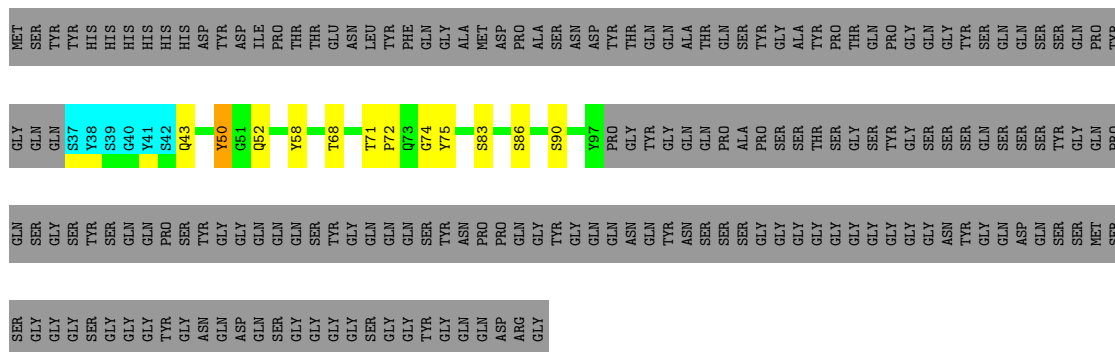
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GLN	SER	GLY	Tyr	SER	GLN	GLN	PRO	SER	Tyr	GLY	GLY	GLN	GLN	GLN	SER	Tyr	GLY	ASN	PRO	PRO	GLN	GLY	Tyr	GLY	GLN	GLN	GLN	GLN	Tyr	ASN	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLN	ASP	GLN	GLN	SER	SER	MET
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SER	GLY	GLY	GLY	SER	GLY	GLY	TYR	GLY	ASN	GLN	ASP	GLN	SER	GLY	GLY	GLY	GLY	SER	GLY	TYR	GLY	GLN	GLN	ASP	ARG	GLY
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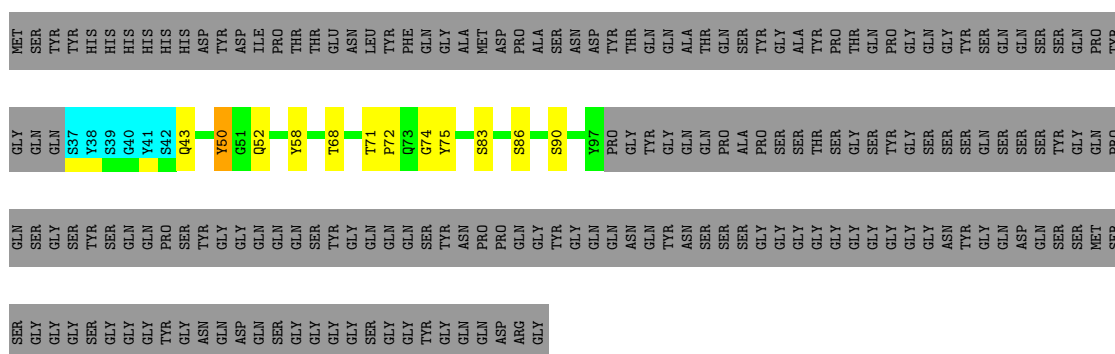
- Molecule 1: RNA-binding protein FUS

Chain F:  18% 5% 77%



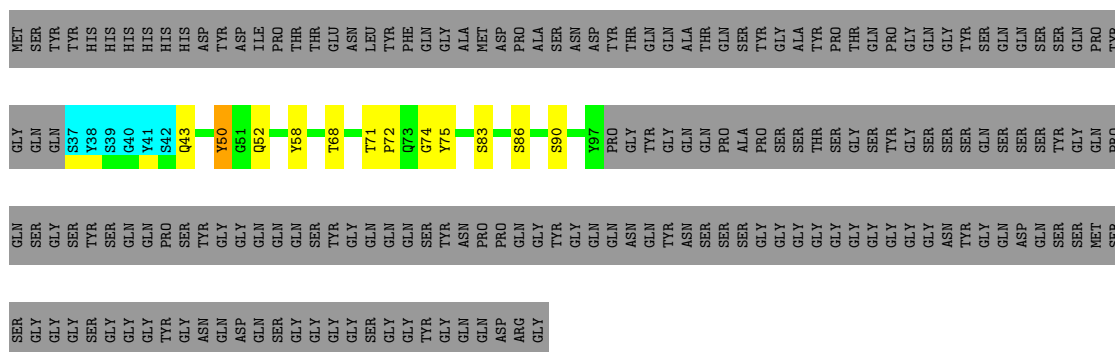
- Molecule 1: RNA-binding protein FUS

Chain G:  18% 5% 77%



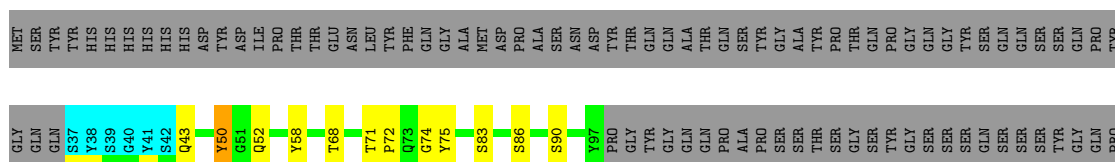
- Molecule 1: RNA-binding protein FUS

Chain H:  18% 5% 77%



- Molecule 1: RNA-binding protein FUS

Chain I:  18% 5% • 77%



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

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

[illegible]

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: 17% ... 75%

MET	TYR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	MET	ASP	ALA	PRO	ALA	SER	ASN	ASP	TYR	THR	GLN	GLN	ALA	ALA	THR	GLN	SER	SER	GLY	ALA	TYR	PRO	PRO	GLN	GLN	PRO	GLY	GLY	GLN	TYR	SER	SER	GLN	GLN	PRO	TYR
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SER	MET	SER	SER	GLY	GLY	SER	GLY	GLY	TYR	GLY	GLY	ASN	GLN	ASP	GLN	SER	GLY	GLY	GLY	SER	GLY	GLY	TYR	GLY	GLN	ASP	ARG	GLY
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- Molecule 1: RNA-binding protein FUS

Chain E:  17% • • • 75%

NET	TYR	TYR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	NET	ASP	PRO	ALA	ALA	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	GLN	SER	SER	GLY	ALA	ALA	TYR	THR	PRO	THR	GLN	PRO	PRO	GLY	GLN	GLY	GLY	TYR	SER	SER	GLN	GLN	PRO	TYR
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[illegible][illegible]

SER	MET	SER	SER	GLY	GLY	GLY	SER	GLY	GLY	TYR	ASN	GLN	ASP	GLN	SER	GLY	GLY	GLY	GLY	SER	GLY	GLY	TYR	GLY	GLN	ASP	GLY	ARG
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- Molecule 1: RNA-binding protein FUS

