



# Full wwPDB NMR Structure Validation Report ⓘ

Sep 26, 2020 – 08:14 AM BST

PDB ID : 6TVM  
Title : LEDGF/p75 dimer (residues 345-467)  
Authors : Lux, V.; Veverka, V.  
Deposited on : 2020-01-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.14.6
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

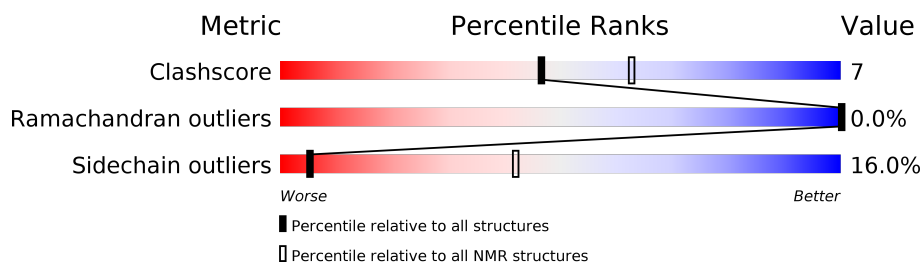
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 44%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	128	<div> <div style="width: 50%;">50%</div> <div style="width: 13%;">13%</div> <div style="width: 37%;">37%</div> </div>
1	B	128	<div> <div style="width: 49%;">49%</div> <div style="width: 14%;">14%</div> <div style="width: 37%;">37%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 22 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:347-A:427, B:347-B:427 (162)	0.15	22

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 6 clusters and 3 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 7, 8, 16, 17, 18, 24, 27, 28
2	2, 11, 13, 25, 30
3	6, 10, 15, 22, 23
4	9, 12
5	20, 26
6	1, 21
Single-model clusters	14; 19; 29

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4152 atoms, of which 2114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			2076	627	1057	187	198	7	
1	B	128	Total	C	H	N	O	S	0
			2076	627	1057	187	198	7	

There are 10 discrepancies between the modelled and reference sequences:

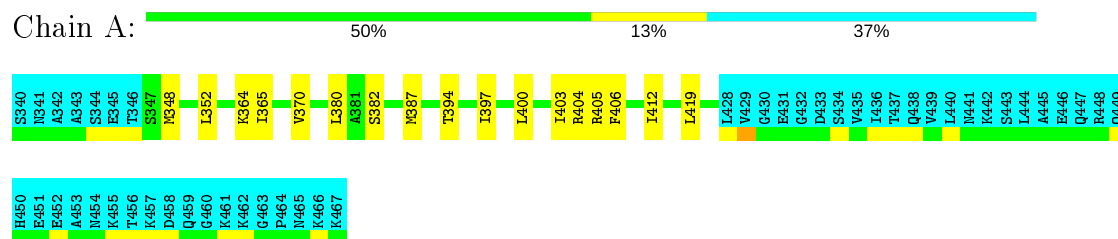
Chain	Residue	Modelled	Actual	Comment	Reference
A	340	SER	-	expression tag	UNP O75475
A	341	ASN	-	expression tag	UNP O75475
A	342	ALA	-	expression tag	UNP O75475
A	343	ALA	-	expression tag	UNP O75475
A	344	SER	-	expression tag	UNP O75475
B	340	SER	-	expression tag	UNP O75475
B	341	ASN	-	expression tag	UNP O75475
B	342	ALA	-	expression tag	UNP O75475
B	343	ALA	-	expression tag	UNP O75475
B	344	SER	-	expression tag	UNP O75475

## 4 Residue-property plots

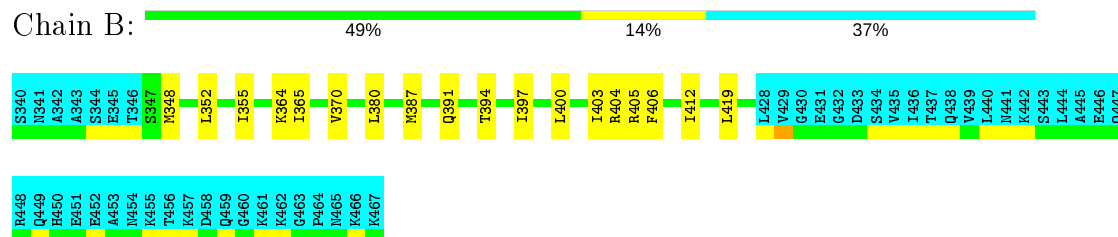
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: PC4 and SFRS1-interacting protein



- Molecule 1: PC4 and SFRS1-interacting protein

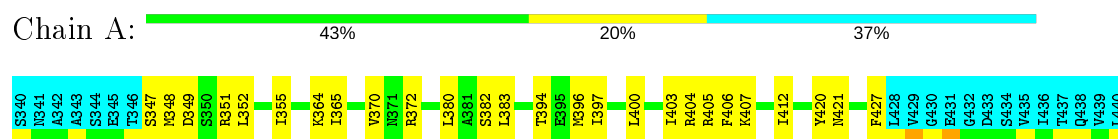


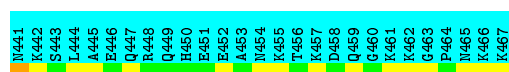
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

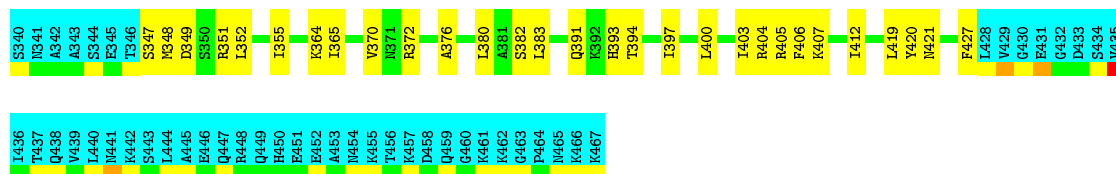
- Molecule 1: PC4 and SFRS1-interacting protein





- Molecule 1: PC4 and SFRS1-interacting protein

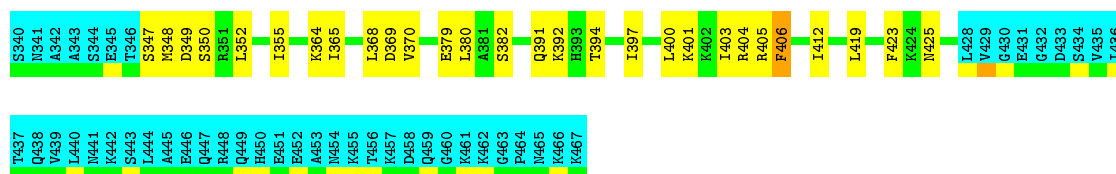
Chain B: 41% 23% 37%



#### 4.2.2 Score per residue for model 2

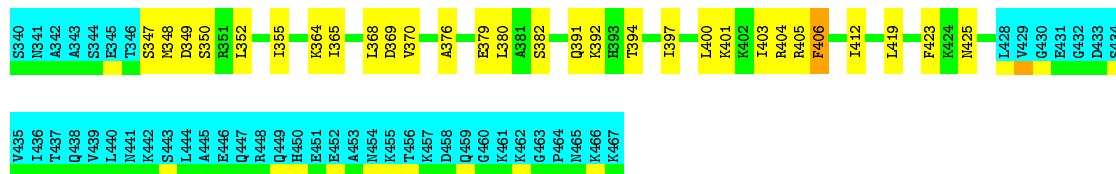
- Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 41% 21% 37%



- Molecule 1: PC4 and SFRS1-interacting protein

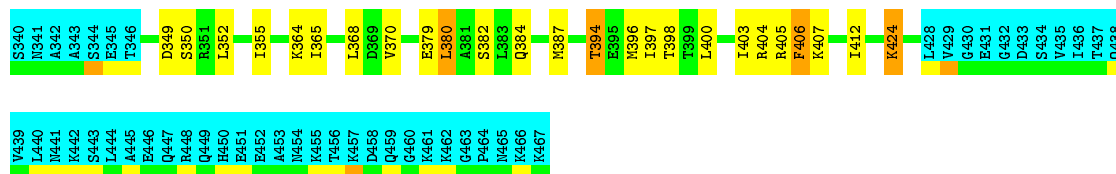
Chain B: 41% 22% 37%



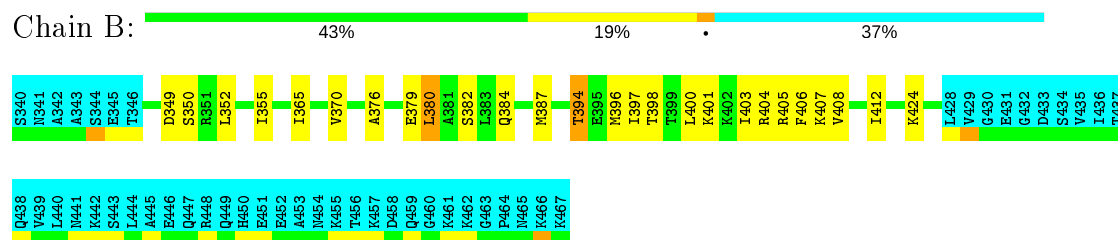
#### 4.2.3 Score per residue for model 3

- Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 44% 16% 37%

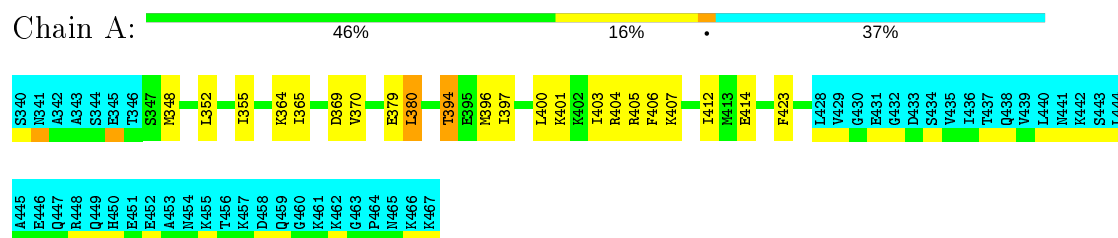


- Molecule 1: PC4 and SFRS1-interacting protein

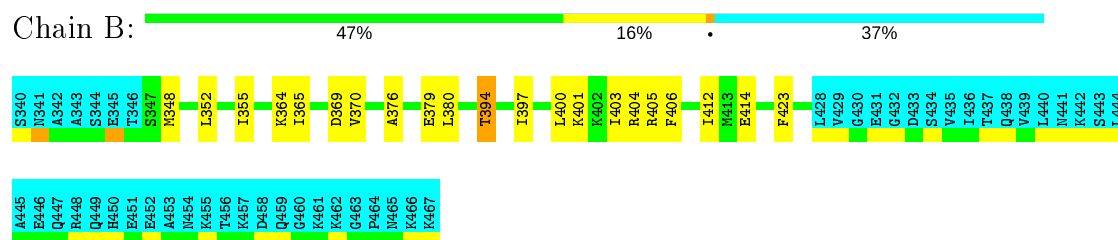


#### 4.2.4 Score per residue for model 4

- Molecule 1: PC4 and SFRS1-interacting protein

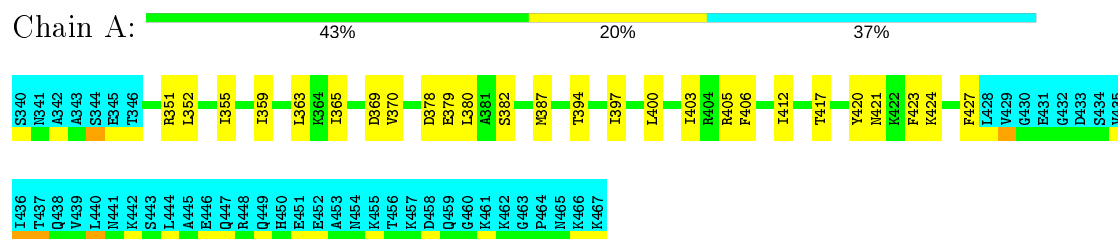


- Molecule 1: PC4 and SFRS1-interacting protein

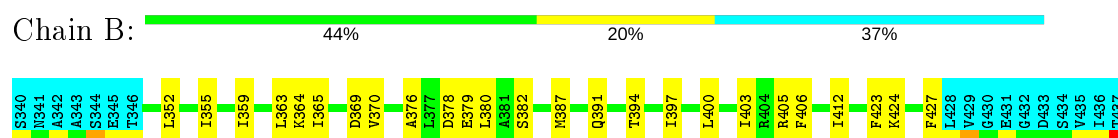


#### 4.2.5 Score per residue for model 5

- Molecule 1: PC4 and SFRS1-interacting protein



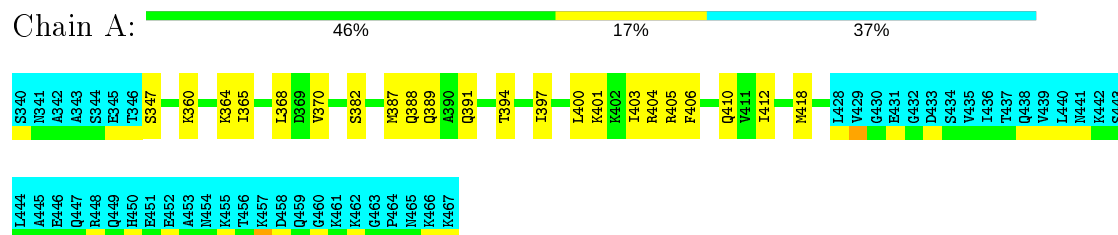
- Molecule 1: PC4 and SFRS1-interacting protein



