



# Full wwPDB NMR Structure Validation Report ⓘ

May 31, 2020 – 10:26 pm BST

PDB ID : 6EMQ  
Title : Solution structure of the LEDGF/p75 IBD - MLL1 (aa 111-160) complex  
Authors : Veverka, V.  
Deposited on : 2017-10-03

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.

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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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

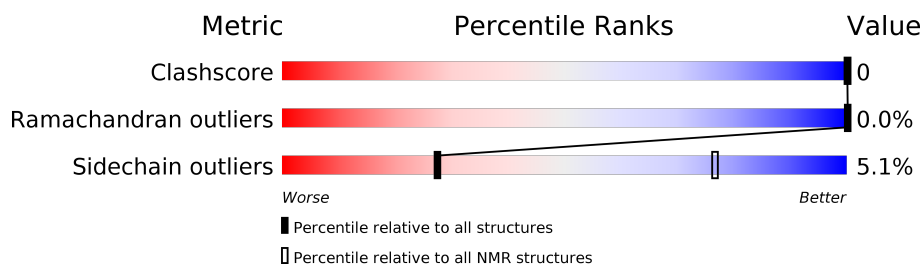
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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	165	

## 2 Ensemble composition and analysis

This entry contains 40 models. Model 10 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:348-A:426, A:497-A:500 (83)	0.18	10

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 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 32, 36, 37, 39, 40
2	15, 31
3	18, 33
4	30, 35
Single-model clusters	21; 34; 38

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2507 atoms, of which 1251 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A.

Mol	Chain	Residues	Atoms						Trace
1	A	165	Total	C	H	N	O	S	0
			2507	771	1251	227	251	7	

There are 16 discrepancies between the modelled and reference sequences:

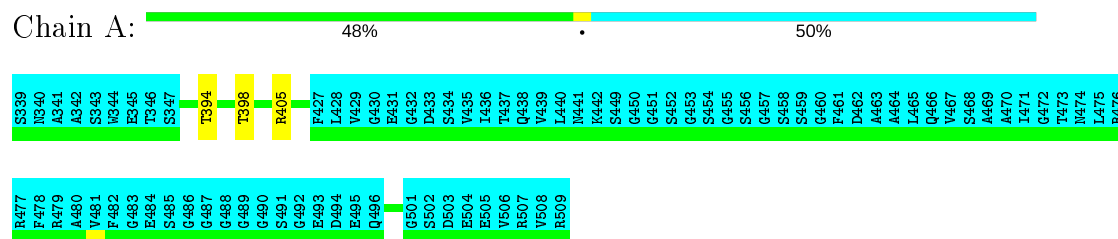
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	SER	-	expression tag	UNP O75475
A	340	ASN	-	expression tag	UNP O75475
A	341	ALA	-	expression tag	UNP O75475
A	342	ALA	-	expression tag	UNP O75475
A	343	SER	-	expression tag	UNP O75475
A	344	TRP	-	expression tag	UNP O75475
A	450	GLY	-	linker	UNP O75475
A	451	GLY	-	linker	UNP O75475
A	452	SER	-	linker	UNP O75475
A	453	GLY	-	linker	UNP O75475
A	454	SER	-	linker	UNP O75475
A	455	GLY	-	linker	UNP O75475
A	456	SER	-	linker	UNP O75475
A	457	GLY	-	linker	UNP O75475
A	458	SER	-	linker	UNP O75475
A	459	SER	PRO	linker	UNP Q03164

## 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: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

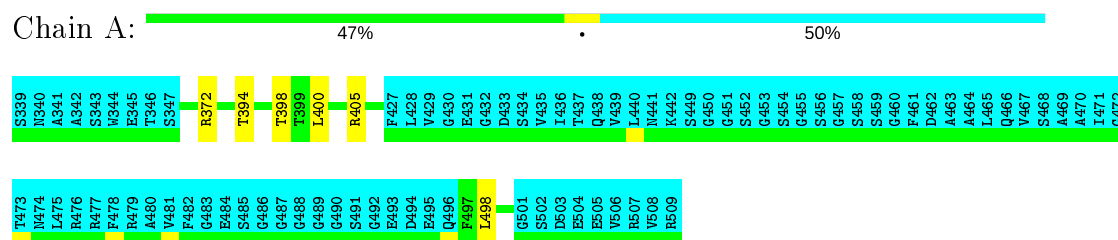


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

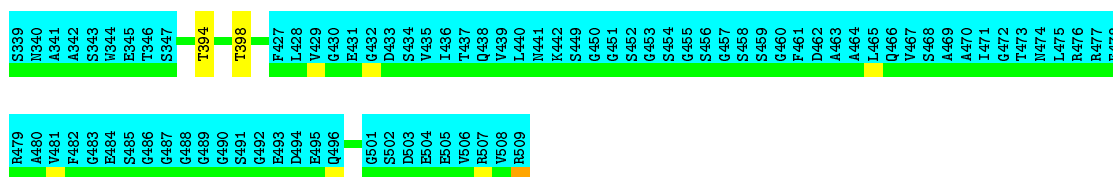
- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