Chain F:  17% • • 75%

NET	TYR	TYR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	NET	ASP	PRO	ALA	ALA	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	GLN	SER	SER	GLY	ALA	ALA	TYR	THR	PRO	THR	GLN	PRO	PRO	GLY	GLY	GLN	GLY	TYR	SER	SER	GLN	GLN	PRO	TYR
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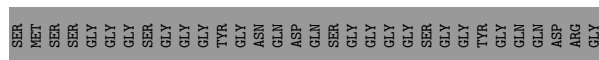
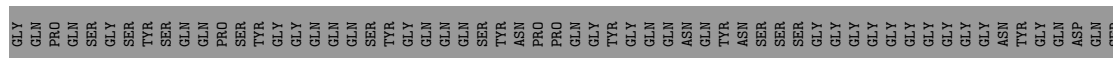
GLY	GLN	GLN	S37	S38	S39	G40	T41	S42	Q43	Y50	G51	Q52		S56	G59	G65	T71	P72	Y75		S83	S84	Q85		Q88		S95	S96	Y97	PRO	PRO	GLY	Tyr	GLY	GLN	GLN	PRO	ALA	PRO	PRO	PRO	SER	SER	THR	SER	GLY	Tyr	GLY	SER	SER	GLN	SER	SER	SER	Thr
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[illegible]

SER	MET	SER	SER	GLY	GLY	GLY	SER	GLY	GLY	TYR	ASN	GLN	ASP	GLN	SER	GLY	GLY	GLY	GLY	SER	GLY	GLY	TYR	GLY	GLN	ASP	GLY	ARG
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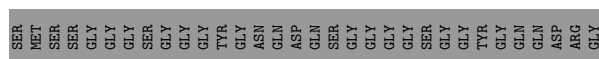
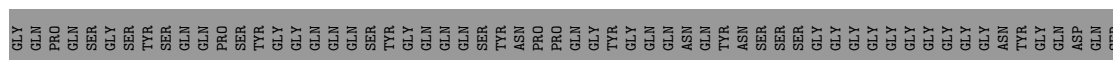
- Molecule 1: RNA-binding protein FUS

Chain G:  17% ... 75%



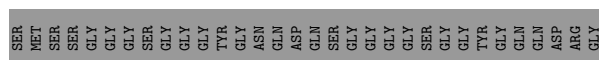
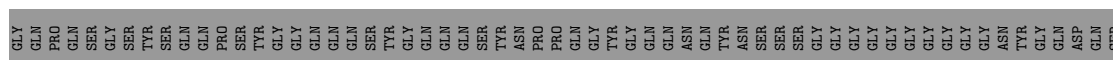
- Molecule 1: RNA-binding protein FUS

Chain B:  17% 6% 75%



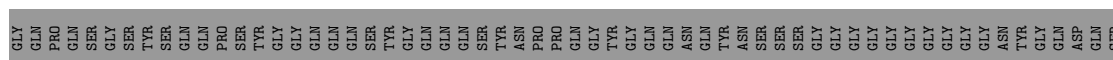
- Molecule 1: RNA-binding protein FUS

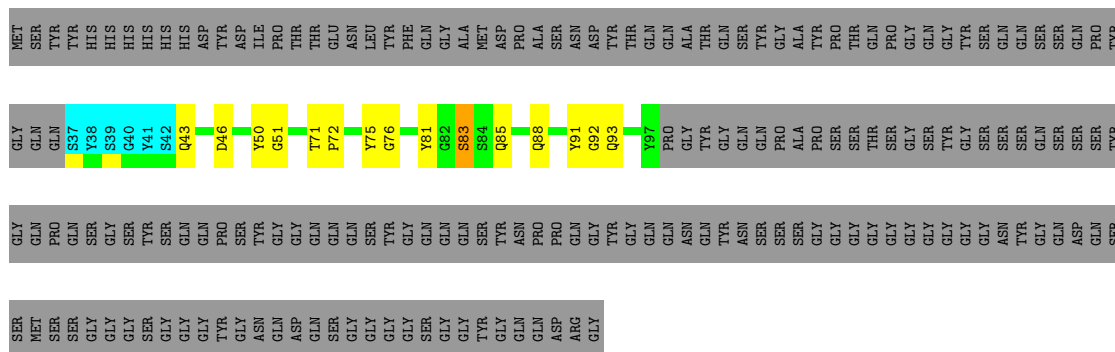
Chain C:  17% 6% 75%



- Molecule 1: RNA-binding protein FUS

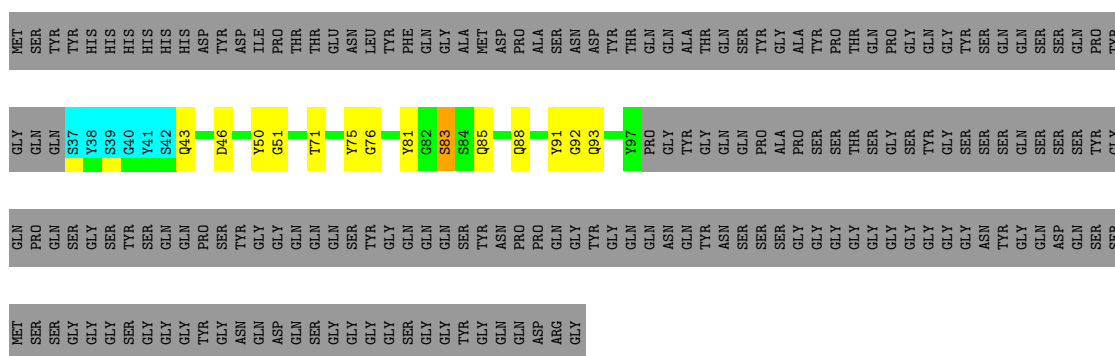
Chain D: 17% 6% 75%





• Molecule 1: RNA-binding protein FUS

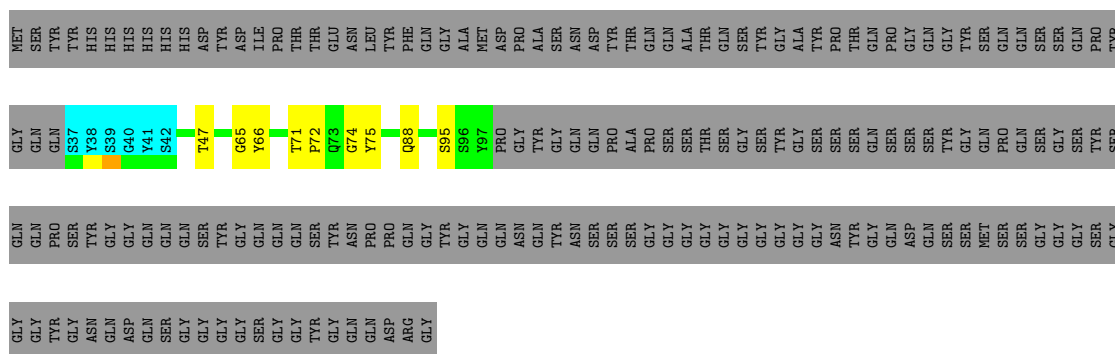
Chain I: 17% 5% 75%



4.2.17 Score per residue for model 17

• Molecule 1: RNA-binding protein FUS

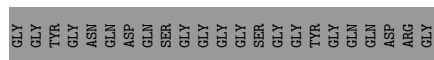
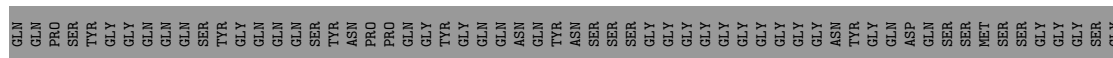
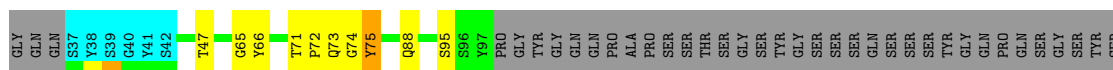
Chain A: 19% 1% 75%