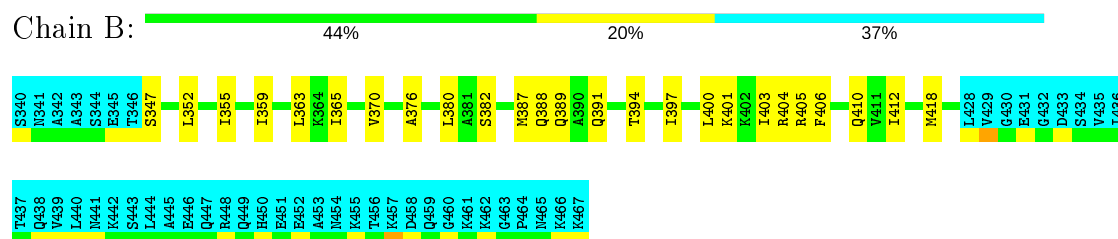


#### 4.2.6 Score per residue for model 6

- Molecule 1: PC4 and SFRS1-interacting protein

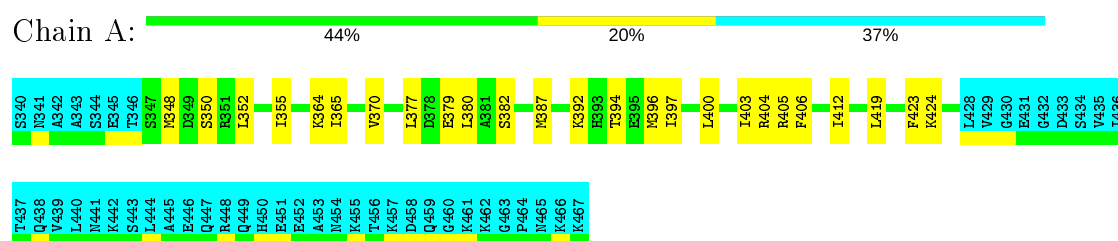


- Molecule 1: PC4 and SFRS1-interacting protein

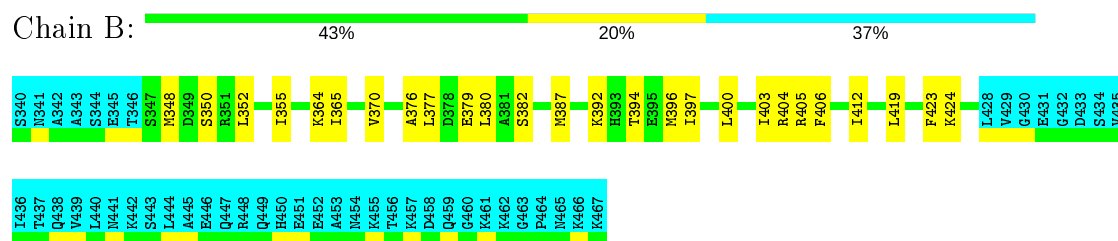


#### 4.2.7 Score per residue for model 7

- Molecule 1: PC4 and SFRS1-interacting protein

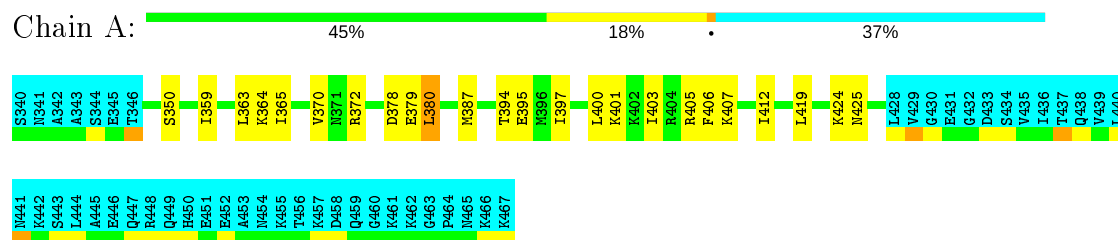


- Molecule 1: PC4 and SFRS1-interacting protein

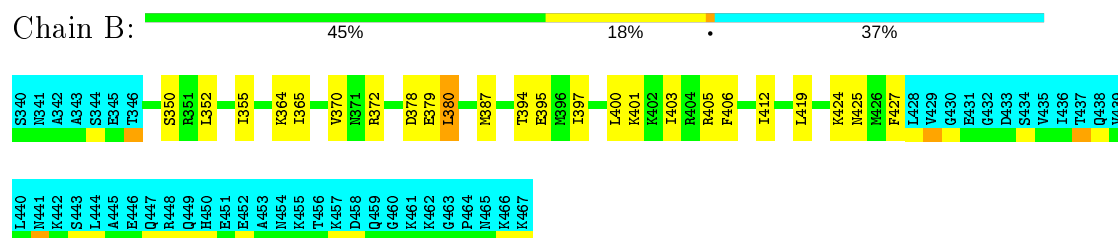






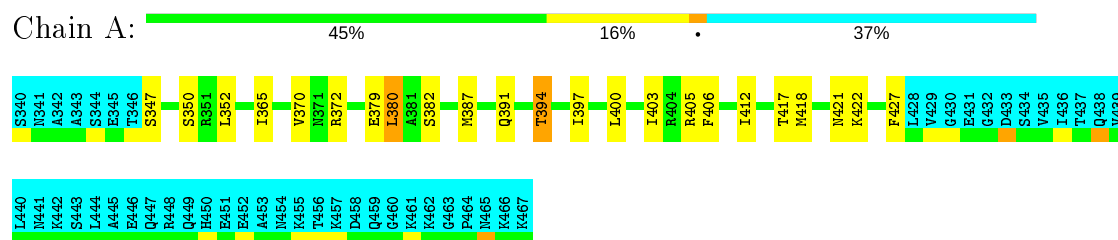


- Molecule 1: PC4 and SFRS1-interacting protein

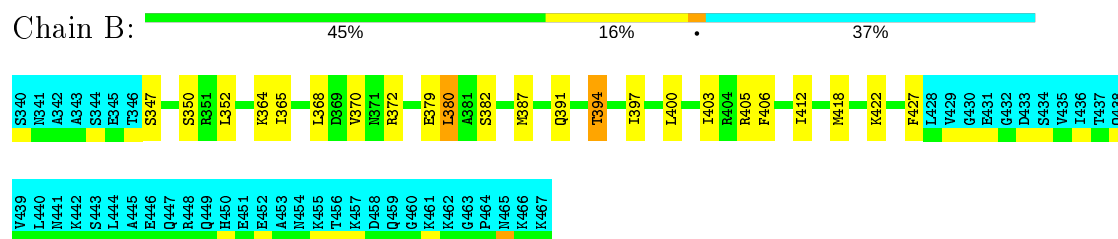


#### 4.2.11 Score per residue for model 11

- Molecule 1: PC4 and SFRS1-interacting protein

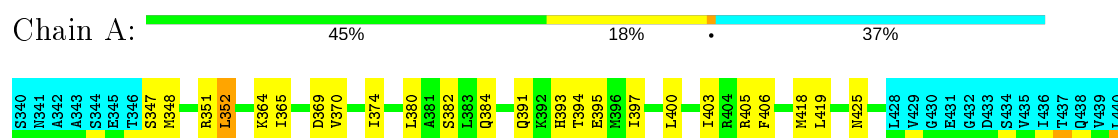


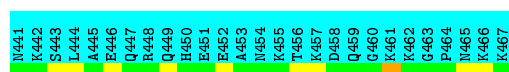
- Molecule 1: PC4 and SFRS1-interacting protein



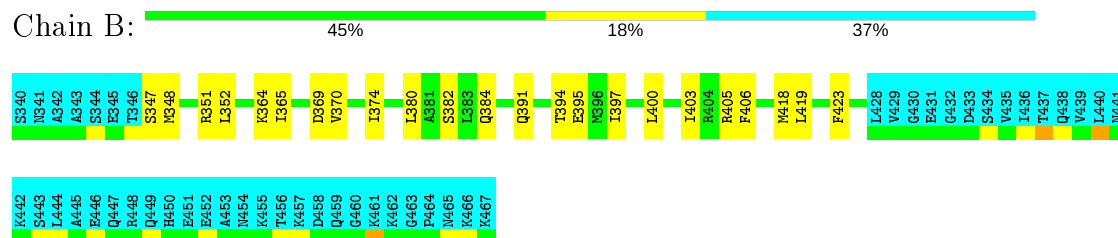
#### 4.2.12 Score per residue for model 12

- Molecule 1: PC4 and SFRS1-interacting protein



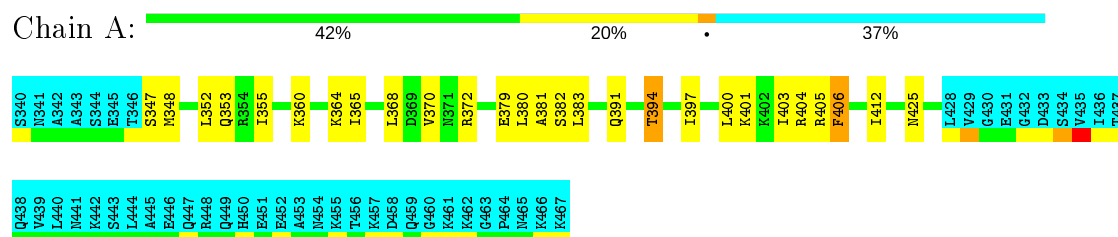


- Molecule 1: PC4 and SFRS1-interacting protein

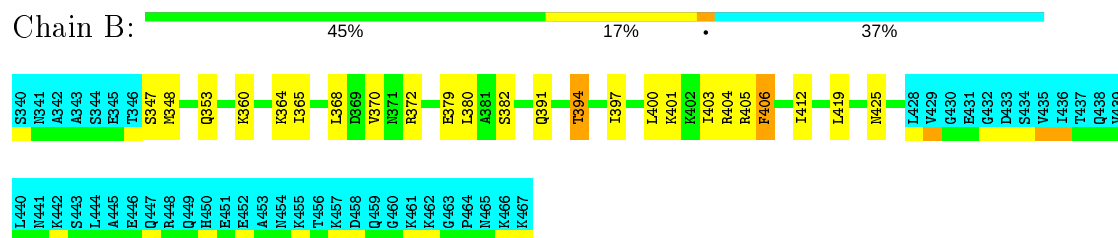


#### 4.2.13 Score per residue for model 13

- Molecule 1: PC4 and SFRS1-interacting protein

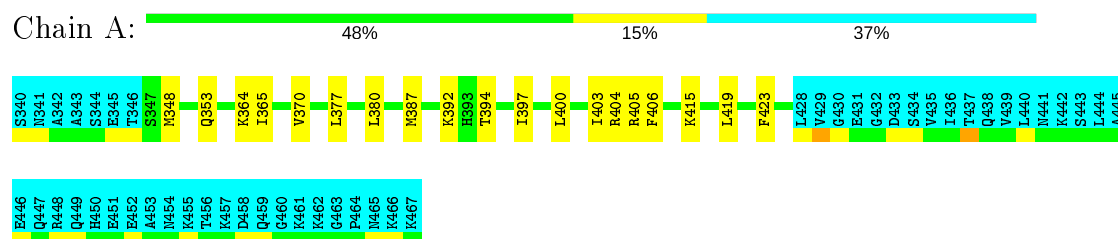


- Molecule 1: PC4 and SFRS1-interacting protein

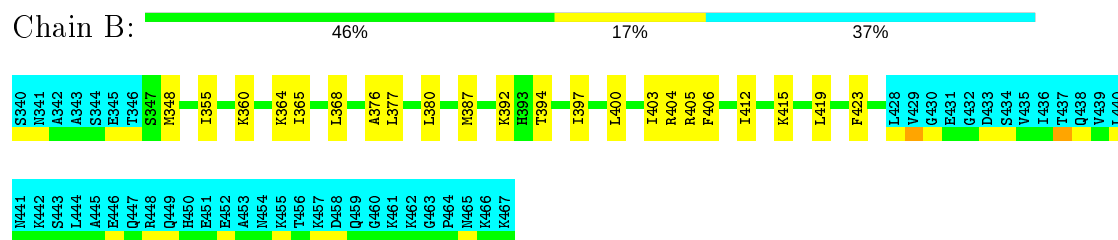


#### 4.2.14 Score per residue for model 14

- Molecule 1: PC4 and SFRS1-interacting protein

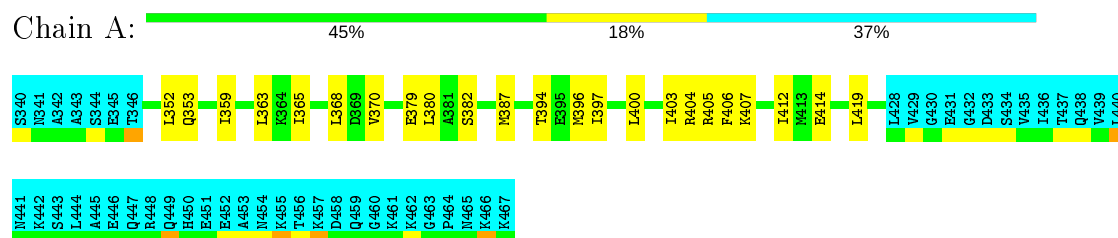


- Molecule 1: PC4 and SFRS1-interacting protein

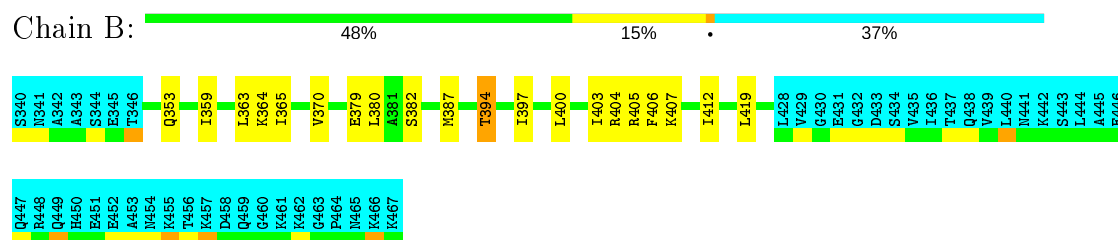


#### 4.2.15 Score per residue for model 15

- Molecule 1: PC4 and SFRS1-interacting protein

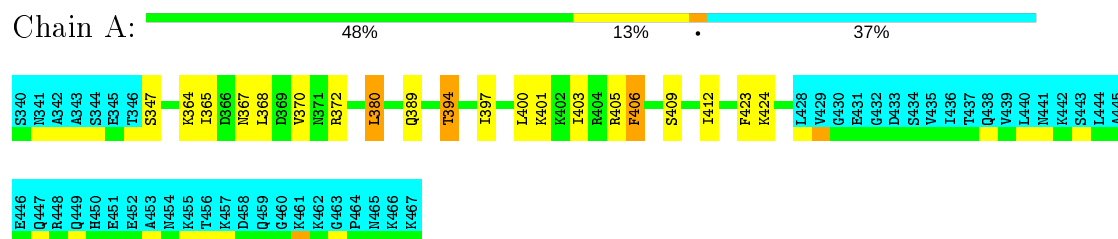


- Molecule 1: PC4 and SFRS1-interacting protein

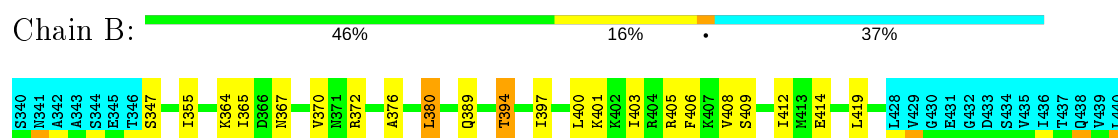


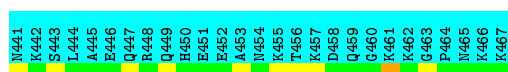
#### 4.2.16 Score per residue for model 16

- Molecule 1: PC4 and SFRS1-interacting protein



- Molecule 1: PC4 and SFRS1-interacting protein

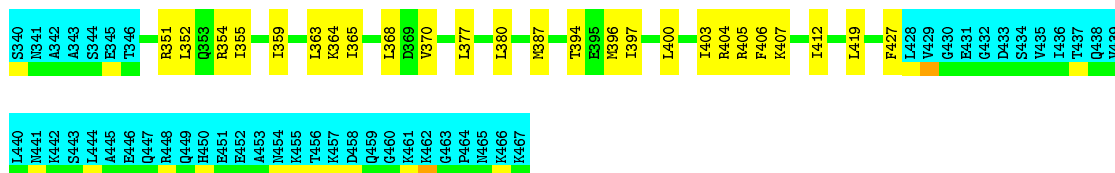




#### 4.2.17 Score per residue for model 17

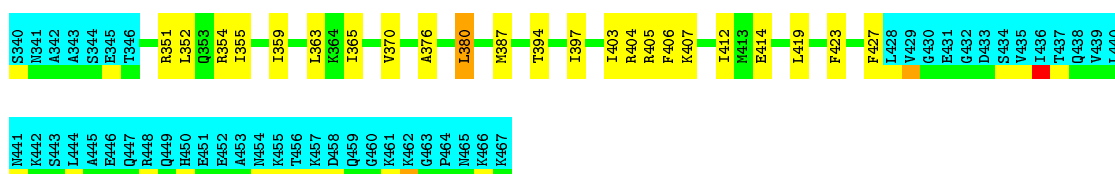
- Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 44% 20% 37%



- Molecule 1: PC4 and SFRS1-interacting protein

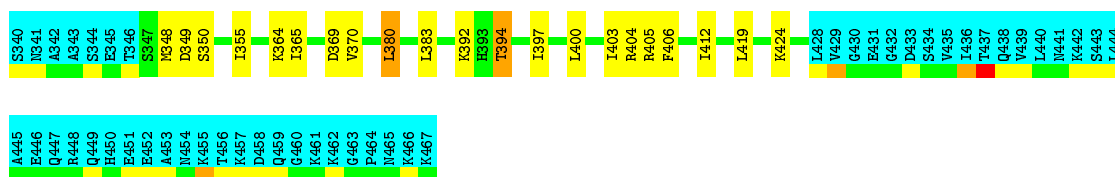
Chain B: 45% 17% 37%



#### 4.2.18 Score per residue for model 18

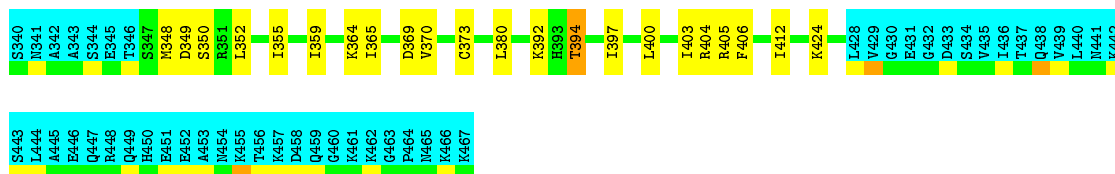
- Molecule 1: PC4 and SFRS1-interacting protein

Chain A: 47% 15% 37%



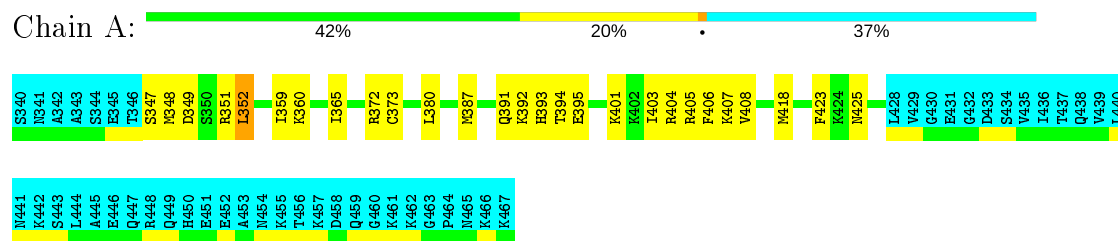
- Molecule 1: PC4 and SFRS1-interacting protein

Chain B: 46% 16% 37%

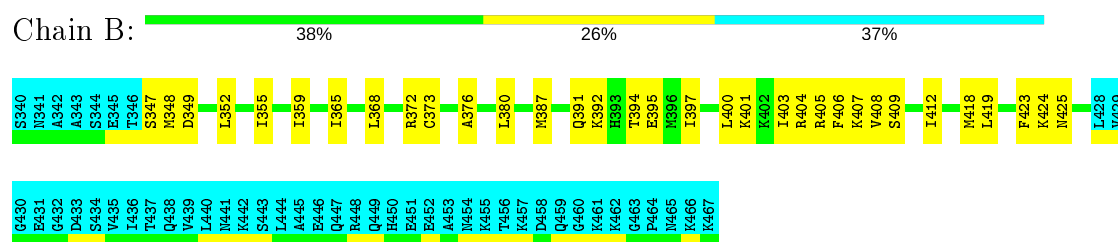


### 4.2.19 Score per residue for model 19

- Molecule 1: PC4 and SFRS1-interacting protein

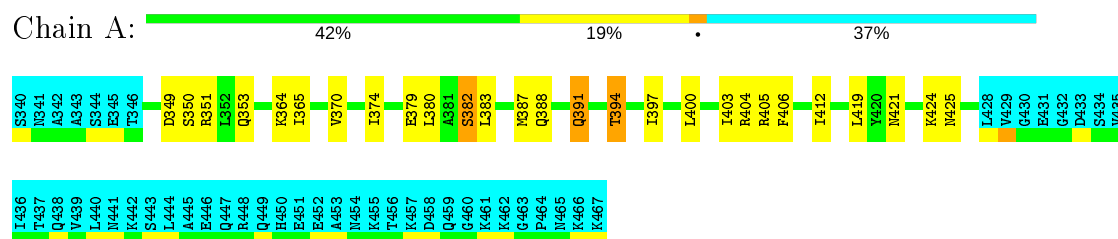


- Molecule 1: PC4 and SFRS1-interacting protein

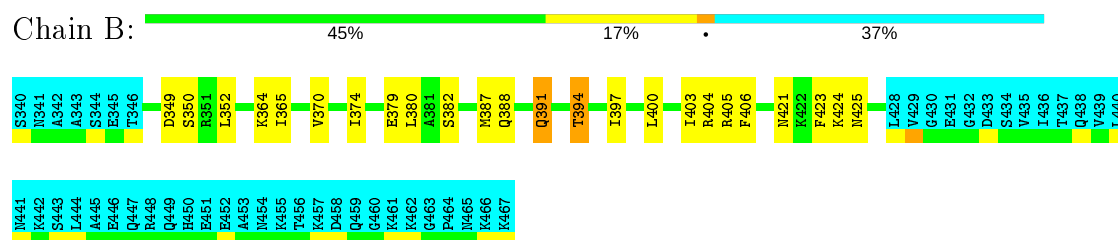


### 4.2.20 Score per residue for model 20

- Molecule 1: PC4 and SFRS1-interacting protein

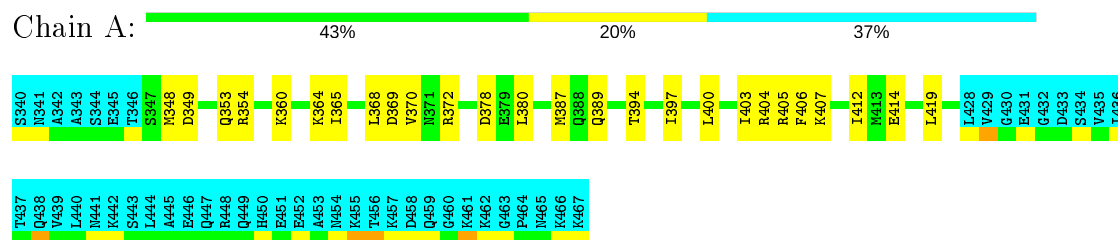


- Molecule 1: PC4 and SFRS1-interacting protein

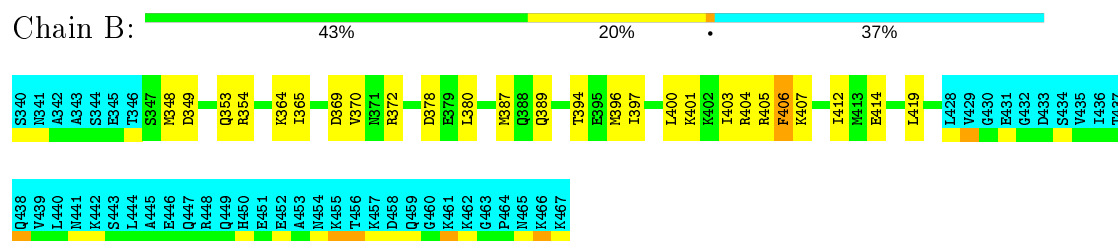


### 4.2.21 Score per residue for model 21

- Molecule 1: PC4 and SFRS1-interacting protein

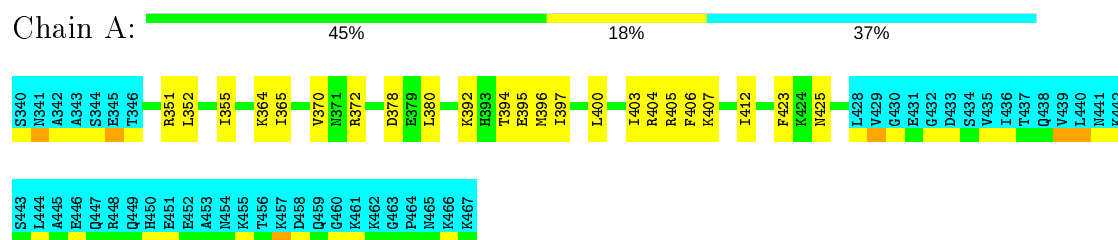


- Molecule 1: PC4 and SFRS1-interacting protein

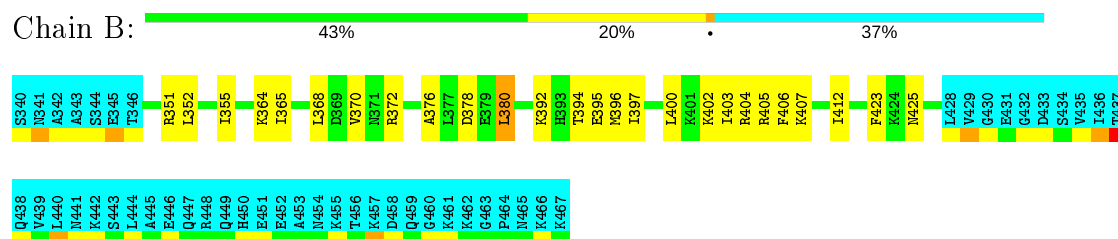


#### 4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: PC4 and SFRS1-interacting protein

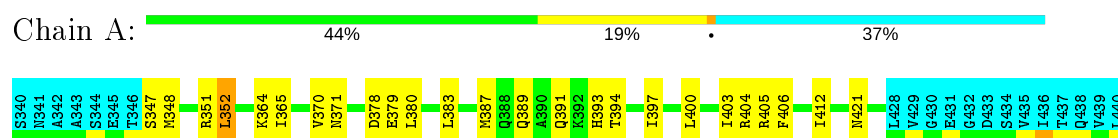


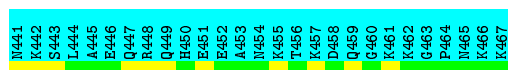
- Molecule 1: PC4 and SFRS1-interacting protein



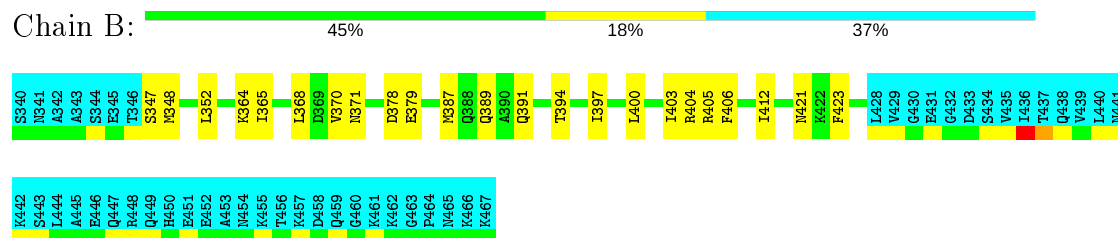
#### 4.2.23 Score per residue for model 23

- Molecule 1: PC4 and SFRS1-interacting protein



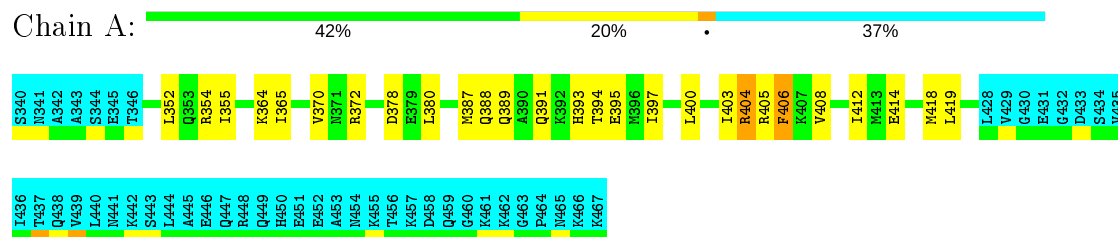


- Molecule 1: PC4 and SFRS1-interacting protein

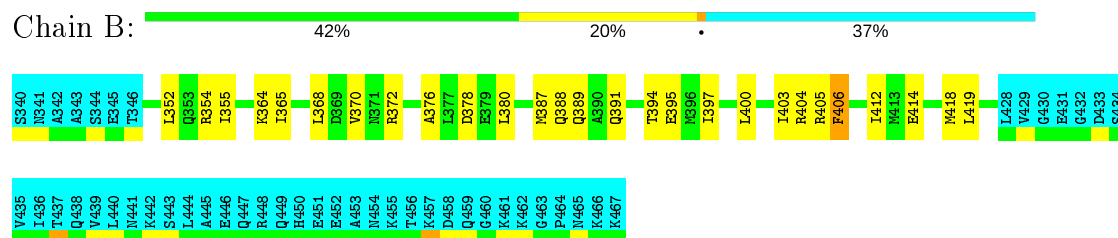


#### 4.2.24 Score per residue for model 24

- Molecule 1: PC4 and SFRS1-interacting protein

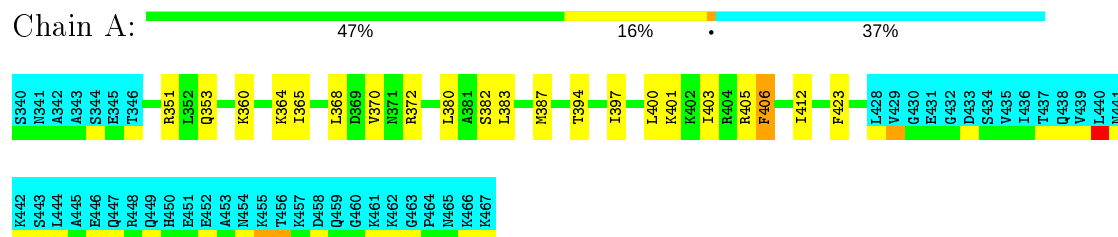


- Molecule 1: PC4 and SFRS1-interacting protein



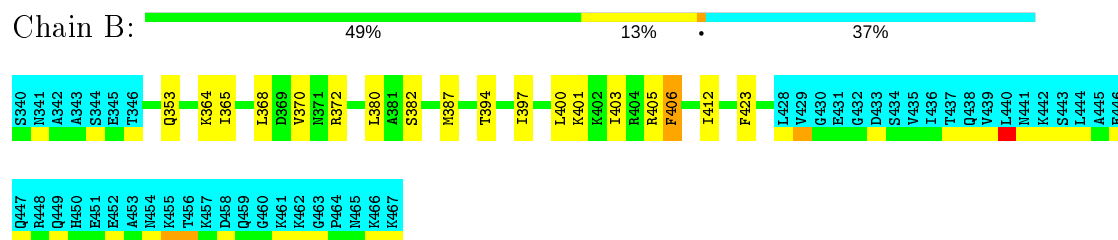
#### 4.2.25 Score per residue for model 25

- Molecule 1: PC4 and SFRS1-interacting protein



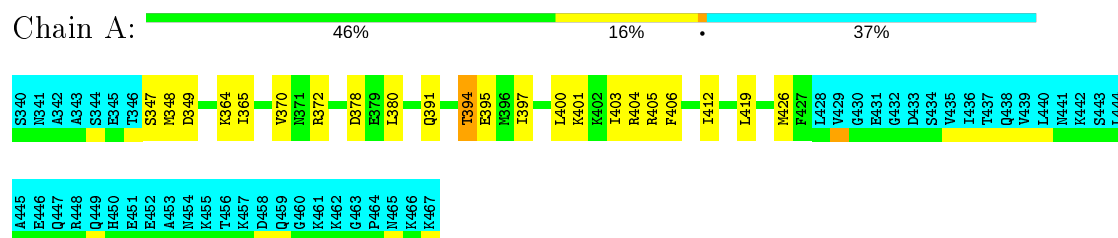
- Molecule 1: PC4 and SFRS1-interacting protein



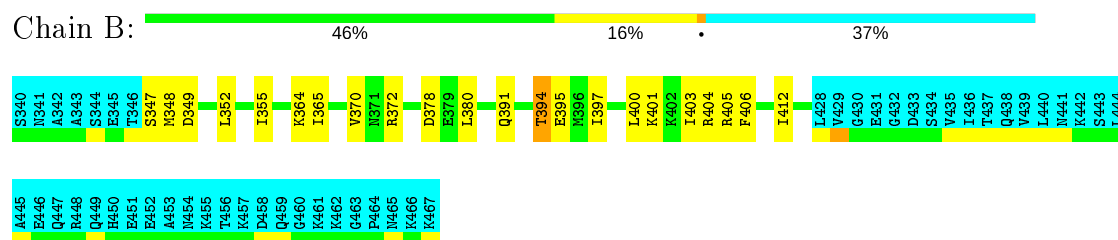


#### 4.2.26 Score per residue for model 26

- Molecule 1: PC4 and SFRS1-interacting protein

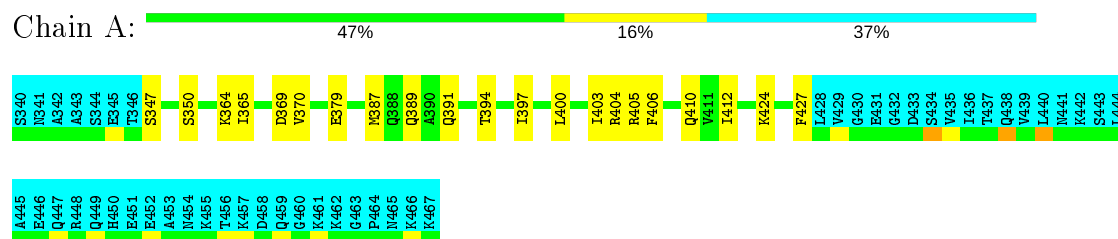


- Molecule 1: PC4 and SFRS1-interacting protein

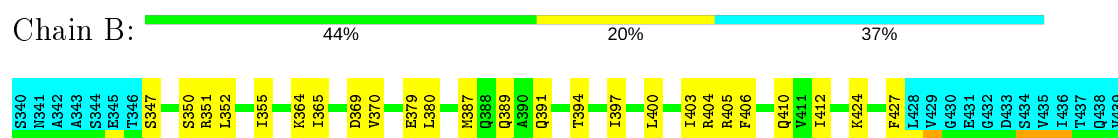


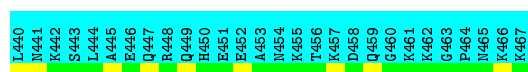
#### 4.2.27 Score per residue for model 27

- Molecule 1: PC4 and SFRS1-interacting protein



- Molecule 1: PC4 and SFRS1-interacting protein



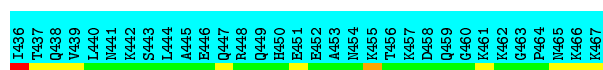


#### 4.2.28 Score per residue for model 28

- Molecule 1: PC4 and SFRS1-interacting protein

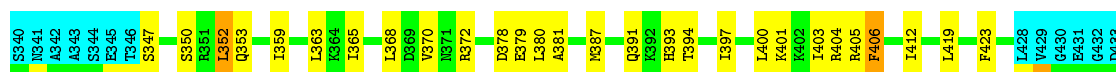


- Molecule 1: PC4 and SFRS1-interacting protein

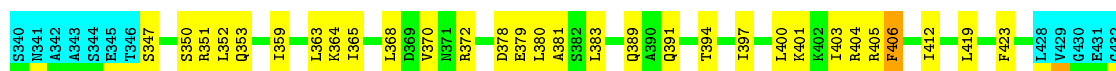


#### 4.2.29 Score per residue for model 29

- Molecule 1: PC4 and SFRS1-interacting protein

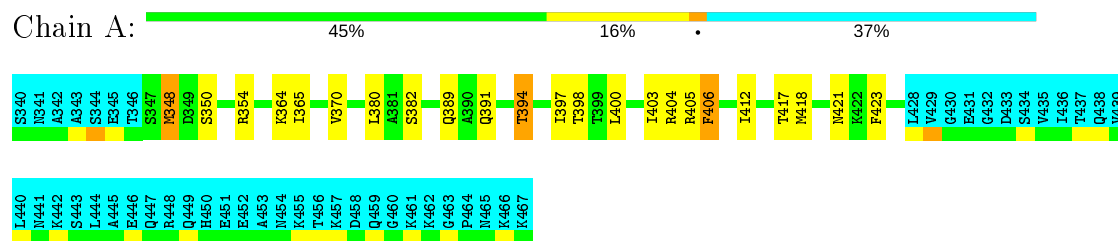


- Molecule 1: PC4 and SFRS1-interacting protein

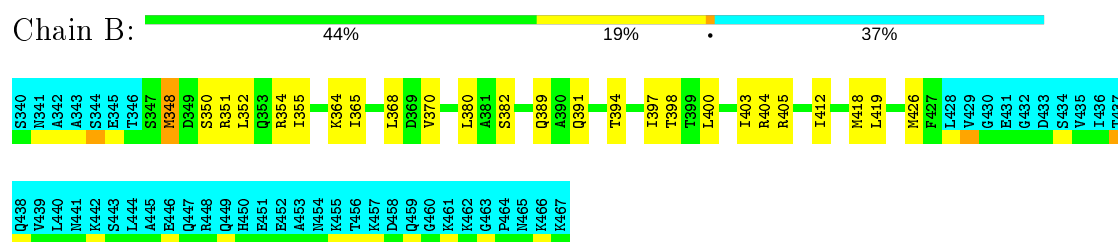


### 4.2.30 Score per residue for model 30

- Molecule 1: PC4 and SFRS1-interacting protein



- Molecule 1: PC4 and SFRS1-interacting protein



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1561
Number of shifts mapped to atoms	1561
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	665	701	701	14±2
1	B	665	701	701	14±2
All	All	39900	42060	42060	535

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:403:ILE:HG22	1:B:365:ILE:HD11	0.94	1.39	3	30
1:A:365:ILE:HD11	1:B:403:ILE:HG22	0.94	1.39	13	30
1:A:380:LEU:HD23	1:B:419:LEU:HD13	0.82	1.50	21	1
1:A:419:LEU:HD13	1:B:380:LEU:HD23	0.82	1.50	18	2
1:A:419:LEU:HD12	1:B:380:LEU:HD12	0.66	1.66	17	4
1:A:419:LEU:HD13	1:B:380:LEU:CD2	0.65	2.21	18	2
1:A:380:LEU:HD21	1:A:396:MET:HE1	0.64	1.69	3	2
1:A:406:PHE:CD2	1:B:368:LEU:HD13	0.63	2.28	19	8
1:A:380:LEU:HD12	1:B:419:LEU:HD12	0.63	1.70	28	3
1:A:412:ILE:HD11	1:B:370:VAL:HB	0.62	1.71	17	26
1:A:380:LEU:CD2	1:B:419:LEU:HD13	0.62	2.24	21	1
1:B:380:LEU:HD21	1:B:396:MET:HE1	0.61	1.72	3	1
1:A:380:LEU:HD12	1:B:419:LEU:HD22	0.61	1.72	12	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:368:LEU:HD13	1:B:406:PHE:CE1	0.61	2.31	15	5
1:A:397:ILE:HD13	1:B:427:PHE:CE2	0.60	2.32	27	3
1:A:406:PHE:CE2	1:B:368:LEU:HD13	0.60	2.32	19	5
1:A:370:VAL:HB	1:B:412:ILE:HD11	0.59	1.72	11	26
1:A:397:ILE:HA	1:A:400:LEU:HD12	0.59	1.74	20	29
1:B:397:ILE:HA	1:B:400:LEU:HD12	0.59	1.74	20	29
1:B:352:LEU:HA	1:B:355:ILE:HD12	0.59	1.74	8	17
1:A:427:PHE:CE2	1:B:397:ILE:HD13	0.59	2.33	27	3
1:B:394:THR:HA	1:B:397:ILE:HD12	0.58	1.74	12	12
1:A:380:LEU:O	1:A:380:LEU:HD13	0.58	1.99	20	6
1:A:380:LEU:HD13	1:A:380:LEU:O	0.57	2.00	25	7
1:A:394:THR:HA	1:A:397:ILE:HD12	0.57	1.74	12	12
1:B:380:LEU:HD13	1:B:380:LEU:O	0.57	2.00	1	6
1:A:365:ILE:CD1	1:B:403:ILE:HG22	0.57	2.26	11	29
1:A:415:LYS:CB	1:B:377:LEU:HD23	0.57	2.30	14	1
1:A:351:ARG:CZ	1:A:383:LEU:HD21	0.56	2.30	23	2
1:B:351:ARG:CZ	1:B:383:LEU:HD21	0.56	2.31	29	2
1:A:419:LEU:HG	1:B:380:LEU:HD12	0.56	1.77	20	1
1:A:381:ALA:HB2	1:B:419:LEU:HD21	0.56	1.78	29	2
1:A:377:LEU:HD23	1:B:419:LEU:HD12	0.56	1.77	17	1
1:B:380:LEU:O	1:B:380:LEU:HD13	0.55	2.02	9	4
1:A:403:ILE:HG22	1:B:365:ILE:CD1	0.55	2.28	6	29
1:A:352:LEU:HD23	1:A:393:HIS:CG	0.55	2.37	8	7
1:B:355:ILE:HG23	1:B:376:ALA:HB1	0.53	1.80	16	15
1:A:419:LEU:HD13	1:B:380:LEU:HD12	0.53	1.78	24	4
1:A:423:PHE:CZ	1:B:380:LEU:HD11	0.52	2.39	2	12
1:A:419:LEU:HD22	1:B:380:LEU:HD12	0.52	1.82	12	3
1:A:377:LEU:HD23	1:B:415:LYS:CB	0.52	2.34	14	1
1:A:377:LEU:HD22	1:B:419:LEU:HD12	0.52	1.80	7	1
1:A:380:LEU:HD11	1:B:423:PHE:CZ	0.52	2.39	29	13
1:A:391:GLN:O	1:A:394:THR:HG23	0.52	2.05	20	10
1:A:406:PHE:CD1	1:B:368:LEU:HD13	0.52	2.40	14	3
1:A:380:LEU:HD21	1:A:396:MET:HE3	0.52	1.82	7	2
1:A:380:LEU:HD12	1:B:419:LEU:HD13	0.51	1.82	19	5
1:A:352:LEU:HA	1:A:355:ILE:HD12	0.51	1.83	28	11
1:B:352:LEU:HD22	1:B:396:MET:HE1	0.50	1.82	22	1
1:A:417:THR:HG22	1:A:421:ASN:OD1	0.50	2.06	11	2
1:B:391:GLN:O	1:B:394:THR:HG23	0.50	2.07	6	12
1:B:380:LEU:HD21	1:B:396:MET:HE3	0.49	1.84	7	1
1:A:394:THR:HG22	1:B:427:PHE:CZ	0.49	2.42	1	1
1:A:419:LEU:CD1	1:B:380:LEU:HD12	0.49	2.36	17	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:419:LEU:HD21	1:B:381:ALA:HB2	0.49	1.83	29	1
1:A:427:PHE:CZ	1:B:394:THR:HG22	0.49	2.42	1	1
1:A:397:ILE:HD13	1:B:427:PHE:CZ	0.48	2.42	11	2
1:A:355:ILE:CD1	1:A:383:LEU:HD11	0.48	2.39	13	2
1:A:368:LEU:HD13	1:B:406:PHE:CD1	0.48	2.43	6	6
1:A:368:LEU:HD13	1:B:406:PHE:CD2	0.47	2.44	25	4
1:A:406:PHE:CE1	1:B:368:LEU:HD13	0.47	2.45	22	2
1:A:380:LEU:HD23	1:A:383:LEU:HD12	0.47	1.85	18	1
1:A:427:PHE:CZ	1:B:397:ILE:HD13	0.47	2.44	27	2
1:A:406:PHE:CE1	1:B:408:VAL:HG13	0.46	2.45	3	2
1:B:370:VAL:O	1:B:374:ILE:HD12	0.46	2.11	20	2
1:A:415:LYS:HB2	1:B:377:LEU:HD23	0.45	1.87	14	1
1:B:359:ILE:HG22	1:B:363:LEU:HD12	0.45	1.89	6	5
1:B:352:LEU:CD2	1:B:380:LEU:HD23	0.45	2.42	20	1
1:A:406:PHE:CD2	1:B:365:ILE:HD13	0.45	2.47	14	1
1:A:380:LEU:HD12	1:B:419:LEU:CD1	0.44	2.42	10	2
1:A:370:VAL:O	1:A:374:ILE:HD12	0.44	2.13	12	2
1:A:359:ILE:HG22	1:A:363:LEU:HD12	0.44	1.88	15	5
1:A:359:ILE:HG23	1:A:373:CYS:SG	0.44	2.52	19	1
1:A:419:LEU:HD12	1:B:377:LEU:HD22	0.43	1.89	7	1
1:A:408:VAL:HG13	1:A:408:VAL:O	0.43	2.13	19	1
1:A:423:PHE:HZ	1:B:380:LEU:HD11	0.43	1.74	9	1
1:A:408:VAL:HG13	1:B:406:PHE:CE2	0.43	2.48	24	1
1:A:352:LEU:HD22	1:A:396:MET:HE1	0.42	1.90	22	1
1:A:365:ILE:HD11	1:B:403:ILE:CG2	0.42	2.29	30	1
1:A:380:LEU:C	1:A:380:LEU:HD13	0.42	2.35	29	4
1:A:368:LEU:HD13	1:B:406:PHE:CE2	0.42	2.50	25	1
1:A:382:SER:O	1:A:383:LEU:HD23	0.42	2.14	20	1
1:A:352:LEU:HD23	1:A:355:ILE:HD12	0.42	1.92	13	1
1:A:380:LEU:HD13	1:A:380:LEU:C	0.42	2.36	24	3
1:A:351:ARG:NH2	1:A:383:LEU:HD22	0.41	2.30	20	1
1:B:408:VAL:HG22	1:B:412:ILE:HB	0.41	1.92	19	2
1:A:351:ARG:HH11	1:A:383:LEU:HD22	0.41	1.75	25	1
1:A:352:LEU:HD22	1:A:396:MET:CE	0.41	2.46	15	2
1:A:417:THR:HG22	1:A:421:ASN:ND2	0.41	2.30	5	1
1:B:380:LEU:HD13	1:B:380:LEU:C	0.41	2.36	13	2
1:B:380:LEU:C	1:B:380:LEU:HD13	0.41	2.35	29	3
1:A:380:LEU:HD11	1:B:423:PHE:HZ	0.41	1.76	17	2
1:A:408:VAL:HG22	1:A:412:ILE:HB	0.41	1.92	28	1
1:B:396:MET:HB3	1:B:396:MET:HE2	0.41	1.86	28	1
1:B:352:LEU:HD23	1:B:393:HIS:CG	0.41	2.51	1	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:370:VAL:CB	1:B:412:ILE:HD11	0.40	2.45	11	1
1:B:359:ILE:HG23	1:B:373:CYS:SG	0.40	2.56	19	2
1:A:412:ILE:HD11	1:B:370:VAL:CB	0.40	2.45	17	1
1:A:403:ILE:CG2	1:B:365:ILE:HD11	0.40	2.28	3	1
1:A:415:LYS:HB3	1:B:377:LEU:HD23	0.40	1.93	14	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	81/128 (63%)	76±1 (93±1%)	5±1 (7±1%)	0±0 (0±0%)	100	100
1	B	81/128 (63%)	76±1 (93±1%)	5±1 (7±1%)	0±0 (0±0%)	100	100
All	All	4860/7680 (63%)	4538 (93%)	321 (7%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	B	409	SER	1

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	77/116 (66%)	65±2 (84±3%)	12±2 (16±3%)	5	42
1	B	77/116 (66%)	65±2 (84±3%)	12±2 (16±3%)	5	42
All	All	4620/6960 (66%)	3883 (84%)	737 (16%)	5	42

All 83 unique residues with a non-rotameric sidechain are listed below. They are sorted by the



frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	405	ARG	30
1	B	405	ARG	30
1	B	364	LYS	26
1	A	406	PHE	25
1	A	364	LYS	24
1	B	406	PHE	24
1	B	404	ARG	22
1	A	404	ARG	22
1	A	387	MET	19
1	B	394	THR	18
1	A	394	THR	18
1	B	387	MET	18
1	A	348	MET	15
1	A	382	SER	15
1	B	382	SER	15
1	B	348	MET	15
1	B	379	GLU	14
1	A	379	GLU	14
1	B	347	SER	13
1	B	372	ARG	13
1	A	347	SER	13
1	A	372	ARG	13
1	B	350	SER	12
1	A	350	SER	12
1	B	401	LYS	12
1	B	389	GLN	11
1	B	380	LEU	10
1	A	407	LYS	10
1	A	389	GLN	10
1	A	401	LYS	10
1	A	378	ASP	8
1	B	407	LYS	8
1	A	380	LEU	8
1	A	392	LYS	8
1	B	392	LYS	8
1	B	378	ASP	8
1	A	418	MET	7
1	A	353	GLN	7
1	A	395	GLU	7
1	A	425	ASN	7
1	A	349	ASP	7
1	B	418	MET	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	B	425	ASN	7
1	B	349	ASP	7
1	B	369	ASP	7
1	A	369	ASP	7
1	B	395	GLU	7
1	A	352	LEU	6
1	B	414	GLU	6
1	A	360	LYS	6
1	B	353	GLN	6
1	A	391	GLN	5
1	A	351	ARG	5
1	A	414	GLU	5
1	B	391	GLN	5
1	B	352	LEU	5
1	A	424	LYS	5
1	A	354	ARG	4
1	B	351	ARG	4
1	B	424	LYS	4
1	B	354	ARG	4
1	A	384	GLN	3
1	B	388	GLN	3
1	B	421	ASN	3
1	A	421	ASN	3
1	A	388	GLN	3
1	B	384	GLN	3
1	B	410	GLN	2
1	B	398	THR	2
1	A	398	THR	2
1	B	360	LYS	2
1	A	410	GLN	2
1	B	371	ASN	1
1	B	402	LYS	1
1	A	409	SER	1
1	A	367	ASN	1
1	B	422	LYS	1
1	B	427	PHE	1
1	B	367	ASN	1
1	B	396	MET	1
1	A	371	ASN	1
1	A	422	LYS	1
1	B	409	SER	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 44% for the well-defined parts and 42% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1561
Number of shifts mapped to atoms	1561
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	126	$-0.69 \pm 0.15$	Should be applied
$^{13}\text{C}_\beta$	121	$0.28 \pm 0.05$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	126	$-0.48 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	122	$-0.42 \pm 0.26$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 44%, i.e. 946 atoms were assigned a chemical shift out of a possible 2162. 12 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	396/810 (49%)	158/324 (49%)	160/324 (49%)	78/162 (48%)
Sidechain	522/1254 (42%)	324/736 (44%)	190/448 (42%)	8/70 (11%)

*Continued on next page...*

Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	28/98 (29%)	20/54 (37%)	8/40 (20%)	0/4 (0%)
Overall	946/2162 (44%)	502/1114 (45%)	358/812 (44%)	86/236 (36%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 42%, i.e. 1389 atoms were assigned a chemical shift out of a possible 3278. 17 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	622/1276 (49%)	248/510 (49%)	252/512 (49%)	122/254 (48%)
Sidechain	739/1890 (39%)	452/1108 (41%)	279/676 (41%)	8/106 (8%)
Aromatic	28/112 (25%)	20/62 (32%)	8/44 (18%)	0/6 (0%)
Overall	1389/3278 (42%)	720/1680 (43%)	539/1232 (44%)	130/366 (36%)

#### 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:

