



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 02:11 AM UTC

PDB ID : 8A6M / pdb_00008a6m
BMRB ID : 34738
Title : Phosphatidylserine-dependent synaptic vesicle membrane sculpting by synaptogyrin
Authors : Yu, T.K.; Eastep, G.N.; Flores, D.; Zweckstetter, M.
Deposited on : 2022-06-18

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

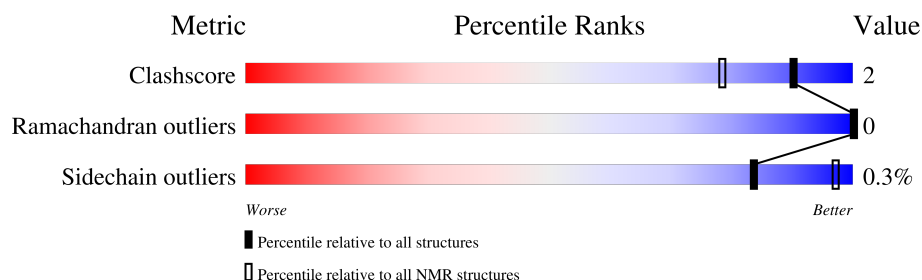
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	210	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:19-A:46, A:67-A:128, A:145-A:176 (122)	1.13	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 5, 8, 9
2	1, 3, 6, 10
Single-model clusters	4; 7

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2535 atoms, of which 1259 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Isoform 1B of Synaptogyrin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2535	841	1259	206	225	4	

There are 19 discrepancies between the modelled and reference sequences:

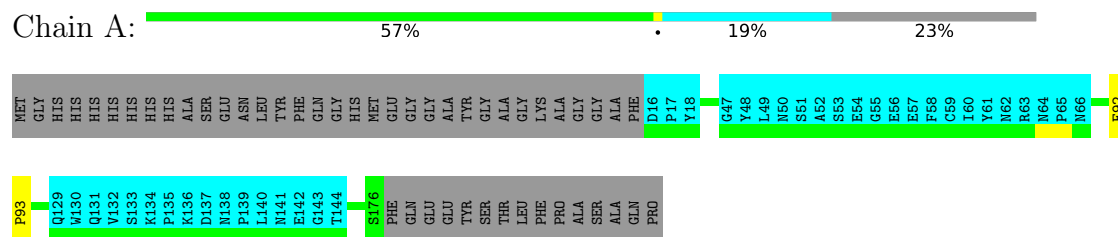
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O43759
A	-17	GLY	-	expression tag	UNP O43759
A	-16	HIS	-	expression tag	UNP O43759
A	-15	HIS	-	expression tag	UNP O43759
A	-14	HIS	-	expression tag	UNP O43759
A	-13	HIS	-	expression tag	UNP O43759
A	-12	HIS	-	expression tag	UNP O43759
A	-11	HIS	-	expression tag	UNP O43759
A	-10	HIS	-	expression tag	UNP O43759
A	-9	ALA	-	expression tag	UNP O43759
A	-8	SER	-	expression tag	UNP O43759
A	-7	GLU	-	expression tag	UNP O43759
A	-6	ASN	-	expression tag	UNP O43759
A	-5	LEU	-	expression tag	UNP O43759
A	-4	TYR	-	expression tag	UNP O43759
A	-3	PHE	-	expression tag	UNP O43759
A	-2	GLN	-	expression tag	UNP O43759
A	-1	GLY	-	expression tag	UNP O43759
A	0	HIS	-	expression tag	UNP O43759

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Isoform 1B of Synaptogyrin-1

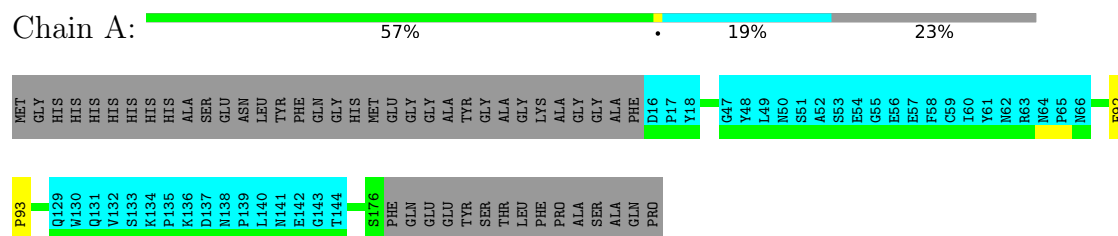


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

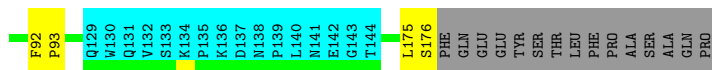
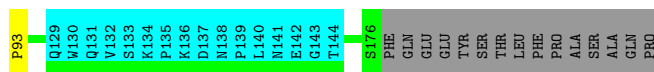
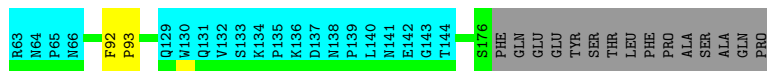
- Molecule 1: Isoform 1B of Synaptogyrin-1

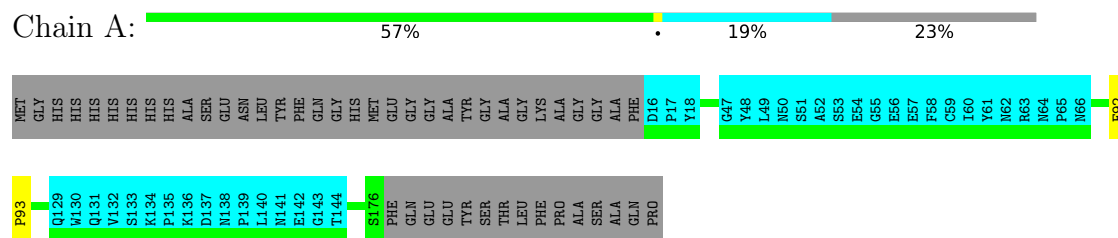


4.2.2 Score per residue for model 2

- Molecule 1: Isoform 1B of Synaptogyrin-1

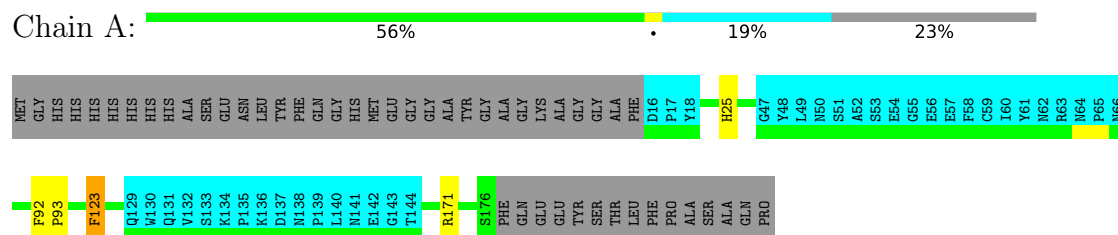






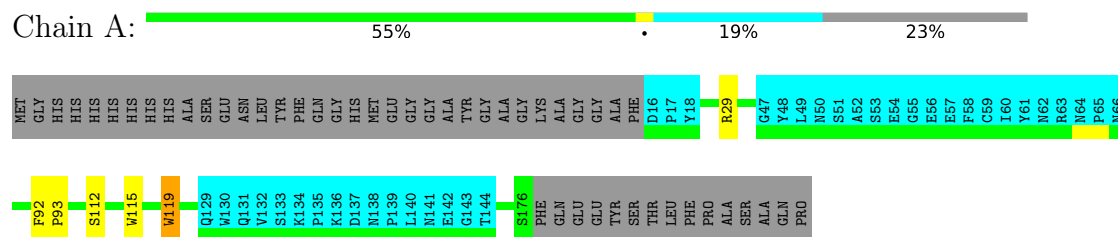
4.2.7 Score per residue for model 7

- Molecule 1: Isoform 1B of Synaptogyrin-1



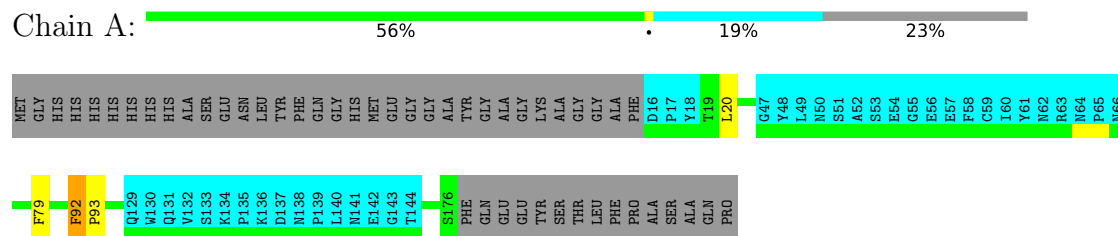
4.2.8 Score per residue for model 8

- Molecule 1: Isoform 1B of Synaptogyrin-1



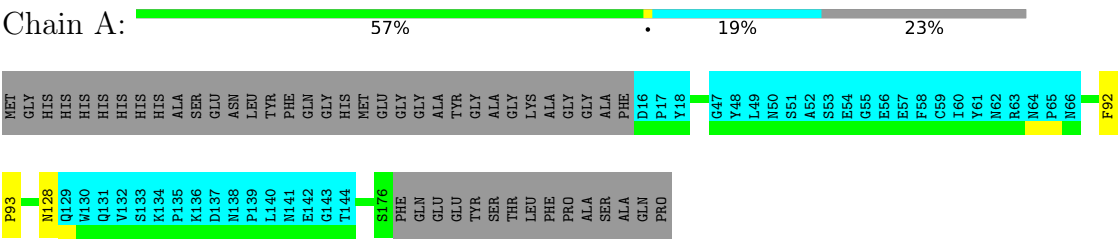
4.2.9 Score per residue for model 9

- Molecule 1: Isoform 1B of Synaptogyrin-1



4.2.10 Score per residue for model 10

- Molecule 1: Isoform 1B of Synaptogyrin-1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 470 calculated structures, 10 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
CS-ROSETTA	structure calculation	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1965
Number of shifts mapped to atoms	1739
Number of unparsed shifts	0
Number of shifts with mapping errors	226
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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	961	979	978	3±2
All	All	9610	9790	9780	32

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:PHE:CD1	1:A:123:PHE:C	0.62	2.78	7	1
1:A:20:LEU:HD23	1:A:20:LEU:C	0.57	2.24	9	2
1:A:92:PHE:N	1:A:93:PRO:CD	0.56	2.67	10	10
1:A:119:TRP:CE3	1:A:119:TRP:HA	0.51	2.41	8	1
1:A:92:PHE:N	1:A:93:PRO:HD2	0.49	2.23	8	8
1:A:25:HIS:HD1	1:A:171:ARG:HH11	0.48	1.51	7	1
1:A:79:PHE:C	1:A:79:PHE:CD1	0.48	2.91	5	2
1:A:29:ARG:NH2	1:A:112:SER:OG	0.48	2.47	8	1
1:A:175:LEU:O	1:A:176:SER:O	0.47	2.32	5	1
1:A:92:PHE:HB3	1:A:93:PRO:HD3	0.46	1.86	3	1
1:A:123:PHE:CD1	1:A:123:PHE:O	0.45	2.70	7	1
1:A:115:TRP:CE3	1:A:115:TRP:HA	0.44	2.48	8	1
1:A:25:HIS:HD1	1:A:171:ARG:HD3	0.42	1.74	7	1
1:A:25:HIS:HD1	1:A:29:ARG:HH12	0.40	1.59	2	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	121/210 (58%)	120±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	1210/2100 (58%)	1197 (99%)	13 (1%)	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	101/170 (59%)	101±0 (100±0%)	0±0 (0±0%)	84	97
All	All	1010/1700 (59%)	1007 (100%)	3 (0%)	84	97

All 3 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	123	PHE	1
1	A	119	TRP	1
1	A	92	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 oligosaccharides 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 78% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1965
Number of shifts mapped to atoms	1739
Number of unparsed shifts	0
Number of shifts with mapping errors	226
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- No matching atom found in the structure. All 226 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	GLU	H	8.179	0.03	1
1	A	2	GLU	HA	4.173	0.03	1
1	A	2	GLU	C	177.036	0.03	1
1	A	2	GLU	CA	56.429	0.03	1
1	A	2	GLU	N	125.92	0.03	1
1	A	3	GLY	H	8.403	0.03	1
1	A	3	GLY	C	174.716	0.03	1
1	A	3	GLY	CA	45.204	0.03	1
1	A	3	GLY	N	110.384	0.03	1
1	A	4	GLY	H	8.168	0.03	1
1	A	4	GLY	C	174.057	0.03	1
1	A	4	GLY	CA	44.971	0.03	1
1	A	4	GLY	N	108.695	0.03	1
1	A	5	ALA	H	8.112	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	ALA	C	175.446	0.03	1
1	A	5	ALA	CA	52.154	0.03	1
1	A	5	ALA	CB	18.597	0.03	1
1	A	5	ALA	N	123.901	0.03	1
1	A	6	TYR	H	8.2	0.03	1
1	A	6	TYR	C	176.618	0.03	1
1	A	6	TYR	CA	58.093	0.03	1
1	A	6	TYR	CB	38.781	0.03	1
1	A	6	TYR	N	118.905	0.03	1
1	A	7	GLY	H	8.13	0.03	1
1	A	7	GLY	C	174.026	0.03	1
1	A	7	GLY	CA	45.132	0.03	1
1	A	7	GLY	N	110.575	0.03	1
1	A	8	ALA	H	8.058	0.03	1
1	A	8	ALA	C	178.291	0.03	1
1	A	8	ALA	CA	52.292	0.03	1
1	A	8	ALA	CB	18.612	0.03	1
1	A	8	ALA	N	123.923	0.03	1
1	A	9	GLY	H	8.281	0.03	1
1	A	9	GLY	HA2	3.998	0.03	1
1	A	9	GLY	C	174.307	0.03	1
1	A	9	GLY	CA	45.118	0.03	1
1	A	9	GLY	N	108.61	0.03	1
1	A	10	LYS	H	8.037	0.03	1
1	A	10	LYS	HA	4.194	0.03	1
1	A	10	LYS	HB2	1.821	0.03	1
1	A	10	LYS	C	176.567	0.03	1
1	A	10	LYS	CA	55.762	0.03	1
1	A	10	LYS	CB	32.324	0.03	1
1	A	10	LYS	N	120.955	0.03	1
1	A	11	ALA	H	8.287	0.03	1
1	A	11	ALA	HA	4.197	0.03	1
1	A	11	ALA	HB1	1.246	0.03	1
1	A	11	ALA	HB2	1.246	0.03	1
1	A	11	ALA	HB3	1.246	0.03	1
1	A	11	ALA	C	178.396	0.03	1
1	A	11	ALA	CA	52.281	0.03	1
1	A	11	ALA	CB	18.796	0.03	1
1	A	11	ALA	N	125.379	0.03	1
1	A	12	GLY	H	8.326	0.03	1
1	A	12	GLY	C	174.759	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	GLY	CA	45.157	0.03	1
1	A	12	GLY	N	108.248	0.03	1
1	A	13	GLY	H	8.162	0.03	1
1	A	13	GLY	HA2	3.976	0.03	1
1	A	13	GLY	C	173.891	0.03	1
1	A	13	GLY	CA	44.964	0.03	1
1	A	13	GLY	N	108.922	0.03	1
1	A	14	ALA	H	8.072	0.03	1
1	A	14	ALA	HA	4.383	0.03	1
1	A	14	ALA	HB1	1.367	0.03	1
1	A	14	ALA	HB2	1.367	0.03	1
1	A	14	ALA	HB3	1.367	0.03	1
1	A	14	ALA	C	177.264	0.03	1
1	A	14	ALA	CA	52.075	0.03	1
1	A	14	ALA	CB	19.175	0.03	1
1	A	14	ALA	N	123.586	0.03	1
1	A	15	PHE	H	8.234	0.03	1
1	A	15	PHE	HA	4.614	0.03	1
1	A	15	PHE	HB2	3.177	0.03	1
1	A	15	PHE	HB3	3.049	0.03	1
1	A	15	PHE	HD1	7.193	0.03	1
1	A	15	PHE	HE1	7.215	0.03	1
1	A	15	PHE	HZ	6.927	0.03	1
1	A	15	PHE	C	174.11	0.03	1
1	A	15	PHE	CA	57.303	0.03	1
1	A	15	PHE	CB	39.001	0.03	1
1	A	15	PHE	CD1	133.374	0.03	1
1	A	15	PHE	CE1	133.072	0.03	1
1	A	15	PHE	CZ	133.351	0.03	1
1	A	15	PHE	N	120.053	0.03	1
1	A	177	PHE	H	8.296	0.03	1
1	A	177	PHE	HA	4.615	0.03	1
1	A	177	PHE	HB2	3.136	0.03	1
1	A	177	PHE	HB3	3.121	0.03	1
1	A	177	PHE	HD1	7.206	0.03	1
1	A	177	PHE	HE1	7.298	0.03	1
1	A	177	PHE	HZ	6.938	0.03	1
1	A	177	PHE	C	176.953	0.03	1
1	A	177	PHE	CA	57.959	0.03	1
1	A	177	PHE	CB	40.866	0.03	1
1	A	177	PHE	N	117.679	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	178	GLN	H	8.112	0.03	1
1	A	178	GLN	HA	4.533	0.03	1
1	A	178	GLN	HB2	2.043	0.03	1
1	A	178	GLN	HB3	2.028	0.03	1
1	A	178	GLN	HE21	7.035	0.03	1
1	A	178	GLN	HE22	6.815	0.03	1
1	A	178	GLN	HG2	2.147	0.03	1
1	A	178	GLN	HG3	2.122	0.03	1
1	A	178	GLN	C	176.625	0.03	1
1	A	178	GLN	CA	56.184	0.03	1
1	A	178	GLN	CB	29.6	0.03	1
1	A	178	GLN	N	120.686	0.03	1
1	A	179	GLU	H	8.134	0.03	1
1	A	179	GLU	HA	4.48	0.03	1
1	A	179	GLU	HB2	2.064	0.03	1
1	A	179	GLU	HB3	2.045	0.03	1
1	A	179	GLU	HG2	2.389	0.03	1
1	A	179	GLU	HG3	2.37	0.03	1
1	A	179	GLU	C	177.163	0.03	1
1	A	179	GLU	CA	56.449	0.03	1
1	A	179	GLU	CB	29.438	0.03	1
1	A	179	GLU	N	120.687	0.03	1
1	A	180	GLU	H	8.141	0.03	1
1	A	180	GLU	HA	4.723	0.03	1
1	A	180	GLU	HB2	2.064	0.03	1
1	A	180	GLU	HB3	2.043	0.03	1
1	A	180	GLU	HG2	2.239	0.03	1
1	A	180	GLU	HG3	2.221	0.03	1
1	A	180	GLU	C	177.229	0.03	1
1	A	180	GLU	CA	53.159	0.03	1
1	A	180	GLU	CB	28.529	0.03	1
1	A	180	GLU	N	121.124	0.03	1
1	A	181	TYR	H	8.134	0.03	1
1	A	181	TYR	HA	4.463	0.03	1
1	A	181	TYR	HB2	2.984	0.03	1
1	A	181	TYR	HB3	2.959	0.03	1
1	A	181	TYR	HD1	7.122	0.03	1
1	A	181	TYR	HE1	6.379	0.03	1
1	A	181	TYR	HH	8.471	0.03	1
1	A	181	TYR	C	176.427	0.03	1
1	A	181	TYR	CA	58.658	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	181	TYR	CB	37.772	0.03	1
1	A	181	TYR	N	119.999	0.03	1
1	A	182	SER	H	8.048	0.03	1
1	A	182	SER	HA	4.415	0.03	1
1	A	182	SER	HB2	3.966	0.03	1
1	A	182	SER	HB3	3.944	0.03	1
1	A	182	SER	HG	5.447	0.03	1
1	A	182	SER	C	175.094	0.03	1
1	A	182	SER	CA	59.045	0.03	1
1	A	182	SER	CB	62.832	0.03	1
1	A	182	SER	N	115.599	0.03	1
1	A	183	THR	H	7.88	0.03	1
1	A	183	THR	HA	4.532	0.03	1
1	A	183	THR	HB	3.99	0.03	1
1	A	183	THR	HG1	5.218	0.03	1
1	A	183	THR	HG21	1.32	0.03	1
1	A	183	THR	HG22	1.32	0.03	1
1	A	183	THR	HG23	1.32	0.03	1
1	A	183	THR	C	174.608	0.03	1
1	A	183	THR	CA	62.295	0.03	1
1	A	183	THR	CB	66.226	0.03	1
1	A	183	THR	N	115.003	0.03	1
1	A	184	LEU	H	7.795	0.03	1
1	A	184	LEU	HA	4.427	0.03	1
1	A	184	LEU	HB2	1.68	0.03	1
1	A	184	LEU	HB3	1.533	0.03	1
1	A	184	LEU	HD11	0.967	0.03	1
1	A	184	LEU	HD12	0.967	0.03	1
1	A	184	LEU	HD13	0.967	0.03	1
1	A	184	LEU	HD21	0.943	0.03	1
1	A	184	LEU	HD22	0.943	0.03	1
1	A	184	LEU	HD23	0.943	0.03	1
1	A	184	LEU	HG	1.499	0.03	1
1	A	184	LEU	C	176.404	0.03	1
1	A	184	LEU	CA	55.239	0.03	1
1	A	184	LEU	CB	41.783	0.03	1
1	A	184	LEU	N	123.063	0.03	1
1	A	185	PHE	H	7.873	0.03	1
1	A	185	PHE	HA	4.994	0.03	1
1	A	185	PHE	HB2	2.934	0.03	1
1	A	185	PHE	HB3	3.001	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	185	PHE	HD1	7.221	0.03	1
1	A	185	PHE	HE1	7.342	0.03	1
1	A	185	PHE	HZ	6.637	0.03	1
1	A	185	PHE	C	175.139	0.03	1
1	A	185	PHE	CA	55.148	0.03	1
1	A	185	PHE	CB	38.349	0.03	1
1	A	185	PHE	N	119.138	0.03	1
1	A	186	PRO	C	177.063	0.03	1
1	A	186	PRO	CA	63.035	0.03	1
1	A	186	PRO	CB	31.297	0.03	1
1	A	187	ALA	H	8.328	0.03	1
1	A	187	ALA	HA	4.378	0.03	1
1	A	187	ALA	HB1	1.336	0.03	1
1	A	187	ALA	HB2	1.336	0.03	1
1	A	187	ALA	HB3	1.336	0.03	1
1	A	187	ALA	C	178.076	0.03	1
1	A	187	ALA	CA	52.344	0.03	1
1	A	187	ALA	CB	18.719	0.03	1
1	A	187	ALA	N	124.353	0.03	1
1	A	188	SER	H	8.135	0.03	1
1	A	188	SER	HA	4.484	0.03	1
1	A	188	SER	HB2	3.944	0.03	1
1	A	188	SER	HB3	3.922	0.03	1
1	A	188	SER	HG	5.444	0.03	1
1	A	188	SER	C	174.213	0.03	1
1	A	188	SER	CA	57.753	0.03	1
1	A	188	SER	CB	62.738	0.03	1
1	A	188	SER	N	114.599	0.03	1
1	A	189	ALA	H	8.176	0.03	1
1	A	189	ALA	HA	4.119	0.03	1
1	A	189	ALA	HB1	1.374	0.03	1
1	A	189	ALA	HB2	1.374	0.03	1
1	A	189	ALA	HB3	1.374	0.03	1
1	A	189	ALA	C	176.6	0.03	1
1	A	189	ALA	CA	52.08	0.03	1
1	A	189	ALA	CB	18.702	0.03	1
1	A	189	ALA	N	125.696	0.03	1
1	A	190	GLN	H	7.875	0.03	1
1	A	190	GLN	HA	4.623	0.03	1
1	A	190	GLN	HB2	1.977	0.03	1
1	A	190	GLN	HB3	1.966	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	190	GLN	HE21	7.424	0.03	1
1	A	190	GLN	HE22	7.18	0.03	1
1	A	190	GLN	HG2	2.403	0.03	1
1	A	190	GLN	HG3	2.382	0.03	1
1	A	190	GLN	CA	53.007	0.03	1
1	A	190	GLN	CB	29.979	0.03	1
1	A	190	GLN	N	119.14	0.03	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	188	-0.73 ± 0.13	Should be checked
$^{13}\text{C}_\beta$	172	1.11 ± 0.09	Should be checked
$^{13}\text{C}'$	185	-0.48 ± 0.12	None needed (< 0.5 ppm)
^{15}N	182	0.35 ± 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 78%, i.e. 1328 atoms were assigned a chemical shift out of a possible 1711. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	604/611 (99%)	244/247 (99%)	240/244 (98%)	120/120 (100%)
Sidechain	671/880 (76%)	545/589 (93%)	126/265 (48%)	0/26 (0%)
Aromatic	53/220 (24%)	53/109 (49%)	0/107 (0%)	0/4 (0%)
Overall	1328/1711 (78%)	842/945 (89%)	366/616 (59%)	120/150 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1693 atoms were assigned a chemical shift out of a possible 2214. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	788/801 (98%)	315/324 (97%)	318/322 (99%)	155/155 (100%)
Sidechain	843/1144 (74%)	679/755 (90%)	164/350 (47%)	0/39 (0%)
Aromatic	62/269 (23%)	62/132 (47%)	0/132 (0%)	0/5 (0%)
Overall	1693/2214 (76%)	1056/1211 (87%)	482/804 (60%)	155/199 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	144	THR	HG1	5.82	0.08 – 2.19	22.2
1	A	81	THR	HG1	5.40	0.08 – 2.19	20.2
1	A	164	THR	HG1	5.39	0.08 – 2.19	20.2
1	A	26	THR	HG1	5.39	0.08 – 2.19	20.1
1	A	183	THR	HG1	5.22	0.08 – 2.19	19.3
1	A	19	THR	HG1	4.99	0.08 – 2.19	18.2

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

