



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:46 PM UTC

PDB ID : 1GO0 / pdb_00001go0
BMRB ID : 5485
Title : NMR Structure of Ribosomal Protein L30e from *Thermococcus celer*
Authors : Chan, S.-H.; Bycroft, M.; Freund, S.M.V.; Wong, K.-B.
Deposited on : 2001-10-15

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

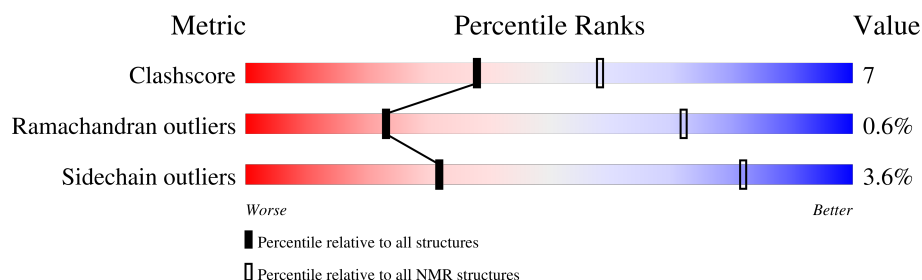
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	102	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:3-A:97 (95)	0.85	4

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 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1328 atoms, of which 555 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L30E.

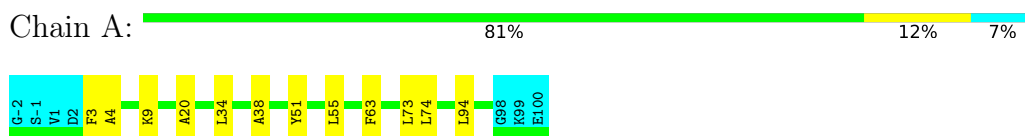
Mol	Chain	Residues	Atoms						Trace
1	A	102	Total	C	H	N	O	S	0
			1328	490	555	135	146	2	

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: 50S RIBOSOMAL PROTEIN L30E

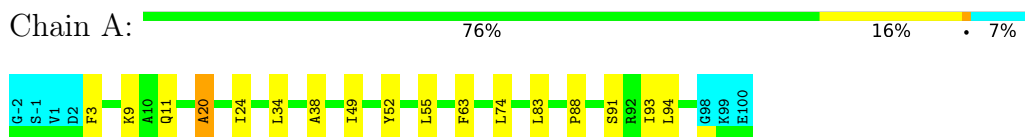


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

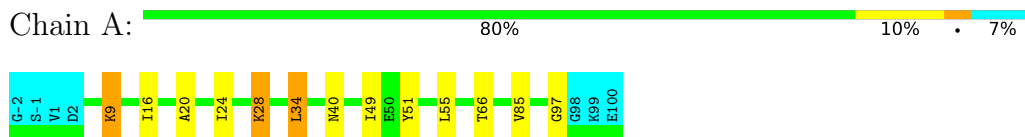
4.2.1 Score per residue for model 1

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E



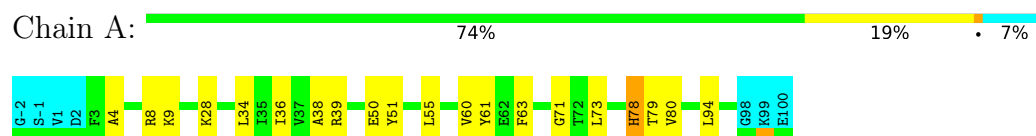
4.2.2 Score per residue for model 2

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E



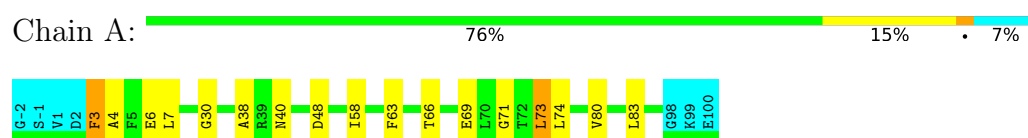
4.2.3 Score per residue for model 3

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E



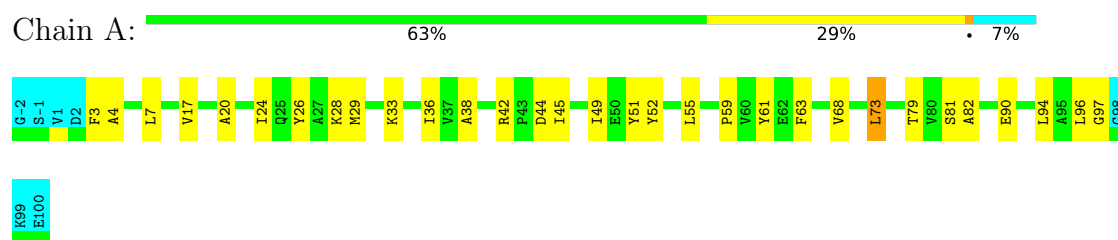
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E



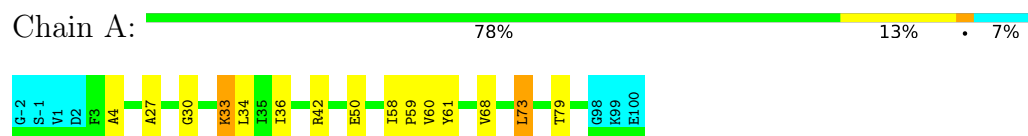
4.2.5 Score per residue for model 5

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E



4.2.6 Score per residue for model 6

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E



4.2.7 Score per residue for model 7

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E





4.2.8 Score per residue for model 8

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E

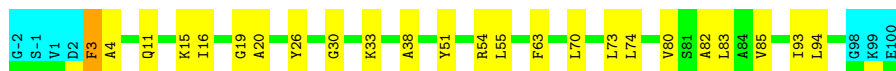
Chain A: 72% 21% 7%



4.2.9 Score per residue for model 9

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E

Chain A: 70% 23% 7%



4.2.10 Score per residue for model 10

- Molecule 1: 50S RIBOSOMAL PROTEIN L30E

Chain A: 68% 25% 7%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING USING AMBIGUOUS NOES*.

Of the 400 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
CNS	refinement	1.1
NMRPipe	structure solution	
NMRView	structure solution	
CNS	structure solution	
ARIA	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1096
Number of shifts mapped to atoms	859
Number of unparsed shifts	0
Number of shifts with mapping errors	237
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.4
All	All	0	2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	52	TYR	Sidechain	2

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	725	526	753	11±3
All	All	7250	5260	7530	109

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LYS:HA	1:A:9:LYS:HE3	0.82	1.49	8	1
1:A:38:ALA:HA	1:A:63:PHE:HB3	0.75	1.58	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:GLY:HA2	1:A:58:ILE:HD11	0.74	1.58	6	4
1:A:16:ILE:HG12	1:A:85:VAL:HG23	0.74	1.57	9	1
1:A:4:ALA:HA	1:A:73:LEU:HD11	0.70	1.61	5	4
1:A:17:VAL:HG12	1:A:84:ALA:HB3	0.70	1.64	10	1
1:A:20:ALA:HA	1:A:82:ALA:HB3	0.68	1.64	9	2
1:A:7:LEU:HD12	1:A:73:LEU:HD12	0.68	1.66	4	1
1:A:34:LEU:HD21	1:A:97:GLY:HA3	0.67	1.65	2	1
1:A:9:LYS:HD3	1:A:90:GLU:HG3	0.67	1.65	7	1
1:A:24:ILE:HG12	1:A:49:ILE:HG12	0.64	1.69	2	2
1:A:71:GLY:HA2	1:A:80:VAL:HG23	0.62	1.72	3	2
1:A:40:ASN:HB2	1:A:66:THR:HA	0.62	1.70	2	2
1:A:16:ILE:HG13	1:A:85:VAL:HA	0.61	1.73	10	1
1:A:66:THR:HG22	1:A:69:GLU:HG2	0.58	1.74	4	1
1:A:7:LEU:HB3	1:A:74:LEU:HD12	0.58	1.76	7	1
1:A:4:ALA:HA	1:A:73:LEU:HD21	0.57	1.75	10	2
1:A:51:TYR:O	1:A:55:LEU:HG	0.55	2.02	3	7
1:A:88:PRO:HG2	1:A:94:LEU:HD23	0.54	1.76	1	1
1:A:26:TYR:HA	1:A:30:GLY:HA3	0.54	1.78	9	1
1:A:22:LYS:HE2	1:A:22:LYS:HA	0.52	1.81	10	1
1:A:9:LYS:HE3	1:A:91:SER:HA	0.52	1.79	1	1
1:A:34:LEU:HD22	1:A:94:LEU:HA	0.52	1.81	8	3
1:A:68:VAL:HA	1:A:79:THR:HG22	0.51	1.83	5	1
1:A:54:ARG:HA	1:A:54:ARG:NE	0.51	2.20	9	1
1:A:70:LEU:HD21	1:A:83:LEU:HD22	0.51	1.82	9	1
1:A:96:LEU:H	1:A:96:LEU:HD23	0.50	1.66	8	1
1:A:94:LEU:HA	1:A:97:GLY:O	0.49	2.06	5	1
1:A:20:ALA:HB2	1:A:81:SER:HB3	0.49	1.84	5	1
1:A:74:LEU:HD12	1:A:80:VAL:HG11	0.48	1.84	8	1
1:A:39:ARG:HG3	1:A:63:PHE:O	0.48	2.08	3	1
1:A:74:LEU:HD21	1:A:83:LEU:HD22	0.48	1.86	1	1
1:A:9:LYS:HA	1:A:9:LYS:HE2	0.48	1.86	2	1
1:A:3:PHE:CD1	1:A:93:ILE:HD11	0.47	2.44	1	1
1:A:20:ALA:O	1:A:24:ILE:HG13	0.47	2.09	1	2
1:A:50:GLU:HG2	1:A:60:VAL:HG11	0.47	1.87	8	3
1:A:38:ALA:HA	1:A:63:PHE:CB	0.47	2.39	7	1
1:A:50:GLU:O	1:A:54:ARG:HG2	0.47	2.10	8	1
1:A:42:ARG:HB3	1:A:44:ASP:OD1	0.46	2.11	5	1
1:A:26:TYR:HA	1:A:29:MET:HG2	0.46	1.86	5	1
1:A:33:LYS:O	1:A:59:PRO:HD2	0.46	2.10	6	2
1:A:68:VAL:HG22	1:A:79:THR:HG22	0.46	1.87	6	1
1:A:14:GLY:HA3	1:A:87:ASP:O	0.46	2.11	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HG12	1:A:61:TYR:HB3	0.45	1.87	3	3
1:A:74:LEU:HD13	1:A:83:LEU:HD22	0.45	1.89	4	1
1:A:18:MET:HB3	1:A:74:LEU:HD23	0.45	1.89	10	1
1:A:78:HIS:H	1:A:78:HIS:CD2	0.44	2.30	3	1
1:A:16:ILE:HG12	1:A:85:VAL:HG22	0.44	1.88	2	1
1:A:76:ARG:HD3	1:A:77:PRO:HD2	0.44	1.90	7	1
1:A:33:LYS:HG3	1:A:94:LEU:HD21	0.44	1.89	9	1
1:A:3:PHE:HD2	1:A:96:LEU:HD11	0.44	1.72	5	2
1:A:28:LYS:HG2	1:A:52:TYR:CD2	0.44	2.48	5	1
1:A:11:GLN:NE2	1:A:16:ILE:HB	0.43	2.27	9	1
1:A:20:ALA:HB1	1:A:45:ILE:HG21	0.43	1.91	5	1
1:A:63:PHE:CE2	1:A:70:LEU:HB2	0.43	2.49	9	1
1:A:3:PHE:HB2	1:A:6:GLU:HB2	0.43	1.90	4	1
1:A:5:PHE:HA	1:A:8:ARG:HG2	0.43	1.91	10	1
1:A:24:ILE:HG12	1:A:49:ILE:HG13	0.42	1.92	5	1
1:A:74:LEU:HD12	1:A:80:VAL:HG21	0.42	1.91	9	1
1:A:4:ALA:O	1:A:8:ARG:HG3	0.42	2.15	3	1
1:A:7:LEU:HD23	1:A:73:LEU:HD12	0.42	1.92	5	1
1:A:71:GLY:HA3	1:A:78:HIS:O	0.42	2.14	7	1
1:A:36:ILE:HA	1:A:61:TYR:O	0.42	2.14	5	1
1:A:93:ILE:HG23	1:A:94:LEU:HD12	0.42	1.91	9	1
1:A:52:TYR:O	1:A:55:LEU:HG	0.41	2.15	1	1
1:A:24:ILE:O	1:A:28:LYS:HG3	0.41	2.16	2	1
1:A:17:VAL:HG21	1:A:26:TYR:CZ	0.41	2.50	5	1
1:A:3:PHE:CD2	1:A:96:LEU:HD22	0.41	2.50	10	1
1:A:42:ARG:HA	1:A:42:ARG:NE	0.41	2.31	6	1
1:A:88:PRO:HB3	1:A:94:LEU:HD13	0.41	1.93	7	1
1:A:92:ARG:NE	1:A:92:ARG:HA	0.41	2.30	7	1
1:A:9:LYS:O	1:A:13:THR:HG22	0.40	2.16	7	1
1:A:24:ILE:HG22	1:A:28:LYS:HE3	0.40	1.94	5	1
1:A:34:LEU:HD12	1:A:59:PRO:O	0.40	2.17	6	1
1:A:34:LEU:HD11	1:A:97:GLY:HA3	0.40	1.93	10	1
1:A:27:ALA:HA	1:A:58:ILE:HD12	0.40	1.92	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	95/102 (93%)	86±2 (90±2%)	9±2 (9±2%)	1±1 (1±1%)	23	72
All	All	950/1020 (93%)	856 (90%)	88 (9%)	6 (1%)	23	72

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	20	ALA	2
1	A	3	PHE	2
1	A	79	THR	1
1	A	19	GLY	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	74/79 (94%)	71±1 (96±1%)	3±1 (4±1%)	32	82
All	All	740/790 (94%)	713 (96%)	27 (4%)	32	82

All 16 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	9	LYS	3
1	A	48	ASP	3
1	A	73	LEU	3
1	A	28	LYS	2
1	A	34	LEU	2
1	A	3	PHE	2
1	A	47	GLU	2
1	A	91	SER	2
1	A	11	GLN	1
1	A	78	HIS	1
1	A	90	GLU	1
1	A	33	LYS	1
1	A	8	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	93	ILE	1
1	A	15	LYS	1
1	A	67	SER	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 80% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_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	1096
Number of shifts mapped to atoms	859
Number of unparsed shifts	0
Number of shifts with mapping errors	237
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 237 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ASP	HB2	2.995	0.02	2
1	A	2	ASP	HB3	2.518	0.02	2
1	A	3	PHE	HB2	3.323	0.02	2
1	A	3	PHE	HB3	3.154	0.02	2
1	A	5	PHE	HB2	3.185	0.02	2
1	A	5	PHE	HB3	2.997	0.02	2
1	A	6	GLU	HB2	1.699	0.02	2
1	A	6	GLU	HB3	1.512	0.02	2
1	A	6	GLU	HG2	2.864	0.02	2
1	A	6	GLU	HG3	2.864	0.02	2
1	A	7	LEU	HB2	1.288	0.02	2
1	A	7	LEU	HB3	0.541	0.02	2
1	A	8	ARG	HB2	1.742	0.02	2
1	A	8	ARG	HB3	1.742	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	ARG	HD2	3.176	0.02	1
1	A	8	ARG	HD3	3.176	0.02	1
1	A	8	ARG	HG2	1.549	0.02	2
1	A	8	ARG	HG3	1.63	0.02	2
1	A	9	LYS	HB2	1.517	0.02	2
1	A	9	LYS	HB3	1.517	0.02	2
1	A	9	LYS	HD2	1.206	0.02	2
1	A	9	LYS	HD3	1.206	0.02	2
1	A	9	LYS	HE2	3.039	0.02	2
1	A	9	LYS	HE3	3.039	0.02	2
1	A	9	LYS	HG2	1.152	0.02	2
1	A	9	LYS	HG3	1.152	0.02	2
1	A	11	GLN	HB2	2.223	0.02	2
1	A	11	GLN	HB3	1.746	0.02	2
1	A	11	GLN	HG2	2.138	0.02	2
1	A	11	GLN	HG3	2.283	0.02	2
1	A	12	ASP	HB2	2.64	0.02	1
1	A	12	ASP	HB3	2.64	0.02	1
1	A	15	LYS	HB2	1.749	0.02	2
1	A	15	LYS	HB3	1.59	0.02	2
1	A	15	LYS	HE2	2.893	0.02	1
1	A	15	LYS	HE3	2.893	0.02	1
1	A	15	LYS	HG2	1.336	0.02	2
1	A	15	LYS	HG3	1.09	0.02	2
1	A	16	ILE	HG12	1.304	0.02	2
1	A	16	ILE	HG13	1.001	0.02	2
1	A	18	MET	HB2	2.167	0.02	2
1	A	18	MET	HB3	1.968	0.02	2
1	A	18	MET	HG2	2.448	0.02	2
1	A	18	MET	HG3	2.404	0.02	2
1	A	21	ARG	HB2	1.798	0.02	2
1	A	21	ARG	HB3	1.921	0.02	2
1	A	21	ARG	HG2	1.601	0.02	2
1	A	21	ARG	HG3	1.75	0.02	2
1	A	22	LYS	HB2	1.576	0.02	1
1	A	22	LYS	HB3	1.576	0.02	1
1	A	22	LYS	HD2	1.908	0.02	1
1	A	22	LYS	HD3	1.908	0.02	1
1	A	22	LYS	HE2	3.179	0.02	1
1	A	22	LYS	HE3	3.179	0.02	1
1	A	22	LYS	HG2	1.695	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	LYS	HG3	1.55	0.02	2
1	A	23	SER	HB2	3.343	0.02	2
1	A	23	SER	HB3	3.343	0.02	2
1	A	24	ILE	HG12	0.847	0.02	2
1	A	24	ILE	HG13	1.834	0.02	4
1	A	25	GLN	HB2	2.073	0.02	1
1	A	25	GLN	HB3	2.073	0.02	1
1	A	25	GLN	HG2	2.139	0.02	2
1	A	25	GLN	HG3	2.295	0.02	2
1	A	26	TYR	HB2	2.773	0.02	2
1	A	26	TYR	HB3	2.419	0.02	2
1	A	28	LYS	HB2	1.511	0.02	2
1	A	28	LYS	HB3	1.297	0.02	2
1	A	28	LYS	HD2	1.122	0.02	2
1	A	28	LYS	HD3	1.192	0.02	2
1	A	28	LYS	HE2	2.374	0.02	1
1	A	28	LYS	HE3	2.374	0.02	1
1	A	28	LYS	HG2	0.986	0.02	2
1	A	28	LYS	HG3	0.605	0.02	2
1	A	29	MET	HB2	1.997	0.02	1
1	A	29	MET	HB3	1.997	0.02	1
1	A	29	MET	HG2	2.495	0.02	1
1	A	29	MET	HG3	2.495	0.02	1
1	A	33	LYS	HB2	1.923	0.02	2
1	A	33	LYS	HB3	1.26	0.02	2
1	A	33	LYS	HD2	1.847	0.02	2
1	A	33	LYS	HD3	1.711	0.02	2
1	A	33	LYS	HE2	2.982	0.02	1
1	A	33	LYS	HE3	2.982	0.02	1
1	A	33	LYS	HG2	1.468	0.02	1
1	A	33	LYS	HG3	1.468	0.02	1
1	A	34	LEU	HB2	1.687	0.02	2
1	A	34	LEU	HB3	1.032	0.02	2
1	A	35	ILE	HG12	1.364	0.02	2
1	A	35	ILE	HG13	1.067	0.02	2
1	A	36	ILE	HG12	1.232	0.02	1
1	A	36	ILE	HG13	1.232	0.02	1
1	A	39	ARG	HB2	1.986	0.02	2
1	A	39	ARG	HB3	1.529	0.02	2
1	A	39	ARG	HD2	3.037	0.02	1
1	A	39	ARG	HD3	3.037	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	39	ARG	HG2	1.529	0.02	1
1	A	39	ARG	HG3	1.529	0.02	1
1	A	40	ASN	HB2	3.188	0.02	2
1	A	40	ASN	HB3	2.554	0.02	2
1	A	42	ARG	HB2	2.049	0.02	2
1	A	42	ARG	HB3	1.762	0.02	2
1	A	42	ARG	HD2	3.316	0.02	1
1	A	42	ARG	HD3	3.316	0.02	1
1	A	42	ARG	HG2	1.822	0.02	2
1	A	42	ARG	HG3	1.978	0.02	2
1	A	43	PRO	HB2	2.406	0.02	2
1	A	43	PRO	HB3	2.034	0.02	2
1	A	43	PRO	HD2	3.182	0.02	2
1	A	43	PRO	HD3	3.182	0.02	2
1	A	43	PRO	HG2	2.183	0.02	2
1	A	43	PRO	HG3	2.183	0.02	2
1	A	44	ASP	HB2	2.586	0.02	2
1	A	44	ASP	HB3	2.647	0.02	2
1	A	45	ILE	HG12	1.585	0.02	2
1	A	45	ILE	HG13	1.144	0.02	2
1	A	46	LYS	HB2	1.854	0.02	2
1	A	46	LYS	HB3	1.747	0.02	2
1	A	46	LYS	HD2	1.654	0.02	1
1	A	46	LYS	HD3	1.654	0.02	1
1	A	46	LYS	HE2	2.892	0.02	2
1	A	46	LYS	HE3	2.98	0.02	2
1	A	46	LYS	HG2	1.387	0.02	2
1	A	46	LYS	HG3	1.201	0.02	2
1	A	47	GLU	HB2	2.337	0.02	2
1	A	47	GLU	HB3	2.017	0.02	2
1	A	47	GLU	HG2	2.28	0.02	2
1	A	47	GLU	HG3	2.371	0.02	2
1	A	48	ASP	HB2	2.913	0.02	2
1	A	48	ASP	HB3	2.586	0.02	2
1	A	49	ILE	HG12	1.911	0.02	4
1	A	49	ILE	HG13	1.911	0.02	4
1	A	50	GLU	HB2	2.101	0.02	1
1	A	50	GLU	HB3	2.101	0.02	1
1	A	50	GLU	HG2	2.213	0.02	2
1	A	50	GLU	HG3	2.487	0.02	2
1	A	51	TYR	HB2	3.126	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	TYR	HB3	2.788	0.02	2
1	A	52	TYR	HB2	2.778	0.02	2
1	A	52	TYR	HB3	2.677	0.02	2
1	A	54	ARG	HB2	1.896	0.02	1
1	A	54	ARG	HB3	1.896	0.02	1
1	A	54	ARG	HD2	3.197	0.02	1
1	A	54	ARG	HD3	3.197	0.02	1
1	A	54	ARG	HG2	1.689	0.02	2
1	A	54	ARG	HG3	1.578	0.02	2
1	A	55	LEU	HB2	1.803	0.02	2
1	A	55	LEU	HB3	1.507	0.02	2
1	A	56	SER	HB2	3.95	0.02	1
1	A	56	SER	HB3	3.95	0.02	1
1	A	58	ILE	HG12	1.081	0.02	1
1	A	58	ILE	HG13	1.081	0.02	1
1	A	59	PRO	HB2	2.319	0.02	2
1	A	59	PRO	HB3	1.822	0.02	2
1	A	59	PRO	HD2	3.883	0.02	1
1	A	59	PRO	HD3	3.883	0.02	1
1	A	59	PRO	HG2	2.026	0.02	2
1	A	59	PRO	HG3	1.676	0.02	2
1	A	61	TYR	HB2	2.746	0.02	1
1	A	61	TYR	HB3	2.746	0.02	1
1	A	62	GLU	HB2	1.749	0.02	2
1	A	62	GLU	HB3	1.556	0.02	2
1	A	62	GLU	HG2	1.746	0.02	2
1	A	62	GLU	HG3	1.901	0.02	2
1	A	63	PHE	HB2	2.56	0.02	1
1	A	64	GLU	HB2	1.837	0.02	2
1	A	64	GLU	HB3	1.679	0.02	2
1	A	64	GLU	HG2	2.111	0.02	2
1	A	64	GLU	HG3	1.968	0.02	2
1	A	67	SER	HB2	3.675	0.02	1
1	A	67	SER	HB3	3.675	0.02	1
1	A	69	GLU	HB2	2.557	0.02	2
1	A	69	GLU	HB3	2.231	0.02	2
1	A	69	GLU	HG2	2.352	0.02	1
1	A	69	GLU	HG3	2.352	0.02	1
1	A	70	LEU	HB2	2.283	0.02	2
1	A	70	LEU	HB3	1.372	0.02	2
1	A	73	LEU	HB2	1.915	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	73	LEU	HB3	1.449	0.02	2
1	A	74	LEU	HB2	1.716	0.02	1
1	A	74	LEU	HB3	1.716	0.02	1
1	A	76	ARG	HB2	1.45	0.02	1
1	A	76	ARG	HB3	1.45	0.02	1
1	A	76	ARG	HD2	3.09	0.02	1
1	A	76	ARG	HD3	3.09	0.02	1
1	A	76	ARG	HG2	0.956	0.02	1
1	A	76	ARG	HG3	0.956	0.02	1
1	A	77	PRO	HB2	2.194	0.02	2
1	A	77	PRO	HB3	1.953	0.02	2
1	A	77	PRO	HD2	3.72	0.02	2
1	A	77	PRO	HD3	3.47	0.02	2
1	A	77	PRO	HG2	1.846	0.02	2
1	A	77	PRO	HG3	2.104	0.02	2
1	A	78	HIS	HB2	3.236	0.02	1
1	A	78	HIS	HB3	3.236	0.02	1
1	A	81	SER	HB2	3.919	0.02	1
1	A	81	SER	HB3	3.919	0.02	1
1	A	83	LEU	HB2	1.548	0.02	1
1	A	83	LEU	HB3	1.548	0.02	1
1	A	87	ASP	HB2	2.632	0.02	1
1	A	87	ASP	HB3	2.632	0.02	1
1	A	88	PRO	HB2	2.063	0.02	2
1	A	88	PRO	HB3	1.66	0.02	2
1	A	88	PRO	HD2	3.159	0.02	1
1	A	88	PRO	HD3	3.159	0.02	1
1	A	88	PRO	HG2	2.075	0.02	1
1	A	88	PRO	HG3	2.075	0.02	1
1	A	90	GLU	HB2	2.236	0.02	2
1	A	90	GLU	HB3	1.579	0.02	2
1	A	90	GLU	HG2	2.228	0.02	1
1	A	90	GLU	HG3	2.228	0.02	1
1	A	91	SER	HB2	3.615	0.02	2
1	A	91	SER	HB3	4.426	0.02	2
1	A	92	ARG	HB2	2.14	0.02	2
1	A	92	ARG	HB3	1.263	0.02	2
1	A	92	ARG	HD2	3.165	0.02	1
1	A	92	ARG	HD3	3.165	0.02	1
1	A	92	ARG	HG2	1.612	0.02	1
1	A	92	ARG	HG3	1.612	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	ILE	HG12	0.885	0.02	2
1	A	93	ILE	HG13	1.238	0.02	2
1	A	94	LEU	HB2	1.63	0.02	2
1	A	94	LEU	HB3	1.511	0.02	2
1	A	96	LEU	HB2	1.454	0.02	2
1	A	96	LEU	HB3	1.07	0.02	2
1	A	99	LYS	HB2	1.861	0.02	2
1	A	99	LYS	HB3	1.695	0.02	2
1	A	99	LYS	HD2	1.532	0.02	2
1	A	99	LYS	HD3	1.646	0.02	2
1	A	99	LYS	HE2	2.982	0.02	1
1	A	99	LYS	HE3	2.982	0.02	1
1	A	99	LYS	HG2	1.409	0.02	1
1	A	99	LYS	HG3	1.409	0.02	1
1	A	100	GLU	HB2	2.02	0.02	2
1	A	100	GLU	HB3	1.844	0.02	2
1	A	100	GLU	HG2	2.159	0.02	1
1	A	100	GLU	HG3	2.159	0.02	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
$^{13}\text{C}_\alpha$	100	1.64 ± 0.11	Should be checked
$^{13}\text{C}_\beta$	89	2.18 ± 0.17	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	96	0.59 ± 0.51	None needed (imprecise)

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 80%, i.e. 1044 atoms were assigned a chemical shift out of a possible 1301. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	382/477 (80%)	196/196 (100%)	95/190 (50%)	91/91 (100%)
Sidechain	630/750 (84%)	440/492 (89%)	190/228 (83%)	0/30 (0%)
Aromatic	32/74 (43%)	32/35 (91%)	0/37 (0%)	0/2 (0%)
Overall	1044/1301 (80%)	668/723 (92%)	285/455 (63%)	91/123 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1096 atoms were assigned a chemical shift out of a possible 1375. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	403/514 (78%)	207/212 (98%)	100/204 (49%)	96/98 (98%)
Sidechain	661/787 (84%)	461/515 (90%)	200/241 (83%)	0/31 (0%)
Aromatic	32/74 (43%)	32/35 (91%)	0/37 (0%)	0/2 (0%)
Overall	1096/1375 (80%)	700/762 (92%)	300/482 (62%)	96/131 (73%)

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	76	ARG	CD	49.06	38.57 – 47.75	6.4

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:

