



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1I17
Title : NMR STRUCTURE OF MOUSE DOPPEL 51-157
Authors : Mo, H.; Moore, R.C.; Cohen, F.E.; Westaway, D.; Prusiner, S.B.; Wright, P.E.;
Dyson, H.J.
Deposited on : 2001-01-31

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

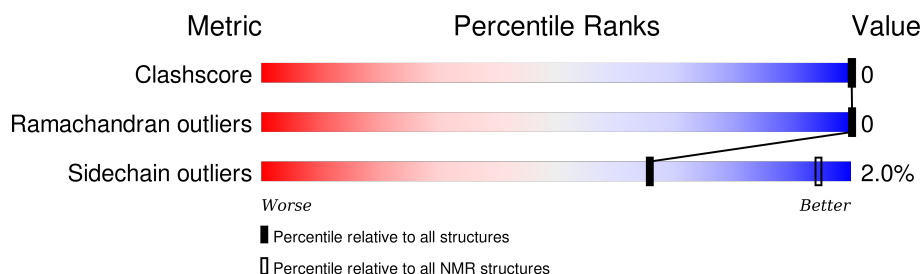
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	107	 88% • 9%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 16 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:101 (97)	0.31	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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1693 atoms, of which 828 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRION-LIKE PROTEIN.

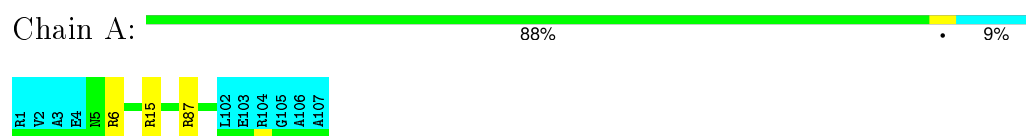
Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1693	542	828	157	161	5	

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: PRION-LIKE PROTEIN

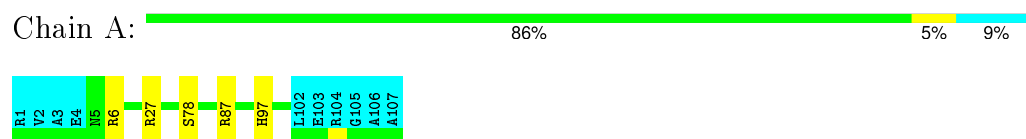


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

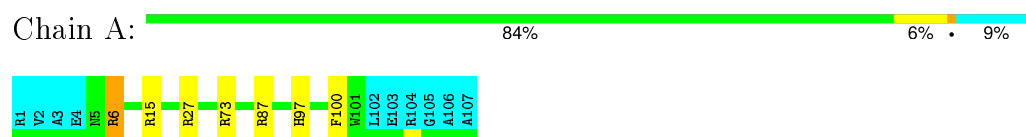
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: PRION-LIKE PROTEIN



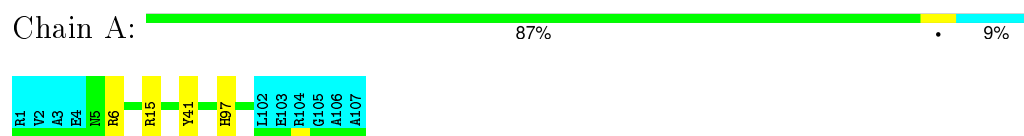
4.2.2 Score per residue for model 2

- Molecule 1: PRION-LIKE PROTEIN



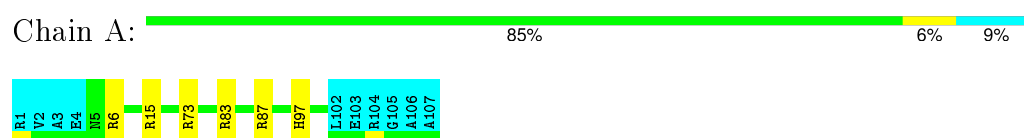
4.2.3 Score per residue for model 3

- Molecule 1: PRION-LIKE PROTEIN



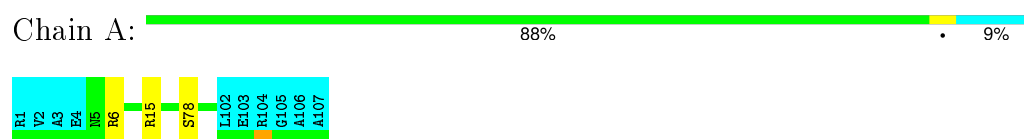
4.2.4 Score per residue for model 4

- Molecule 1: PRION-LIKE PROTEIN



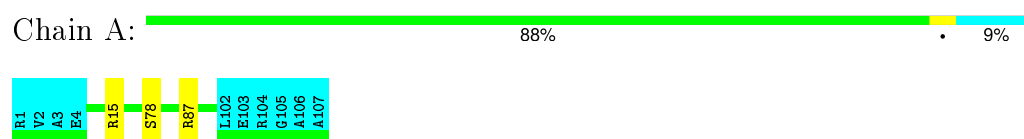
4.2.5 Score per residue for model 5

- Molecule 1: PRION-LIKE PROTEIN



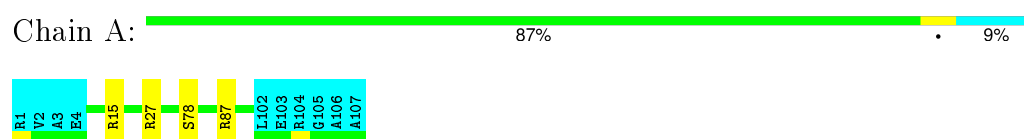
4.2.6 Score per residue for model 6

- Molecule 1: PRION-LIKE PROTEIN



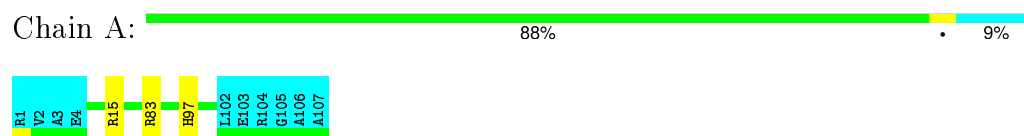
4.2.7 Score per residue for model 7

- Molecule 1: PRION-LIKE PROTEIN



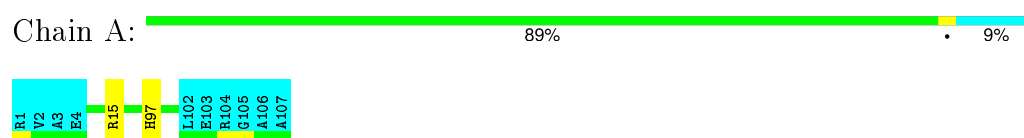
4.2.8 Score per residue for model 8

- Molecule 1: PRION-LIKE PROTEIN



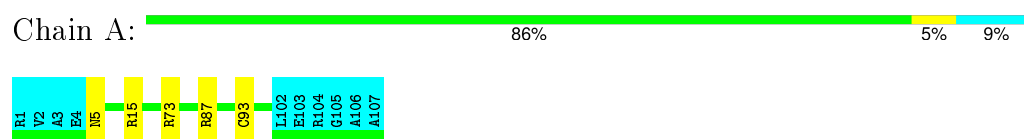
4.2.9 Score per residue for model 9

- Molecule 1: PRION-LIKE PROTEIN



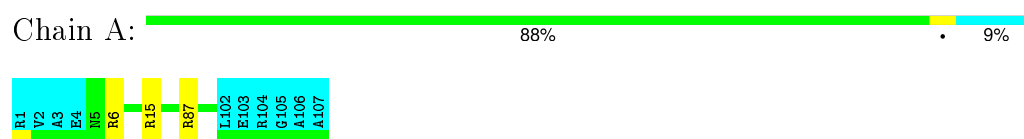
4.2.10 Score per residue for model 10

- Molecule 1: PRION-LIKE PROTEIN



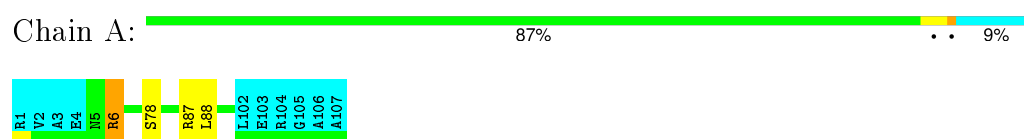
4.2.11 Score per residue for model 11

- Molecule 1: PRION-LIKE PROTEIN



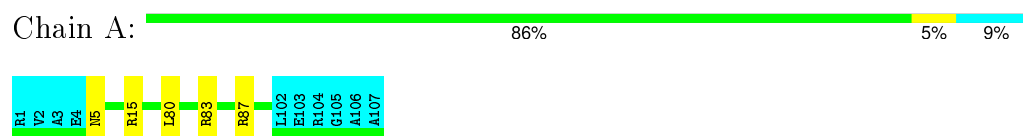
4.2.12 Score per residue for model 12

- Molecule 1: PRION-LIKE PROTEIN



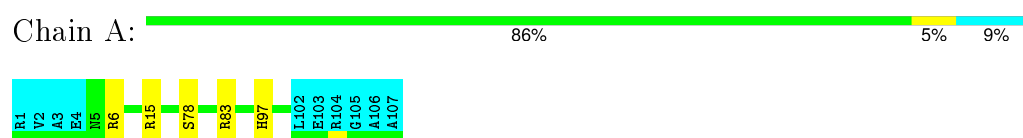
4.2.13 Score per residue for model 13

- Molecule 1: PRION-LIKE PROTEIN



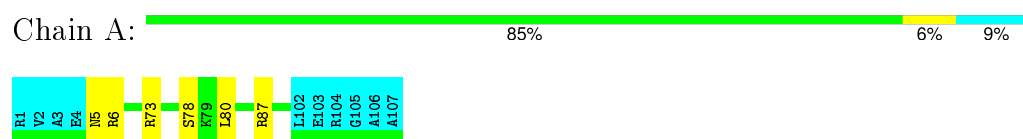
4.2.14 Score per residue for model 14

- Molecule 1: PRION-LIKE PROTEIN



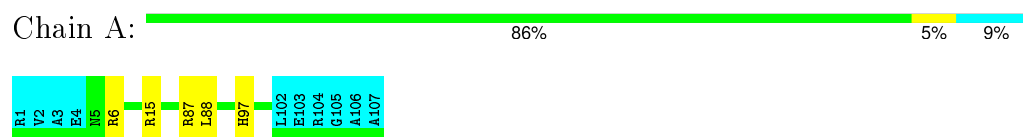
4.2.15 Score per residue for model 15

- Molecule 1: PRION-LIKE PROTEIN



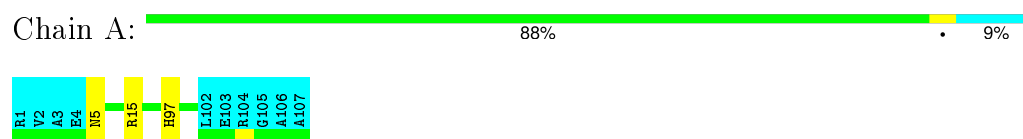
4.2.16 Score per residue for model 16

- Molecule 1: PRION-LIKE PROTEIN




4.2.17 Score per residue for model 17

- Molecule 1: PRION-LIKE PROTEIN



4.2.18 Score per residue for model 18


- Molecule 1: PRION-LIKE PROTEIN

Chain A:  86% 5% 9%



4.2.19 Score per residue for model 19


- Molecule 1: PRION-LIKE PROTEIN

Chain A:  87% 0% 9%



4.2.20 Score per residue for model 20

- Molecule 1: PRION-LIKE PROTEIN

Chain A:  85% 6% 9%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
DYANA	structure solution	1.5
amber	refinement	7

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)	BMRB entry 4938
Number of chemical shift lists	1
Total number of shifts	1685
Number of shifts mapped to atoms	1361
Number of unparsed shifts	11
Number of shifts with mapping errors	313
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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

6 Model quality

6.1 Standard geometry

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	0.75±0.00	0±0/810 (0.0±0.0%)	1.02±0.02	3±1/1093 (0.3±0.1%)
All	All	0.75	0/16200 (0.0%)	1.02	56/21860 (0.3%)

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	0.1±0.2
All	All	0	1

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	73	ARG	NE-CZ-NH1	7.39	124.00	120.30	4	5
1	A	83	ARG	NE-CZ-NH1	7.18	123.89	120.30	13	6
1	A	6	ARG	NE-CZ-NH1	6.78	123.69	120.30	18	13
1	A	15	ARG	NE-CZ-NH1	6.37	123.49	120.30	16	16
1	A	87	ARG	NE-CZ-NH1	5.92	123.26	120.30	1	13
1	A	27	ARG	NE-CZ-NH1	5.90	123.25	120.30	2	3

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	41	TYR	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
All	All	15800	15000	14960	-

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 -.

There are no clashes.

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	97/107 (91%)	90±2 (93±2%)	7±2 (7±2%)	0±0 (0±0%)	100	100
All	All	1940/2140 (91%)	1796 (93%)	144 (7%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	81/87 (93%)	79±1 (98±1%)	2±1 (2±1%)	66	94
All	All	1620/1740 (93%)	1587 (98%)	33 (2%)	66	94

All 9 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	97	HIS	10
1	A	78	SER	8
1	A	5	ASN	5
1	A	88	LEU	2
1	A	80	LEU	2
1	A	50	VAL	2
1	A	6	ARG	2
1	A	93	CYS	1
1	A	100	PHE	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

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4938

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	1685
Number of shifts mapped to atoms	1361
Number of unparsed shifts	11
Number of shifts with mapping errors	313
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- Chemical shift has been reported more than once. All 11 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
618	A	24	GLU	H	8.77	0.02	1
619	A	24	GLU	HA	4.12	0.02	1
620	A	24	GLU	HB2	2.04	0.02	1
621	A	24	GLU	HB3	2.04	0.02	1
622	A	24	GLU	HG2	2.36	0.02	1
623	A	24	GLU	HG3	2.36	0.02	1
624	A	24	GLU	C	174.8	0.2	1
625	A	24	GLU	CA	59.8	0.2	1
626	A	24	GLU	CB	29.5	0.2	1
627	A	24	GLU	CG	37	0.2	1
628	A	24	GLU	N	118	0.1	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 313 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	9	LYS	HD2	1.68	0.02	2
A	6	HIS	HB3	3.03	0.02	2
A	14	VAL	CG1	20.9	0.2	2
A	17	SER	HB3	3.9	0.02	2
A	7	ARG	HD3	3.11	0.02	1
A	17	SER	HA	4.49	0.02	1
A	9	LYS	C	175.7	0.2	1
A	13	LYS	CG	24.7	0.2	1
A	20	GLY	CA	45.1	0.2	1
A	17	SER	H	8.4	0.02	1
A	10	TRP	H	8.1	0.02	1
A	8	PHE	HE2	7.2	0.02	1
A	25	ALA	N	125.5	0.1	1
A	8	PHE	HD2	7.18	0.02	1
A	9	LYS	CB	33.2	0.2	1
A	19	GLY	HA2	4.04	0.02	1
A	7	ARG	CA	56.2	0.2	1
A	14	VAL	HG21	0.92	0.02	1
A	23	THR	C	174.4	0.2	1
A	5	LYS	CD	29.1	0.2	1
A	25	ALA	HA	4.3	0.02	1
A	17	SER	CB	64.0	0.2	1
A	12	ARG	NE	84.8	0.1	1
A	12	ARG	HB3	1.7	0.02	2
A	5	LYS	H	8.43	0.02	1
A	12	ARG	HG2	1.53	0.02	1
A	21	GLN	CB	29.7	0.2	1
A	19	GLY	H	8.46	0.02	1
A	9	LYS	H	8.23	0.02	1
A	10	TRP	CE3	120.9	0.2	1
A	13	LYS	H	8.33	0.02	1
A	16	PRO	C	177.1	0.2	1
A	6	HIS	HA	4.61	0.02	1
A	10	TRP	HA	4.65	0.02	1
A	22	ILE	HD13	0.88	0.02	1
A	8	PHE	CD1	131.9	0.2	1
A	7	ARG	N	122.9	0.1	1
A	4	ILE	CG1	27.0	0.2	1
A	10	TRP	HE1	10.17	0.02	1
A	10	TRP	CZ2	114.8	0.2	1
A	10	TRP	CD1	127.2	0.2	1
A	23	THR	HA	4.37	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	GLY	CA	45.2	0.2	1
A	4	ILE	HG12	1.41	0.02	2
A	4	ILE	HB	1.81	0.02	1
A	10	TRP	C	175.8	0.2	1
A	22	ILE	HA	4.26	0.02	1
A	8	PHE	C	175.4	0.2	1
A	13	LYS	HD3	1.65	0.02	1
A	2	ARG	HG2	1.67	0.02	1
A	3	GLY	HA2	4.01	0.02	2
A	15	LEU	HD11	0.97	0.02	9
A	4	ILE	CD1	12.8	0.2	1
A	12	ARG	HD3	3.11	0.02	1
A	14	VAL	CG2	21.3	0.2	2
A	8	PHE	H	8.33	0.02	1
A	9	LYS	N	123.3	0.1	1
A	25	ALA	HB1	1.4	0.02	1
A	11	ASN	HD21	7.55	0.02	2
A	3	GLY	N	110.7	0.1	1
A	14	VAL	HG13	0.92	0.02	1
A	10	TRP	HH2	7.21	0.02	1
A	22	ILE	CB	38.9	0.2	1
A	12	ARG	HA	4.17	0.02	1
A	15	LEU	HD22	0.91	0.02	2
A	19	GLY	C	174.7	0.2	1
A	12	ARG	H	8.01	0.02	1
A	23	THR	CG2	21.6	0.2	1
A	20	GLY	H	8.3	0.02	1
A	7	ARG	CB	31.1	0.2	1
A	14	VAL	HG22	0.92	0.02	1
A	1	ALA	CB	19.0	0.2	9
A	2	ARG	HB3	1.85	0.02	1
A	9	LYS	HB3	1.62	0.02	1
A	10	TRP	NE1	129.6	0.1	1
A	16	PRO	HG2	2.05	0.02	2
A	5	LYS	HD3	1.67	0.02	1
A	17	SER	C	174.9	0.2	1
A	18	SER	CA	58.6	0.2	1
A	21	GLN	CG	34.0	0.2	1
A	16	PRO	HB3	1.97	0.02	2
A	20	GLY	HA2	3.99	0.02	1
A	5	LYS	HE2	2.97	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	23	THR	H	8.24	0.02	1
A	2	ARG	HE	7.18	0.02	1
A	22	ILE	HG13	1.23	0.02	2
A	10	TRP	HZ3	7.15	0.02	1
A	21	GLN	HA	4.38	0.02	1
A	7	ARG	H	8.35	0.02	1
A	17	SER	CA	58.5	0.2	1
A	10	TRP	HB2	3.3	0.02	2
A	6	HIS	C	176.2	0.2	1
A	15	LEU	CD2	25.0	0.2	2
A	21	GLN	HG3	2.37	0.02	1
A	23	THR	CB	70.1	0.2	1
A	16	PRO	HB2	2.31	0.02	2
A	11	ASN	N	121.2	0.1	1
A	21	GLN	NE2	112.2	0.1	1
A	15	LEU	HD12	0.97	0.02	9
A	9	LYS	HG3	1.24	0.02	2
A	17	SER	N	115.7	0.1	1
A	4	ILE	HG21	0.82	0.02	1
A	16	PRO	HD3	3.69	0.02	2
A	22	ILE	CA	61.6	0.2	1
A	15	LEU	HB2	1.65	0.02	2
A	11	ASN	HB3	2.67	0.02	2
A	1	ALA	HB1	1.55	0.02	9
A	4	ILE	N	120.4	0.1	1
A	9	LYS	HD3	1.62	0.02	2
A	6	HIS	HB2	3.06	0.02	2
A	25	ALA	CB	19.4	0.2	1
A	22	ILE	CD1	12.9	0.2	1
A	2	ARG	CB	31.0	0.2	1
A	7	ARG	CG	27.0	0.2	1
A	13	LYS	CD	29.1	0.2	1
A	23	THR	N	118.7	0.1	1
A	1	ALA	HA	4.13	0.02	9
A	22	ILE	CG1	27.2	0.2	1
A	23	THR	HG23	1.22	0.02	1
A	7	ARG	HD2	3.11	0.02	1
A	4	ILE	HD13	0.85	0.02	1
A	8	PHE	HE1	7.2	0.02	1
A	22	ILE	HG21	0.93	0.02	1
A	15	LEU	CD1	23.4	0.2	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	5	LYS	CE	42.3	0.2	1
A	12	ARG	HB2	1.77	0.02	2
A	12	ARG	HG3	1.53	0.02	1
A	3	GLY	C	173.8	0.2	1
A	7	ARG	C	175.7	0.2	1
A	23	THR	CA	61.9	0.2	1
A	11	ASN	HA	4.64	0.02	1
A	16	PRO	CG	27.3	0.2	1
A	7	ARG	HB3	1.68	0.02	1
A	21	GLN	HE21	7.55	0.02	2
A	8	PHE	CA	57.6	0.2	1
A	23	THR	HB	4.22	0.02	1
A	2	ARG	HD3	3.22	0.02	1
A	2	ARG	HA	4.4	0.02	1
A	10	TRP	CH2	125.0	0.2	1
A	13	LYS	HB2	1.8	0.02	2
A	10	TRP	CZ3	121.3	0.2	1
A	20	GLY	N	108.7	0.1	1
A	4	ILE	HG13	1.15	0.02	2
A	4	ILE	C	176.3	0.2	1
A	1	ALA	HB2	1.55	0.02	9
A	21	GLN	HB2	2.1	0.02	2
A	7	ARG	HG3	1.5	0.02	1
A	20	GLY	HA3	3.99	0.02	1
A	12	ARG	C	175.9	0.2	1
A	2	ARG	HG3	1.67	0.02	1
A	25	ALA	CA	52.7	0.2	1
A	3	GLY	H	8.56	0.02	1
A	6	HIS	N	120.9	0.1	1
A	14	VAL	CB	33.2	0.2	1
A	14	VAL	HG12	0.92	0.02	1
A	15	LEU	HD21	0.91	0.02	2
A	7	ARG	HB2	1.68	0.02	1
A	11	ASN	H	8.29	0.02	1
A	15	LEU	CA	52.8	0.2	1
A	12	ARG	CG	27.1	0.2	1
A	14	VAL	HG23	0.92	0.02	1
A	2	ARG	HB2	1.85	0.02	1
A	13	LYS	HE3	2.98	0.02	1
A	8	PHE	HB2	2.93	0.02	2
A	5	LYS	C	176.2	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	4	ILE	H	8.11	0.02	1
A	22	ILE	HG12	1.5	0.02	2
A	10	TRP	HZ2	7.43	0.02	1
A	9	LYS	CG	24.5	0.2	1
A	15	LEU	N	127.9	0.1	1
A	10	TRP	CB	29.9	0.2	1
A	8	PHE	CE1	132.0	0.2	1
A	6	HIS	CB	30.2	0.2	1
A	5	LYS	CA	56.2	0.2	1
A	21	GLN	HG2	2.37	0.02	1
A	6	HIS	HE1	8.24	0.02	1
A	22	ILE	C	176.5	0.2	1
A	4	ILE	CB	39.1	0.2	1
A	12	ARG	HD2	3.11	0.02	1
A	21	GLN	C	176.2	0.2	1
A	12	ARG	CD	43.4	0.2	1
A	15	LEU	HD13	0.97	0.02	9
A	9	LYS	HG2	1.28	0.02	2
A	25	ALA	HB3	1.4	0.02	1
A	5	LYS	HG3	1.35	0.02	2
A	13	LYS	CB	33.1	0.2	1
A	5	LYS	N	125.7	0.1	1
A	15	LEU	HB3	1.6	0.02	2
A	6	HIS	CD2	119.9	0.2	1
A	14	VAL	HB	2.04	0.02	1
A	13	LYS	HG3	1.4	0.02	1
A	13	LYS	CA	56.2	0.2	1
A	2	ARG	CA	56.4	0.2	1
A	15	LEU	CB	41.8	0.2	1
A	7	ARG	CD	43.4	0.2	1
A	13	LYS	CE	42.3	0.2	1
A	21	GLN	H	8.29	0.02	1
A	6	HIS	HD2	7.05	0.02	1
A	18	SER	HB3	3.9	0.02	2
A	8	PHE	CE2	132.0	0.2	1
A	12	ARG	N	121.2	0.1	1
A	22	ILE	CG2	17.8	0.2	1
A	23	THR	HG22	1.22	0.02	1
A	18	SER	HA	4.52	0.02	1
A	14	VAL	H	8.15	0.02	1
A	4	ILE	HD12	0.85	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	9	LYS	CD	29.2	0.2	1
A	22	ILE	HG22	0.93	0.02	1
A	22	ILE	N	122.6	0.1	1
A	5	LYS	HG2	1.42	0.02	3
A	4	ILE	CA	61.0	0.2	1
A	21	GLN	HE22	6.87	0.02	2
A	6	HIS	CE1	137.2	0.2	1
A	8	PHE	CB	39.9	0.2	1
A	5	LYS	HB2	1.73	0.02	1
A	7	ARG	HE	7.18	0.02	1
A	2	ARG	HD2	3.22	0.02	1
A	15	LEU	HA	4.68	0.02	1
A	25	ALA	C	177.7	0.2	1
A	22	ILE	HD11	0.88	0.02	1
A	13	LYS	HB3	1.72	0.02	2
A	4	ILE	HG23	0.82	0.02	1
A	21	GLN	CA	56.1	0.2	1
A	13	LYS	C	176.2	0.2	1
A	1	ALA	HB3	1.55	0.02	9
A	21	GLN	HB3	2.0	0.02	2
A	7	ARG	HG2	1.5	0.02	1
A	14	VAL	HA	4.13	0.02	1
A	16	PRO	HA	4.47	0.02	1
A	12	ARG	CB	30.9	0.2	1
A	2	ARG	CD	43.5	0.2	1
A	15	LEU	CG	27.4	0.2	1
A	17	SER	HB2	3.96	0.02	2
A	11	ASN	ND2	112.4	0.1	1
A	14	VAL	HG11	0.92	0.02	1
A	8	PHE	N	121.8	0.1	1
A	10	TRP	HD1	7.27	0.02	1
A	15	LEU	H	8.4	0.02	1
A	4	ILE	HD11	0.85	0.02	1
A	19	GLY	CA	45.6	0.2	1
A	8	PHE	HD1	7.18	0.02	1
A	14	VAL	C	175.7	0.2	1
A	9	LYS	CA	56.3	0.2	1
A	19	GLY	HA3	4.04	0.02	1
A	10	TRP	N	122.4	0.1	1
A	10	TRP	HE3	7.62	0.02	1
A	13	LYS	HE2	2.98	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	8	PHE	HB3	2.89	0.02	2
A	9	LYS	HE2	2.94	0.02	1
A	14	VAL	CA	62.1	0.2	1
A	5	LYS	HA	4.29	0.02	1
A	16	PRO	CA	63.5	0.2	1
A	18	SER	C	175.1	0.2	1
A	2	ARG	N	119.8	0.1	1
A	19	GLY	N	110.8	0.1	1
A	10	TRP	CA	57.1	0.2	1
A	13	LYS	HA	4.31	0.02	1
A	22	ILE	HD12	0.88	0.02	1
A	8	PHE	CD2	131.9	0.2	1
A	13	LYS	N	122.8	0.1	1
A	6	HIS	CA	55.6	0.2	1
A	5	LYS	CB	33.3	0.2	1
A	4	ILE	HA	4.17	0.02	1
A	18	SER	N	117.5	0.1	1
A	21	GLN	N	119.9	0.1	1
A	22	ILE	HB	1.91	0.02	1
A	25	ALA	H	8.36	0.02	1
A	13	LYS	HD2	1.65	0.02	1
A	2	ARG	H	8.23	0.02	1
A	7	ARG	HA	4.27	0.02	1
A	3	GLY	HA3	3.97	0.02	2
A	2	ARG	CG	27.1	0.2	1
A	25	ALA	HB2	1.4	0.02	1
A	4	ILE	CG2	17.4	0.2	1
A	11	ASN	HD22	6.88	0.02	2
A	2	ARG	C	176.6	0.2	1
A	7	ARG	NE	84.8	0.1	1
A	15	LEU	HD23	0.91	0.02	2
A	1	ALA	C	177.6	0.2	9
A	11	ASN	CA	52.9	0.2	1
A	13	LYS	HG2	1.4	0.02	1
A	1	ALA	CA	52.0	0.2	9
A	11	ASN	C	174.6	0.2	1
A	9	LYS	HB2	1.62	0.02	1
A	16	PRO	HG3	2.02	0.02	2
A	5	LYS	HD2	1.67	0.02	1
A	18	SER	CB	64.0	0.2	1
A	18	SER	HB2	3.96	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	16	PRO	CB	32.0	0.2	1
A	23	THR	HG21	1.22	0.02	1
A	5	LYS	HE3	2.97	0.02	1
A	15	LEU	HG	1.67	0.02	1
A	9	LYS	CE	42.2	0.2	1
A	22	ILE	HG23	0.93	0.02	1
A	22	ILE	H	8.35	0.02	1
A	9	LYS	HE3	2.94	0.02	1
A	10	TRP	HB3	3.21	0.02	2
A	14	VAL	N	122.2	0.1	1
A	18	SER	H	8.38	0.02	1
A	5	LYS	CG	24.7	0.2	1
A	8	PHE	HA	4.59	0.02	1
A	16	PRO	CD	50.5	0.2	1
A	5	LYS	HB3	1.73	0.02	1
A	9	LYS	HA	4.24	0.02	1
A	2	ARG	NE	84.8	0.1	1
A	4	ILE	HG22	0.82	0.02	1
A	16	PRO	HD2	3.86	0.02	2
A	11	ASN	HB2	2.7	0.02	2
A	6	HIS	H	8.42	0.02	1
A	12	ARG	HE	7.18	0.02	1
A	11	ASN	CB	39.0	0.2	1
A	20	GLY	C	174.1	0.2	1
A	12	ARG	CA	56.2	0.2	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
$^{13}\text{C}_\alpha$	131	-0.44 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	121	0.19 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	126	-0.33 ± 0.07	None needed (< 0.5 ppm)
^{15}N	127	-0.28 ± 0.25	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 93%, i.e. 1140 atoms were assigned a chemical shift out of a possible 1232. 3 out of 9 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	478/481 (99%)	192/192 (100%)	191/194 (98%)	95/95 (100%)
Sidechain	533/614 (87%)	336/363 (93%)	180/214 (84%)	17/37 (46%)
Aromatic	129/137 (94%)	67/71 (94%)	59/59 (100%)	3/7 (43%)
Overall	1140/1232 (93%)	595/626 (95%)	430/467 (92%)	115/139 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1241 atoms were assigned a chemical shift out of a possible 1353. 3 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	527/531 (99%)	212/212 (100%)	210/214 (98%)	105/105 (100%)
Sidechain	585/685 (85%)	368/404 (91%)	200/238 (84%)	17/43 (40%)
Aromatic	129/137 (94%)	67/71 (94%)	59/59 (100%)	3/7 (43%)
Overall	1241/1353 (92%)	647/687 (94%)	469/511 (92%)	125/155 (81%)

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	98	CYS	HB3	0.00	5.25 – 0.55	-6.2
1	A	98	CYS	H	4.73	11.75 – 5.05	-5.5
1	A	16	LYS	HB3	0.37	3.10 – 0.40	-5.1

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:

