



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:49 PM BST

PDB ID : 1R7F
Title : NMR structure of the membrane anchor domain (1-31) of the nonstructural protein 5A (NS5A) of hepatitis C virus (Ensemble of 43 structures. Sample in 100mM SDS)
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Deposited on : 2003-10-21

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

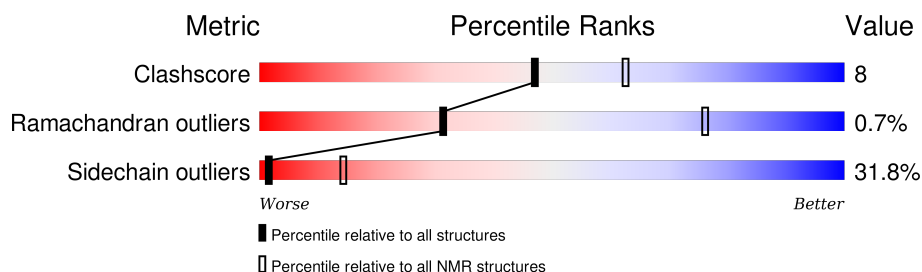
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	31	

2 Ensemble composition and analysis

This entry contains 43 models. Model 8 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:5-A:27 (23)	0.58	8

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 7 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 8, 10, 11, 31, 33, 34, 36, 37, 42
2	2, 12, 18, 22, 27, 35, 41, 43
3	1, 7, 16, 21, 26, 28, 30
4	4, 13, 20, 24, 38, 39
5	9, 14, 15, 25, 32, 40
6	5, 6, 23
7	17, 19
Single-model clusters	29

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 532 atoms, of which 266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Genome polyprotein.

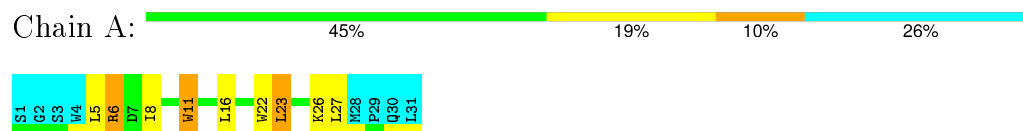
Mol	Chain	Residues	Atoms						Trace
1	A	31	Total	C	H	N	O	S	0
			532	177	266	42	45	2	

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: Genome polyprotein

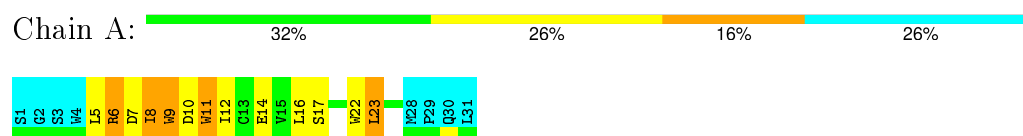


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

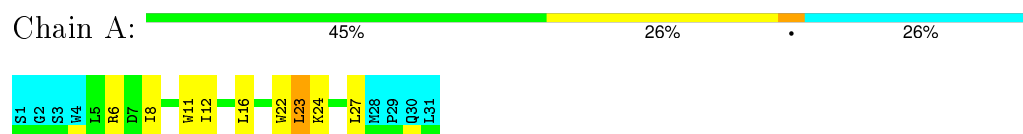
4.2.1 Score per residue for model 1

- Molecule 1: Genome polyprotein



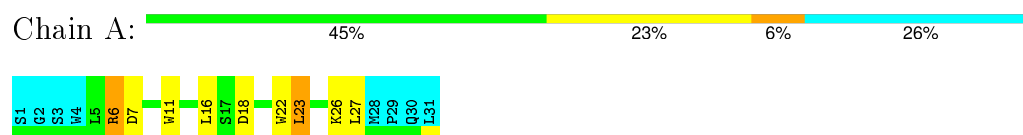
4.2.2 Score per residue for model 2

- Molecule 1: Genome polyprotein



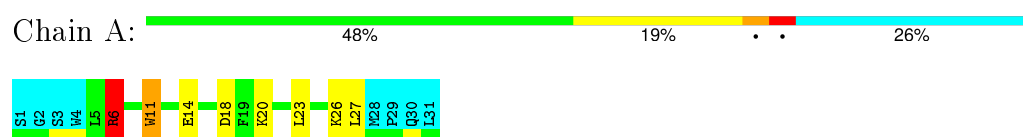
4.2.3 Score per residue for model 3

- Molecule 1: Genome polyprotein



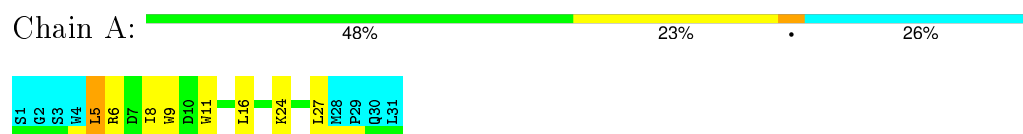
4.2.4 Score per residue for model 4

- Molecule 1: Genome polyprotein



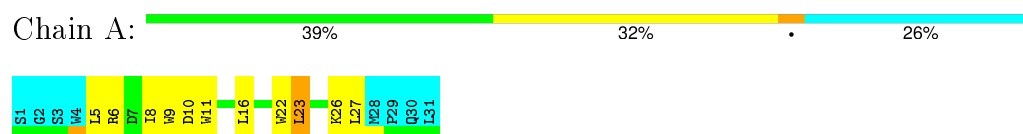
4.2.5 Score per residue for model 5

- Molecule 1: Genome polyprotein



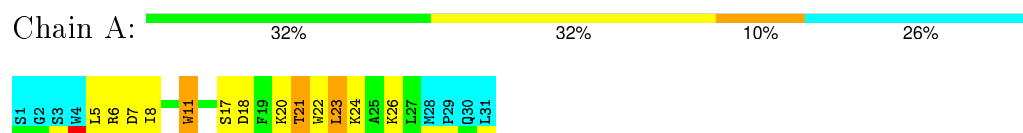
4.2.6 Score per residue for model 6

- Molecule 1: Genome polyprotein



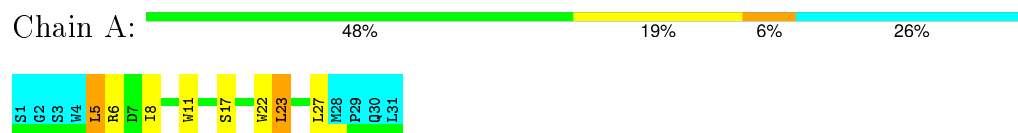
4.2.7 Score per residue for model 7

- Molecule 1: Genome polyprotein



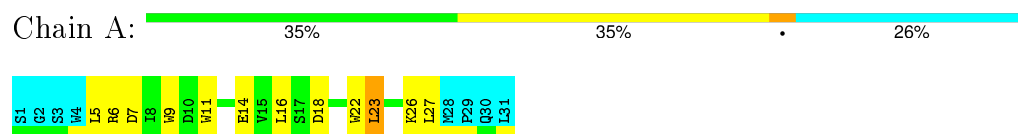
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Genome polyprotein



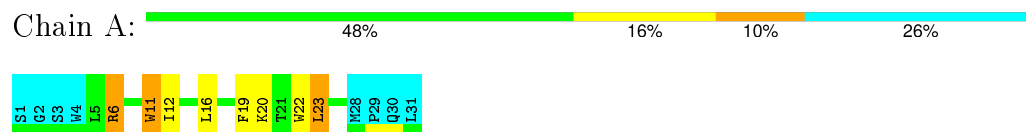
4.2.9 Score per residue for model 9

- Molecule 1: Genome polyprotein



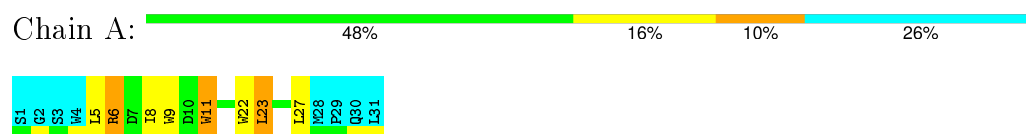
4.2.10 Score per residue for model 10

- Molecule 1: Genome polyprotein



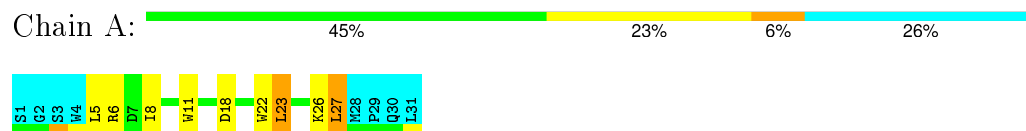
4.2.11 Score per residue for model 11

- Molecule 1: Genome polyprotein



4.2.12 Score per residue for model 12

- Molecule 1: Genome polyprotein



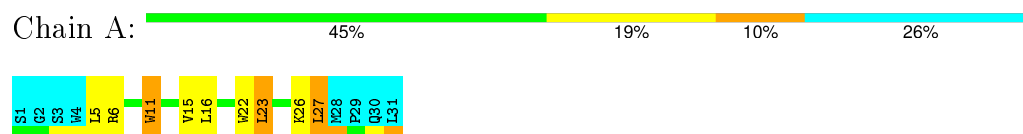
4.2.13 Score per residue for model 13

- Molecule 1: Genome polypeptide



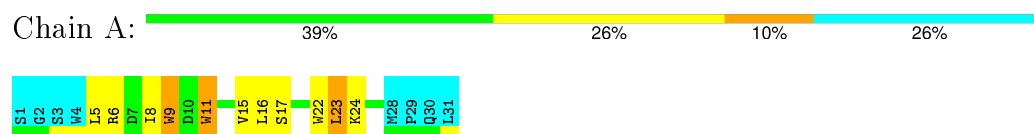
4.2.14 Score per residue for model 14

- Molecule 1: Genome polypeptide



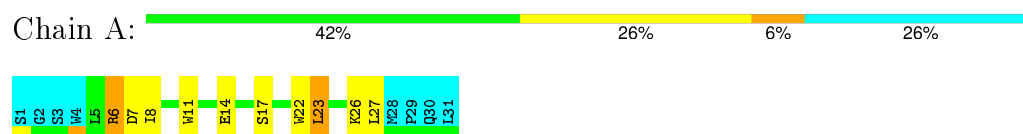
4.2.15 Score per residue for model 15

- Molecule 1: Genome polypeptide



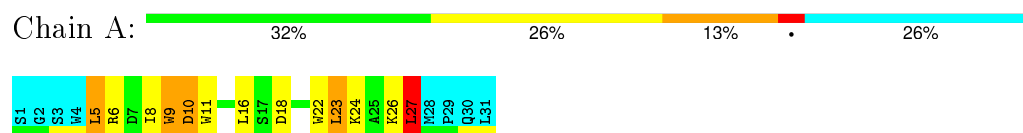
4.2.16 Score per residue for model 16

- Molecule 1: Genome polypeptide



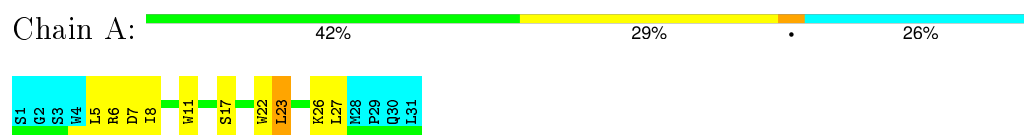
4.2.17 Score per residue for model 17

- Molecule 1: Genome polypeptide



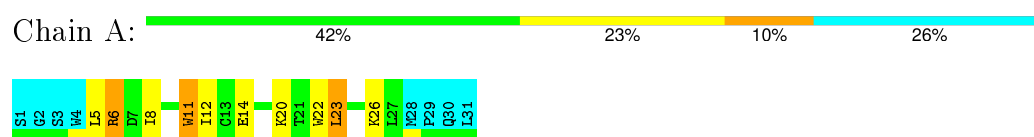
4.2.18 Score per residue for model 18

- Molecule 1: Genome polyprotein



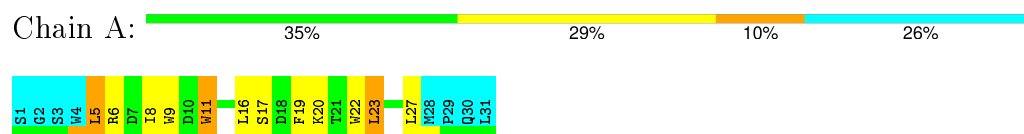
4.2.19 Score per residue for model 19

- Molecule 1: Genome polyprotein



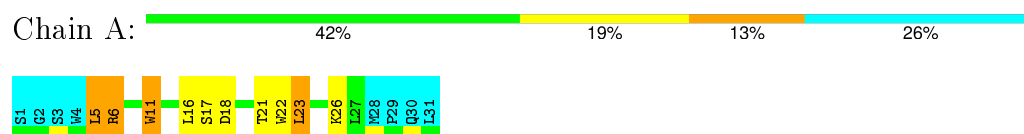
4.2.20 Score per residue for model 20

- Molecule 1: Genome polyprotein



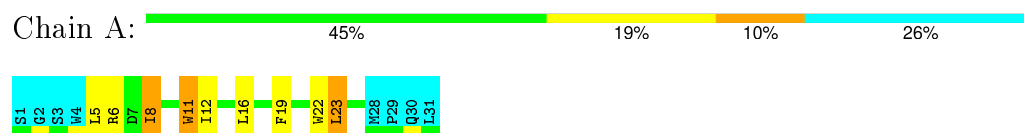
4.2.21 Score per residue for model 21

- Molecule 1: Genome polyprotein



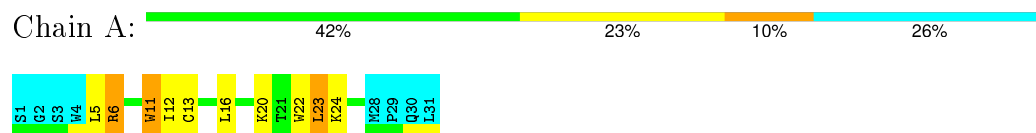
4.2.22 Score per residue for model 22

- Molecule 1: Genome polyprotein



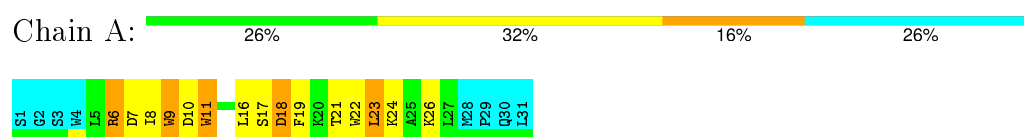
4.2.23 Score per residue for model 23

- Molecule 1: Genome polyprotein



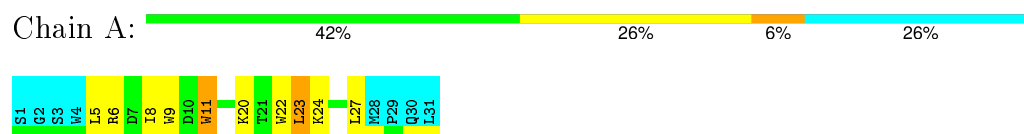
4.2.24 Score per residue for model 24

- Molecule 1: Genome polyprotein



4.2.25 Score per residue for model 25

- Molecule 1: Genome polyprotein



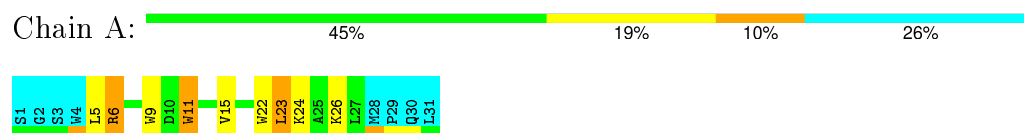
4.2.26 Score per residue for model 26

- Molecule 1: Genome polyprotein



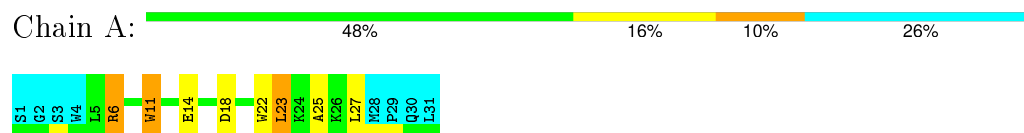
4.2.27 Score per residue for model 27

- Molecule 1: Genome polyprotein



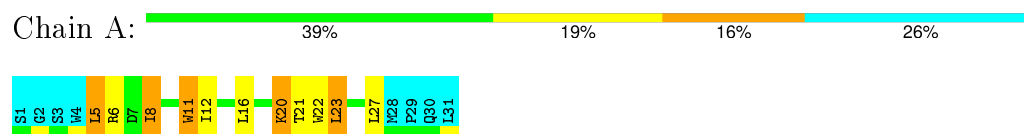
4.2.28 Score per residue for model 28

- Molecule 1: Genome polyprotein



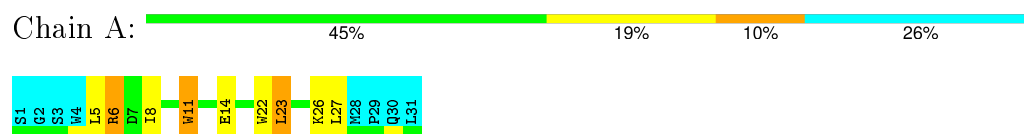
4.2.29 Score per residue for model 29

- Molecule 1: Genome polyprotein



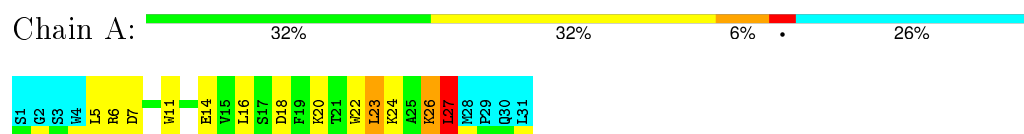
4.2.30 Score per residue for model 30

- Molecule 1: Genome polyprotein



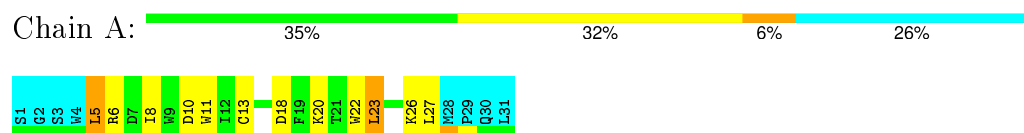
4.2.31 Score per residue for model 31

- Molecule 1: Genome polyprotein



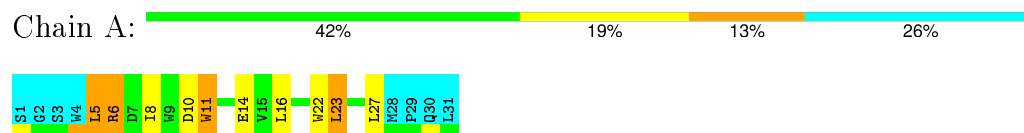
4.2.32 Score per residue for model 32

- Molecule 1: Genome polyprotein



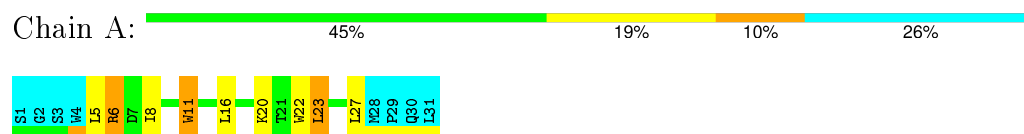
4.2.33 Score per residue for model 33

- Molecule 1: Genome polyprotein



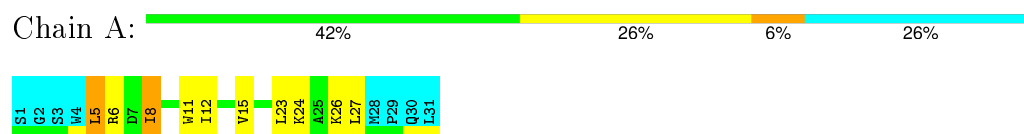
4.2.34 Score per residue for model 34

- Molecule 1: Genome polyprotein



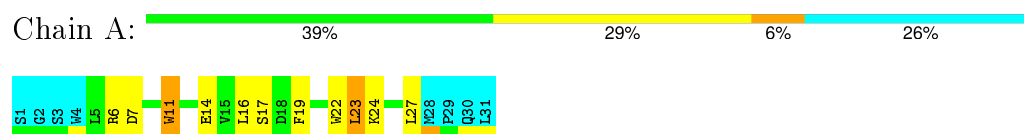
4.2.35 Score per residue for model 35

- Molecule 1: Genome polyprotein



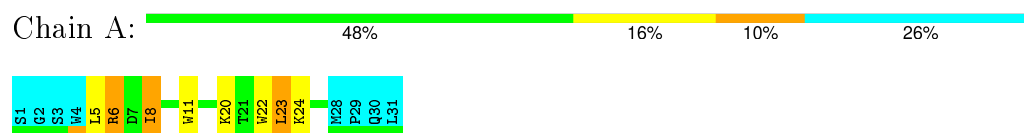
4.2.36 Score per residue for model 36

- Molecule 1: Genome polyprotein



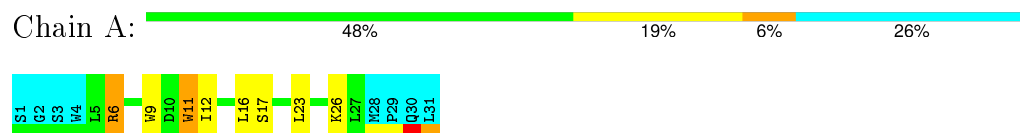
4.2.37 Score per residue for model 37

- Molecule 1: Genome polyprotein



4.2.38 Score per residue for model 38

- Molecule 1: Genome polypeptide



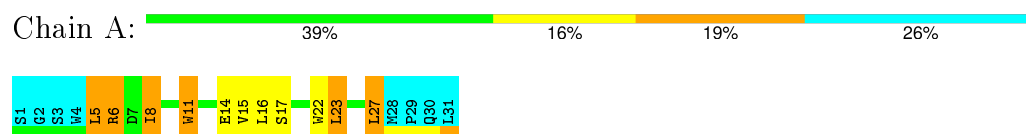
4.2.39 Score per residue for model 39

- Molecule 1: Genome polypeptide



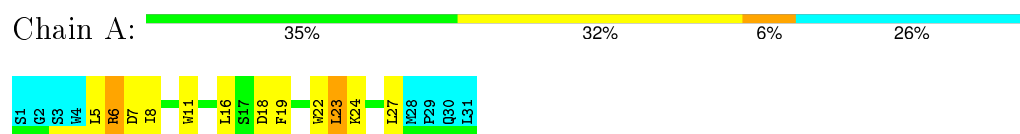
4.2.40 Score per residue for model 40

- Molecule 1: Genome polypeptide



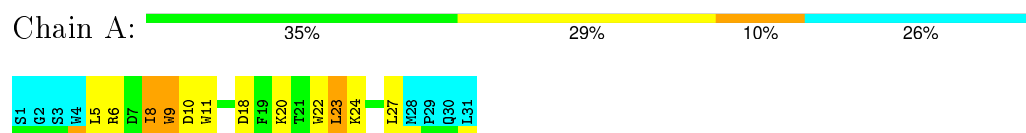
4.2.41 Score per residue for model 41

- Molecule 1: Genome polypeptide



4.2.42 Score per residue for model 42

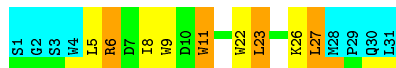
- Molecule 1: Genome polypeptide



4.2.43 Score per residue for model 43

- Molecule 1: Genome polyprotein

Chain A: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, simulated annealing, molecular dynamics, energy minimization*.

Of the 100 calculated structures, 43 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
X-PLOR	structure solution	3.85
X-PLOR	refinement	3.85

No chemical shift data was provided. 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.

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	1.0±0.0
All	All	0	43

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	6	ARG	Sidechain	43

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	203	206	206	3±1
All	All	8729	8858	8858	137

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HA	1:A:8:ILE:HG22	0.76	1.56	20	11
1:A:22:TRP:HE3	1:A:23:LEU:HD22	0.66	1.51	16	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:TRP:CE3	1:A:23:LEU:HD22	0.64	2.27	16	15
1:A:5:LEU:HD13	1:A:8:ILE:HB	0.63	1.70	15	1
1:A:11:TRP:C	1:A:11:TRP:CD1	0.61	2.72	24	8
1:A:11:TRP:CD1	1:A:11:TRP:C	0.60	2.75	4	7
1:A:19:PHE:O	1:A:23:LEU:HD12	0.59	1.97	39	1
1:A:5:LEU:HB3	1:A:8:ILE:HB	0.56	1.78	1	3
1:A:8:ILE:O	1:A:12:ILE:HD12	0.55	2.01	2	1
1:A:12:ILE:HG23	1:A:16:LEU:HD12	0.54	1.79	23	1
1:A:16:LEU:HD13	1:A:16:LEU:C	0.54	2.23	3	1
1:A:5:LEU:HD23	1:A:9:TRP:CZ2	0.53	2.37	6	1
1:A:22:TRP:CZ2	1:A:23:LEU:HD22	0.53	2.39	20	1
1:A:11:TRP:CZ3	1:A:15:VAL:HG21	0.52	2.39	27	6
1:A:12:ILE:CG2	1:A:16:LEU:HD12	0.52	2.34	23	1
1:A:5:LEU:HD13	1:A:8:ILE:HG21	0.52	1.81	25	1
1:A:5:LEU:O	1:A:8:ILE:HG22	0.51	2.06	33	4
1:A:22:TRP:CZ3	1:A:23:LEU:HG	0.48	2.44	2	19
1:A:5:LEU:HA	1:A:8:ILE:CG2	0.47	2.39	22	7
1:A:6:ARG:O	1:A:9:TRP:CD1	0.47	2.67	1	1
1:A:9:TRP:CD1	1:A:10:ASP:N	0.47	2.82	1	3
1:A:8:ILE:O	1:A:8:ILE:HD13	0.46	2.10	37	1
1:A:11:TRP:CE2	1:A:12:ILE:HD13	0.46	2.46	22	1
1:A:12:ILE:HA	1:A:15:VAL:HG12	0.45	1.87	35	1
1:A:9:TRP:C	1:A:9:TRP:CD1	0.45	2.88	1	1
1:A:16:LEU:O	1:A:16:LEU:HD13	0.45	2.11	3	1
1:A:5:LEU:O	1:A:5:LEU:HD12	0.45	2.12	5	1
1:A:26:LYS:O	1:A:27:LEU:HB2	0.44	2.12	17	1
1:A:20:LYS:HG3	1:A:21:THR:N	0.44	2.27	29	1
1:A:11:TRP:CD1	1:A:12:ILE:HG12	0.43	2.48	1	6
1:A:22:TRP:CH2	1:A:23:LEU:HG	0.43	2.49	10	2
1:A:5:LEU:HG	1:A:6:ARG:N	0.42	2.29	34	1
1:A:5:LEU:HD12	1:A:9:TRP:CG	0.42	2.50	15	1
1:A:27:LEU:HD13	1:A:27:LEU:O	0.41	2.15	25	2
1:A:18:ASP:O	1:A:21:THR:HG22	0.41	2.16	21	3
1:A:5:LEU:HD12	1:A:5:LEU:O	0.41	2.14	23	1
1:A:26:LYS:O	1:A:27:LEU:CB	0.41	2.69	31	1
1:A:9:TRP:CG	1:A:10:ASP:N	0.41	2.87	24	1
1:A:23:LEU:HD13	1:A:23:LEU:HA	0.40	1.77	17	1
1:A:8:ILE:HG13	1:A:11:TRP:CZ3	0.40	2.51	24	1
1:A:8:ILE:HD13	1:A:8:ILE:O	0.40	2.16	40	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	23/31 (74%)	22±1 (97±3%)	1±1 (2±3%)	0±0 (1±2%)	31	76
All	All	989/1333 (74%)	958 (97%)	24 (2%)	7 (1%)	31	76

All 2 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	27	LEU	6
1	A	5	LEU	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	22/29 (76%)	15±2 (68±9%)	7±2 (32±9%)	1	14
All	All	946/1247 (76%)	645 (68%)	301 (32%)	1	14

All 19 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	11	TRP	42
1	A	23	LEU	41
1	A	27	LEU	27
1	A	16	LEU	22
1	A	6	ARG	21
1	A	26	LYS	20
1	A	24	LYS	15
1	A	5	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	17	SER	13
1	A	9	TRP	13
1	A	20	LYS	13
1	A	14	GLU	12
1	A	7	ASP	12
1	A	8	ILE	11
1	A	18	ASP	11
1	A	19	PHE	6
1	A	10	ASP	4
1	A	13	CYS	2
1	A	21	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided