



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2KCA  
Title : GP16  
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Deposited on : 2008-12-18

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:

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 : 2.23.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

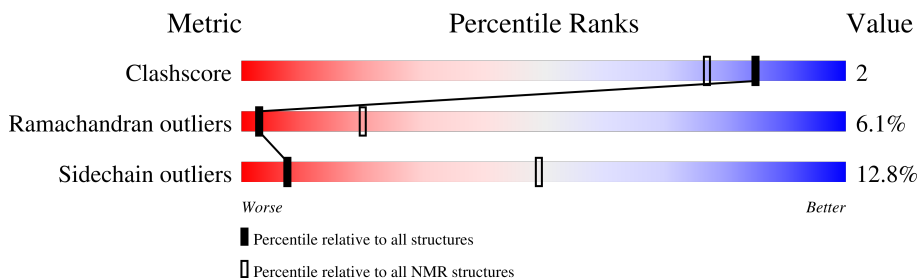
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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	109	 42% 10% . 45%

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 6 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:41-A:48, A:62-A:75, A:91-A:123, A:129-A:133 (60)	0.53	6

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 5 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1749 atoms, of which 859 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bacteriophage SPP1 complete nucleotide sequence.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	109	1749	569	859	145	174	2	0

There is a discrepancy between the modelled and reference sequences:

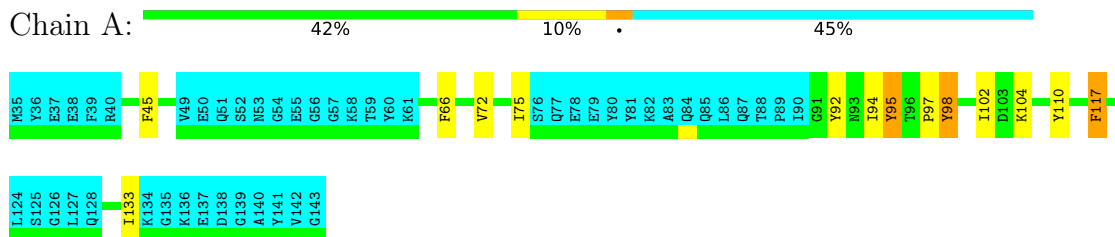
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ARG	PRO	engineered mutation	UNP O48446

## 4 Residue-property plots [i](#)

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

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

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence

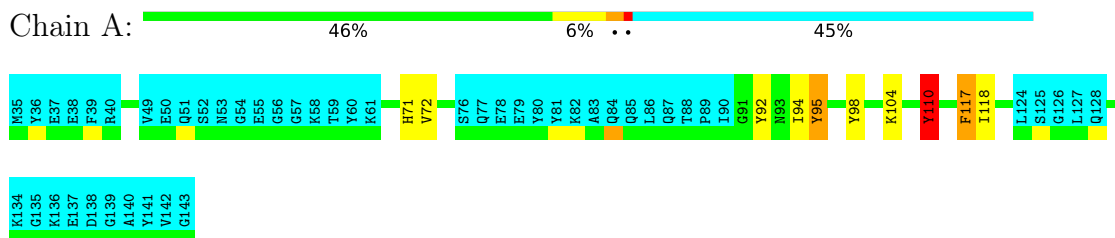


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

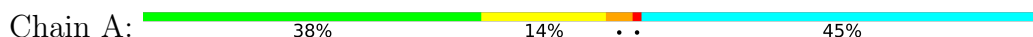
#### 4.2.1 Score per residue for model 1

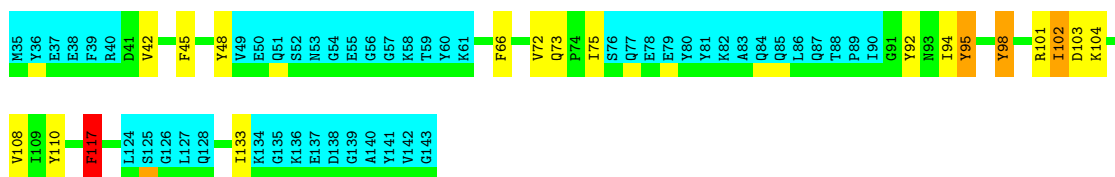
- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