#### 4.2.2 Score per residue for model 2

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

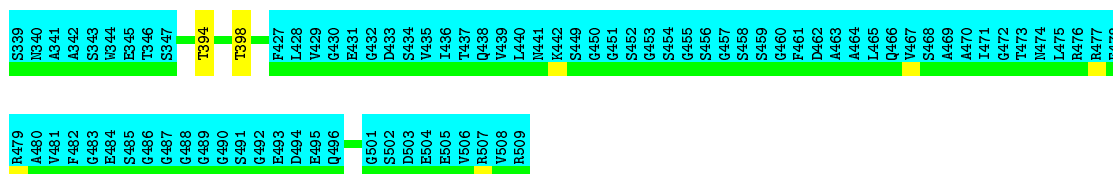




### 4.2.3 Score per residue for model 3

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

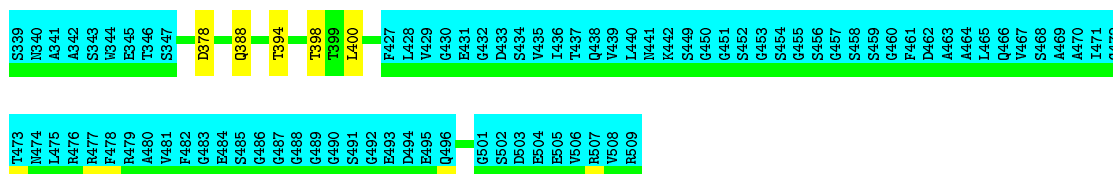
Chain A: 49% 50%



### 4.2.4 Score per residue for model 4

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

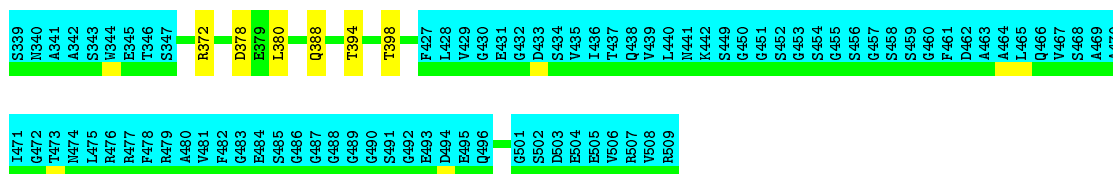
Chain A: 47% 50%



### 4.2.5 Score per residue for model 5

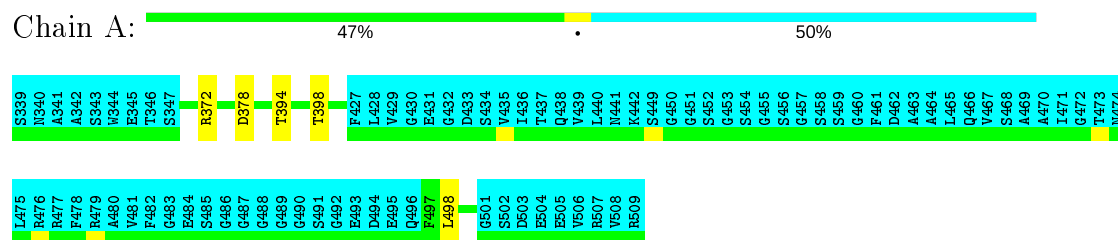
- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

Chain A: 47% 50%



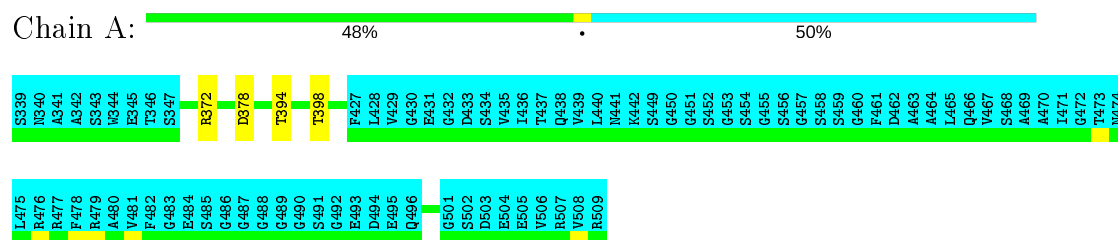
### 4.2.6 Score per residue for model 6

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



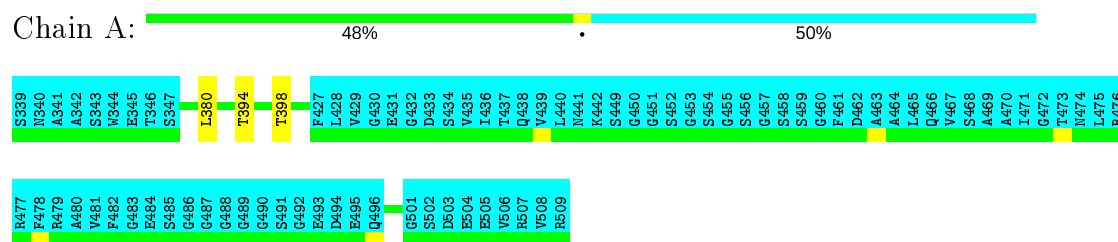
#### 4.2.7 Score per residue for model 7

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



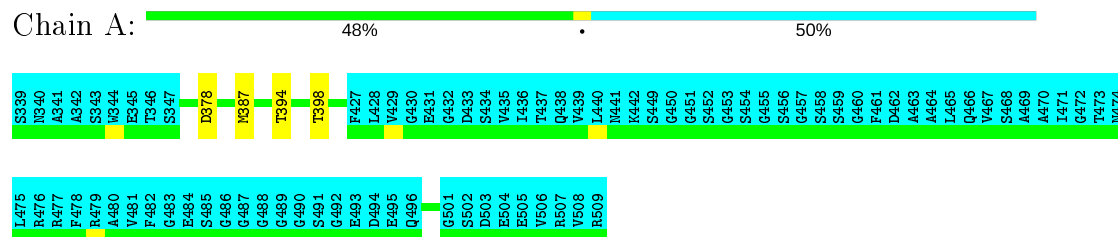
#### 4.2.8 Score per residue for model 8

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



#### 4.2.9 Score per residue for model 9

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



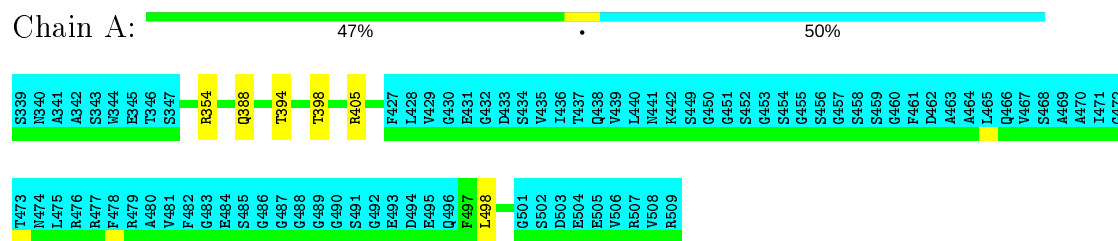






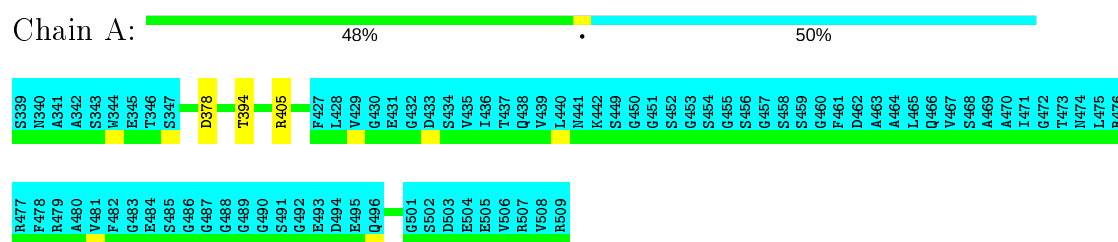
### 4.2.18 Score per residue for model 18

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



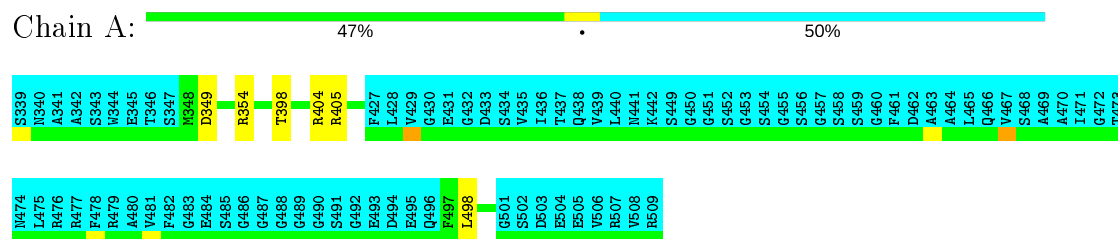
### 4.2.19 Score per residue for model 19

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



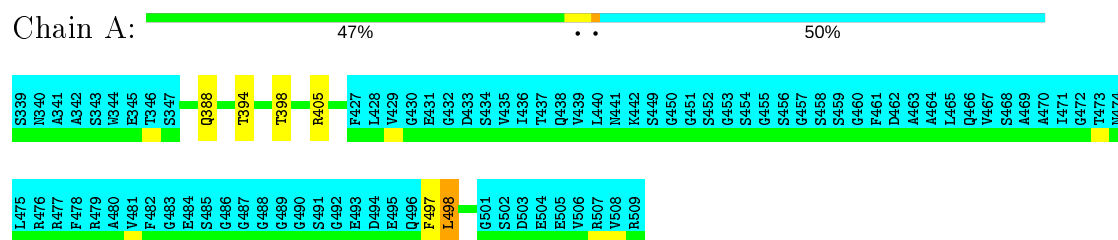
### 4.2.20 Score per residue for model 20

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



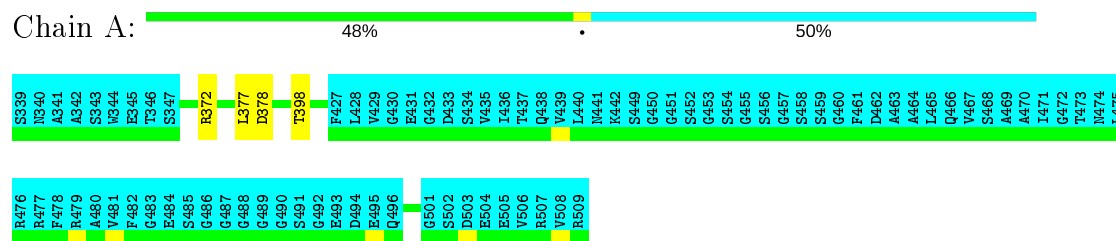
### 4.2.21 Score per residue for model 21

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



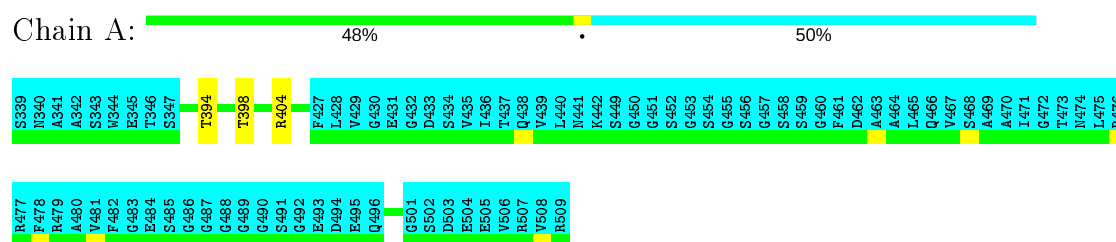
### 4.2.22 Score per residue for model 22

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



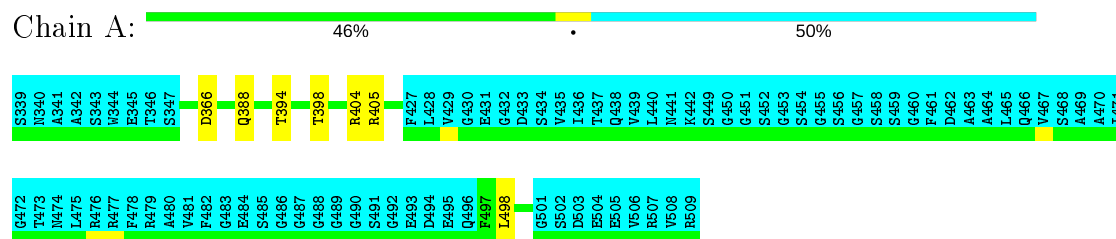
### 4.2.23 Score per residue for model 23

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



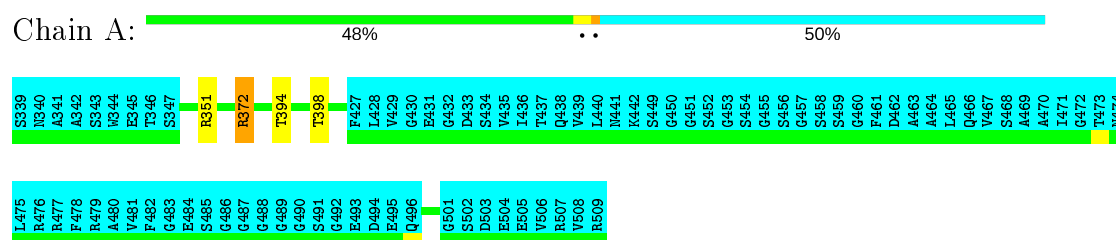
### 4.2.24 Score per residue for model 24

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



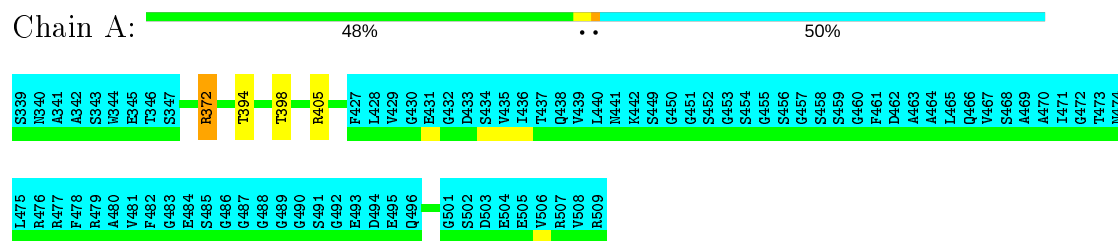
### 4.2.25 Score per residue for model 25

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



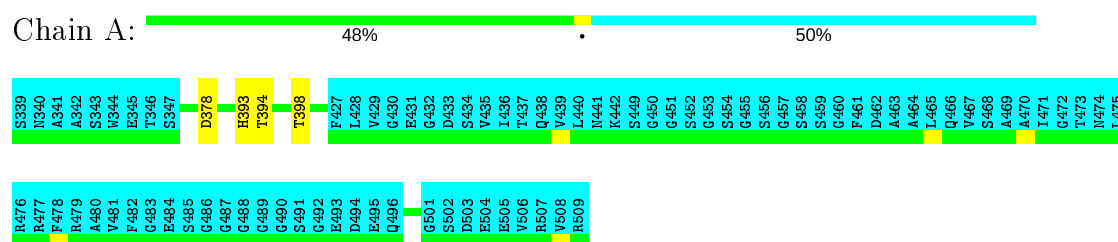
### 4.2.26 Score per residue for model 26

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



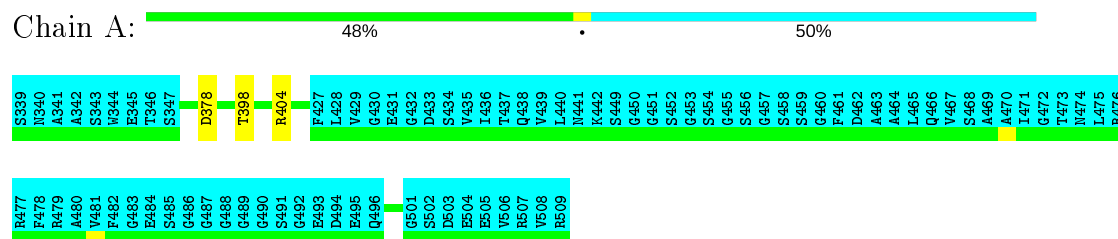
### 4.2.27 Score per residue for model 27

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



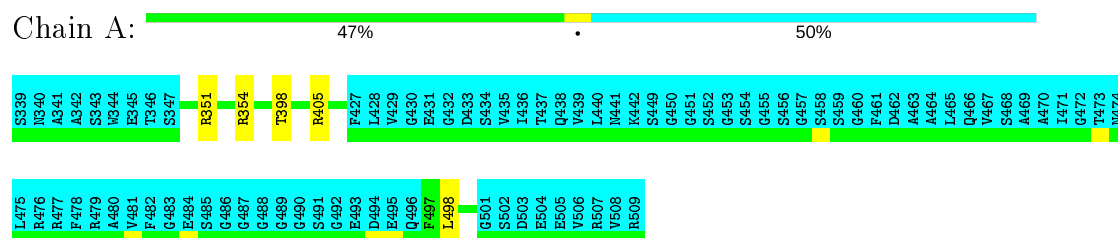
### 4.2.28 Score per residue for model 28

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



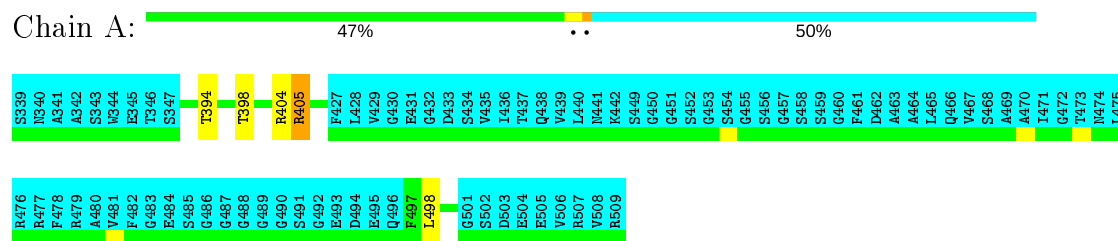
### 4.2.29 Score per residue for model 29

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



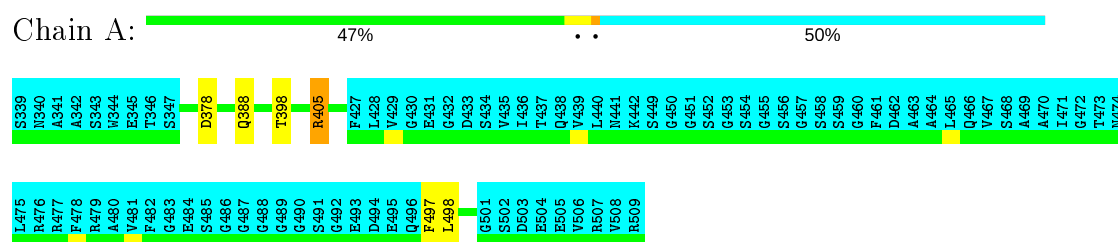
### 4.2.30 Score per residue for model 30

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



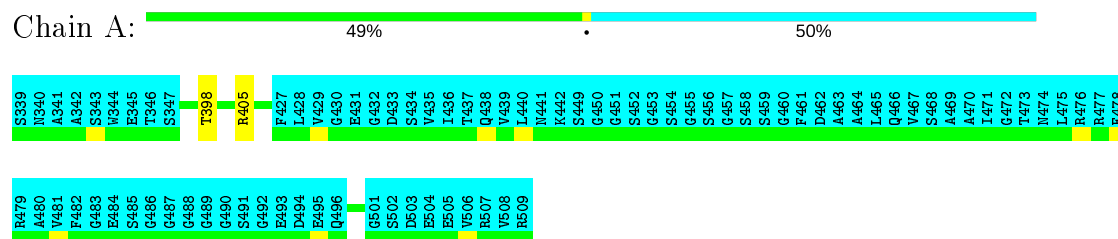
### 4.2.31 Score per residue for model 31

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



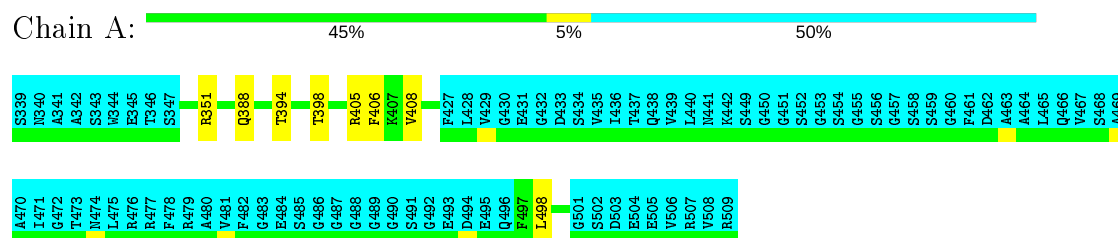
### 4.2.32 Score per residue for model 32

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



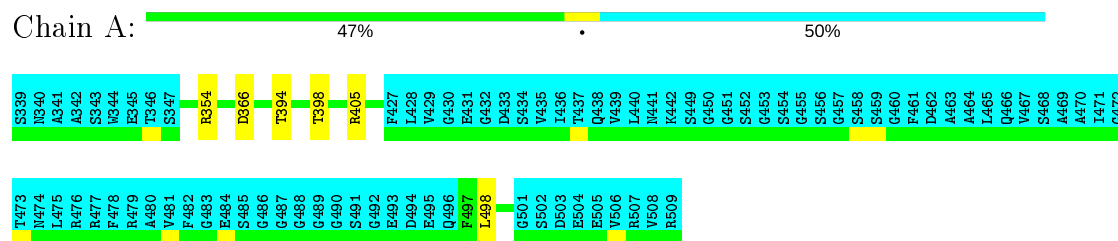
### 4.2.33 Score per residue for model 33

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



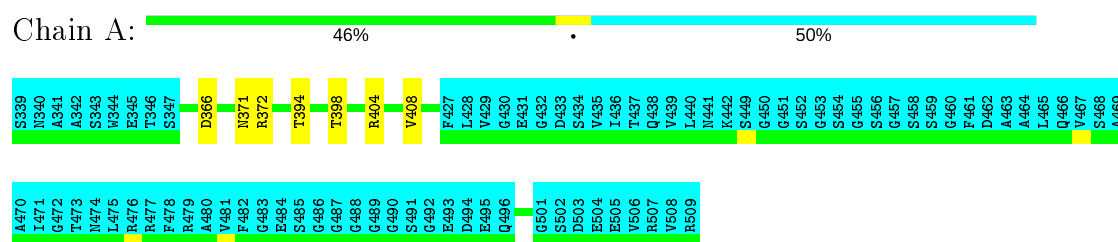
#### 4.2.34 Score per residue for model 34

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



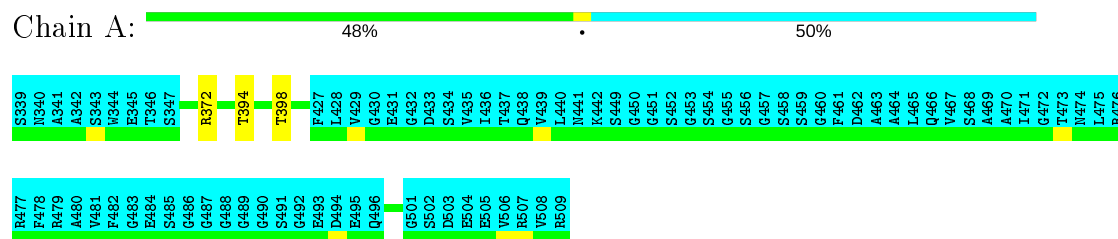
#### 4.2.35 Score per residue for model 35

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



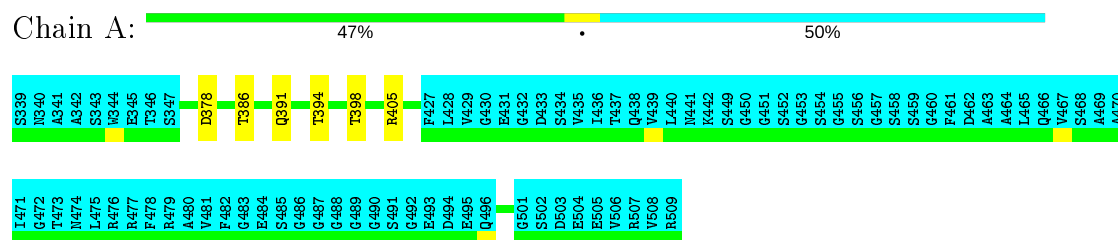
#### 4.2.36 Score per residue for model 36

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



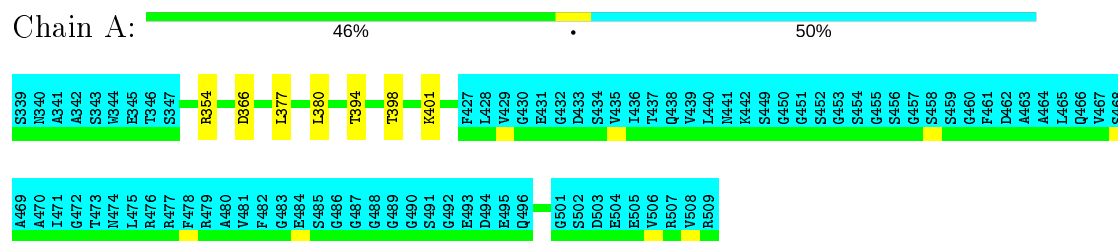
#### 4.2.37 Score per residue for model 37

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



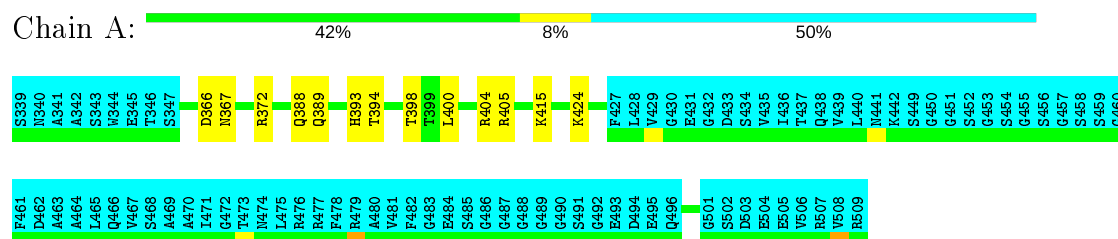
### 4.2.38 Score per residue for model 38

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



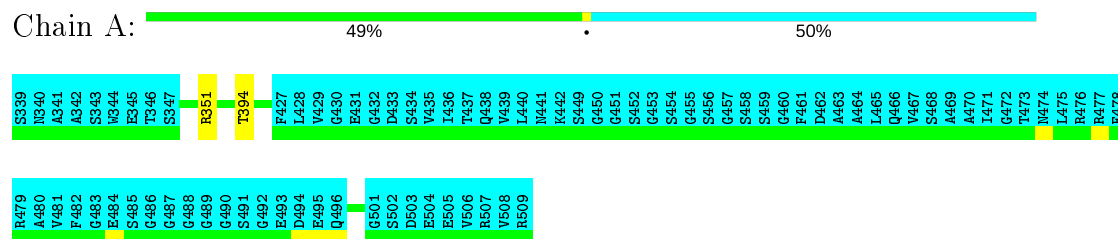
### 4.2.39 Score per residue for model 39

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



### 4.2.40 Score per residue for model 40

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 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
YASARA	refinement	
TopSpin	structure solution	
Sparky	structure solution	
CYANA	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1837
Number of shifts mapped to atoms	1837
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	682	719	719	0±0
All	All	27280	28760	28760	1

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 0.



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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:406:PHE:CE1	1:A:408:VAL:HG22	0.41	2.50	33	1

## 5.2 Torsion angles [i](#)

### 5.2.1 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	83/165 (50%)	82±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
All	All	3320/6600 (50%)	3269 (98%)	50 (2%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	498	LEU	1

### 5.2.2 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	78/136 (57%)	74±2 (95±2%)	4±2 (5±2%)	27	77
All	All	3120/5440 (57%)	2962 (95%)	158 (5%)	27	77

All 26 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	398	THR	38
1	A	394	THR	33
1	A	378	ASP	14

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Mol	Chain	Res	Type	Models (Total)
1	A	498	LEU	13
1	A	405	ARG	10
1	A	388	GLN	8
1	A	372	ARG	7
1	A	366	ASP	6
1	A	380	LEU	4
1	A	400	LEU	4
1	A	377	LEU	2
1	A	497	PHE	2
1	A	393	HIS	2
1	A	371	ASN	2
1	A	387	MET	2
1	A	389	GLN	1
1	A	354	ARG	1
1	A	401	LYS	1
1	A	415	LYS	1
1	A	404	ARG	1
1	A	386	THR	1
1	A	424	LYS	1
1	A	391	GLN	1
1	A	349	ASP	1
1	A	408	VAL	1
1	A	367	ASN	1

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

## 5.6 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 6 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 84% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *str*

#### 6.1.1 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	1837
Number of shifts mapped to atoms	1837
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

#### 6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	$-0.62 \pm 0.13$	Should be applied
$^{13}\text{C}_\beta$	138	$0.22 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	142	$-0.39 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	144	$-0.27 \pm 0.18$	None needed ( $< 0.5$ ppm)

#### 6.1.3 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 90%, i.e. 999 atoms were assigned a chemical shift out of a possible 1109. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	402/415 (97%)	163/166 (98%)	159/166 (96%)	80/83 (96%)
Sidechain	544/636 (86%)	340/373 (91%)	193/228 (85%)	11/35 (31%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	53/58 (91%)	30/32 (94%)	23/24 (96%)	0/2 (0%)
Overall	999/1109 (90%)	533/571 (93%)	375/418 (90%)	91/120 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1648 atoms were assigned a chemical shift out of a possible 1965. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	723/825 (88%)	288/330 (87%)	291/330 (88%)	144/165 (87%)
Sidechain	826/1034 (80%)	511/604 (85%)	301/373 (81%)	14/57 (25%)
Aromatic	99/106 (93%)	54/58 (93%)	44/45 (98%)	1/3 (33%)
Overall	1648/1965 (84%)	853/992 (86%)	636/748 (85%)	159/225 (71%)

#### 6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 6.1.5 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:

