



# wwPDB NMR Structure Validation Summary Report ⓘ

Dec 6, 2016 – 07:33 PM EST

PDB ID : 5LG9  
Title : Structure of PfIMP2 (Immune Mapped Protein 2 from Plasmodium falciparum) - an antigenic protein  
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Deposited on : 2016-07-06

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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-20028442
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

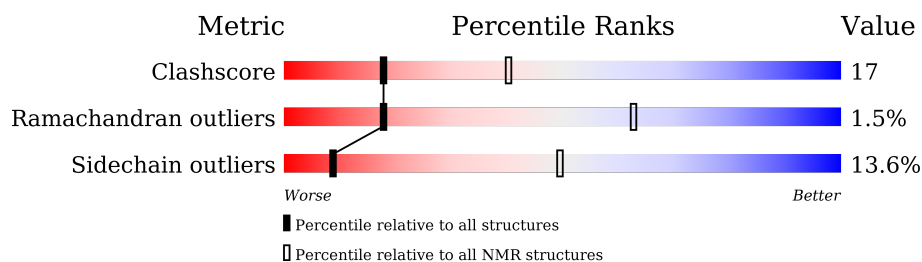
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 88%.

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	156	

## 2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 2 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:5-A:90, A:94-A:158 (151)	0.25	2

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	2, 3, 5, 7, 9, 11, 12, 15
2	4, 8, 13, 14
3	1, 6
Single-model clusters	10

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2515 atoms, of which 1277 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

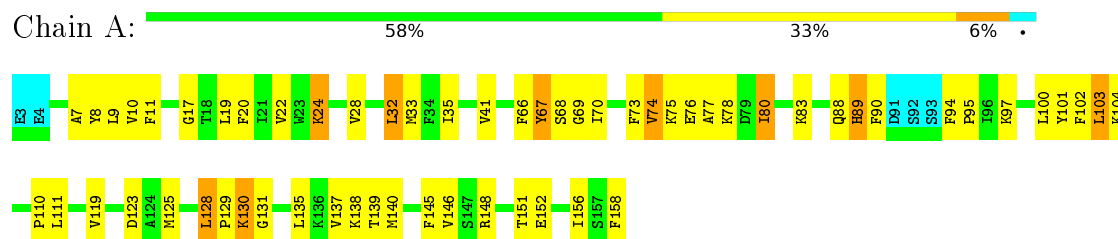
Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2515	802	1277	202	228	6	

## 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.

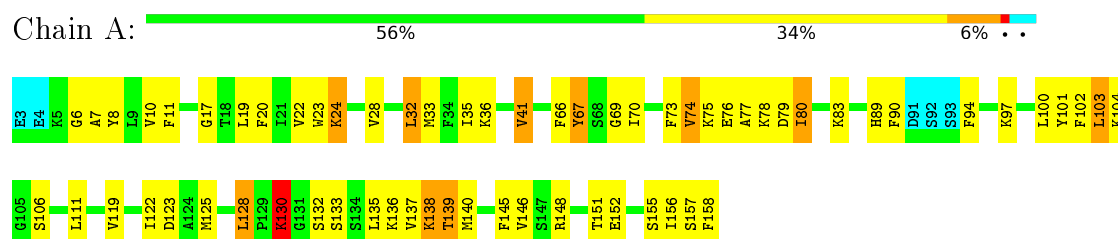
- Molecule 1: Uncharacterized protein



### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: Uncharacterized protein



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 15 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	refinement	

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)	5lg9_cs.cif
Number of chemical shift lists	1
Total number of shifts	1925
Number of shifts mapped to atoms	1925
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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 [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	1200	1249	1248	43±6
All	All	18000	18735	18720	642

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 17.

5 of 167 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LYS:HD2	1:A:122:ILE:HG22	0.84	1.49	13	5
1:A:102:PHE:HE1	1:A:125:MET:SD	0.79	1.99	12	9
1:A:74:VAL:HG11	1:A:125:MET:SD	0.75	2.21	15	9
1:A:102:PHE:CE1	1:A:125:MET:SD	0.74	2.80	12	9
1:A:74:VAL:HG21	1:A:125:MET:SD	0.70	2.27	12	9

### 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	150/156 (96%)	138±2 (92±1%)	10±2 (7±1%)	2±1 (1±0%)	18	63
All	All	2250/2340 (96%)	2065 (92%)	152 (7%)	33 (1%)	18	63

All 5 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	89	HIS	15
1	A	130	LYS	14
1	A	131	GLY	2
1	A	14	ALA	1
1	A	81	LYS	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	134/139 (96%)	116±2 (86±2%)	18±2 (14±2%)	9	49
All	All	2010/2085 (96%)	1737 (86%)	273 (14%)	9	49

5 of 39 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	TYR	15
1	A	20	PHE	15
1	A	80	ILE	15
1	A	139	THR	15
1	A	111	LEU	15

### 6.3.3 RNA ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: 5lg9\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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	1925
Number of shifts mapped to atoms	1925
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	235

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	156	$-0.20 \pm 0.18$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	146	$-0.10 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	151	$0.17 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	144	$0.09 \pm 0.40$	None needed ( $< 0.5$ ppm)

#### 7.1.3 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 88%, i.e. 1685 atoms were assigned a chemical shift out of a possible 1916. 27 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	729/743 (98%)	291/296 (98%)	298/302 (99%)	140/145 (97%)
Sidechain	879/1012 (87%)	545/596 (91%)	334/373 (90%)	0/43 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	77/161 (48%)	40/87 (46%)	36/71 (51%)	1/3 (33%)
Overall	1685/1916 (88%)	876/979 (89%)	668/746 (90%)	141/191 (74%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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	90	PHE	CD1	35.19	137.63 – 125.43	-79.0
1	A	20	PHE	CD1	35.73	137.63 – 125.43	-78.5
1	A	11	PHE	CD1	35.73	137.63 – 125.43	-78.5
1	A	73	PHE	CD1	35.73	137.63 – 125.43	-78.5
1	A	34	PHE	CD1	35.85	137.63 – 125.43	-78.4
1	A	44	PHE	CD1	35.95	137.63 – 125.43	-78.3
1	A	145	PHE	CD1	35.95	137.63 – 125.43	-78.3
1	A	117	PHE	CD1	35.95	137.63 – 125.43	-78.3
1	A	158	PHE	CD1	35.95	137.63 – 125.43	-78.3
1	A	66	PHE	CD1	36.05	137.63 – 125.43	-78.3
1	A	102	PHE	CD1	36.15	137.63 – 125.43	-78.2
1	A	94	PHE	CD1	36.23	137.63 – 125.43	-78.1
1	A	46	PHE	CD1	36.35	137.63 – 125.43	-78.0
1	A	8	TYR	CD1	35.47	139.11 – 126.41	-76.6
1	A	101	TYR	CD1	35.95	139.11 – 126.41	-76.2
1	A	67	TYR	CD1	36.48	139.11 – 126.41	-75.8
1	A	20	PHE	CE1	32.48	137.92 – 123.42	-67.7
1	A	11	PHE	CE1	33.45	137.92 – 123.42	-67.0
1	A	158	PHE	CE1	34.23	137.92 – 123.42	-66.5
1	A	90	PHE	CE1	35.23	137.92 – 123.42	-65.8
1	A	44	PHE	CE1	35.65	137.92 – 123.42	-65.5
1	A	117	PHE	CE1	35.73	137.92 – 123.42	-65.5
1	A	34	PHE	CE1	35.85	137.92 – 123.42	-65.4
1	A	145	PHE	CE1	35.95	137.92 – 123.42	-65.3
1	A	46	PHE	CE1	35.98	137.92 – 123.42	-65.3
1	A	66	PHE	CE1	36.15	137.92 – 123.42	-65.2
1	A	102	PHE	CE1	36.15	137.92 – 123.42	-65.2
1	A	46	PHE	CZ	33.23	137.04 – 121.44	-61.5
1	A	34	PHE	CZ	35.75	137.04 – 121.44	-59.9
1	A	23	TRP	CH2	26.65	133.06 – 114.56	-52.5
1	A	67	TYR	CE1	53.84	124.14 – 111.74	-51.7
1	A	101	TYR	CE1	54.67	124.14 – 111.74	-51.0

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	8	TYR	CE1	54.67	124.14 – 111.74	-51.0
1	A	23	TRP	CD1	30.42	136.18 – 116.78	-49.5
1	A	23	TRP	CZ2	50.24	121.76 – 106.66	-42.4
1	A	23	TRP	CZ3	56.34	129.20 – 113.60	-41.7
1	A	89	HIS	CE1	42.98	149.70 – 125.30	-38.7
1	A	23	TRP	CE3	56.47	129.06 – 111.96	-37.5
1	A	85	THR	CG2	54.19	27.15 – 15.95	29.1
1	A	151	THR	CG2	53.57	27.15 – 15.95	28.6
1	A	38	THR	CG2	53.56	27.15 – 15.95	28.6
1	A	113	THR	CG2	53.53	27.15 – 15.95	28.5
1	A	52	LYS	CG	57.71	30.67 – 19.17	28.5
1	A	5	LYS	CG	57.71	30.67 – 19.17	28.5
1	A	139	THR	CG2	53.48	27.15 – 15.95	28.5
1	A	36	LYS	CG	57.70	30.67 – 19.17	28.5
1	A	64	LYS	CG	57.69	30.67 – 19.17	28.5
1	A	18	THR	CG2	53.32	27.15 – 15.95	28.4
1	A	81	LYS	CG	57.47	30.67 – 19.17	28.3
1	A	63	LYS	CG	57.44	30.67 – 19.17	28.3
1	A	104	LYS	CG	57.40	30.67 – 19.17	28.2
1	A	75	LYS	CG	57.38	30.67 – 19.17	28.2
1	A	78	LYS	CG	57.28	30.67 – 19.17	28.1
1	A	138	LYS	CG	57.27	30.67 – 19.17	28.1
1	A	136	LYS	CG	57.25	30.67 – 19.17	28.1
1	A	107	LYS	CG	57.18	30.67 – 19.17	28.1
1	A	142	LYS	CG	57.13	30.67 – 19.17	28.0
1	A	97	LYS	CG	56.80	30.67 – 19.17	27.7
1	A	39	LYS	CG	56.54	30.67 – 19.17	27.5
1	A	59	LEU	CG	57.73	32.55 – 21.05	26.9
1	A	130	LYS	CG	55.55	30.67 – 19.17	26.6
1	A	74	VAL	CG1	55.95	28.40 – 14.60	25.0
1	A	57	ARG	CG	56.50	33.23 – 21.23	24.4
1	A	81	LYS	CD	57.57	34.86 – 23.06	24.2
1	A	98	VAL	CG1	54.82	28.40 – 14.60	24.1
1	A	146	VAL	CG1	54.78	28.40 – 14.60	24.1
1	A	122	ILE	CG2	51.65	24.63 – 10.43	24.0
1	A	108	VAL	CG1	54.52	28.40 – 14.60	23.9
1	A	127	VAL	CG1	54.09	28.40 – 14.60	23.6
1	A	22	VAL	CG1	53.94	28.40 – 14.60	23.5
1	A	45	LYS	CD	56.58	34.86 – 23.06	23.4
1	A	119	VAL	CG1	53.66	28.40 – 14.60	23.3
1	A	70	ILE	CG2	50.53	24.63 – 10.43	23.2
1	A	96	ILE	CG2	50.50	24.63 – 10.43	23.2

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	15	SER	CB	29.20	71.24 – 56.34	-23.2
1	A	28	VAL	CG1	53.39	28.40 – 14.60	23.1
1	A	10	VAL	CG1	53.33	28.40 – 14.60	23.1
1	A	118	VAL	CG1	53.31	28.40 – 14.60	23.1
1	A	47	VAL	CG1	53.29	28.40 – 14.60	23.0
1	A	35	ILE	CG2	50.23	24.63 – 10.43	23.0
1	A	41	VAL	CG1	53.23	28.40 – 14.60	23.0
1	A	56	ILE	CG2	49.45	24.63 – 10.43	22.5
1	A	80	ILE	CG2	49.44	24.63 – 10.43	22.5
1	A	68	SER	CB	30.47	71.24 – 56.34	-22.4
1	A	21	ILE	CG2	49.01	24.63 – 10.43	22.2
1	A	147	SER	CB	30.88	71.24 – 56.34	-22.1
1	A	134	SER	CB	30.94	71.24 – 56.34	-22.0
1	A	132	SER	CB	31.15	71.24 – 56.34	-21.9
1	A	137	VAL	CG1	51.41	28.40 – 14.60	21.7
1	A	156	ILE	CG2	48.29	24.63 – 10.43	21.7
1	A	133	SER	CB	31.94	71.24 – 56.34	-21.4
1	A	61	SER	CB	31.99	71.24 – 56.34	-21.3
1	A	110	PRO	CA	30.05	71.13 – 55.53	-21.3
1	A	119	VAL	CG2	54.68	29.20 – 13.40	21.1
1	A	92	SER	CB	32.40	71.24 – 56.34	-21.1
1	A	74	VAL	CG2	54.58	29.20 – 13.40	21.1
1	A	108	VAL	CG2	54.50	29.20 – 13.40	21.0
1	A	106	SER	CB	32.59	71.24 – 56.34	-20.9
1	A	42	PRO	CA	30.97	71.13 – 55.53	-20.7
1	A	127	VAL	CG2	54.06	29.20 – 13.40	20.7
1	A	22	VAL	CG2	54.06	29.20 – 13.40	20.7
1	A	28	VAL	CG2	54.02	29.20 – 13.40	20.7
1	A	157	SER	CB	32.97	71.24 – 56.34	-20.7
1	A	129	PRO	CA	31.08	71.13 – 55.53	-20.7
1	A	37	PRO	CA	31.08	71.13 – 55.53	-20.7
1	A	10	VAL	CG2	53.95	29.20 – 13.40	20.7
1	A	116	PRO	CA	31.26	71.13 – 55.53	-20.6
1	A	137	VAL	CG2	53.77	29.20 – 13.40	20.6
1	A	93	SER	CB	33.19	71.24 – 56.34	-20.5
1	A	154	ALA	CB	55.96	28.03 – 9.93	20.4
1	A	65	LEU	CD1	57.60	32.77 – 16.57	20.3
1	A	100	LEU	CD1	57.53	32.77 – 16.57	20.3
1	A	118	VAL	CG2	53.34	29.20 – 13.40	20.3
1	A	19	LEU	CD1	57.49	32.77 – 16.57	20.3
1	A	47	VAL	CG2	53.29	29.20 – 13.40	20.2
1	A	41	VAL	CG2	53.23	29.20 – 13.40	20.2

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	146	VAL	CG2	53.12	29.20 – 13.40	20.1
1	A	56	ILE	CD1	46.91	21.91 – 5.01	19.8
1	A	59	LEU	CD2	57.70	32.60 – 15.60	19.8
1	A	156	ILE	CD1	46.82	21.91 – 5.01	19.7
1	A	113	THR	CB	36.74	78.10 – 61.30	-19.6
1	A	122	ILE	CD1	46.60	21.91 – 5.01	19.6
1	A	111	LEU	CD1	56.35	32.77 – 16.57	19.6
1	A	124	ALA	CB	54.24	28.03 – 9.93	19.5
1	A	80	ILE	CD1	46.36	21.91 – 5.01	19.5
1	A	151	THR	CB	37.24	78.10 – 61.30	-19.3
1	A	21	ILE	CD1	46.01	21.91 – 5.01	19.3
1	A	95	PRO	CA	33.29	71.13 – 55.53	-19.3
1	A	55	LEU	CD1	55.80	32.77 – 16.57	19.2
1	A	84	LEU	CD2	56.67	32.60 – 15.60	19.2
1	A	128	LEU	CD1	55.71	32.77 – 16.57	19.2
1	A	135	LEU	CD2	56.61	32.60 – 15.60	19.1
1	A	38	THR	CB	37.59	78.10 – 61.30	-19.1
1	A	31	ALA	CB	53.46	28.03 – 9.93	19.0
1	A	155	SER	CB	35.54	71.24 – 56.34	-19.0
1	A	9	LEU	CD1	55.35	32.77 – 16.57	18.9
1	A	103	LEU	CD1	55.21	32.77 – 16.57	18.9
1	A	126	SER	CB	35.75	71.24 – 56.34	-18.8
1	A	70	ILE	CD1	45.26	21.91 – 5.01	18.8
1	A	32	LEU	CD2	55.79	32.60 – 15.60	18.6
1	A	98	VAL	CG2	50.71	29.20 – 13.40	18.6
1	A	55	LEU	CD2	55.70	32.60 – 15.60	18.6
1	A	35	ILE	CD1	44.63	21.91 – 5.01	18.4
1	A	96	ILE	CD1	44.58	21.91 – 5.01	18.4
1	A	9	LEU	CD2	55.38	32.60 – 15.60	18.4
1	A	103	LEU	CD2	55.24	32.60 – 15.60	18.3
1	A	141	ALA	CB	51.88	28.03 – 9.93	18.2
1	A	19	LEU	CD2	54.79	32.60 – 15.60	18.1
1	A	32	LEU	CD1	53.79	32.77 – 16.57	18.0
1	A	7	ALA	CB	51.51	28.03 – 9.93	18.0
1	A	14	ALA	CB	51.49	28.03 – 9.93	18.0
1	A	65	LEU	CD2	54.61	32.60 – 15.60	17.9
1	A	85	THR	CB	39.61	78.10 – 61.30	-17.9
1	A	87	LEU	CD2	54.33	32.60 – 15.60	17.8
1	A	139	THR	CB	40.39	78.10 – 61.30	-17.4
1	A	77	ALA	CB	50.17	28.03 – 9.93	17.2
1	A	18	THR	CB	41.11	78.10 – 61.30	-17.0
1	A	33	MET	CE	50.48	26.97 – 7.37	17.0

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	122	ILE	CG1	57.58	36.54 – 18.94	17.0
1	A	144	MET	CE	49.72	26.97 – 7.37	16.6
1	A	106	SER	CA	25.80	69.25 – 48.25	-15.7
1	A	126	SER	CA	26.48	69.25 – 48.25	-15.4
1	A	133	SER	CA	26.99	69.25 – 48.25	-15.1
1	A	132	SER	CA	27.37	69.25 – 48.25	-14.9
1	A	29	GLU	CA	25.99	67.86 – 46.86	-14.9
1	A	93	SER	CA	27.39	69.25 – 48.25	-14.9
1	A	3	GLU	CA	26.08	67.86 – 46.86	-14.9
1	A	54	GLU	CA	26.34	67.86 – 46.86	-14.8
1	A	61	SER	CA	27.75	69.25 – 48.25	-14.8
1	A	43	GLU	CA	26.78	67.86 – 46.86	-14.6
1	A	60	GLN	CA	25.75	67.31 – 45.91	-14.4
1	A	76	GLU	CA	27.43	67.86 – 46.86	-14.3
1	A	92	SER	CA	28.89	69.25 – 48.25	-14.2
1	A	147	SER	CA	29.48	69.25 – 48.25	-13.9
1	A	134	SER	CA	29.55	69.25 – 48.25	-13.9
1	A	72	GLN	CA	26.95	67.31 – 45.91	-13.9
1	A	59	LEU	CA	26.08	66.36 – 44.96	-13.8
1	A	138	LYS	CA	26.68	67.97 – 45.97	-13.8
1	A	144	MET	CA	25.73	67.38 – 44.88	-13.5
1	A	68	SER	CA	30.47	69.25 – 48.25	-13.5
1	A	49	ARG	CA	25.72	68.35 – 45.25	-13.5
1	A	139	THR	CA	26.85	75.37 – 49.07	-13.4
1	A	64	LYS	CA	27.46	67.97 – 45.97	-13.4
1	A	78	LYS	CA	27.48	67.97 – 45.97	-13.4
1	A	63	LYS	CA	27.66	67.97 – 45.97	-13.3
1	A	142	LYS	CA	28.43	67.97 – 45.97	-13.0
1	A	75	LYS	CA	28.62	67.97 – 45.97	-12.9
1	A	148	ARG	CA	27.22	68.35 – 45.25	-12.8
1	A	35	ILE	CA	27.32	75.08 – 48.18	-12.8
1	A	90	PHE	CA	25.84	70.99 – 45.29	-12.6
1	A	56	ILE	CA	27.92	75.08 – 48.18	-12.5
1	A	156	ILE	CA	28.22	75.08 – 48.18	-12.4
1	A	18	THR	CA	29.59	75.37 – 49.07	-12.4
1	A	122	ILE	CA	28.32	75.08 – 48.18	-12.4
1	A	96	ILE	CA	28.34	75.08 – 48.18	-12.4
1	A	41	VAL	CA	26.85	76.93 – 48.03	-12.3
1	A	85	THR	CA	29.85	75.37 – 49.07	-12.3
1	A	98	VAL	CA	26.95	76.93 – 48.03	-12.3
1	A	80	ILE	CA	28.60	75.08 – 48.18	-12.3
1	A	21	ILE	CA	28.63	75.08 – 48.18	-12.3

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	89	HIS	CA	27.82	68.24 – 44.74	-12.2
1	A	137	VAL	CA	27.31	76.93 – 48.03	-12.2
1	A	67	TYR	CA	27.33	70.88 – 45.38	-12.1
1	A	158	PHE	CA	27.12	70.99 – 45.29	-12.1
1	A	46	PHE	CA	27.21	70.99 – 45.29	-12.0
1	A	38	THR	CA	30.65	75.37 – 49.07	-12.0
1	A	23	TRP	CE2	56.42	173.31 – 104.01	-11.9
1	A	127	VAL	CA	28.19	76.93 – 48.03	-11.9
1	A	22	VAL	CA	28.29	76.93 – 48.03	-11.8
1	A	44	PHE	CA	28.26	70.99 – 45.29	-11.6
1	A	28	VAL	CA	28.89	76.93 – 48.03	-11.6
1	A	10	VAL	CA	29.06	76.93 – 48.03	-11.6
1	A	119	VAL	CA	29.77	76.93 – 48.03	-11.3
1	A	113	THR	CA	33.00	75.37 – 49.07	-11.1
1	A	108	VAL	CA	30.64	76.93 – 48.03	-11.0
1	A	145	PHE	CA	30.06	70.99 – 45.29	-10.9
1	A	66	PHE	CA	30.15	70.99 – 45.29	-10.9
1	A	73	PHE	CA	30.43	70.99 – 45.29	-10.8
1	A	151	THR	CA	33.90	75.37 – 49.07	-10.8
1	A	70	ILE	CA	32.87	75.08 – 48.18	-10.7
1	A	118	VAL	CA	31.61	76.93 – 48.03	-10.7
1	A	47	VAL	CA	31.94	76.93 – 48.03	-10.6
1	A	146	VAL	CA	33.42	76.93 – 48.03	-10.1
1	A	74	VAL	CA	35.13	76.93 – 48.03	-9.5
1	A	140	MET	CE	32.50	26.97 – 7.37	7.8
1	A	71	CYS	CA	32.31	75.07 – 41.27	-7.6
1	A	7	ALA	HB2	-0.36	2.61 – 0.11	-6.9
1	A	7	ALA	HB1	-0.36	2.61 – 0.11	-6.9
1	A	7	ALA	HB3	-0.36	2.61 – 0.11	-6.9
1	A	45	LYS	HB3	0.03	3.10 – 0.40	-6.4
1	A	95	PRO	HD2	1.45	5.45 – 1.85	-6.1
1	A	45	LYS	HD3	0.21	2.75 – 0.45	-6.0
1	A	82	GLY	N	131.04	129.07 – 90.27	5.5
1	A	149	GLY	N	130.26	129.07 – 90.27	5.3
1	A	51	GLY	N	130.25	129.07 – 90.27	5.3

### 7.1.5 Random Coil Index (RCI) plots

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:

