



# Full wwPDB NMR Structure Validation Report ⓘ

Oct 6, 2016 – 05:11 PM EDT

PDB ID : 3ZD0  
Title : The Solution Structure of Monomeric Hepatitis C Virus p7 Yields Potent Inhibitors of Virion Release  
Authors : Foster, T.L.; Sthompson, G.; Kalverda, A.P.; Kankanala, J.; Thompson, J.; Barker, A.M.; Clarke, D.; Noerenberg, M.; Pearson, A.R.; Rowlands, D.J.; Homans, S.W.; Harris, M.; Foster, R.; Griffin, S.D.C.  
Deposited on : 2012-11-23

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

<http://wwpdb.org/validation/2016/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
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-20027939
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

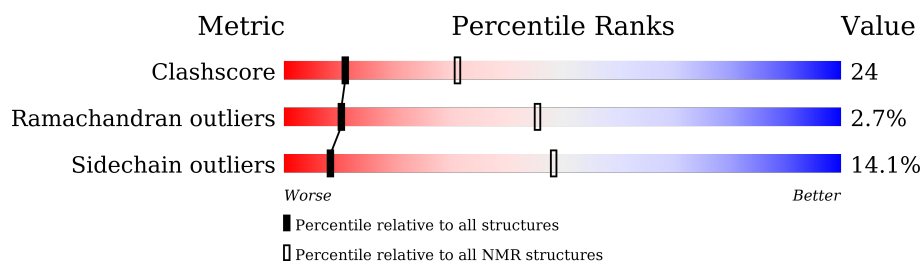
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 72%.

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  $\geq 3$ , 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	86	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:6-A:76 (71)	0.19	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 3 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1276 atoms, of which 637 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called P7 PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	85	Total	C	H	N	O	S	0
			1276	426	637	100	111	2	

There are 23 discrepancies between the modelled and reference sequences:

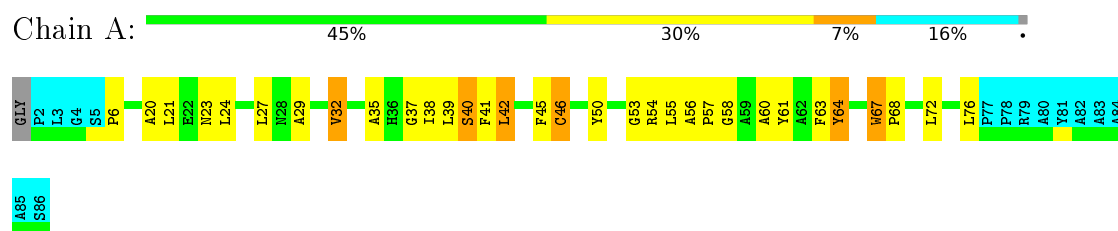
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q9WLK8
A	2	PRO	-	EXPRESSION TAG	UNP Q9WLK8
A	3	LEU	-	EXPRESSION TAG	UNP Q9WLK8
A	4	GLY	-	EXPRESSION TAG	UNP Q9WLK8
A	5	SER	-	EXPRESSION TAG	UNP Q9WLK8
A	6	PRO	-	EXPRESSION TAG	UNP Q9WLK8
A	7	GLU	-	EXPRESSION TAG	UNP Q9WLK8
A	8	PHE	-	EXPRESSION TAG	UNP Q9WLK8
A	9	ALA	-	EXPRESSION TAG	UNP Q9WLK8
A	10	ALA	-	EXPRESSION TAG	UNP Q9WLK8
A	11	MET	-	EXPRESSION TAG	UNP Q9WLK8
A	12	ASP	-	EXPRESSION TAG	UNP Q9WLK8
A	13	TYR	-	EXPRESSION TAG	UNP Q9WLK8
A	14	LYS	-	EXPRESSION TAG	UNP Q9WLK8
A	15	ASP	-	EXPRESSION TAG	UNP Q9WLK8
A	16	ASP	-	EXPRESSION TAG	UNP Q9WLK8
A	17	ASP	-	EXPRESSION TAG	UNP Q9WLK8
A	18	ASP	-	EXPRESSION TAG	UNP Q9WLK8
A	19	LYS	-	EXPRESSION TAG	UNP Q9WLK8
A	83	ALA	-	EXPRESSION TAG	UNP Q9WLK8
A	84	ALA	-	EXPRESSION TAG	UNP Q9WLK8
A	85	ALA	-	EXPRESSION TAG	UNP Q9WLK8
A	86	SER	-	EXPRESSION TAG	UNP Q9WLK8

## 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: P7 PROTEIN

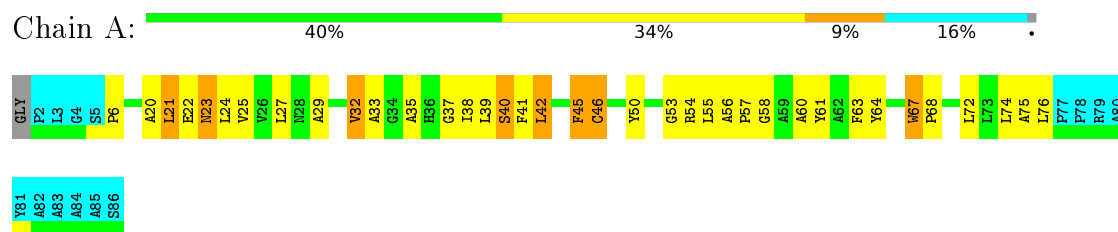


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

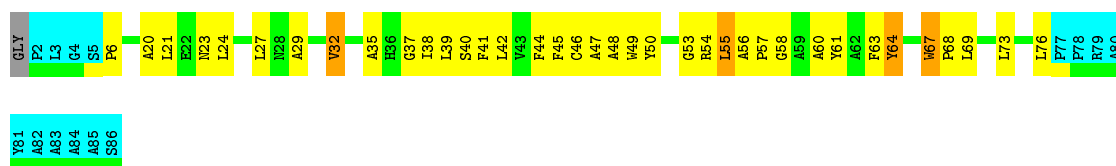
- Molecule 1: P7 PROTEIN



#### 4.2.2 Score per residue for model 2

- Molecule 1: P7 PROTEIN

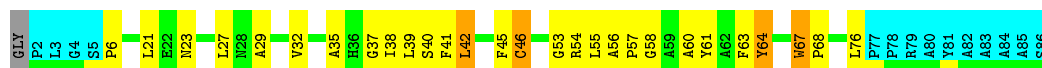




#### 4.2.3 Score per residue for model 3

- Molecule 1: P7 PROTEIN

Chain A: 50% 28% 5% 16%



#### 4.2.4 Score per residue for model 4

- Molecule 1: P7 PROTEIN

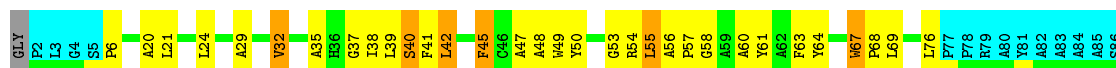
Chain A: 47% 28% 8% 16%



#### 4.2.5 Score per residue for model 5

- Molecule 1: P7 PROTEIN

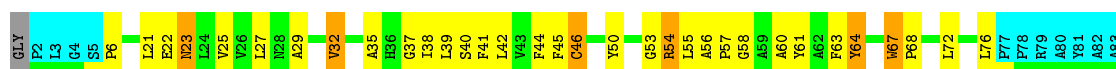
Chain A: 45% 30% 7% 16%



#### 4.2.6 Score per residue for model 6

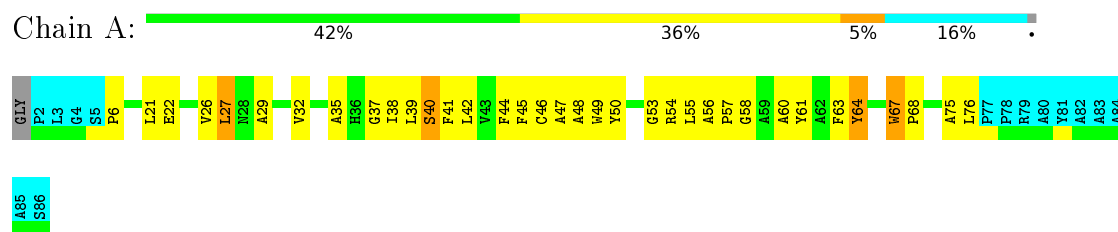
- Molecule 1: P7 PROTEIN

Chain A: 44% 31% 7% 16%



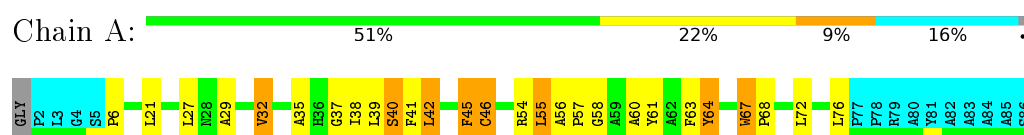
### 4.2.7 Score per residue for model 7

- Molecule 1: P7 PROTEIN



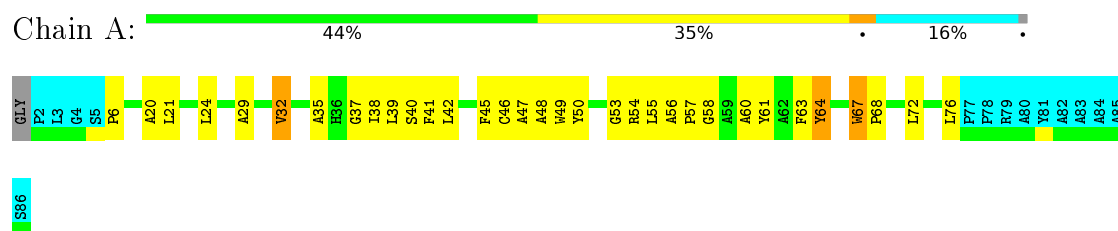
### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: P7 PROTEIN



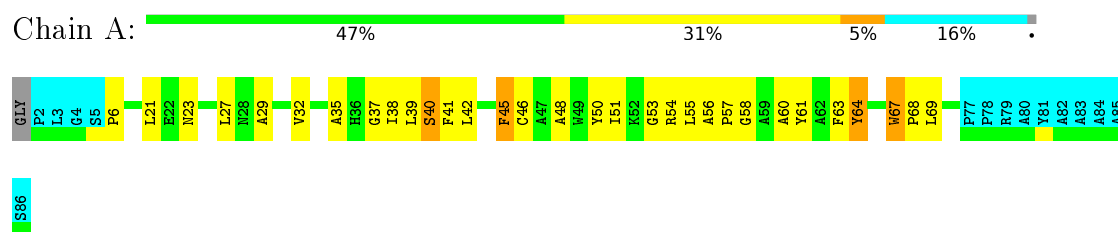
### 4.2.9 Score per residue for model 9

- Molecule 1: P7 PROTEIN



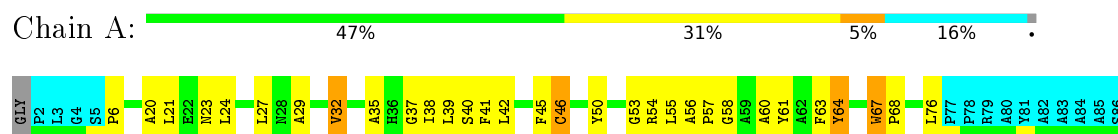
### 4.2.10 Score per residue for model 10

- Molecule 1: P7 PROTEIN



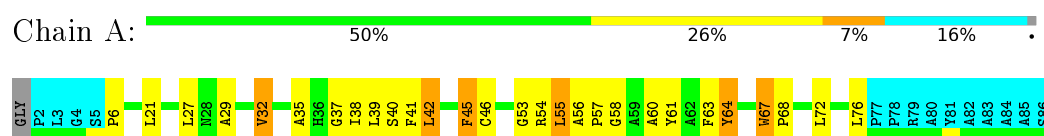
### 4.2.11 Score per residue for model 11

- Molecule 1: P7 PROTEIN



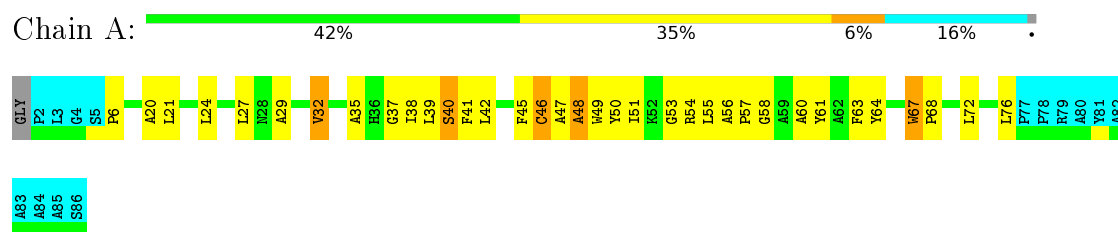
### 4.2.12 Score per residue for model 12

- Molecule 1: P7 PROTEIN



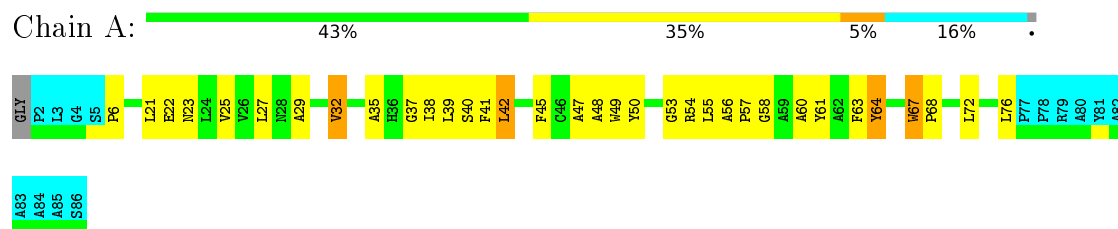
### 4.2.13 Score per residue for model 13

- Molecule 1: P7 PROTEIN



### 4.2.14 Score per residue for model 14

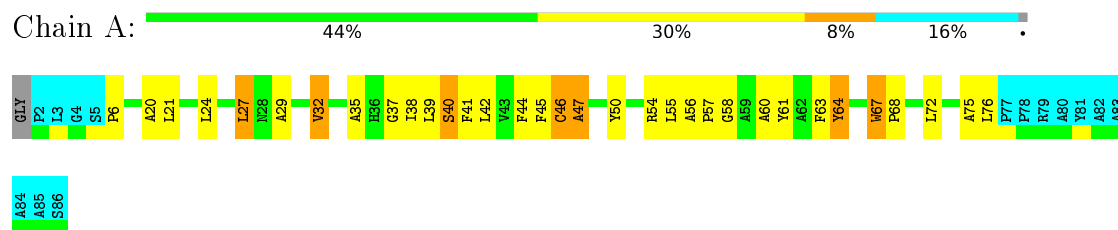
- Molecule 1: P7 PROTEIN



### 4.2.15 Score per residue for model 15

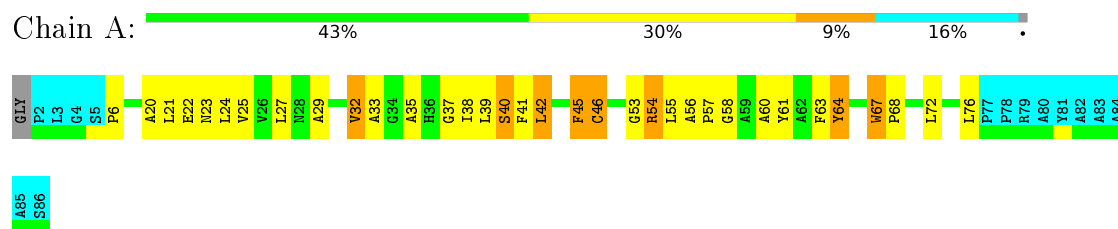
- Molecule 1: P7 PROTEIN





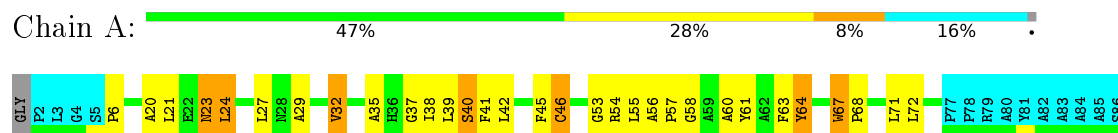
#### 4.2.16 Score per residue for model 16

- Molecule 1: P7 PROTEIN



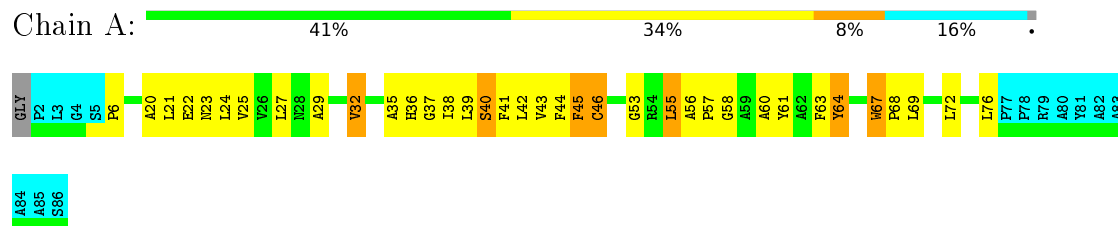
#### 4.2.17 Score per residue for model 17

- Molecule 1: P7 PROTEIN



#### 4.2.18 Score per residue for model 18

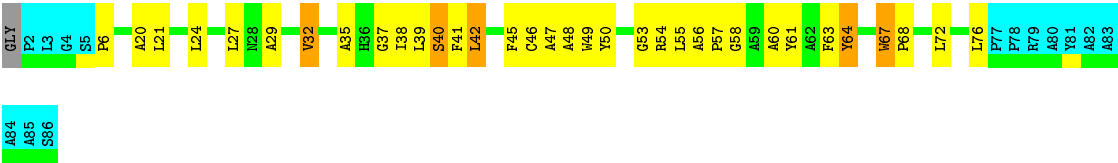
- Molecule 1: P7 PROTEIN



#### 4.2.19 Score per residue for model 19

- Molecule 1: P7 PROTEIN

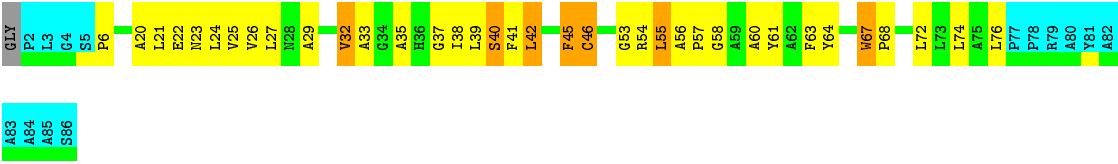




4.2.20 Score per residue for model 20

- Molecule 1: P7 PROTEIN

Chain A: 41% 34% 8% 16%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA MEMBRANE CS ROSETTA*.

Of the 30 calculated structures, 20 were deposited, based on the following criterion: *ENERGY*.

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

Software name	Classification	Version
MEMBRANE CS ROSETTA,ARIA 2.2U3,CNS	refinement	
CCPNMR ANALYSIS 1.15	structure solution	
CCPNMR ANALYSIS 2.2	structure solution	
TALOS 2007.068.09.0	structure solution	
CNS 1.1	structure solution	
CS ROSETTA 1.01	structure solution	
ROSETTA 3.3	structure solution	
ARIA 2.2U3	structure solution	

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

Chemical shift file(s)	3zd0_cs.cif
Number of chemical shift lists	1
Total number of shifts	769
Number of shifts mapped to atoms	768
Number of unparsed shifts	1
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

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

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	545	545	544	26±3
All	All	10900	10900	10880	520

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD12	1:A:40:SER:N	0.79	1.90	10	20
1:A:64:TYR:O	1:A:68:PRO:HD3	0.78	1.79	5	20
1:A:64:TYR:O	1:A:68:PRO:CD	0.71	2.38	17	20
1:A:29:ALA:O	1:A:32:VAL:HG12	0.63	1.94	11	20
1:A:21:LEU:O	1:A:25:VAL:HG13	0.62	1.93	6	3
1:A:21:LEU:HG	1:A:22:GLU:N	0.61	2.11	6	4
1:A:63:PHE:O	1:A:67:TRP:HB2	0.61	1.96	11	20
1:A:38:ILE:O	1:A:42:LEU:HD13	0.60	1.96	2	7
1:A:67:TRP:N	1:A:68:PRO:HD2	0.60	2.12	1	20
1:A:41:PHE:CD2	1:A:60:ALA:HB1	0.58	2.32	1	20
1:A:42:LEU:HD22	1:A:61:TYR:CE1	0.58	2.34	1	4
1:A:23:ASN:O	1:A:27:LEU:HD13	0.58	1.98	1	4
1:A:45:PHE:HB3	1:A:57:PRO:HG3	0.58	1.75	7	7
1:A:21:LEU:O	1:A:25:VAL:HG23	0.57	1.99	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD12	1:A:72:LEU:N	0.55	2.16	17	1
1:A:57:PRO:HB3	1:A:61:TYR:OH	0.55	2.00	2	20
1:A:37:GLY:HA3	1:A:64:TYR:CD2	0.53	2.39	2	20
1:A:35:ALA:O	1:A:38:ILE:HG22	0.52	2.04	7	19
1:A:23:ASN:O	1:A:27:LEU:HG	0.51	2.05	18	7
1:A:35:ALA:HA	1:A:38:ILE:HG22	0.50	1.84	14	14
1:A:42:LEU:HD12	1:A:61:TYR:CD1	0.50	2.42	2	5
1:A:46:CYS:HB2	1:A:61:TYR:OH	0.50	2.06	2	12
1:A:72:LEU:O	1:A:76:LEU:HB2	0.50	2.07	16	11
1:A:54:ARG:HG3	1:A:54:ARG:O	0.49	2.07	3	5
1:A:54:ARG:O	1:A:54:ARG:HG2	0.49	2.07	1	4
1:A:56:ALA:HB3	1:A:57:PRO:HD3	0.49	1.83	6	18
1:A:20:ALA:O	1:A:24:LEU:HG	0.48	2.09	17	12
1:A:42:LEU:HD12	1:A:61:TYR:CE1	0.48	2.44	5	9
1:A:38:ILE:O	1:A:42:LEU:HD23	0.47	2.08	16	5
1:A:55:LEU:O	1:A:58:GLY:N	0.47	2.48	16	20
1:A:54:ARG:O	1:A:54:ARG:HG3	0.46	2.10	17	3
1:A:27:LEU:HG	1:A:75:ALA:HB3	0.46	1.87	1	1
1:A:67:TRP:N	1:A:68:PRO:CD	0.46	2.78	1	20
1:A:27:LEU:HD21	1:A:75:ALA:O	0.46	2.11	15	3
1:A:27:LEU:HD23	1:A:72:LEU:HD12	0.45	1.87	1	1
1:A:47:ALA:C	1:A:49:TRP:H	0.45	2.15	2	7
1:A:35:ALA:O	1:A:39:LEU:HG	0.45	2.11	17	20
1:A:22:GLU:O	1:A:25:VAL:HG22	0.45	2.11	6	5
1:A:42:LEU:O	1:A:46:CYS:HB3	0.45	2.12	18	11
1:A:54:ARG:HG2	1:A:54:ARG:O	0.45	2.12	6	5
1:A:55:LEU:O	1:A:56:ALA:C	0.45	2.55	15	20
1:A:54:ARG:O	1:A:54:ARG:CG	0.45	2.65	6	3
1:A:55:LEU:H	1:A:55:LEU:CD1	0.44	2.24	2	4
1:A:55:LEU:HD22	1:A:55:LEU:C	0.44	2.33	8	1
1:A:42:LEU:HD22	1:A:61:TYR:CD1	0.44	2.48	19	2
1:A:45:PHE:HB3	1:A:57:PRO:CG	0.44	2.43	7	7
1:A:67:TRP:CE3	1:A:67:TRP:HA	0.44	2.48	16	9
1:A:50:TYR:HB2	1:A:57:PRO:HG2	0.44	1.89	11	2
1:A:21:LEU:CG	1:A:22:GLU:N	0.44	2.81	16	4
1:A:32:VAL:CG1	1:A:33:ALA:N	0.43	2.81	16	3
1:A:45:PHE:CD1	1:A:57:PRO:HG3	0.43	2.49	4	9
1:A:67:TRP:HA	1:A:67:TRP:CE3	0.43	2.49	4	4
1:A:54:ARG:CG	1:A:54:ARG:O	0.43	2.67	16	4
1:A:72:LEU:O	1:A:76:LEU:CB	0.43	2.66	6	2
1:A:42:LEU:O	1:A:46:CYS:SG	0.43	2.76	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:VAL:HG23	1:A:27:LEU:HD13	0.43	1.90	4	1
1:A:21:LEU:HD23	1:A:22:GLU:N	0.42	2.30	1	1
1:A:69:LEU:O	1:A:73:LEU:HD13	0.41	2.15	2	1
1:A:22:GLU:HG3	1:A:23:ASN:HD22	0.41	1.75	6	1
1:A:46:CYS:SG	1:A:46:CYS:O	0.41	2.78	13	1
1:A:26:VAL:HG23	1:A:27:LEU:HD12	0.41	1.92	20	1
1:A:48:ALA:O	1:A:51:ILE:HG12	0.41	2.15	10	2
1:A:45:PHE:HB3	1:A:57:PRO:CB	0.41	2.46	6	1
1:A:55:LEU:CD1	1:A:55:LEU:H	0.41	2.29	12	1
1:A:21:LEU:HG	1:A:22:GLU:H	0.41	1.75	16	1
1:A:46:CYS:O	1:A:47:ALA:C	0.41	2.60	15	1
1:A:36:HIS:HA	1:A:39:LEU:HG	0.40	1.93	18	1
1:A:43:VAL:HG23	1:A:44:PHE:N	0.40	2.31	18	1
1:A:55:LEU:N	1:A:55:LEU:CD1	0.40	2.84	2	1
1:A:47:ALA:C	1:A:49:TRP:N	0.40	2.75	2	1
1:A:26:VAL:HG13	1:A:27:LEU:HD13	0.40	1.93	7	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	71/86 (83%)	67±0 (94±1%)	2±0 (3±1%)	2±0 (3±0%)	10	45
All	All	1420/1720 (83%)	1332 (94%)	49 (3%)	39 (3%)	10	45

All 4 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	53	GLY	18
1	A	46	CYS	13
1	A	48	ALA	7
1	A	47	ALA	1

### 6.3.2 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	52/60 (87%)	45±1 (86±3%)	7±1 (14±3%)	8 48
All	All	1040/1200 (87%)	893 (86%)	147 (14%)	8 48

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	67	TRP	20
1	A	32	VAL	17
1	A	21	LEU	16
1	A	64	TYR	16
1	A	40	SER	13
1	A	45	PHE	13
1	A	50	TYR	11
1	A	42	LEU	10
1	A	27	LEU	6
1	A	55	LEU	6
1	A	44	PHE	4
1	A	54	ARG	3
1	A	23	ASN	3
1	A	69	LEU	3
1	A	74	LEU	2
1	A	46	CYS	1
1	A	24	LEU	1
1	A	22	GLU	1
1	A	51	ILE	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 69% for the entire structure.

### 7.1 Chemical shift list 1

File name: 3zd0\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list*

#### 7.1.1 Bookkeeping

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

Total number of shifts	769
Number of shifts mapped to atoms	768
Number of unparsed shifts	1
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. The only occurrence is reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
81	A	22	GLU	HB2	2.095	0.027	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	77	$-1.98 \pm 0.19$	Should be applied
$^{13}\text{C}_\beta$	59	$-1.16 \pm 0.07$	Should be applied
$^{13}\text{C}'$	68	$-1.49 \pm 0.15$	Should be applied
$^{15}\text{N}$	74	$0.09 \pm 0.17$	None needed ( $< 0.5$ ppm)

### 7.1.3 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 72%, i.e. 598 atoms were assigned a chemical shift out of a possible 836. 10 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	303/349 (87%)	118/139 (85%)	122/142 (86%)	63/68 (93%)
Sidechain	220/378 (58%)	132/218 (61%)	86/152 (57%)	2/8 (25%)
Aromatic	75/109 (69%)	39/57 (68%)	34/48 (71%)	2/4 (50%)
Overall	598/836 (72%)	289/414 (70%)	242/342 (71%)	67/80 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 679 atoms were assigned a chemical shift out of a possible 981. 10 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	357/413 (86%)	138/164 (84%)	145/170 (85%)	74/79 (94%)
Sidechain	239/451 (53%)	143/263 (54%)	94/177 (53%)	2/11 (18%)
Aromatic	83/117 (71%)	43/61 (70%)	38/52 (73%)	2/4 (50%)
Overall	679/981 (69%)	324/488 (66%)	277/399 (69%)	78/94 (83%)

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

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