#### 4.2.2 Score per residue for model 2

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence

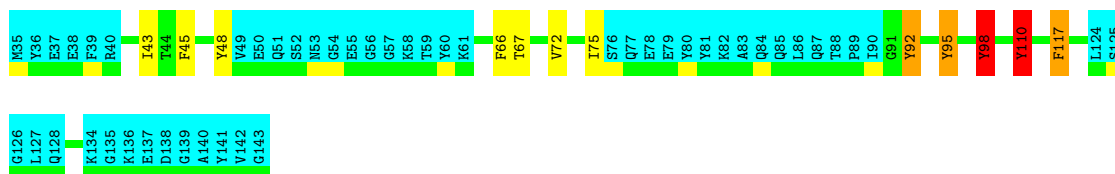




#### 4.2.3 Score per residue for model 3

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence

Chain A: 44% 6% 50%



#### 4.2.4 Score per residue for model 4

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence

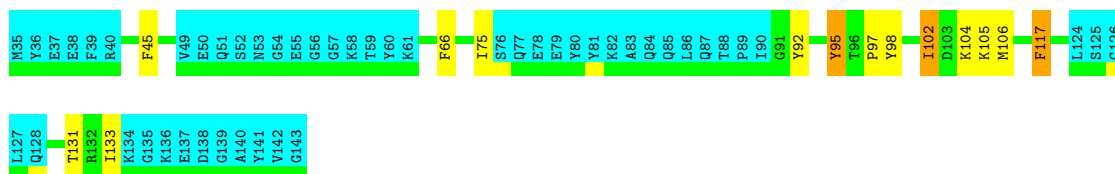
Chain A: 43% 9% 48%



#### 4.2.5 Score per residue for model 5

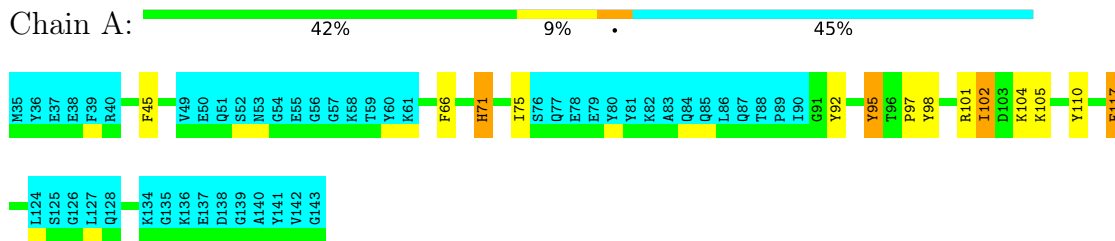
- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence

Chain A: 42% 10% 48%



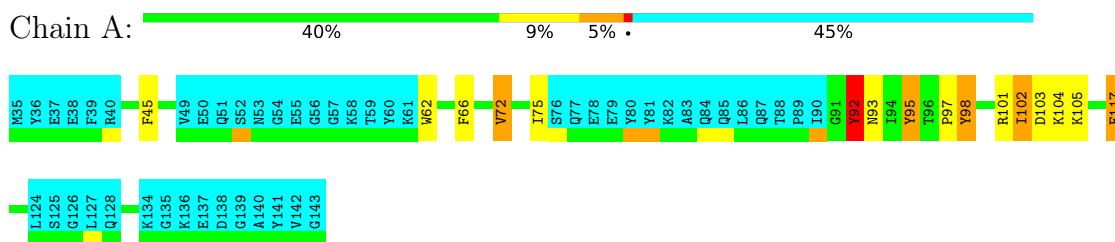
#### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



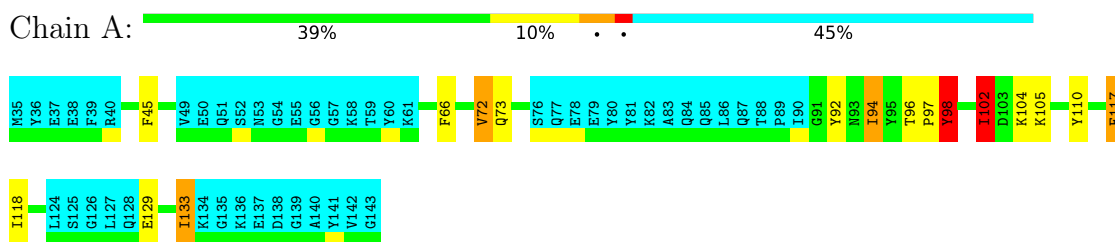
#### 4.2.7 Score per residue for model 7

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



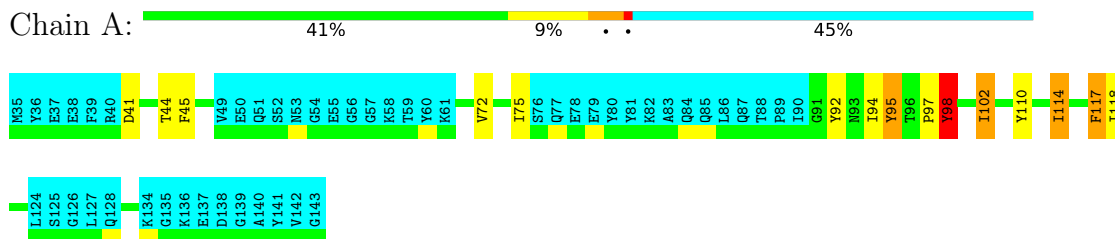
#### 4.2.8 Score per residue for model 8

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



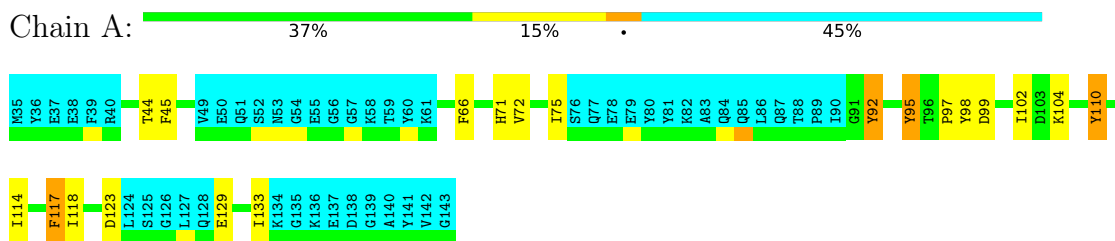
#### 4.2.9 Score per residue for model 9

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



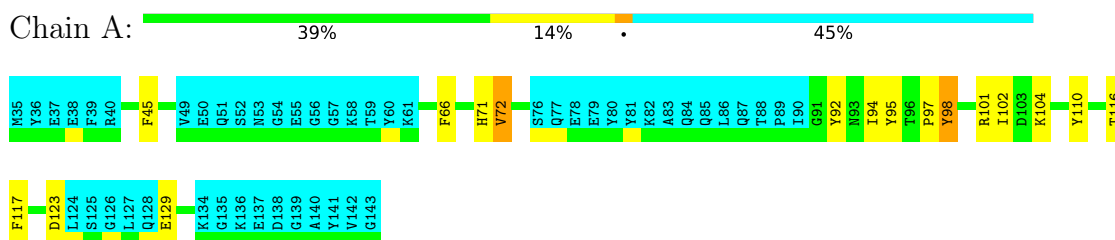
#### 4.2.10 Score per residue for model 10

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



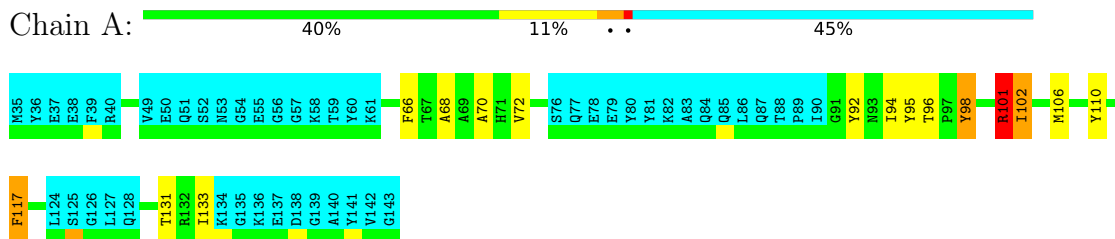
#### 4.2.11 Score per residue for model 11

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



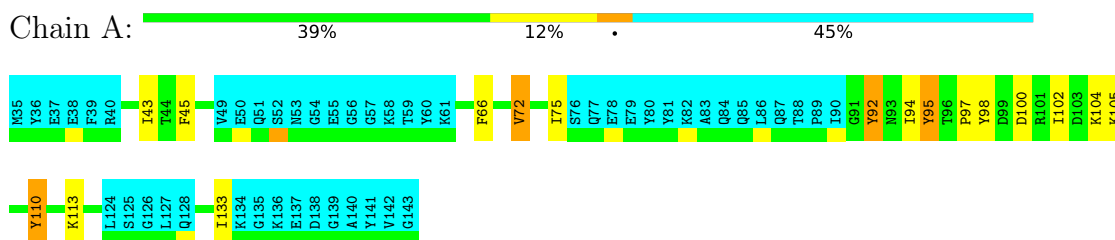
#### 4.2.12 Score per residue for model 12

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



#### 4.2.13 Score per residue for model 13

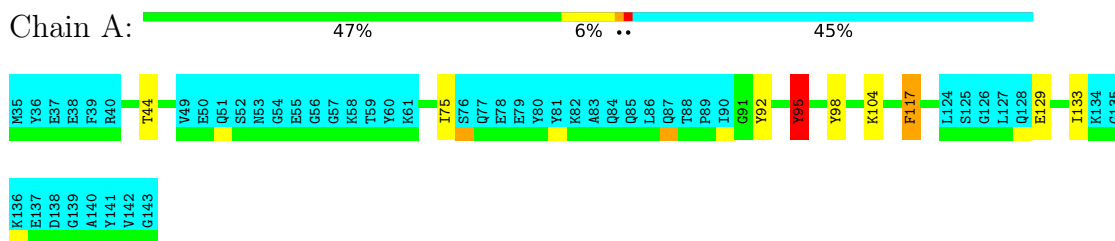
- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence





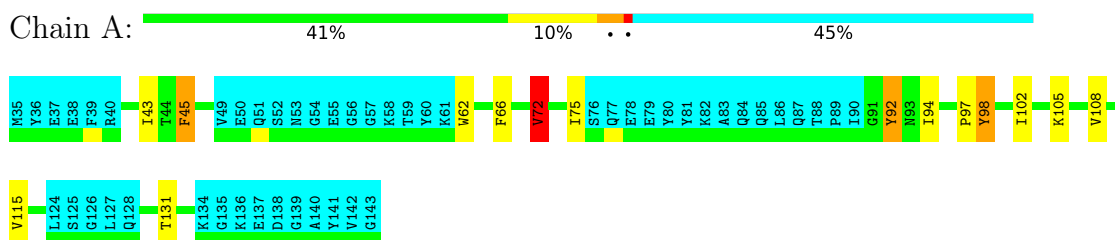
#### 4.2.14 Score per residue for model 14

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



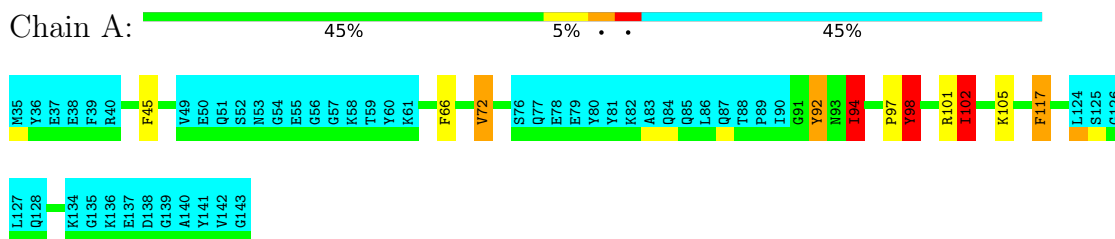
#### 4.2.15 Score per residue for model 15

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



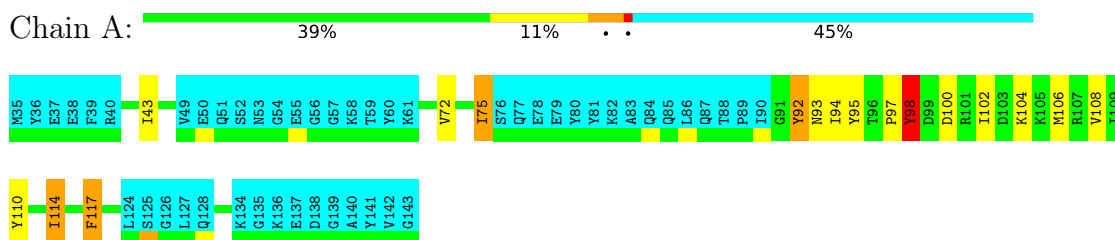
#### 4.2.16 Score per residue for model 16

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



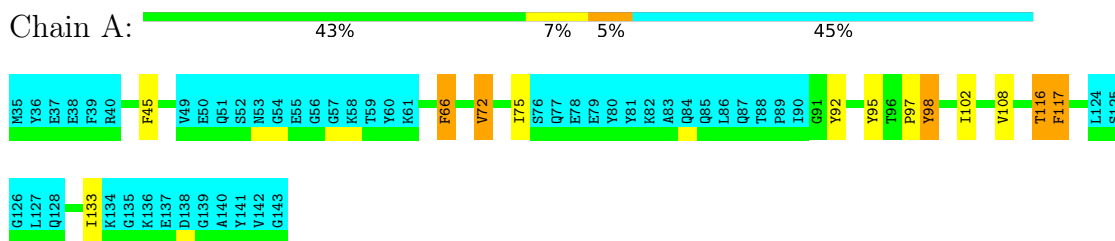
#### 4.2.17 Score per residue for model 17

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



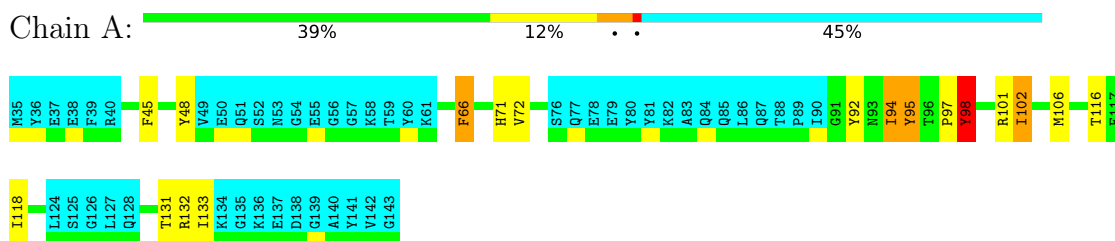
### 4.2.18 Score per residue for model 18

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



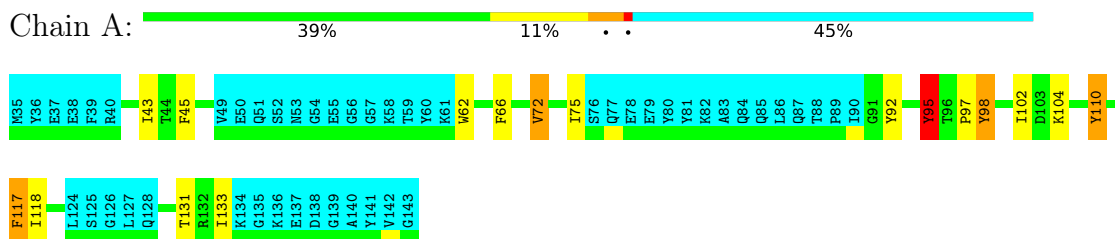
### 4.2.19 Score per residue for model 19

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



### 4.2.20 Score per residue for model 20

- Molecule 1: Bacteriophage SPP1 complete nucleotide sequence



## 5 Refinement protocol and experimental data overview

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

Of the 6000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.97±0.01	0±0/513 ( 0.0± 0.0%)	1.45±0.05	6±2/700 ( 0.9± 0.3%)
All	All	0.97	0/10260 ( 0.0%)	1.45	125/14000 ( 0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.6±0.7
All	All	0	32

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	92	TYR	CB-CG-CD2	-11.80	113.92	121.00	13	15
1	A	92	TYR	CB-CG-CD1	11.16	127.69	121.00	13	13
1	A	117	PHE	CB-CG-CD1	10.98	128.49	120.80	12	14
1	A	117	PHE	CB-CG-CD2	-9.72	113.99	120.80	12	13
1	A	110	TYR	CB-CG-CD1	-9.03	115.58	121.00	1	4
1	A	72	VAL	CA-CB-CG1	8.44	123.57	110.90	10	5
1	A	72	VAL	CA-CB-CG2	7.90	122.75	110.90	20	8
1	A	45	PHE	CB-CG-CD2	6.79	125.56	120.80	15	1
1	A	97	PRO	C-N-CA	6.74	138.54	121.70	19	15
1	A	98	TYR	CB-CG-CD2	-6.57	117.06	121.00	19	2
1	A	98	TYR	CB-CG-CD1	6.40	124.84	121.00	3	2
1	A	72	VAL	CG1-CB-CG2	-6.33	100.77	110.90	12	3
1	A	116	THR	N-CA-C	6.30	128.02	111.00	18	1
1	A	110	TYR	CB-CG-CD2	-6.29	117.23	121.00	20	1
1	A	131	THR	N-CA-CB	5.88	121.47	110.30	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	101	ARG	C-N-CA	5.74	136.06	121.70	6	3
1	A	48	TYR	CB-CG-CD2	-5.72	117.57	121.00	19	3
1	A	95	TYR	CB-CA-C	5.57	121.55	110.40	20	3
1	A	48	TYR	CB-CG-CD1	5.53	124.32	121.00	3	1
1	A	98	TYR	N-CA-C	5.53	125.93	111.00	16	6
1	A	72	VAL	CB-CA-C	5.41	121.67	111.40	20	1
1	A	62	TRP	CB-CG-CD1	5.30	133.89	127.00	20	3
1	A	72	VAL	N-CA-C	-5.28	96.75	111.00	12	3
1	A	95	TYR	N-CA-C	-5.28	96.75	111.00	20	1
1	A	110	TYR	CA-CB-CG	-5.18	103.55	113.40	13	1
1	A	94	ILE	CA-CB-CG1	5.12	120.72	111.00	16	1
1	A	117	PHE	N-CA-CB	5.05	119.69	110.60	18	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	95	TYR	Sidechain	11
1	A	92	TYR	Sidechain	8
1	A	110	TYR	Sidechain	7
1	A	66	PHE	Sidechain	4
1	A	101	ARG	Sidechain	1
1	A	117	PHE	Sidechain	1

## 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	A	499	489	489	2±1
All	All	9980	9780	9780	44

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ILE:HD12	1:A:102:ILE:H	0.71	1.44	7	2
1:A:94:ILE:HG23	1:A:133:ILE:HG23	0.59	1.75	8	1
1:A:102:ILE:H	1:A:102:ILE:CD1	0.58	2.12	7	3
1:A:72:VAL:HG12	1:A:92:TYR:CD2	0.57	2.34	13	2
1:A:94:ILE:HD11	1:A:102:ILE:HG21	0.53	1.80	8	1
1:A:45:PHE:CE1	1:A:102:ILE:HG22	0.53	2.38	8	1
1:A:102:ILE:HD13	1:A:133:ILE:HG21	0.53	1.81	8	1
1:A:114:ILE:H	1:A:114:ILE:HD13	0.51	1.64	9	2
1:A:45:PHE:CE2	1:A:102:ILE:HG22	0.49	2.42	9	2
1:A:72:VAL:HG12	1:A:110:TYR:CE2	0.49	2.42	17	1
1:A:45:PHE:CD2	1:A:66:PHE:CZ	0.48	3.02	11	8
1:A:68:ALA:HB3	1:A:101:ARG:HE	0.47	1.70	12	1
1:A:110:TYR:CD1	1:A:110:TYR:N	0.45	2.84	3	2
1:A:66:PHE:CE1	1:A:101:ARG:HB2	0.45	2.47	11	2
1:A:72:VAL:HG21	1:A:108:VAL:HG21	0.44	1.90	18	1
1:A:72:VAL:HG22	1:A:94:ILE:HG13	0.44	1.89	19	1
1:A:66:PHE:CZ	1:A:101:ARG:HB3	0.43	2.48	19	1
1:A:108:VAL:HG11	1:A:117:PHE:CZ	0.43	2.49	2	1
1:A:45:PHE:CG	1:A:66:PHE:CZ	0.43	3.07	4	2
1:A:45:PHE:CD1	1:A:66:PHE:CZ	0.42	3.06	5	3
1:A:72:VAL:HG11	1:A:108:VAL:HG11	0.42	1.90	15	1
1:A:70:ALA:HB2	1:A:101:ARG:CD	0.41	2.44	12	1
1:A:72:VAL:HG22	1:A:94:ILE:HG12	0.41	1.92	11	1
1:A:72:VAL:HG12	1:A:92:TYR:HE2	0.40	1.76	7	1
1:A:45:PHE:CD1	1:A:45:PHE:N	0.40	2.90	15	1
1:A:94:ILE:HD11	1:A:102:ILE:HG22	0.40	1.93	16	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	60/109 (55%)	53±1 (89±2%)	3±1 (5±2%)	4±1 (6±2%)	3	20
All	All	1200/2180 (55%)	1067 (89%)	60 (5%)	73 (6%)	3	20

All 9 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	98	TYR	20
1	A	104	LYS	12
1	A	75	ILE	12
1	A	102	ILE	12
1	A	105	LYS	7
1	A	129	GLU	5
1	A	116	THR	2
1	A	117	PHE	2
1	A	99	ASP	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	54/94 (57%)	47±3 (87±5%)	7±3 (13±5%)	7	49
All	All	1080/1880 (57%)	942 (87%)	138 (13%)	7	49

All 32 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	95	TYR	16
1	A	117	PHE	15
1	A	98	TYR	13
1	A	102	ILE	11
1	A	133	ILE	11
1	A	94	ILE	10
1	A	118	ILE	6
1	A	110	TYR	5
1	A	43	ILE	5
1	A	106	MET	4
1	A	131	THR	4
1	A	93	ASN	3
1	A	71	HIS	3
1	A	72	VAL	3
1	A	44	THR	3
1	A	114	ILE	3
1	A	73	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	103	ASP	2
1	A	67	THR	2
1	A	96	THR	2
1	A	123	ASP	2
1	A	75	ILE	2
1	A	100	ASP	2
1	A	42	VAL	1
1	A	92	TYR	1
1	A	41	ASP	1
1	A	101	ARG	1
1	A	113	LYS	1
1	A	115	VAL	1
1	A	108	VAL	1
1	A	116	THR	1
1	A	132	ARG	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

No chemical shift data were provided