• Molecule 1: RNA-binding protein FUS

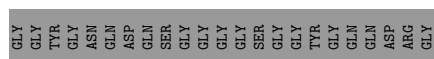
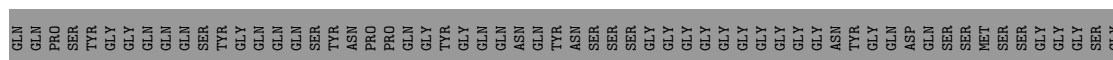
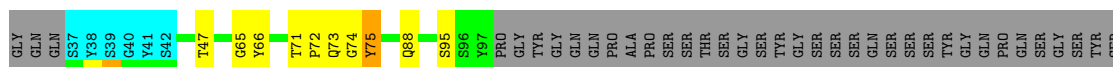
Chain B: 19% 1% 75%





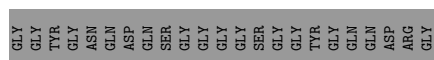
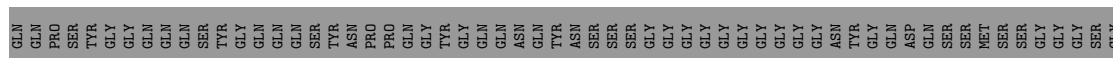
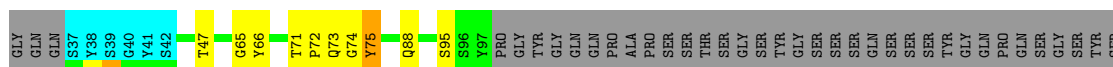
- Molecule 1: RNA-binding protein FUS

Chain C:  19% . . 75%



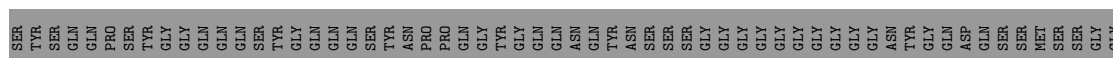
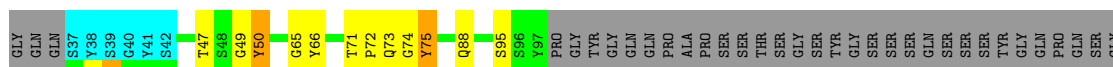
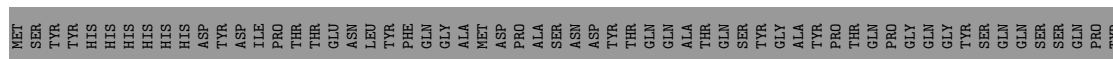
- Molecule 1: RNA-binding protein FUS

Chain D:  19% 2% 75%



- Molecule 1: RNA-binding protein FUS

Chain E:  18% • • 75%



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

- Molecule 1: RNA-binding protein FUS

Chain F: 19% 2% 2% 77%

MET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	ASP	TYR	ASP	ILE	PRO	THR	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	MET	ASP	ASP	PRO	PRO	ALA	SER	ASN	ASP	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	GLN	GLN	PRO	GLY	GLY	GLY	TYR	SER	SER	SER	SER	GLN	GLN	PRO
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	GLY	GLN	GLN	S37	Y38	S39	G40	Y41	S42	T47	G65	Y66	T71	P72	Q73	G74	Y75	Q88	S95	S96	Y97	PRO	PRO	GLY	TYR	GLY	GLN	GLN	PRO	ALA	PRO	PRO	SER	SER	THR	SER	SER	SER	GLY	SER	TYR	GLY	SER	SER	GLN	SER	SER	TYR	GLY	GLN	GLN	PRO	GLN	SER	SER	GLY	TYR
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[illegible]

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: 19% . . 75%

[illegible]

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

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: 19% 75%

[illegible]

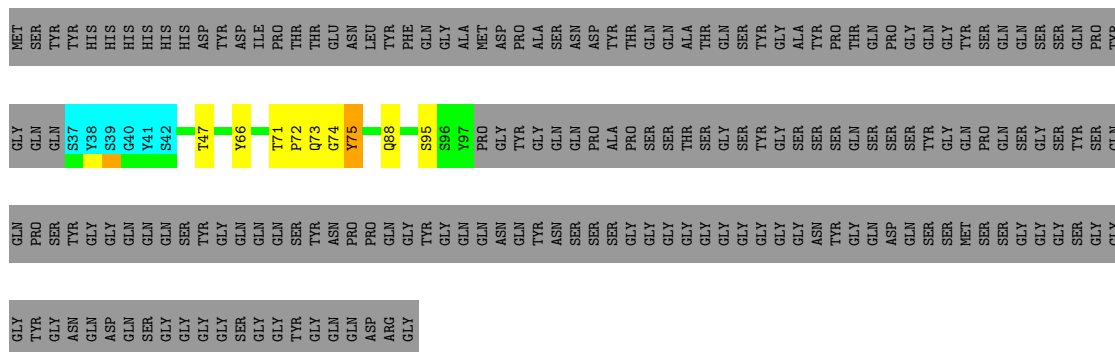
GLY	GLN	GLM	S37	Y38	S39	G40	Y41	S42	T47	G65	Y66	T71	P72	Q73	G74	Y75	Q88	S95	S96	Y97	PRO	GLY	GLY	TYR	GLY	GLN	GLM	GLN	PRO	PRO	ALA	PRO	PRO	SER	SER	SER	THR	SER	SER	GLY	SER	SER	TYR	GLY	SER	GLN	GLM	GLN	GLM	GLN	PRO	GLY	SER	TYR
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GLN	GLN	PRO	SER	TYR	GLY	GLN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

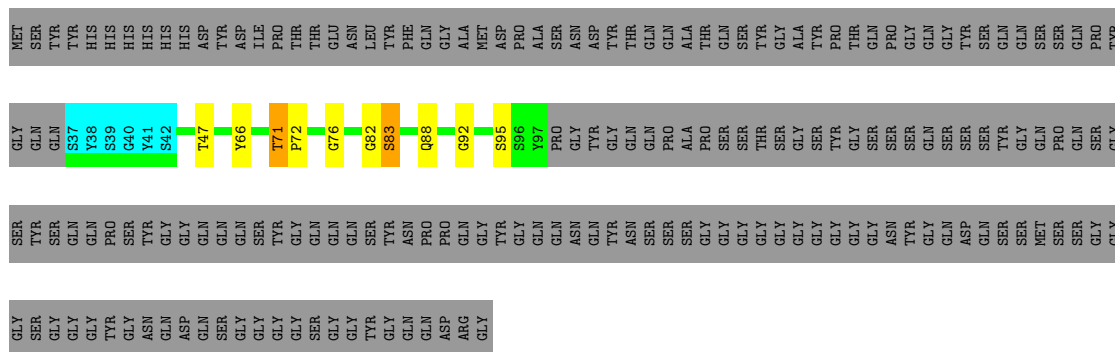
- Molecule 1: RNA-binding protein FUS

Chain I: 19% 2% 75%

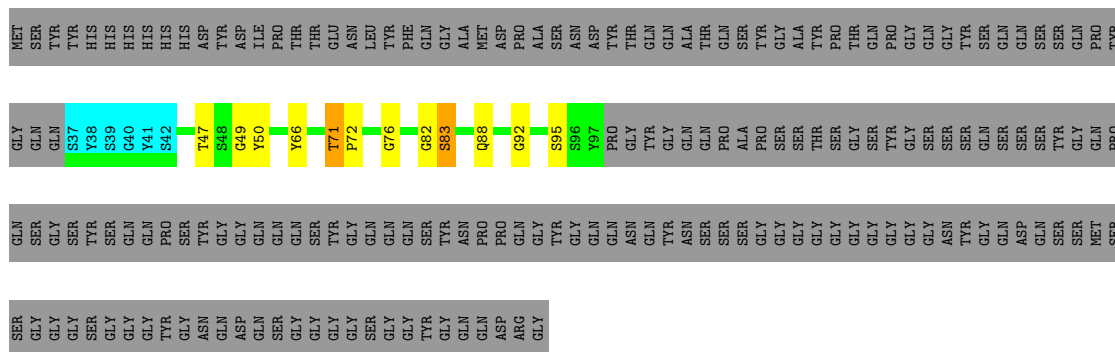


4.2.18 Score per residue for model 18

- Molecule 1: RNA-binding protein FUS

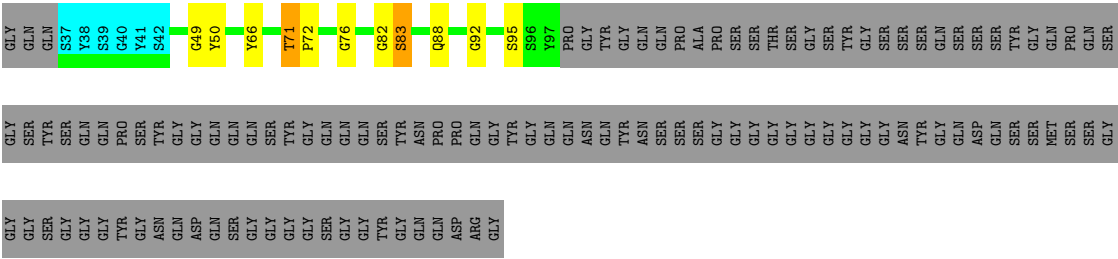


- Molecule 1: RNA-binding protein FUS

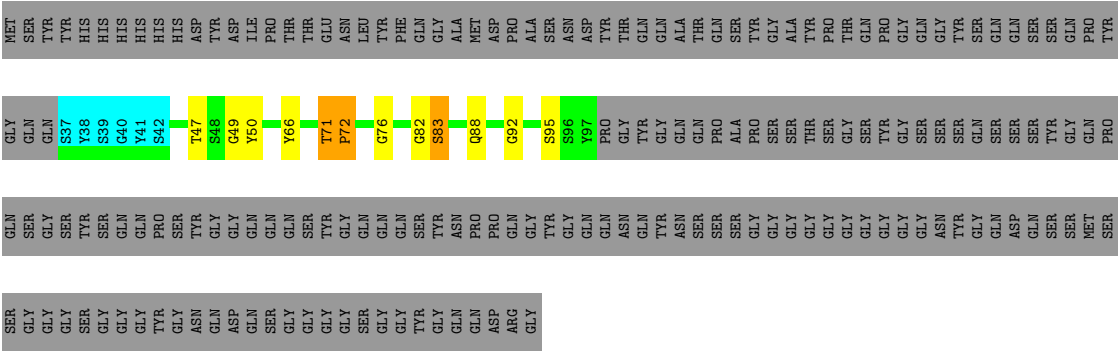


- Molecule 1: RNA-binding protein FUS

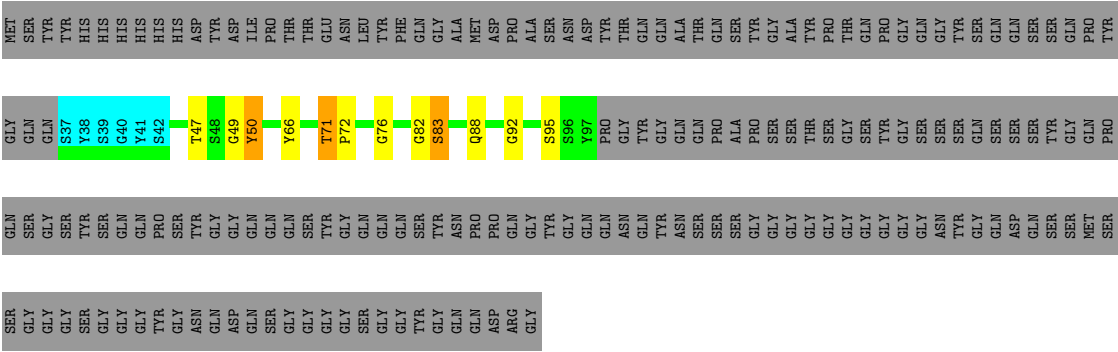




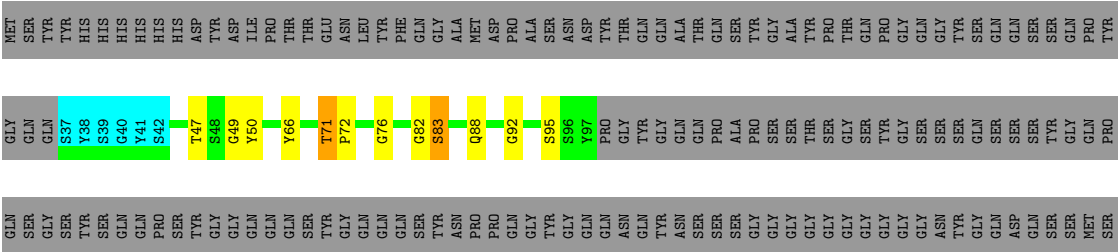
• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



• Molecule 1: RNA-binding protein FUS



SER GLY GLY GLY SER 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:  18% ... 75%

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

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%

NET	TYR	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ILE	PRO	THR	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	NET	ASP	ALA	PRO	ASP	SER	ASN	GLN	GLN	THR	THR	GLN	ALA	ALA	THR	GLN	SER	SER	GLY	ALA	TYR	PRO	PRO	GLN	GLN	GLY	GLY	TYR	SER	SER	GLN	GLN	PRO	TYR
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[illegible][illegible]

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

- Molecule 1: RNA-binding protein FUS

Chain I:

NET	TYR	TYR	TYR	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	NET	ASP	ALA	PRO	ASP	SER	ASN	GLN	GLN	THR	THR	GLN	ALA	ALA	THR	GLN	SER	TYR	PRO	THR	GLN	PRO	GLY	GLN	GLY	TYR	TYR	GLY	GLN	GLN	GLN	GLN	GLN	PRO	TYR
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GLY	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	PRO	ALA	ALA	PRO	PRO	SER	SER	SER	THR	SER	SER	SER	GLY	TYR	GLY	GLN	PRO	PRO	GLN	SER
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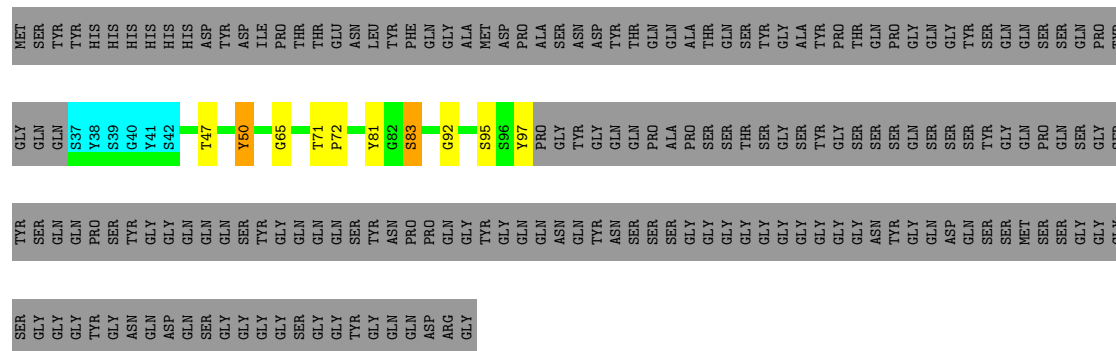
[illegible]

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

4.2.19 Score per residue for model 19

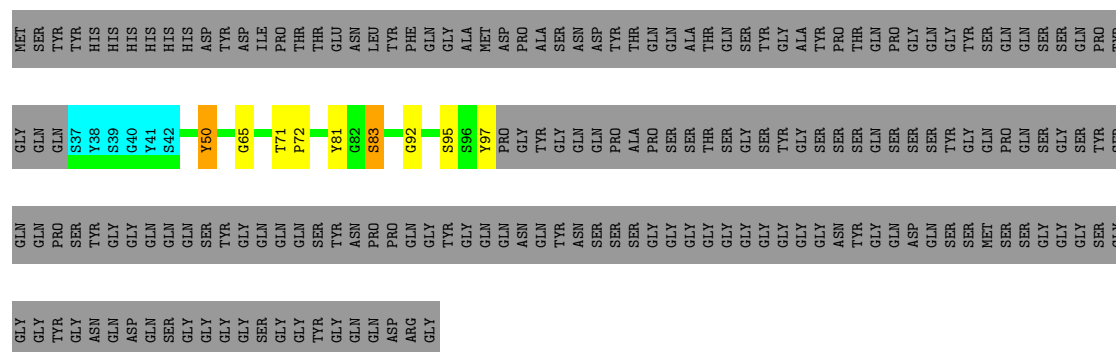
- Molecule 1: RNA-binding protein FUS

Chain A: 19% ... 75%



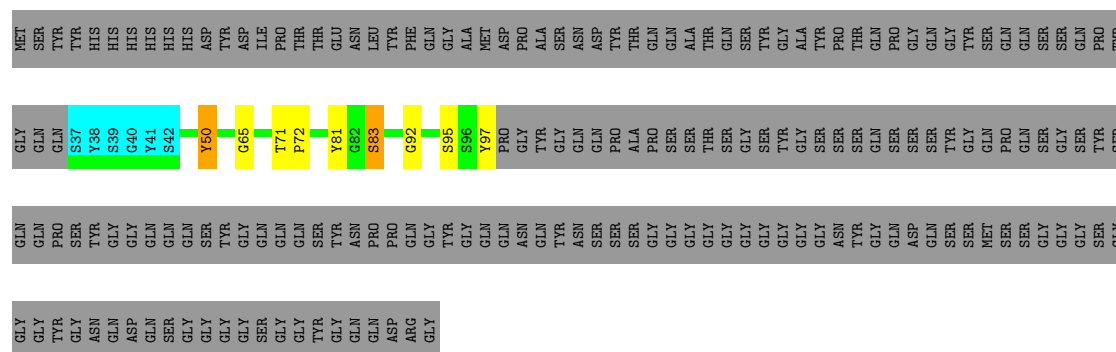
- Molecule 1: RNA-binding protein FUS

Chain B: 



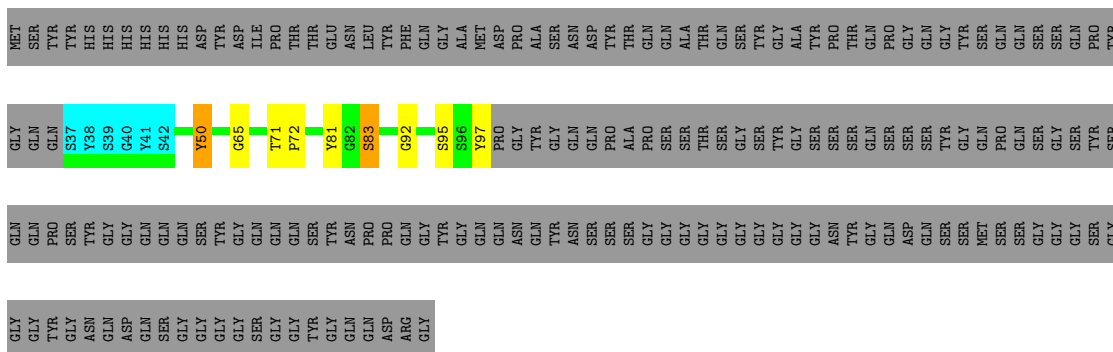
- Molecule 1: RNA-binding protein FUS

Chain C:  19% ... 75%



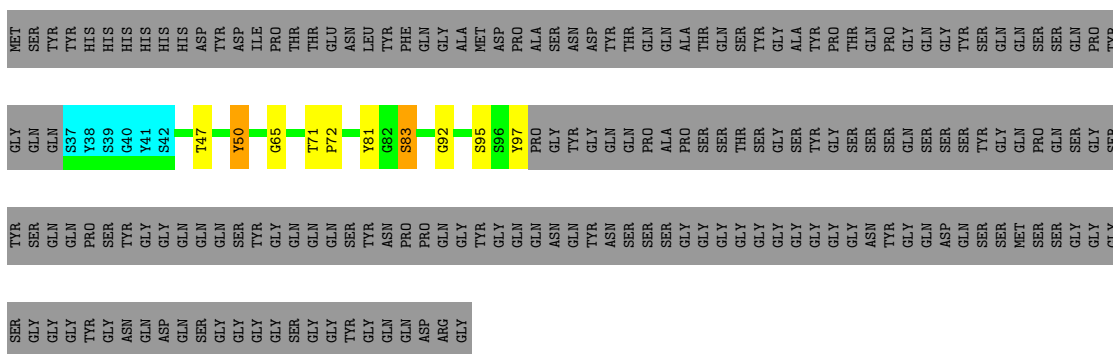
- Molecule 1: RNA-binding protein FUS

Chain D:  19% ... 75%



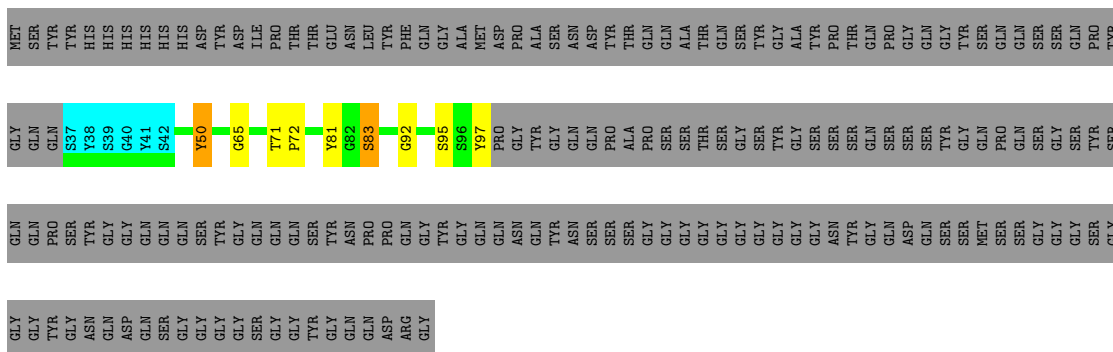
- Molecule 1: RNA-binding protein FUS

Chain E: 19% . . . 75%



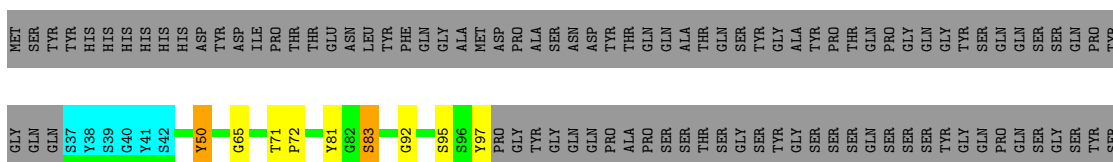
- Molecule 1: RNA-binding protein FUS

Chain F: 19% ... 75%



- Molecule 1: RNA-binding protein FUS

Chain G: 19% ... 75%



[illegible]

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:  19% ... 75%

MET	SER	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	PRO	THR	GLU	ASN	PHE	GLN	GLY	ALA	MET	ASP	PRO	ALA	SER	ASN	ASP	TYR	THR	GLN	GLN	ALA	ALA	THR	GLN	SER	SER	GLY	ALA	TYR	PRO	THR	GLN	PRO	GLY	GLN	GLY	SER	SER	GLN	PRO
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[illegible][illegible]

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

- Molecule 1: RNA-binding protein FUS

Chain I:  19% 1% 1% 75%

NET	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	ASP	ASP	PRO	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	ALA	PRO	ASP	ASP	PRO	ALA	PRO	SER	ASN	ASP	TYR	THR	THR	GLN	GLN	ALA	ALA	THR	THR	PRO	PRO	GLN	GLN	GLY	GLY	ALA	TYR	TYR	PRO	THR	THR	THR	GLN	GLN	GLY	GLY	PRO	TYR
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[illegible][illegible]

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

4.2.20 Score per residue for model 20

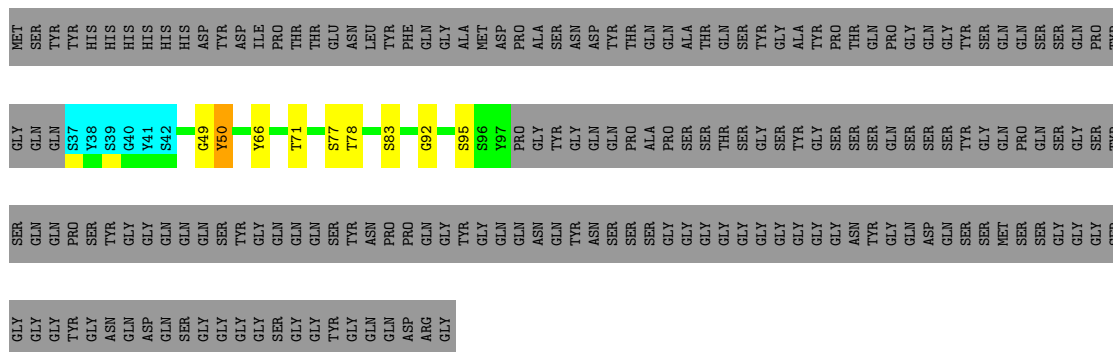
- Molecule 1: RNA-binding protein FUS

Chain A: 20% 75%

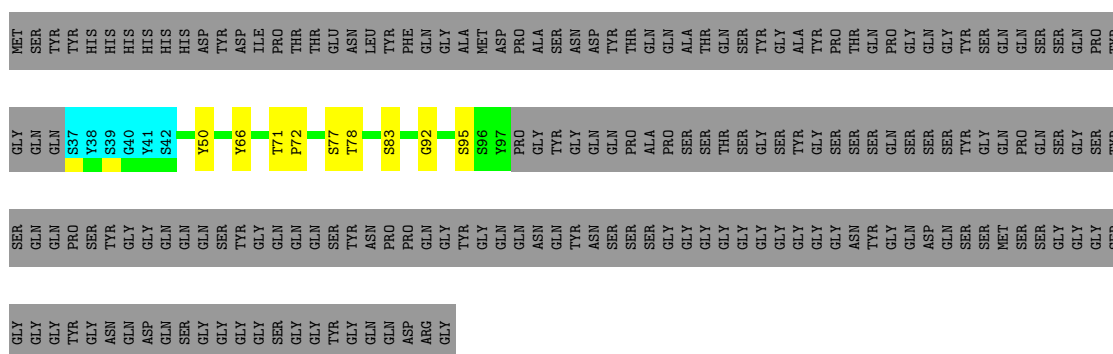
NET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	TYR	ASP	ILE	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	THR	GLN	GLY	ALA	MET	ASP	ALA	PRO	SER	ASN	ASP	TYR	THR	GLN	GLN	ALA	THR	GLN	SER	SER	TYR	GLY	ALA	TYR	PRO	THR	THR	GLN	PRO	GLY	GLN	GLY	TYR	SER	SER	GLN	GLN	PRO	TYR
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GLY	GLN	GLN	S37	S38	S39	G40	Y41	S42		Y66	T71	P72		S77	T78	S83		G92		S95	S96	I97	PRO	PRO	GLY	TYR	GLY	GLN	GLN	PRO	PRO	ALA	ALA	PRO	PRO	SER	SER	SER	THR	SER	GLY	GLY	TYR	GLY	SER	SER	SER	TYR	GLN	GLM	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	TYR	GLN	CYS
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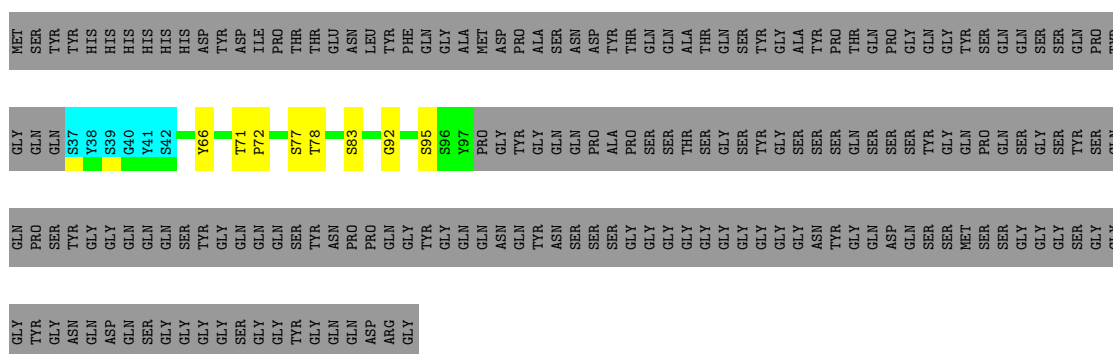
GLN	PRO	SER	TYR	GLY	GLN	GLN	GLN	SER	SER	TYR	GLY	GLN	GLN	GLN	ASN	ASN	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLN	ASP	GLN	GLN	SER	SER	SER	MET	MET	SER	SER	GLY	GLY	GLY	GLY	TYR
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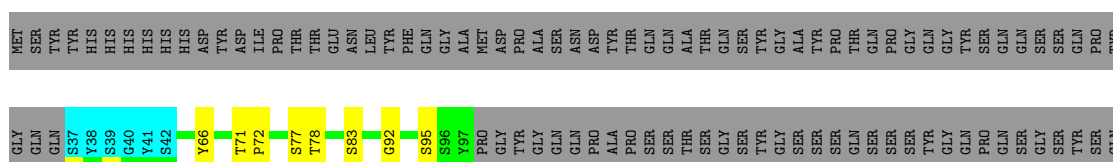
- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



- Molecule 1: RNA-binding protein FUS



[illegible]

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% 2% 79%

NET	SER	TYR	TYR	HIS	HIS	HIS	HIS	HIS	HIS	ASP	ASP	TYR	TYR	THR	THR	THR	GLU	ASN	LEU	LEU	TYR	PHE	GLN	GLY	ALA	ALA	NET	ASP	ASP	PRO	ALA	PRO	SER	SER	ASN	ASP	TYR	TYR	THR	THR	GLN	GLN	GLN	ALA	ALA	THR	THR	GLN	SER	SER	SER	SER	TYR	TYR	GLY	GLY	ALA	TYR	PRO	PRO	THR	THR	GLN	GLN	PRO	PRO	GLY	GLY	GLN	GLN	SER	SER	SER	SER	GLN	GLN	PRO	PRO	TYR	TYR
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GLY	GLN	S37	S38	S39	S40	S41	S42	G43	Y60	Y66	T71	P72	S77	T78	S83	G82	S95	S96	Y97	PRO	PRO	GLY	TYR	GLY	GLN	GLN	PRO	ALA	PRO	PRO	SER	SER	THR	SER	SER	GLY	TYR	GLY	SER	SER	GLN	GLN	PRO	PRO	GLY	SER
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[illegible]

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

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)	5w3n_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.

No validations of the models with respect to experimental NMR restraints is performed at this time.

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:H:71:THR:HG22	1:H:72:PRO:CD	0.46	2.40	10	3
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: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:I:49:GLY:O	1:I:50:TYR:C	0.42	2.57	11	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:49:GLY:O	1:F:50:TYR:C	0.42	2.57	11	8
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: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:B:73:GLN:O	1:B: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	11
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	10
1	F	54/241 (22%)	35±2 (65±5%)	13±2 (25±5%)	5±2 (10±4%)	1	11
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	11
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	G	72	PRO	14
1	E	83	SER	14
1	B	83	SER	14
1	A	83	SER	14
1	H	83	SER	14
1	D	83	SER	14
1	F	83	SER	14
1	G	83	SER	14
1	C	83	SER	14
1	D	72	PRO	14
1	I	83	SER	14
1	B	72	PRO	13
1	F	50	TYR	13
1	C	72	PRO	13
1	H	72	PRO	13
1	F	72	PRO	13
1	I	72	PRO	13
1	B	50	TYR	12
1	C	50	TYR	12
1	D	50	TYR	12
1	A	72	PRO	12
1	G	50	TYR	12
1	H	50	TYR	12

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

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Mol	Chain	Res	Type	Models (Total)
1	I	85	GLN	3
1	E	65	GLY	3
1	C	81	TYR	3
1	A	81	TYR	3
1	E	85	GLN	3
1	A	85	GLN	3
1	H	81	TYR	3
1	B	81	TYR	3
1	F	81	TYR	3
1	B	85	GLN	3
1	D	85	GLN	3
1	F	65	GLY	3
1	C	65	GLY	3
1	G	65	GLY	3
1	I	81	TYR	3
1	F	85	GLN	3
1	C	85	GLN	3
1	G	85	GLN	3
1	D	81	TYR	3
1	H	85	GLN	3
1	G	81	TYR	3
1	E	81	TYR	3
1	B	74	GLY	2
1	H	74	GLY	2
1	F	43	GLN	2
1	G	74	GLY	2
1	F	93	GLN	2
1	B	43	GLN	2
1	E	75	TYR	2
1	C	93	GLN	2
1	H	75	TYR	2
1	D	58	TYR	2
1	B	75	TYR	2
1	I	51	GLY	2
1	I	93	GLN	2
1	A	75	TYR	2
1	F	74	GLY	2
1	E	74	GLY	2
1	C	60	GLN	2
1	D	74	GLY	2
1	I	43	GLN	2
1	G	58	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	93	GLN	2
1	A	58	TYR	2
1	F	75	TYR	2
1	G	60	GLN	2
1	E	43	GLN	2
1	I	75	TYR	2
1	A	43	GLN	2
1	H	51	GLY	2
1	D	43	GLN	2
1	B	60	GLN	2
1	E	93	GLN	2
1	F	60	GLN	2
1	H	58	TYR	2
1	C	58	TYR	2
1	D	51	GLY	2
1	B	51	GLY	2
1	H	60	GLN	2
1	I	58	TYR	2
1	G	93	GLN	2
1	A	60	GLN	2
1	G	51	GLY	2
1	A	51	GLY	2
1	H	43	GLN	2
1	G	75	TYR	2
1	C	51	GLY	2
1	I	60	GLN	2
1	C	74	GLY	2
1	C	43	GLN	2
1	D	93	GLN	2
1	F	51	GLY	2
1	F	58	TYR	2
1	E	60	GLN	2
1	G	43	GLN	2
1	B	58	TYR	2
1	I	74	GLY	2
1	D	60	GLN	2
1	H	93	GLN	2
1	B	93	GLN	2
1	D	75	TYR	2
1	C	75	TYR	2
1	I	65	GLY	2
1	E	58	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	E	51	GLY	2
1	A	74	GLY	2
1	G	59	GLY	1
1	C	80	GLY	1
1	H	57	SER	1
1	H	62	GLN	1
1	F	62	GLN	1
1	C	79	GLY	1
1	B	91	TYR	1
1	D	61	SER	1
1	C	91	TYR	1
1	D	79	GLY	1
1	F	61	SER	1
1	A	61	SER	1
1	B	59	GLY	1
1	B	61	SER	1
1	I	79	GLY	1
1	F	91	TYR	1
1	H	59	GLY	1
1	A	56	SER	1
1	D	57	SER	1
1	E	62	GLN	1
1	B	79	GLY	1
1	A	62	GLN	1
1	A	57	SER	1
1	F	57	SER	1
1	H	80	GLY	1
1	E	79	GLY	1
1	I	57	SER	1
1	I	62	GLN	1
1	B	80	GLY	1
1	A	79	GLY	1
1	I	61	SER	1
1	F	59	GLY	1
1	C	56	SER	1
1	B	57	SER	1
1	I	59	GLY	1
1	H	79	GLY	1
1	E	59	GLY	1
1	C	59	GLY	1
1	C	62	GLN	1
1	G	91	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	E	91	TYR	1
1	I	56	SER	1
1	E	57	SER	1
1	D	56	SER	1
1	C	57	SER	1
1	E	61	SER	1
1	B	62	GLN	1
1	A	91	TYR	1
1	H	61	SER	1
1	F	79	GLY	1
1	I	91	TYR	1
1	G	79	GLY	1
1	E	56	SER	1
1	D	91	TYR	1
1	H	91	TYR	1
1	F	56	SER	1
1	D	62	GLN	1
1	D	80	GLY	1
1	G	62	GLN	1
1	G	56	SER	1
1	D	59	GLY	1
1	B	56	SER	1
1	H	56	SER	1
1	A	80	GLY	1
1	G	57	SER	1
1	I	80	GLY	1
1	F	80	GLY	1
1	A	59	GLY	1
1	G	61	SER	1
1	G	80	GLY	1
1	C	61	SER	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	7 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	7	46
1	C	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	7	47
1	D	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	7	46
1	E	44/182 (24%)	38±2 (85±4%)	6±2 (15±4%)	7	46
1	F	44/182 (24%)	38±2 (86±4%)	6±2 (14±4%)	7	46
1	G	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	7	47
1	H	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	7	46
1	I	44/182 (24%)	38±2 (86±5%)	6±2 (14±5%)	7	47
All	All	7920/32760 (24%)	6774 (86%)	1146 (14%)	7	46

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

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

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Mol	Chain	Res	Type	Models (Total)
1	A	78	THR	6
1	G	83	SER	6
1	C	83	SER	6
1	I	83	SER	6
1	I	47	THR	6
1	E	50	TYR	5
1	B	91	TYR	5
1	I	91	TYR	5
1	B	50	TYR	5
1	F	91	TYR	5
1	C	50	TYR	5
1	G	91	TYR	5
1	F	50	TYR	5
1	D	50	TYR	5
1	E	91	TYR	5
1	G	50	TYR	5
1	A	50	TYR	5
1	C	91	TYR	5
1	A	91	TYR	5
1	D	91	TYR	5
1	H	91	TYR	5
1	H	50	TYR	5
1	I	50	TYR	5
1	A	77	SER	4
1	E	77	SER	4
1	H	77	SER	4
1	I	77	SER	4
1	I	43	GLN	4
1	D	77	SER	4
1	B	77	SER	4
1	E	43	GLN	4
1	A	43	GLN	4
1	C	77	SER	4
1	F	77	SER	4
1	B	43	GLN	4
1	D	43	GLN	4
1	F	43	GLN	4
1	H	43	GLN	4
1	G	77	SER	4
1	C	43	GLN	4
1	G	43	GLN	4
1	C	69	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	E	97	TYR	3
1	G	97	TYR	3
1	F	86	SER	3
1	D	97	TYR	3
1	H	69	GLN	3
1	D	69	GLN	3
1	H	97	TYR	3
1	F	90	SER	3
1	F	69	GLN	3
1	B	90	SER	3
1	G	90	SER	3
1	I	86	SER	3
1	H	86	SER	3
1	E	90	SER	3
1	A	69	GLN	3
1	B	97	TYR	3
1	A	86	SER	3
1	B	86	SER	3
1	I	69	GLN	3
1	A	90	SER	3
1	I	97	TYR	3
1	G	86	SER	3
1	B	69	GLN	3
1	G	69	GLN	3
1	F	97	TYR	3
1	E	69	GLN	3
1	A	97	TYR	3
1	C	97	TYR	3
1	C	90	SER	3
1	C	86	SER	3
1	D	90	SER	3
1	E	86	SER	3
1	I	90	SER	3
1	D	86	SER	3
1	H	90	SER	3
1	A	68	THR	2
1	D	73	GLN	2
1	H	96	SER	2
1	B	96	SER	2
1	E	84	SER	2
1	F	84	SER	2
1	I	93	GLN	2

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

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Mol	Chain	Res	Type	Models (Total)
1	H	93	GLN	2
1	B	93	GLN	2
1	B	56	SER	2
1	H	56	SER	2
1	C	96	SER	2
1	B	46	ASP	1
1	G	94	GLN	1
1	H	57	SER	1
1	A	94	GLN	1
1	A	61	SER	1
1	H	94	GLN	1
1	C	94	GLN	1
1	B	61	SER	1
1	C	81	TYR	1
1	H	46	ASP	1
1	I	81	TYR	1
1	D	94	GLN	1
1	A	57	SER	1
1	F	94	GLN	1
1	F	57	SER	1
1	A	81	TYR	1
1	D	46	ASP	1
1	C	46	ASP	1
1	I	61	SER	1
1	B	57	SER	1
1	A	46	ASP	1
1	B	94	GLN	1
1	I	94	GLN	1
1	C	61	SER	1
1	I	46	ASP	1
1	B	81	TYR	1
1	F	81	TYR	1
1	G	46	ASP	1
1	E	57	SER	1
1	C	57	SER	1
1	I	57	SER	1
1	E	61	SER	1
1	D	57	SER	1
1	H	61	SER	1
1	E	94	GLN	1
1	F	46	ASP	1
1	G	57	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	H	81	TYR	1
1	D	81	TYR	1
1	E	46	ASP	1
1	G	61	SER	1
1	D	61	SER	1
1	G	81	TYR	1
1	F	61	SER	1
1	E	81	TYR	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 carbohydrates 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: 5w3n_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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	46	-0.06 ± 0.38	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	35	-0.55 ± 0.28	None needed (imprecise)
$^{13}\text{C}'$	44	0.30 ± 0.24	None needed (< 0.5 ppm)
^{15}N	45	-1.69 ± 1.01	None needed (imprecise)

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. 199 atoms were assigned a chemical shift out of a possible 5004. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	129/2457 (5%)	0/981 (0%)	87/990 (9%)	42/486 (9%)
Sidechain	50/1971 (3%)	0/1206 (0%)	50/666 (8%)	0/99 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	20/576 (3%)	0/288 (0%)	20/288 (7%)	0/0 (—%)
Overall	199/5004 (4%)	0/2475 (0%)	157/1944 (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. 205 atoms were assigned a chemical shift out of a possible 5553. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	134/2727 (5%)	0/1089 (0%)	90/1098 (8%)	44/540 (8%)
Sidechain	51/2106 (2%)	0/1296 (0%)	51/711 (7%)	0/99 (0%)
Aromatic	20/720 (3%)	0/360 (0%)	20/360 (6%)	0/0 (—%)
Overall	205/5553 (4%)	0/2745 (0%)	161/2169 (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.

Random coil index (RCI) for chain A:

