



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 11:53 am BST

PDB ID : 6SDW
Title : Solution structure of Staufen1 dsRBD3+4 - hARF1 SBS dsRNA complex.
Authors : Yadav, D.K.; Lukavsky, P.J.
Deposited on : 2019-07-29

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 : 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

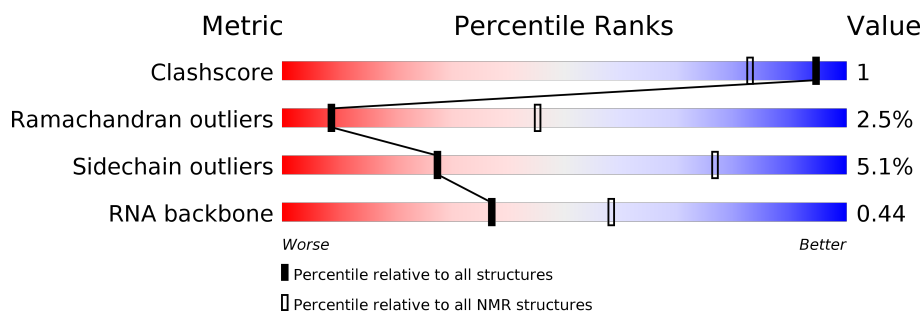
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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
RNA backbone	4643	676

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	177	 59% 5% • 35%
2	B	34	 6% 71% 21% •

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:103-A:121, A:137-A:148, A:157-A:169, A:204-A:274 (115)	0.71	1

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 8, 9, 10, 11, 12, 13, 14, 15, 17
2	3, 7, 16, 18
3	19, 20
Single-model clusters	6

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3949 atoms, of which 1842 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Double-stranded RNA-binding protein Staufen homolog 1.

Mol	Chain	Residues	Atoms						Trace
1	A	177	Total	C	H	N	O	S	0
			2863	879	1476	254	250	4	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	GLY	-	expression tag	UNP O95793
A	99	SER	-	expression tag	UNP O95793
A	100	HIS	-	expression tag	UNP O95793
A	101	MET	-	expression tag	UNP O95793

- Molecule 2 is a RNA chain called hARF1 SBS dsRNA.

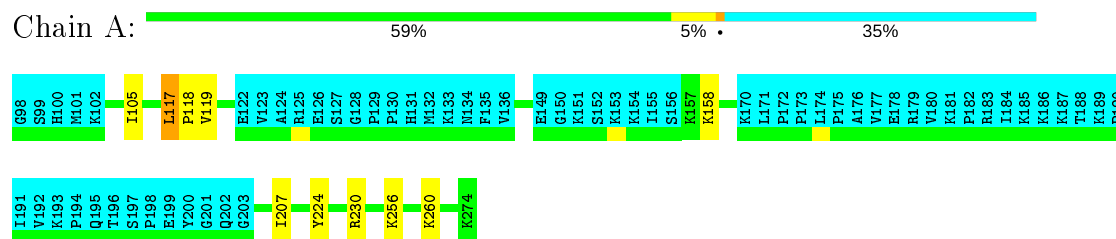
Mol	Chain	Residues	Atoms						Trace
2	B	34	Total	C	H	N	O	P	0
			1086	322	366	126	239	33	

4 Residue-property plots [i](#)

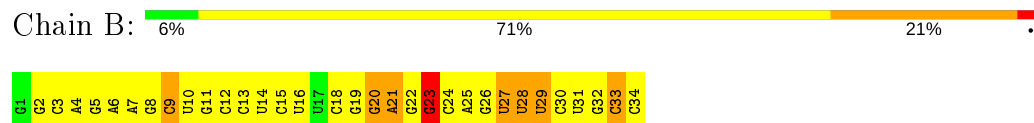
4.1 Average score per residue in the NMR ensemble

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: Double-stranded RNA-binding protein Staufen homolog 1



- Molecule 2: hARF1 SBS dsRNA

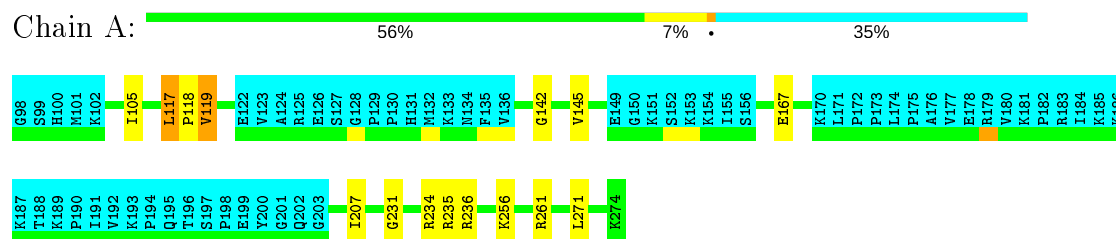


4.2 Scores per residue for each member of the ensemble

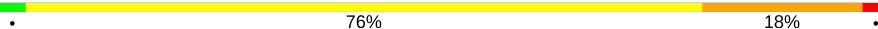
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1



- Molecule 2: hARF1 SBS dsRNA

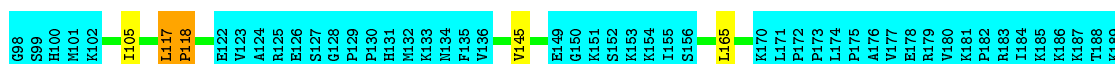
Chain B: 



4.2.2 Score per residue for model 2

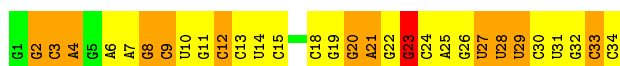
- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 



- Molecule 2: hARF1 SBS dsRNA

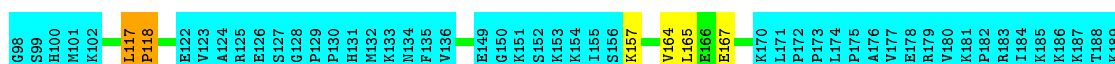
Chain B: 



4.2.3 Score per residue for model 3

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 



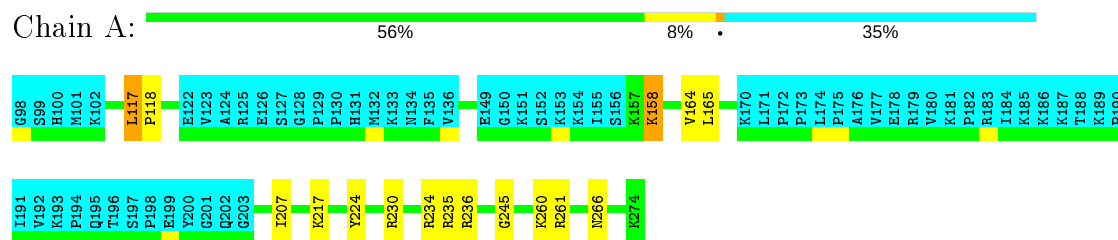
- Molecule 2: hARF1 SBS dsRNA

Chain B: 

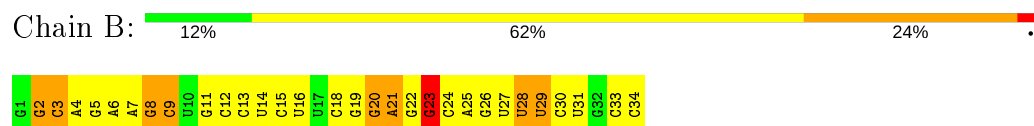


4.2.4 Score per residue for model 4

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

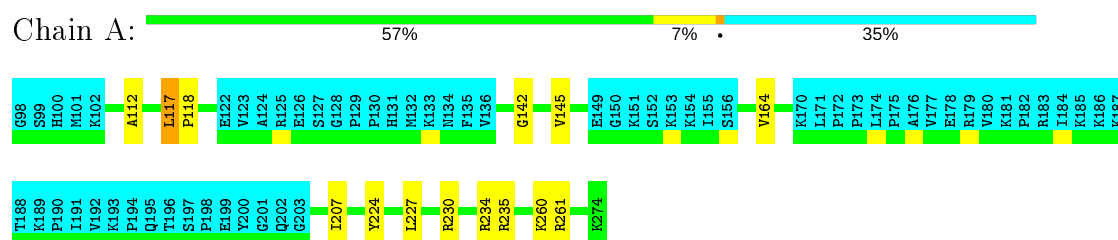


- Molecule 2: hARF1 SBS dsRNA

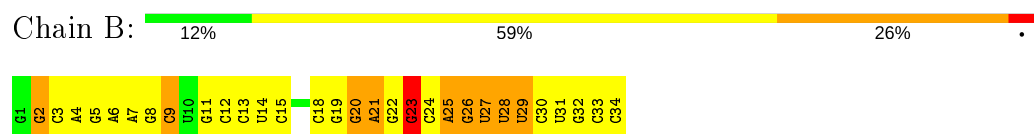


4.2.5 Score per residue for model 5

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

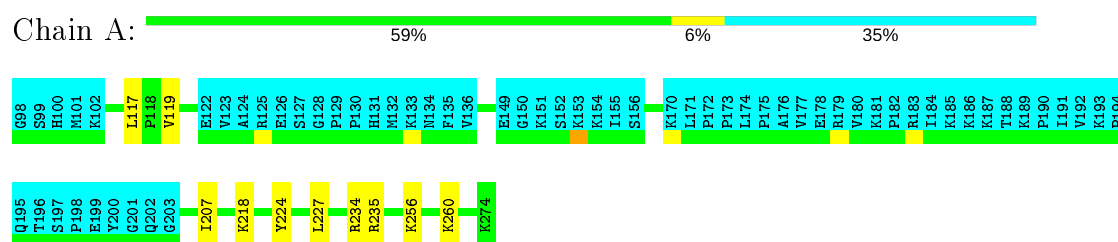


- Molecule 2: hARF1 SBS dsRNA

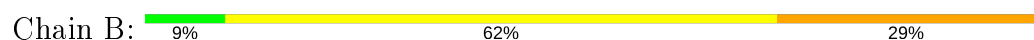


4.2.6 Score per residue for model 6

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1



- Molecule 2: hARF1 SBS dsRNA

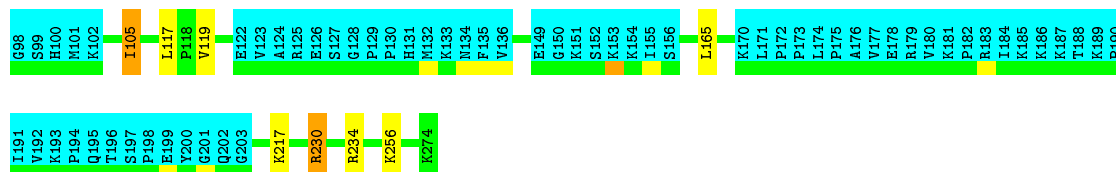




4.2.7 Score per residue for model 7

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 60% 35%



- Molecule 2: hARF1 SBS dsRNA

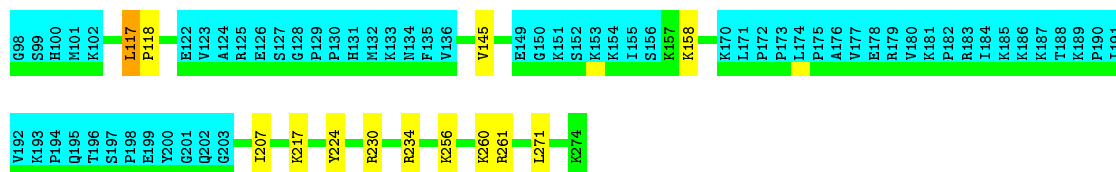
Chain B: 12% 56% 26% 6%



4.2.8 Score per residue for model 8

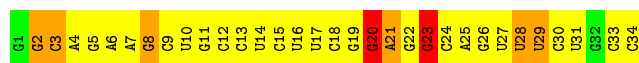
- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 58% 7% 35%



- Molecule 2: hARF1 SBS dsRNA

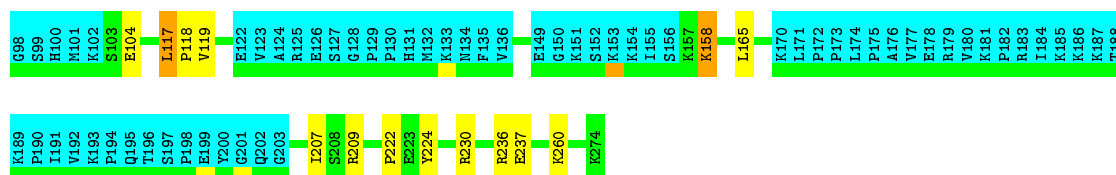
Chain B: 6% 71% 18% 6%



4.2.9 Score per residue for model 9

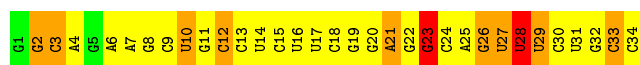
- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 57% 7% 35%



- Molecule 2: hARF1 SBS dsRNA

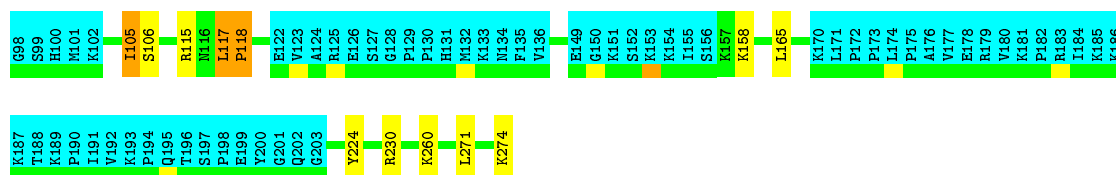
Chain B: 6% 62% 26% 6%



4.2.10 Score per residue for model 10

- Molecule 1: Double-stranded RNA-binding protein Staufens homolog 1

Chain A: 58% 5% 35%



- Molecule 2: hARF1 SBS dsRNA

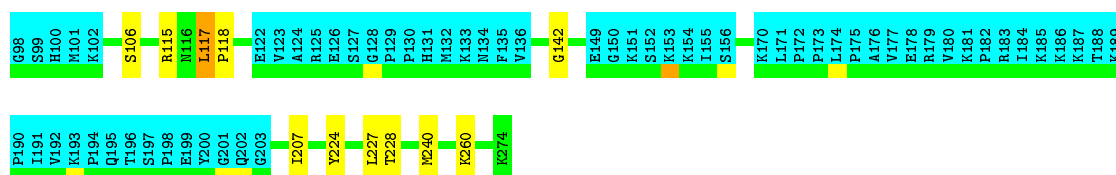
Chain B: 6% 65% 24% 6%



4.2.11 Score per residue for model 11

- Molecule 1: Double-stranded RNA-binding protein Staufens homolog 1

Chain A: 59% 6% 35%



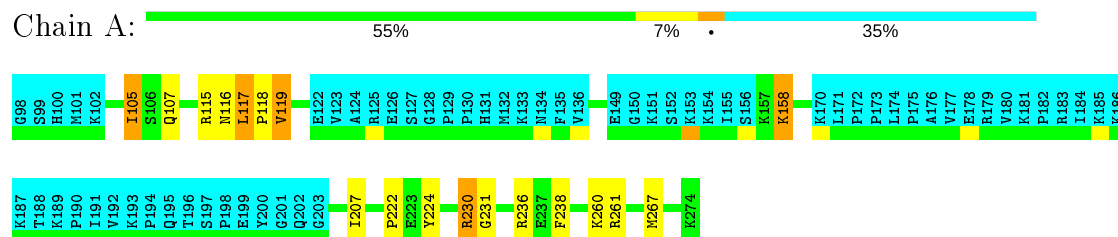
- Molecule 2: hARF1 SBS dsRNA

Chain B: 9% 59% 21% 12%

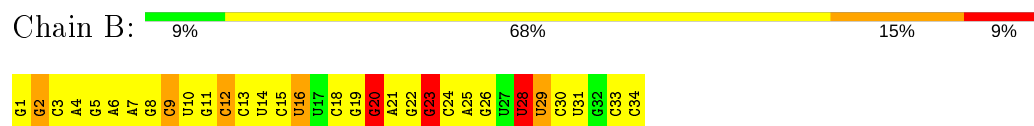


4.2.12 Score per residue for model 12

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

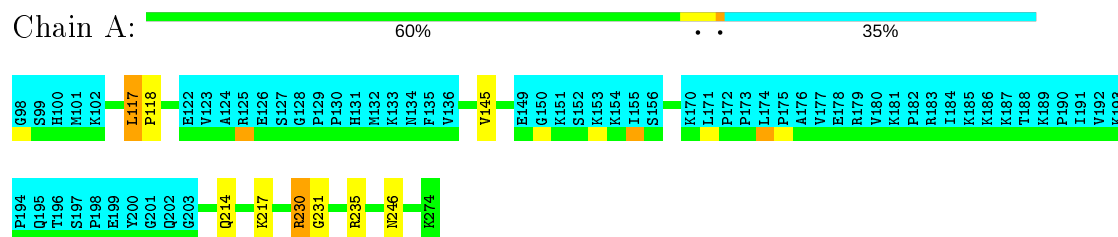


- Molecule 2: hARF1 SBS dsRNA

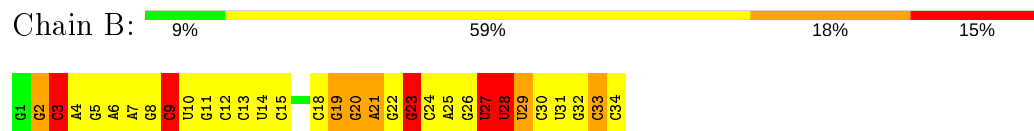


4.2.13 Score per residue for model 13

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1



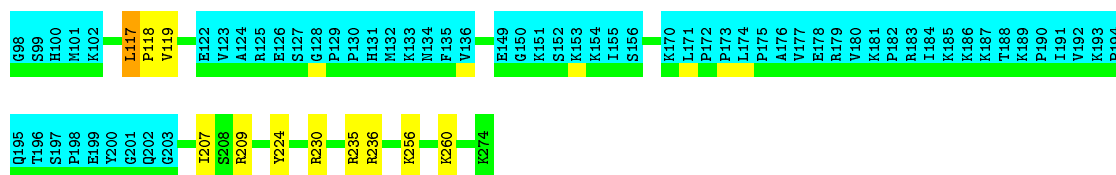
- Molecule 2: hARF1 SBS dsRNA



4.2.14 Score per residue for model 14

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1





- Molecule 2: hARF1 SBS dsRNA

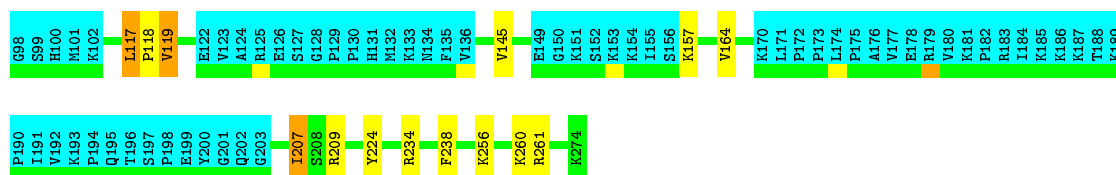
Chain B: 6% 68% 24%



4.2.15 Score per residue for model 15

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 57% 6% 35%



- Molecule 2: hARF1 SBS dsRNA

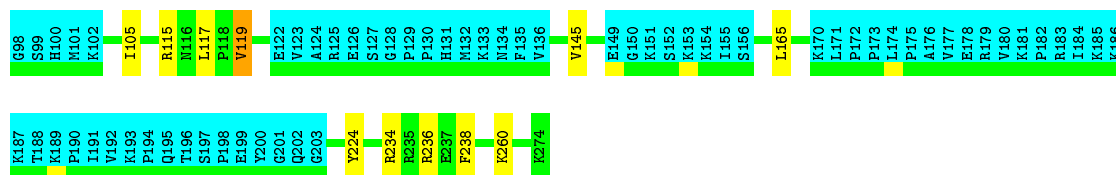
Chain B: 9% 62% 26%



4.2.16 Score per residue for model 16

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 59% 6% 35%



- Molecule 2: hARF1 SBS dsRNA

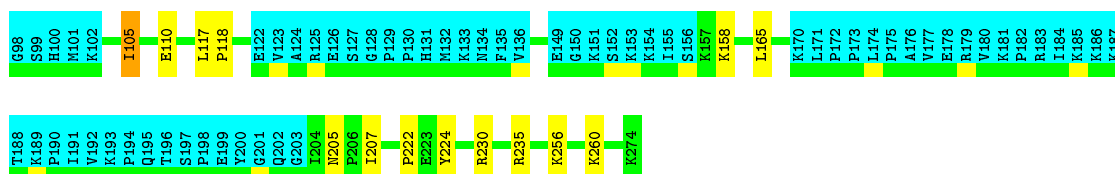
Chain B: 6% 65% 26%



4.2.17 Score per residue for model 17

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 57% 7% 35%



- Molecule 2: hARF1 SBS dsRNA

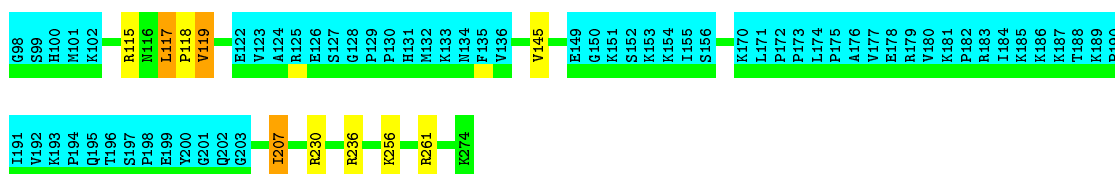
Chain B: 6% 65% 26%



4.2.18 Score per residue for model 18

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 59% 35%



- Molecule 2: hARF1 SBS dsRNA

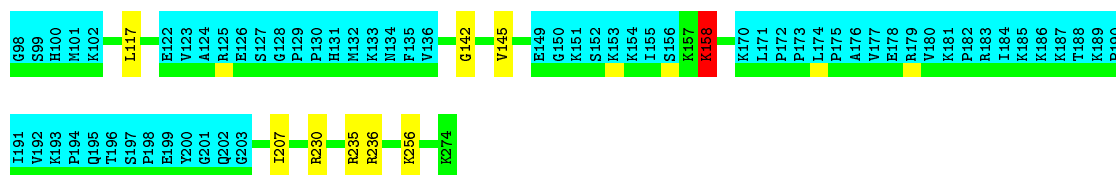
Chain B: 9% 47% 35% 9%



4.2.19 Score per residue for model 19

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 60% 5% 35%



- Molecule 2: hARF1 SBS dsRNA

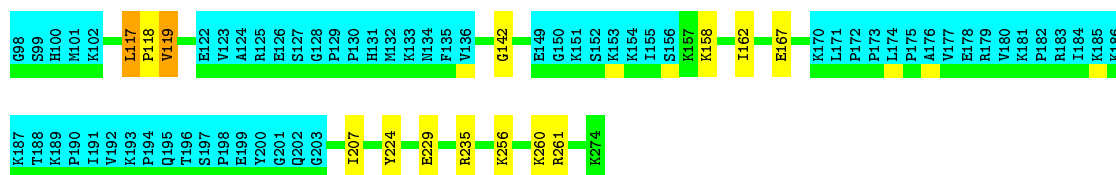
Chain B: 12% 56% 18% 15%



4.2.20 Score per residue for model 20

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1

Chain A: 57% 7% 35%



- Molecule 2: hARF1 SBS dsRNA

Chain B: 9% 62% 26%



5 Refinement protocol and experimental data overview i

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy and restraint violation*.

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

Software name	Classification	Version
Amber	refinement	AMBER14
CYANA	structure calculation	cyana-3.98.5
ATNOS-CANDID	structure calculation	UNIO 2.0.3
PROCHECK / PROCHECK-NMR	refinement	

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	2
Total number of shifts	2385
Number of shifts mapped to atoms	2385
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	A	904	952	952	3±1
2	B	720	366	366	1±1
All	All	32480	26360	26372	62

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:A:224:TYR:CZ	1:A:260:LYS:HE3	0.51	2.40	20	15
1:A:117:LEU:H	1:A:118:PRO:CD	0.49	2.21	11	15
1:A:256:LYS:HE3	2:B:23:G:H5''	0.48	1.85	1	11
1:A:158:LYS:HE3	1:A:158:LYS:HA	0.48	1.85	9	2
1:A:207:ILE:HG21	2:B:7:A:H5'	0.48	1.83	6	2
1:A:105:ILE:HD11	1:A:158:LYS:HA	0.47	1.85	10	2
1:A:105:ILE:HD12	2:B:27:U:C5'	0.46	2.40	1	1
1:A:158:LYS:HE2	2:B:27:U:H5''	0.45	1.89	19	1
1:A:105:ILE:HG22	2:B:26:G:O2'	0.44	2.13	7	1
1:A:158:LYS:HB3	1:A:162:ILE:CD1	0.43	2.42	20	1
1:A:158:LYS:HA	1:A:158:LYS:HE3	0.43	1.90	4	1
2:B:9:C:N4	2:B:26:G:H1	0.43	2.10	3	1
2:B:7:A:H2'	2:B:8:G:C8	0.42	2.49	3	2
2:B:27:U:H2'	2:B:28:U:C6	0.42	2.50	18	3
2:B:26:G:H2'	2:B:27:U:C6	0.41	2.50	11	1
1:A:105:ILE:HD13	1:A:158:LYS:CE	0.41	2.45	12	1
1:A:207:ILE:CG2	2:B:7:A:H5'	0.41	2.45	15	1
2:B:27:U:O5'	2:B:27:U:C6	0.40	2.75	3	1

5.2 Torsion angles ⓘ

5.2.1 Protein backbone ⓘ

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	114/177 (64%)	97±3 (85±3%)	14±3 (12±3%)	3±1 (2±1%)	9	45
All	All	2280/3540 (64%)	1944 (85%)	280 (12%)	56 (2%)	9	45

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	117	LEU	20
1	A	119	VAL	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	142	GLY	5
1	A	118	PRO	4
1	A	231	GLY	3
1	A	222	PRO	3
1	A	267	MET	1
1	A	107	GLN	1
1	A	205	ASN	1
1	A	228	THR	1
1	A	157	LYS	1
1	A	204	ILE	1
1	A	245	GLY	1
1	A	236	ARG	1
1	A	106	SER	1
1	A	112	ALA	1
1	A	214	GLN	1

5.2.2 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	97/152 (64%)	92±1 (95±1%)	5±1 (5±1%)	27	77
All	All	1940/3040 (64%)	1842 (95%)	98 (5%)	27	77

All 29 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	207	ILE	15
1	A	145	VAL	9
1	A	165	LEU	8
1	A	234	ARG	7
1	A	119	VAL	6
1	A	105	ILE	6
1	A	158	LYS	5
1	A	217	LYS	5
1	A	164	VAL	4
1	A	230	ARG	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	227	LEU	3
1	A	238	PHE	3
1	A	271	LEU	3
1	A	167	GLU	3
1	A	237	GLU	2
1	A	209	ARG	2
1	A	274	LYS	1
1	A	266	ASN	1
1	A	110	GLU	1
1	A	246	ASN	1
1	A	256	LYS	1
1	A	157	LYS	1
1	A	104	GLU	1
1	A	106	SER	1
1	A	116	ASN	1
1	A	240	MET	1
1	A	218	LYS	1
1	A	229	GLU	1
1	A	235	ARG	1

5.2.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	33/34 (97%)	3±1 (8±4%)	2±1 (6±2%)	0.44±0.03
All	All	660/680 (97%)	54 (8%)	38 (6%)	0.44

The overall RNA backbone suiteness is 0.44.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	28	U	17
2	B	29	U	16
2	B	20	G	9
2	B	24	C	3
2	B	34	C	2
2	B	2	G	2
2	B	33	C	2
2	B	23	G	1
2	B	3	C	1
2	B	27	U	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	23	G	19
2	B	28	U	16
2	B	33	C	2
2	B	2	G	1

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

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 74% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *starch_output_dsRNA-hARF1*

6.1.1 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	443
Number of shifts mapped to atoms	443
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

6.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

6.1.3 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 20%, i.e. 427 atoms were assigned a chemical shift out of a possible 2109. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/567 (0%)	0/226 (0%)	0/230 (0%)	0/111 (0%)
Sidechain	0/841 (0%)	0/492 (0%)	0/302 (0%)	0/47 (0%)
Aromatic	0/60 (0%)	0/33 (0%)	0/26 (0%)	0/1 (0%)
Overall	427/2109 (20%)	249/1120 (22%)	178/785 (23%)	0/204 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 427 atoms were assigned a chemical shift out of a possible 2915. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/859 (0%)	0/341 (0%)	0/354 (0%)	0/164 (0%)
Sidechain	0/1324 (0%)	0/785 (0%)	0/468 (0%)	0/71 (0%)
Aromatic	0/91 (0%)	0/50 (0%)	0/38 (0%)	0/3 (0%)
Overall	427/2915 (15%)	249/1545 (16%)	178/1087 (16%)	0/283 (0%)

6.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	18	C	H5''	2.82	5.47 – 2.87	-5.2

6.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (starch_output_dsRNA_hARF1). RCI is only applicable to proteins.

6.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: starch_output_prot_RBD3

6.2.1 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	1942
Number of shifts mapped to atoms	1942
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

6.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	151	-0.35 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	-0.03 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	132	0.05 ± 0.14	None needed (< 0.5 ppm)
^{15}N	139	0.02 ± 0.45	None needed (< 0.5 ppm)

6.2.3 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 62%, i.e. 1311 atoms were assigned a chemical shift out of a possible 2109. 20 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	551/567 (97%)	222/226 (98%)	221/230 (96%)	108/111 (97%)
Sidechain	715/841 (85%)	444/492 (90%)	256/302 (85%)	15/47 (32%)
Aromatic	45/60 (75%)	31/33 (94%)	14/26 (54%)	0/1 (0%)
Overall	1311/2109 (62%)	697/1120 (62%)	491/785 (63%)	123/204 (60%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 1737 atoms were assigned a chemical shift out of a possible 2915. 26 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	711/859 (83%)	289/341 (85%)	283/354 (80%)	139/164 (85%)
Sidechain	966/1324 (73%)	602/785 (77%)	347/468 (74%)	17/71 (24%)
Aromatic	60/91 (66%)	40/50 (80%)	20/38 (53%)	0/3 (0%)
Overall	1737/2915 (60%)	931/1545 (60%)	650/1087 (60%)	156/283 (55%)

6.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	260	LYS	HE3	1.51	3.86 – 1.96	-7.4
1	A	260	LYS	HE2	1.87	3.87 – 1.97	-5.5
1	A	175	PRO	CA	54.92	71.13 – 55.53	-5.4

6.2.5 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:

