



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:34 PM UTC

PDB ID : 8DGH / pdb_00008dgh
BMRB ID : 51447
Title : NMR Structure of calmodulin bound to C-terminal site in the beta-subunit of cyclic nucleotide-gated channel
Authors : Bej, A.; Ames, J.B.
Deposited on : 2022-06-23

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

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

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

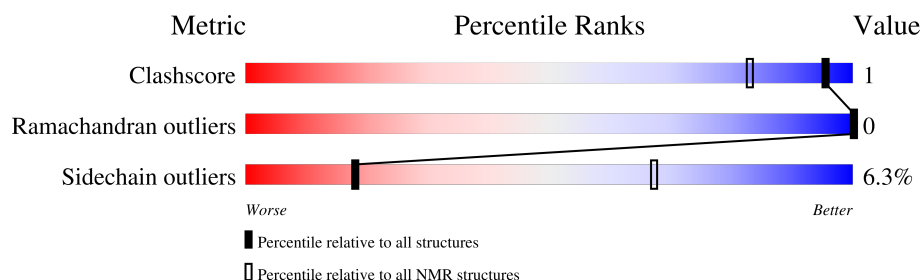
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 69%.

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	149	
2	B	12	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:84-A:149, B:1128-B:1136 (75)	0.52	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 2 clusters and 5 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1271 atoms, of which 625 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1051	333	506	90	118	4	

- Molecule 2 is a protein called Cyclic nucleotide-gated cation channel beta-1.

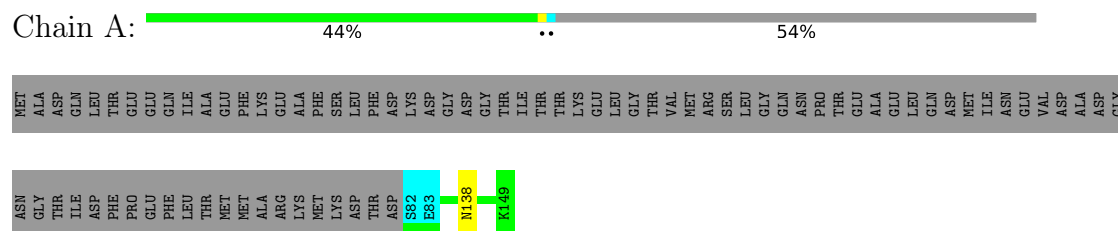
Mol	Chain	Residues	Atoms					Trace
2	B	12	Total	C	H	N	O	0
			220	65	119	22	14	

4 Residue-property plots [i](#)

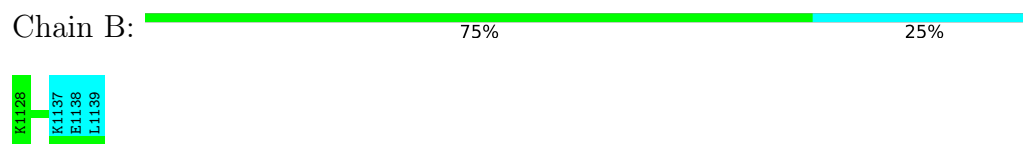
4.1 Average score per residue in the NMR ensemble

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: Calmodulin-1



- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

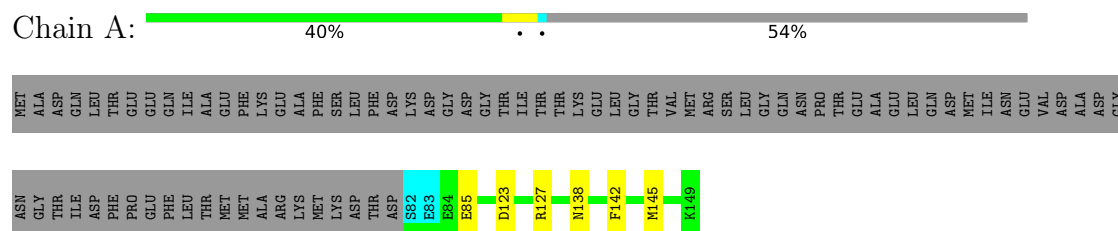


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Calmodulin-1

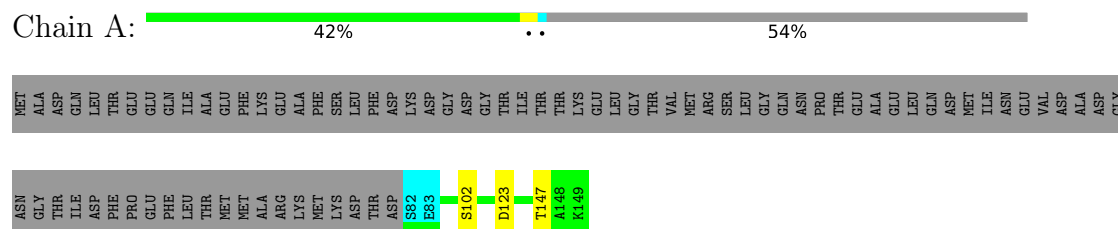


- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

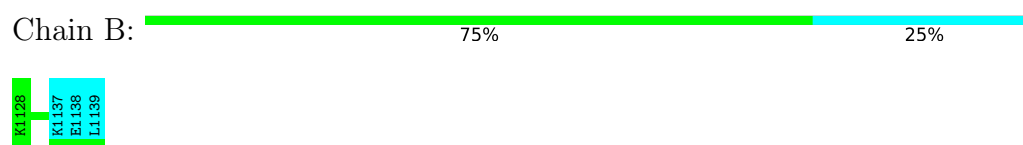


4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin-1

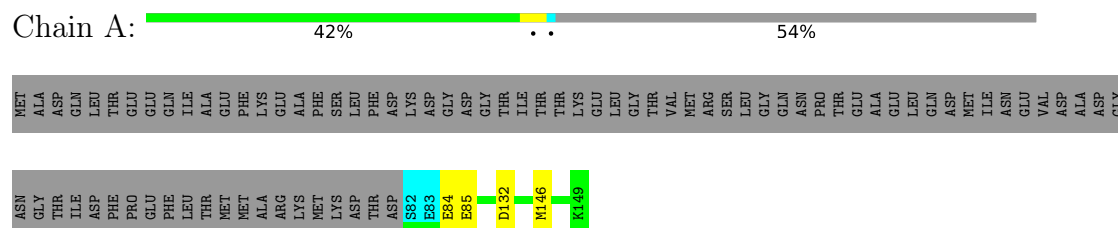


- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

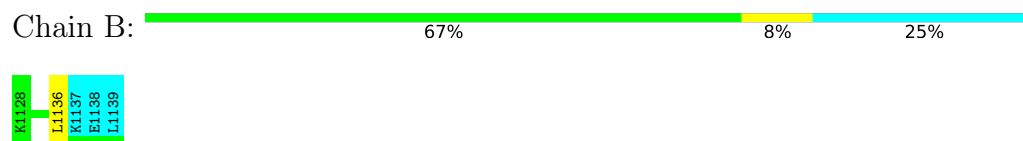


4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin-1



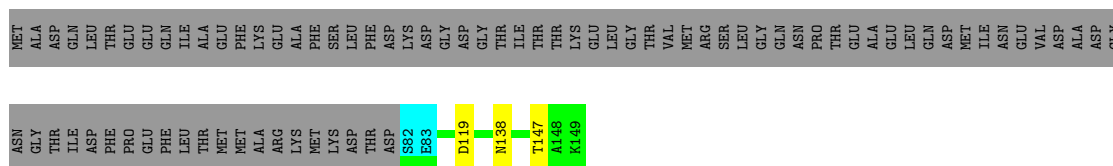
- Molecule 2: Cyclic nucleotide-gated cation channel beta-1



4.2.4 Score per residue for model 4

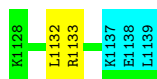
- Molecule 1: Calmodulin-1

Chain A:  42% .. 54%



- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

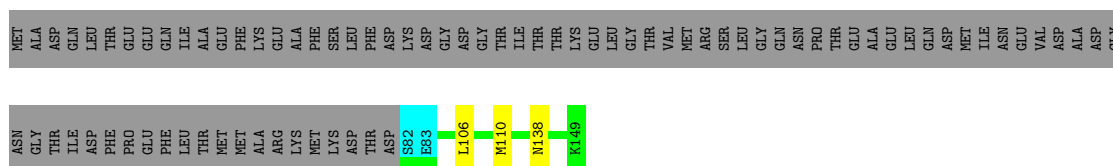
Chain B:  58% 17% 25%



4.2.5 Score per residue for model 5

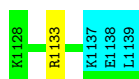
- Molecule 1: Calmodulin-1

Chain A:  42% .. 54%



- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

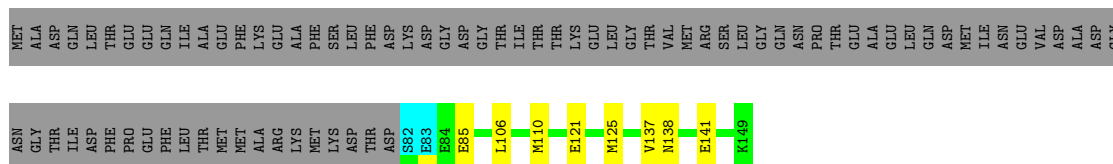
Chain B:  67% 8% 25%



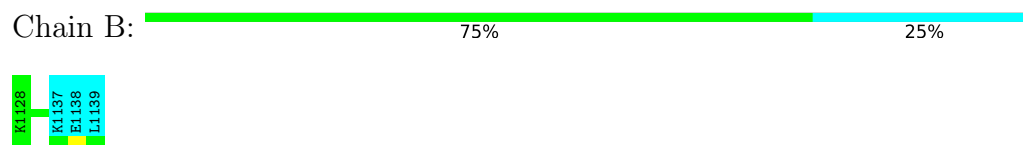
4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin-1

Chain A:  39% 5% . 54%

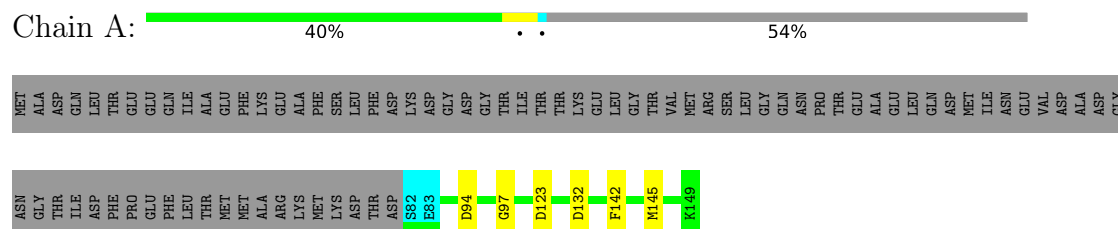


- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

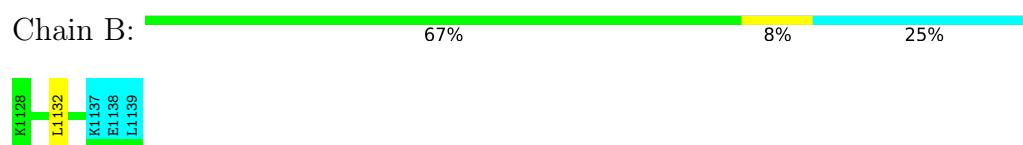


4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin-1

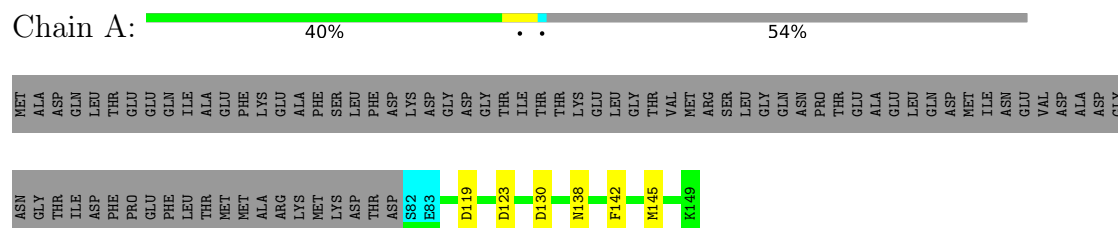


- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

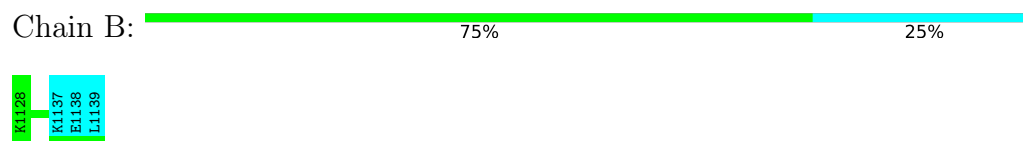


4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin-1

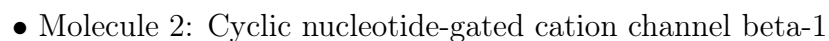


- Molecule 2: Cyclic nucleotide-gated cation channel beta-1

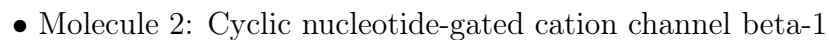


4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin-1



- Molecule 1: Calmodulin-1



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
HADDOCK	refinement	
HADDOCK	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	1450
Number of shifts mapped to atoms	733
Number of unparsed shifts	0
Number of shifts with mapping errors	717
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

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	530	495	495	1±1
2	B	75	89	88	0±0
All	All	6050	5840	5830	12

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ASP:OD1	1:A:97:GLY:HA2	0.47	2.09	7	1
1:A:142:PHE:O	1:A:145:MET:HG2	0.47	2.10	9	4
1:A:123:ASP:O	1:A:127:ARG:HG3	0.45	2.11	1	1
1:A:106:LEU:O	1:A:110:MET:HG2	0.45	2.12	6	2
1:A:107:ARG:HD3	1:A:122:VAL:HG21	0.42	1.91	10	1
1:A:146:MET:HA	2:B:1133:ARG:NH2	0.42	2.29	10	1
1:A:85:GLU:HB3	2:B:1133:ARG:NH1	0.42	2.29	1	1
1:A:121:GLU:O	1:A:125:MET:HG3	0.41	2.16	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	65/149 (44%)	64±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
2	B	8/12 (67%)	8±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	730/1610 (45%)	716 (98%)	14 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	56/127 (44%)	53±1 (95±2%)	3±1 (5±2%)	23	74
2	B	7/10 (70%)	6±1 (83±14%)	1±1 (17±14%)	4	38
All	All	630/1370 (46%)	590 (94%)	40 (6%)	18	67

All 19 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	138	ASN	7
2	B	1132	LEU	4
2	B	1133	ARG	3
1	A	123	ASP	3
1	A	147	THR	3
2	B	1129	LEU	2
1	A	85	GLU	2
1	A	132	ASP	2
2	B	1136	LEU	2
1	A	119	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	141	GLU	2
1	A	102	SER	1
1	A	84	GLU	1
1	A	146	MET	1
1	A	137	VAL	1
1	A	130	ASP	1
1	A	144	GLN	1
2	B	1131	HIS	1
1	A	140	GLU	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 69% for the well-defined parts and 66% 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	1450
Number of shifts mapped to atoms	733
Number of unparsed shifts	0
Number of shifts with mapping errors	717
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 717 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	ASP	HA	4.614	0.002	1
1	A	3	ASP	HB2	2.667	0.010	2
1	A	3	ASP	HB3	2.542	0.015	2
1	A	3	ASP	C	175.621	0.000	1
1	A	3	ASP	CA	54.658	0.000	1
1	A	3	ASP	CB	41.394	0.025	1
1	A	4	GLN	H	8.319	0.006	1
1	A	4	GLN	HA	4.362	0.004	1
1	A	4	GLN	HB2	1.965	0.005	2
1	A	4	GLN	HB3	2.067	0.009	2
1	A	4	GLN	HG2	2.341	0.000	1
1	A	4	GLN	HG3	2.341	0.000	1
1	A	4	GLN	C	175.601	0.000	1
1	A	4	GLN	CA	55.678	0.077	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	GLN	CB	29.77	0.011	1
1	A	4	GLN	N	119.902	0.086	1
1	A	5	LEU	H	8.258	0.002	1
1	A	5	LEU	HA	4.652	0.004	1
1	A	5	LEU	HB2	1.724	0.006	2
1	A	5	LEU	HB3	1.497	0.003	2
1	A	5	LEU	HD11	0.943	0.000	1
1	A	5	LEU	HD12	0.943	0.000	1
1	A	5	LEU	HD13	0.943	0.000	1
1	A	5	LEU	HD21	0.953	0.022	1
1	A	5	LEU	HD22	0.953	0.022	1
1	A	5	LEU	HD23	0.953	0.022	1
1	A	5	LEU	C	177.646	0.000	1
1	A	5	LEU	CA	54.471	0.037	1
1	A	5	LEU	CB	43.563	0.031	1
1	A	5	LEU	CD1	23.699	0.025	1
1	A	5	LEU	CD2	26.831	0.021	1
1	A	5	LEU	N	123.306	0.048	1
1	A	6	THR	H	8.654	0.022	1
1	A	6	THR	HA	4.46	0.008	1
1	A	6	THR	HB	4.771	0.005	1
1	A	6	THR	HG21	1.335	0.009	1
1	A	6	THR	HG22	1.335	0.009	1
1	A	6	THR	HG23	1.335	0.009	1
1	A	6	THR	C	175.496	0.000	1
1	A	6	THR	CA	60.564	0.087	1
1	A	6	THR	CB	71.166	0.022	1
1	A	6	THR	CG2	21.767	0.002	1
1	A	6	THR	N	113.006	0.042	1
1	A	7	GLU	H	8.994	0.001	1
1	A	7	GLU	HA	3.968	0.003	1
1	A	7	GLU	HB2	2.037	0.014	1
1	A	7	GLU	HB3	2.037	0.014	1
1	A	7	GLU	HG2	2.349	0.000	1
1	A	7	GLU	HG3	2.349	0.000	1
1	A	7	GLU	C	179.455	0.000	1
1	A	7	GLU	CA	60.142	0.130	1
1	A	7	GLU	CB	29.243	0.004	1
1	A	7	GLU	N	120.521	0.044	1
1	A	8	GLU	H	8.684	0.008	1
1	A	8	GLU	HA	4.071	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	GLU	CA	59.996	0.043	1
1	A	8	GLU	CB	29.145	0.000	1
1	A	8	GLU	N	119.36	0.046	1
1	A	9	GLN	H	7.71	0.001	1
1	A	9	GLN	HA	3.842	0.006	1
1	A	9	GLN	HB2	1.686	0.005	2
1	A	9	GLN	HB3	2.36	0.000	2
1	A	9	GLN	C	178.21	0.000	1
1	A	9	GLN	CA	58.655	0.036	1
1	A	9	GLN	CB	29.329	0.000	1
1	A	9	GLN	N	120.335	0.017	1
1	A	10	ILE	H	8.356	0.005	1
1	A	10	ILE	HA	3.704	0.004	1
1	A	10	ILE	HB	1.949	0.005	1
1	A	10	ILE	HD11	0.881	0.000	1
1	A	10	ILE	HD12	0.881	0.000	1
1	A	10	ILE	HD13	0.881	0.000	1
1	A	10	ILE	HG21	1.125	0.013	1
1	A	10	ILE	HG22	1.125	0.013	1
1	A	10	ILE	HG23	1.125	0.013	1
1	A	10	ILE	C	177.726	0.000	1
1	A	10	ILE	CA	66.204	0.053	1
1	A	10	ILE	CB	37.752	0.051	1
1	A	10	ILE	CD1	13.04	0.115	1
1	A	10	ILE	CG2	17.463	0.018	1
1	A	10	ILE	N	119.635	0.040	1
1	A	11	ALA	H	8.005	0.006	1
1	A	11	ALA	HA	4.106	0.005	1
1	A	11	ALA	HB1	1.521	0.010	1
1	A	11	ALA	HB2	1.521	0.010	1
1	A	11	ALA	HB3	1.521	0.010	1
1	A	11	ALA	C	180.925	0.000	1
1	A	11	ALA	CA	55.574	0.033	1
1	A	11	ALA	CB	17.88	0.032	1
1	A	11	ALA	N	121.201	0.061	1
1	A	12	GLU	H	7.714	0.016	1
1	A	12	GLU	HA	4.21	0.010	1
1	A	12	GLU	HB2	1.868	0.017	2
1	A	12	GLU	HB3	2.062	0.004	2
1	A	12	GLU	HG2	2.265	0.000	1
1	A	12	GLU	HG3	2.265	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	GLU	C	179.886	0.000	1
1	A	12	GLU	CA	59.182	0.000	1
1	A	12	GLU	CB	28.928	0.048	1
1	A	12	GLU	N	119.725	0.059	1
1	A	13	PHE	H	8.537	0.022	1
1	A	13	PHE	HA	4.989	0.012	1
1	A	13	PHE	HB2	3.45	0.013	1
1	A	13	PHE	HB3	3.45	0.013	1
1	A	13	PHE	HD1	7.152	0.000	1
1	A	13	PHE	HD2	7.152	0.000	1
1	A	13	PHE	HE1	7.256	0.000	1
1	A	13	PHE	HE2	7.256	0.000	1
1	A	13	PHE	C	178.832	0.000	1
1	A	13	PHE	CA	59.532	0.055	1
1	A	13	PHE	CB	37.827	0.039	1
1	A	13	PHE	N	119.423	0.104	1
1	A	14	LYS	H	9.161	0.011	1
1	A	14	LYS	HA	4.018	0.000	1
1	A	14	LYS	HB2	1.9	0.000	1
1	A	14	LYS	HB3	1.9	0.000	1
1	A	14	LYS	C	179.225	0.056	1
1	A	14	LYS	CA	60.07	0.091	1
1	A	14	LYS	CB	31.877	0.017	1
1	A	14	LYS	N	123.374	0.063	1
1	A	15	GLU	H	7.83	0.044	1
1	A	15	GLU	CA	59.643	0.033	1
1	A	15	GLU	CB	29.216	0.029	1
1	A	15	GLU	N	120.612	0.108	1
1	A	16	ALA	H	8.073	0.010	1
1	A	16	ALA	HA	4.137	0.002	1
1	A	16	ALA	HB1	1.912	0.006	1
1	A	16	ALA	HB2	1.912	0.006	1
1	A	16	ALA	HB3	1.912	0.006	1
1	A	16	ALA	C	178.636	0.000	1
1	A	16	ALA	CA	55.397	0.039	1
1	A	16	ALA	CB	17.993	0.109	1
1	A	16	ALA	N	122.082	0.104	1
1	A	17	PHE	H	8.765	0.015	1
1	A	17	PHE	HA	3.255	0.010	1
1	A	17	PHE	HB2	2.929	0.006	1
1	A	17	PHE	HB3	2.929	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	PHE	HD1	6.618	0.000	1
1	A	17	PHE	HD2	6.618	0.000	1
1	A	17	PHE	HE1	7.01	0.000	1
1	A	17	PHE	HE2	7.01	0.000	1
1	A	17	PHE	C	177.636	0.000	1
1	A	17	PHE	CA	62.123	0.080	1
1	A	17	PHE	CB	39.624	0.044	1
1	A	17	PHE	N	118.951	0.022	1
1	A	18	SER	H	7.966	0.016	1
1	A	18	SER	HA	4.12	0.004	1
1	A	18	SER	HB2	4.034	0.014	1
1	A	18	SER	HB3	4.034	0.014	1
1	A	18	SER	C	174.679	0.000	1
1	A	18	SER	CA	61.597	0.141	1
1	A	18	SER	CB	63.365	0.008	1
1	A	18	SER	N	113.156	0.176	1
1	A	19	LEU	H	7.407	0.009	1
1	A	19	LEU	HA	3.977	0.024	1
1	A	19	LEU	HB2	1.639	0.010	1
1	A	19	LEU	HB3	1.639	0.010	1
1	A	19	LEU	HD21	0.757	0.018	1
1	A	19	LEU	HD22	0.757	0.018	1
1	A	19	LEU	HD23	0.757	0.018	1
1	A	19	LEU	HG	1.396	0.000	1
1	A	19	LEU	C	177.537	0.000	1
1	A	19	LEU	CA	57.218	0.072	1
1	A	19	LEU	CB	41.435	0.103	1
1	A	19	LEU	CD2	24.067	0.000	1
1	A	19	LEU	CG	26.943	0.000	1
1	A	19	LEU	N	120.776	0.233	1
1	A	20	PHE	H	7.113	0.008	1
1	A	20	PHE	HA	4.193	0.000	1
1	A	20	PHE	HB2	2.645	0.000	1
1	A	20	PHE	HB3	2.645	0.000	1
1	A	20	PHE	HD1	7.293	0.000	1
1	A	20	PHE	HD2	7.293	0.000	1
1	A	20	PHE	HE1	7.284	0.000	1
1	A	20	PHE	HE2	7.284	0.000	1
1	A	20	PHE	C	176.825	0.000	1
1	A	20	PHE	CA	59.154	0.051	1
1	A	20	PHE	CB	41.27	0.134	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	PHE	N	113.978	0.040	1
1	A	21	ASP	H	7.804	0.013	1
1	A	21	ASP	C	177.16	0.000	1
1	A	21	ASP	CA	52.519	0.110	1
1	A	21	ASP	CB	39.181	0.029	1
1	A	21	ASP	N	117.304	0.059	1
1	A	22	LYS	H	7.667	0.016	1
1	A	22	LYS	HA	3.985	0.004	1
1	A	22	LYS	HB2	1.877	0.004	1
1	A	22	LYS	HB3	1.877	0.004	1
1	A	22	LYS	HG2	1.521	0.000	1
1	A	22	LYS	HG3	1.521	0.000	1
1	A	22	LYS	C	178.14	0.000	1
1	A	22	LYS	CA	58.341	0.014	1
1	A	22	LYS	CB	32.465	0.082	1
1	A	22	LYS	N	124.221	0.045	1
1	A	23	ASP	H	8.032	0.020	1
1	A	23	ASP	HA	4.588	0.011	1
1	A	23	ASP	HB2	3.058	0.006	2
1	A	23	ASP	HB3	2.61	0.005	2
1	A	23	ASP	C	177.677	0.000	1
1	A	23	ASP	CA	52.886	0.065	1
1	A	23	ASP	CB	39.554	0.058	1
1	A	23	ASP	N	114.078	0.044	1
1	A	24	GLY	H	7.657	0.002	1
1	A	24	GLY	HA2	3.861	0.005	1
1	A	24	GLY	HA3	3.861	0.005	1
1	A	24	GLY	C	175.143	0.000	1
1	A	24	GLY	CA	47.33	0.065	1
1	A	24	GLY	N	109.212	0.030	1
1	A	25	ASP	H	8.409	0.006	1
1	A	25	ASP	HA	4.504	0.008	1
1	A	25	ASP	HB2	3.048	0.006	2
1	A	25	ASP	HB3	2.436	0.007	2
1	A	25	ASP	C	177.438	0.000	1
1	A	25	ASP	CA	53.862	0.097	1
1	A	25	ASP	CB	40.454	0.021	1
1	A	25	ASP	N	120.726	0.038	1
1	A	26	GLY	H	10.545	0.004	1
1	A	26	GLY	HA2	3.696	0.001	2
1	A	26	GLY	HA3	4.345	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	GLY	C	173.72	0.000	1
1	A	26	GLY	CA	45.582	0.131	1
1	A	26	GLY	N	112.991	0.041	1
1	A	27	THR	H	8.147	0.012	1
1	A	27	THR	HA	5.325	0.002	1
1	A	27	THR	HB	3.833	0.006	1
1	A	27	THR	HG21	1.038	0.013	1
1	A	27	THR	HG22	1.038	0.013	1
1	A	27	THR	HG23	1.038	0.013	1
1	A	27	THR	C	173.067	0.000	1
1	A	27	THR	CA	59.855	0.054	1
1	A	27	THR	CB	72.694	0.022	1
1	A	27	THR	CG2	21.623	0.001	1
1	A	27	THR	N	112.678	0.062	1
1	A	28	ILE	H	9.798	0.009	1
1	A	28	ILE	HA	4.91	0.006	1
1	A	28	ILE	HB	1.728	0.010	1
1	A	28	ILE	HD11	0.218	0.006	1
1	A	28	ILE	HD12	0.218	0.006	1
1	A	28	ILE	HD13	0.218	0.006	1
1	A	28	ILE	HG21	0.871	0.013	1
1	A	28	ILE	HG22	0.871	0.013	1
1	A	28	ILE	HG23	0.871	0.013	1
1	A	28	ILE	C	176.052	0.000	1
1	A	28	ILE	CA	60.968	0.112	1
1	A	28	ILE	CB	39.748	0.065	1
1	A	28	ILE	CD1	15.576	0.000	1
1	A	28	ILE	CG2	17.779	0.000	1
1	A	28	ILE	N	126.949	0.040	1
1	A	29	THR	H	8.411	0.009	1
1	A	29	THR	HA	4.83	0.014	1
1	A	29	THR	HG21	1.296	0.017	1
1	A	29	THR	HG22	1.296	0.017	1
1	A	29	THR	HG23	1.296	0.017	1
1	A	29	THR	C	176.732	0.000	1
1	A	29	THR	CA	59.601	0.069	1
1	A	29	THR	CB	72.548	0.022	1
1	A	29	THR	CG2	21.88	0.049	1
1	A	29	THR	N	116.473	0.048	1
1	A	30	THR	H	9.174	0.014	1
1	A	30	THR	HA	3.788	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	THR	HB	4.198	0.006	1
1	A	30	THR	HG21	1.281	0.017	1
1	A	30	THR	HG22	1.281	0.017	1
1	A	30	THR	HG23	1.281	0.017	1
1	A	30	THR	C	177.404	0.000	1
1	A	30	THR	CA	66.479	0.090	1
1	A	30	THR	CB	67.972	0.040	1
1	A	30	THR	CG2	23.321	0.084	1
1	A	30	THR	N	112.567	0.065	1
1	A	31	LYS	H	7.613	0.005	1
1	A	31	LYS	HA	4.131	0.013	1
1	A	31	LYS	HB2	1.823	0.009	1
1	A	31	LYS	HB3	1.823	0.009	1
1	A	31	LYS	C	179.915	0.000	1
1	A	31	LYS	CA	59.344	0.044	1
1	A	31	LYS	CB	32.469	0.017	1
1	A	31	LYS	N	121.119	0.048	1
1	A	32	GLU	H	7.698	0.009	1
1	A	32	GLU	HA	4.038	0.008	1
1	A	32	GLU	HB2	2.64	0.000	2
1	A	32	GLU	HB3	2.385	0.000	2
1	A	32	GLU	C	179.394	0.000	1
1	A	32	GLU	CA	59.676	0.066	1
1	A	32	GLU	CB	29.686	0.021	1
1	A	32	GLU	N	121.904	0.077	1
1	A	33	LEU	H	8.622	0.009	1
1	A	33	LEU	HA	4.137	0.010	1
1	A	33	LEU	HB2	1.774	0.006	2
1	A	33	LEU	HB3	1.588	0.009	2
1	A	33	LEU	HD11	0.775	0.009	1
1	A	33	LEU	HD12	0.775	0.009	1
1	A	33	LEU	HD13	0.775	0.009	1
1	A	33	LEU	HD21	0.877	0.024	1
1	A	33	LEU	HD22	0.877	0.024	1
1	A	33	LEU	HD23	0.877	0.024	1
1	A	33	LEU	C	178.979	0.000	1
1	A	33	LEU	CA	58.289	0.019	1
1	A	33	LEU	CB	42.867	0.153	1
1	A	33	LEU	CD2	26.044	0.000	1
1	A	33	LEU	N	120.445	0.068	1
1	A	34	GLY	H	8.679	0.033	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	GLY	HA2	3.569	0.006	2
1	A	34	GLY	HA3	3.958	0.001	2
1	A	34	GLY	C	175.171	0.000	1
1	A	34	GLY	CA	48.414	0.066	1
1	A	34	GLY	N	105.43	0.312	1
1	A	35	THR	H	7.999	0.012	1
1	A	35	THR	HA	3.917	0.007	1
1	A	35	THR	HB	4.329	0.004	1
1	A	35	THR	HG21	1.276	0.011	1
1	A	35	THR	HG22	1.276	0.011	1
1	A	35	THR	HG23	1.276	0.011	1
1	A	35	THR	C	177.098	0.000	1
1	A	35	THR	CA	67.059	0.036	1
1	A	35	THR	CB	68.811	0.009	1
1	A	35	THR	CG2	21.488	0.109	1
1	A	35	THR	N	118.181	0.116	1
1	A	36	VAL	H	7.535	0.054	1
1	A	36	VAL	HA	3.606	0.017	1
1	A	36	VAL	HB	1.999	0.011	1
1	A	36	VAL	HG11	0.755	0.023	1
1	A	36	VAL	HG12	0.755	0.023	1
1	A	36	VAL	HG13	0.755	0.023	1
1	A	36	VAL	HG21	0.482	0.016	1
1	A	36	VAL	HG22	0.482	0.016	1
1	A	36	VAL	HG23	0.482	0.016	1
1	A	36	VAL	C	178.953	0.000	1
1	A	36	VAL	CA	66.568	0.155	1
1	A	36	VAL	CB	31.454	0.024	1
1	A	36	VAL	CG1	23.047	0.031	1
1	A	36	VAL	CG2	20.486	0.100	1
1	A	36	VAL	N	121.884	0.066	1
1	A	37	MET	H	8.355	0.040	1
1	A	37	MET	HA	4.019	0.009	1
1	A	37	MET	HB2	1.992	0.000	2
1	A	37	MET	HB3	1.846	0.000	2
1	A	37	MET	HE1	1.995	0.000	1
1	A	37	MET	HE2	1.995	0.000	1
1	A	37	MET	HE3	1.995	0.000	1
1	A	37	MET	HG2	2.632	0.000	1
1	A	37	MET	HG3	2.632	0.000	1
1	A	37	MET	C	179.067	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	MET	CA	59.519	0.064	1
1	A	37	MET	CB	31.728	0.010	1
1	A	37	MET	CE	17.506	0.000	1
1	A	37	MET	N	118.146	0.032	1
1	A	38	ARG	H	8.607	0.026	1
1	A	38	ARG	HA	4.787	0.006	1
1	A	38	ARG	HB2	1.886	0.026	1
1	A	38	ARG	HB3	1.886	0.026	1
1	A	38	ARG	C	181.326	0.000	1
1	A	38	ARG	CA	59.285	0.099	1
1	A	38	ARG	CB	29.964	0.035	1
1	A	38	ARG	N	118.815	0.188	1
1	A	39	SER	H	7.93	0.019	1
1	A	39	SER	HA	4.376	0.005	1
1	A	39	SER	HB2	4.046	0.021	1
1	A	39	SER	HB3	4.046	0.021	1
1	A	39	SER	C	174.82	0.000	1
1	A	39	SER	CA	61.716	0.021	1
1	A	39	SER	CB	62.763	0.012	1
1	A	39	SER	N	118.92	0.030	1
1	A	40	LEU	H	7.326	0.010	1
1	A	40	LEU	HA	4.406	0.005	1
1	A	40	LEU	HB2	1.801	0.003	1
1	A	40	LEU	HB3	1.801	0.003	1
1	A	40	LEU	HD11	0.839	0.027	1
1	A	40	LEU	HD12	0.839	0.027	1
1	A	40	LEU	HD13	0.839	0.027	1
1	A	40	LEU	HD21	0.742	0.002	1
1	A	40	LEU	HD22	0.742	0.002	1
1	A	40	LEU	HD23	0.742	0.002	1
1	A	40	LEU	C	177.079	0.000	1
1	A	40	LEU	CA	54.465	0.035	1
1	A	40	LEU	CB	41.944	0.022	1
1	A	40	LEU	CD1	25.97	0.136	1
1	A	40	LEU	CD2	22.709	0.000	1
1	A	40	LEU	N	120.541	0.122	1
1	A	41	GLY	H	7.807	0.028	1
1	A	41	GLY	HA2	3.765	0.003	2
1	A	41	GLY	HA3	4.244	0.003	2
1	A	41	GLY	C	174.396	0.000	1
1	A	41	GLY	CA	45.701	0.055	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	GLY	N	106.475	0.294	1
1	A	42	GLN	H	7.762	0.023	1
1	A	42	GLN	HB2	1.6	0.000	2
1	A	42	GLN	HB3	2.104	0.003	2
1	A	42	GLN	CA	54.377	0.053	1
1	A	42	GLN	CB	30.595	0.075	1
1	A	42	GLN	CG	33.641	0.000	1
1	A	42	GLN	N	118.214	0.043	1
1	A	43	ASN	H	8.667	0.009	1
1	A	43	ASN	CA	51.43	0.000	1
1	A	43	ASN	CB	39.285	0.000	1
1	A	43	ASN	N	116.485	0.073	1
1	A	44	PRO	C	177.704	0.000	1
1	A	44	PRO	CA	62.454	0.036	1
1	A	44	PRO	CB	31.991	0.000	1
1	A	45	THR	H	8.716	0.013	1
1	A	45	THR	HA	4.45	0.000	1
1	A	45	THR	HB	4.7	0.000	1
1	A	45	THR	HG21	1.357	0.015	1
1	A	45	THR	HG22	1.357	0.015	1
1	A	45	THR	HG23	1.357	0.015	1
1	A	45	THR	C	175.205	0.000	1
1	A	45	THR	CA	60.423	0.211	1
1	A	45	THR	CB	71.173	0.011	1
1	A	45	THR	CG2	21.871	0.033	1
1	A	45	THR	N	112.876	0.046	1
1	A	46	GLU	H	8.764	0.007	1
1	A	46	GLU	HA	3.974	0.003	1
1	A	46	GLU	HB2	2.028	0.000	1
1	A	46	GLU	HB3	2.028	0.000	1
1	A	46	GLU	C	178.951	0.000	1
1	A	46	GLU	CA	60.052	0.000	1
1	A	46	GLU	CB	28.966	0.000	1
1	A	46	GLU	N	120.645	0.079	1
1	A	47	ALA	H	8.213	0.007	1
1	A	47	ALA	HA	4.093	0.000	1
1	A	47	ALA	HB1	1.394	0.011	1
1	A	47	ALA	HB2	1.394	0.011	1
1	A	47	ALA	HB3	1.394	0.011	1
1	A	47	ALA	C	180.146	0.000	1
1	A	47	ALA	CA	55.194	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	ALA	CB	18.211	0.039	1
1	A	47	ALA	N	120.613	0.022	1
1	A	48	GLU	H	7.678	0.000	1
1	A	48	GLU	HA	4.024	0.000	1
1	A	48	GLU	HB2	2.319	0.005	2
1	A	48	GLU	HB3	1.909	0.001	2
1	A	48	GLU	C	180.067	0.000	1
1	A	48	GLU	CA	59.15	0.061	1
1	A	48	GLU	CB	29.791	0.015	1
1	A	48	GLU	N	118.72	0.053	1
1	A	49	LEU	H	8.049	0.002	1
1	A	49	LEU	HA	4.107	0.023	1
1	A	49	LEU	HB2	2.084	0.012	2
1	A	49	LEU	HB3	1.228	0.016	2
1	A	49	LEU	HD11	0.88	0.012	1
1	A	49	LEU	HD12	0.88	0.012	1
1	A	49	LEU	HD13	0.88	0.012	1
1	A	49	LEU	HD21	0.836	0.002	1
1	A	49	LEU	HD22	0.836	0.002	1
1	A	49	LEU	HD23	0.836	0.002	1
1	A	49	LEU	C	178.557	0.000	1
1	A	49	LEU	CA	57.942	0.063	1
1	A	49	LEU	CB	42.454	0.046	1
1	A	49	LEU	CD1	26.037	0.004	1
1	A	49	LEU	CD2	23.643	0.000	1
1	A	49	LEU	N	120.032	0.041	1
1	A	50	GLN	H	8.237	0.005	1
1	A	50	GLN	HA	3.799	0.001	1
1	A	50	GLN	HB2	2.159	0.003	1
1	A	50	GLN	HB3	2.159	0.003	1
1	A	50	GLN	HG2	2.43	0.000	1
1	A	50	GLN	HG3	2.43	0.000	1
1	A	50	GLN	C	178.463	0.000	1
1	A	50	GLN	CA	58.564	0.003	1
1	A	50	GLN	CB	28.245	0.000	1
1	A	50	GLN	CG	34.15	0.000	1
1	A	50	GLN	N	118.445	0.068	1
1	A	51	ASP	H	8.125	0.002	1
1	A	51	ASP	HA	4.406	0.005	1
1	A	51	ASP	HB2	2.801	0.002	2
1	A	51	ASP	HB3	2.656	0.008	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	ASP	C	178.689	0.000	1
1	A	51	ASP	CA	57.671	0.069	1
1	A	51	ASP	CB	40.553	0.032	1
1	A	51	ASP	N	120.031	0.036	1
1	A	52	MET	H	7.785	0.010	1
1	A	52	MET	HA	4.047	0.024	1
1	A	52	MET	HB2	2.275	0.006	2
1	A	52	MET	HB3	1.993	0.008	2
1	A	52	MET	HE1	2.077	0.001	1
1	A	52	MET	HE2	2.077	0.001	1
1	A	52	MET	HE3	2.077	0.001	1
1	A	52	MET	HG2	2.752	0.000	2
1	A	52	MET	HG3	2.517	0.000	2
1	A	52	MET	C	178.749	0.000	1
1	A	52	MET	CA	59.657	0.011	1
1	A	52	MET	CB	33.63	0.003	1
1	A	52	MET	CE	17.093	0.000	1
1	A	52	MET	N	119.151	0.238	1
1	A	53	ILE	H	7.648	0.016	1
1	A	53	ILE	HA	3.502	0.012	1
1	A	53	ILE	HB	1.942	0.002	1
1	A	53	ILE	HD11	0.75	0.001	1
1	A	53	ILE	HD12	0.75	0.001	1
1	A	53	ILE	HD13	0.75	0.001	1
1	A	53	ILE	HG12	1.028	0.000	1
1	A	53	ILE	HG13	1.028	0.000	1
1	A	53	ILE	HG21	0.701	0.000	1
1	A	53	ILE	HG22	0.701	0.000	1
1	A	53	ILE	HG23	0.701	0.000	1
1	A	53	ILE	C	177.953	0.000	1
1	A	53	ILE	CA	64.702	0.013	1
1	A	53	ILE	CB	37.058	0.075	1
1	A	53	ILE	CD1	12.883	0.000	1
1	A	53	ILE	CG2	16.066	0.048	1
1	A	53	ILE	N	117.884	0.024	1
1	A	54	ASN	H	8.633	0.001	1
1	A	54	ASN	HA	4.367	0.002	1
1	A	54	ASN	HB2	2.991	0.004	2
1	A	54	ASN	HB3	2.871	0.005	2
1	A	54	ASN	C	177.258	0.000	1
1	A	54	ASN	CA	55.937	0.062	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	ASN	CB	38.05	0.040	1
1	A	54	ASN	N	117.92	0.062	1
1	A	55	GLU	H	7.5	0.007	1
1	A	55	GLU	HA	4.017	0.006	1
1	A	55	GLU	HB2	2.132	0.001	2
1	A	55	GLU	HB3	2.005	0.004	2
1	A	55	GLU	HG2	2.454	0.000	1
1	A	55	GLU	HG3	2.454	0.000	1
1	A	55	GLU	CA	58.986	0.062	1
1	A	55	GLU	CB	30.404	0.080	1
1	A	55	GLU	CG	36.265	0.000	1
1	A	55	GLU	N	116.353	0.033	1
1	A	56	VAL	H	7.181	0.006	1
1	A	56	VAL	HA	4.458	0.031	1
1	A	56	VAL	HB	2.359	0.000	1
1	A	56	VAL	HG11	0.839	0.010	1
1	A	56	VAL	HG12	0.839	0.010	1
1	A	56	VAL	HG13	0.839	0.010	1
1	A	56	VAL	HG21	0.93	0.002	1
1	A	56	VAL	HG22	0.93	0.002	1
1	A	56	VAL	HG23	0.93	0.002	1
1	A	56	VAL	C	175.634	0.000	1
1	A	56	VAL	CA	60.774	0.051	1
1	A	56	VAL	CB	32.835	0.140	1
1	A	56	VAL	CG1	21.889	0.090	1
1	A	56	VAL	CG2	19.479	0.109	1
1	A	56	VAL	N	108.605	0.132	1
1	A	57	ASP	H	7.652	0.018	1
1	A	57	ASP	HA	4.595	0.008	1
1	A	57	ASP	HB2	2.725	0.000	2
1	A	57	ASP	HB3	2.557	0.000	2
1	A	57	ASP	C	176.054	0.000	1
1	A	57	ASP	CA	54.011	0.068	1
1	A	57	ASP	CB	40.476	0.042	1
1	A	57	ASP	N	121.588	0.132	1
1	A	58	ALA	H	8.406	0.032	1
1	A	58	ALA	HA	4.202	0.000	1
1	A	58	ALA	HB1	1.531	0.014	1
1	A	58	ALA	HB2	1.531	0.014	1
1	A	58	ALA	HB3	1.531	0.014	1
1	A	58	ALA	C	178.621	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	ALA	CA	54.303	0.056	1
1	A	58	ALA	CB	19.655	0.096	1
1	A	58	ALA	N	131.75	0.038	1
1	A	59	ASP	H	8.181	0.004	1
1	A	59	ASP	HA	4.621	0.000	1
1	A	59	ASP	C	177.855	0.000	1
1	A	59	ASP	CA	52.778	0.087	1
1	A	59	ASP	CB	39.814	0.000	1
1	A	59	ASP	N	113.985	0.030	1
1	A	60	GLY	H	7.56	0.001	1
1	A	60	GLY	HA2	3.879	0.000	2
1	A	60	GLY	HA3	3.767	0.000	2
1	A	60	GLY	C	174.952	0.000	1
1	A	60	GLY	CA	47.286	0.054	1
1	A	60	GLY	N	108.438	0.020	1
1	A	61	ASN	H	8.099	0.010	1
1	A	61	ASN	HA	4.628	0.006	1
1	A	61	ASN	HB2	3.301	0.000	2
1	A	61	ASN	HB3	2.647	0.000	2
1	A	61	ASN	C	176.845	0.000	1
1	A	61	ASN	CA	52.745	0.063	1
1	A	61	ASN	CB	37.644	0.018	1
1	A	61	ASN	N	118.517	0.036	1
1	A	62	GLY	H	10.548	0.021	1
1	A	62	GLY	HA2	3.482	0.006	2
1	A	62	GLY	HA3	4.197	0.004	2
1	A	62	GLY	C	173.265	0.000	1
1	A	62	GLY	CA	45.779	0.000	1
1	A	62	GLY	N	113.313	0.057	1
1	A	63	THR	H	7.66	0.002	1
1	A	63	THR	HA	4.748	0.004	1
1	A	63	THR	HB	4.006	0.012	1
1	A	63	THR	HG21	1.128	0.002	1
1	A	63	THR	HG22	1.128	0.002	1
1	A	63	THR	HG23	1.128	0.002	1
1	A	63	THR	CA	59.673	0.000	1
1	A	63	THR	CB	72.192	0.038	1
1	A	63	THR	CG2	22.443	0.035	1
1	A	63	THR	N	108.756	0.048	1
1	A	64	ILE	H	8.795	0.032	1
1	A	64	ILE	HA	5.134	0.017	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	ILE	HB	2.009	0.000	1
1	A	64	ILE	HD11	0.809	0.002	1
1	A	64	ILE	HD12	0.809	0.002	1
1	A	64	ILE	HD13	0.809	0.002	1
1	A	64	ILE	HG21	1.234	0.016	1
1	A	64	ILE	HG22	1.234	0.016	1
1	A	64	ILE	HG23	1.234	0.016	1
1	A	64	ILE	C	175.547	0.000	1
1	A	64	ILE	CA	59.998	0.046	1
1	A	64	ILE	CB	39.811	0.000	1
1	A	64	ILE	CD1	13.619	0.000	1
1	A	64	ILE	CG1	27.393	0.000	1
1	A	64	ILE	CG2	18.522	0.044	1
1	A	64	ILE	N	123.463	0.026	1
1	A	65	ASP	H	8.89	0.012	1
1	A	65	ASP	HA	5.39	0.001	1
1	A	65	ASP	HB2	3.08	0.000	2
1	A	65	ASP	HB3	2.834	0.000	2
1	A	65	ASP	C	176.335	0.000	1
1	A	65	ASP	CA	52.27	0.001	1
1	A	65	ASP	CB	42.309	0.001	1
1	A	65	ASP	N	128.376	0.055	1
1	A	66	PHE	H	8.945	0.003	1
1	A	66	PHE	HA	4.029	0.000	1
1	A	66	PHE	HD1	6.74	0.000	1
1	A	66	PHE	HD2	6.74	0.000	1
1	A	66	PHE	HE1	7.191	0.000	1
1	A	66	PHE	HE2	7.191	0.000	1
1	A	66	PHE	CA	63.616	0.000	1
1	A	66	PHE	CB	35.993	0.037	1
1	A	66	PHE	N	118.871	0.041	1
1	A	67	PRO	HA	3.898	0.000	1
1	A	67	PRO	HB2	2.234	0.000	2
1	A	67	PRO	HB3	1.918	0.000	2
1	A	67	PRO	C	180.066	0.000	1
1	A	67	PRO	CA	66.713	0.158	1
1	A	67	PRO	CB	30.614	0.061	1
1	A	67	PRO	CG	28.646	0.000	1
1	A	68	GLU	H	8.027	0.041	1
1	A	68	GLU	HA	4.098	0.000	1
1	A	68	GLU	HB2	2.598	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	GLU	HB3	2.079	0.000	2
1	A	68	GLU	HG2	2.93	0.000	2
1	A	68	GLU	HG3	2.538	0.000	2
1	A	68	GLU	CA	59.013	0.077	1
1	A	68	GLU	CB	29.631	0.023	1
1	A	68	GLU	CG	36.905	0.000	1
1	A	68	GLU	N	117.722	0.037	1
1	A	69	PHE	H	8.786	0.028	1
1	A	69	PHE	HA	3.928	0.000	1
1	A	69	PHE	HB2	3.502	0.000	2
1	A	69	PHE	HB3	3.177	0.000	2
1	A	69	PHE	CA	61.484	0.000	1
1	A	69	PHE	CB	40.15	0.000	1
1	A	69	PHE	N	123.607	0.054	1
1	A	70	LEU	HA	3.367	0.010	1
1	A	70	LEU	HB2	1.574	0.004	2
1	A	70	LEU	HB3	1.18	0.014	2
1	A	70	LEU	HD11	0.634	0.001	1
1	A	70	LEU	HD12	0.634	0.001	1
1	A	70	LEU	HD13	0.634	0.001	1
1	A	70	LEU	HD21	0.657	0.004	1
1	A	70	LEU	HD22	0.657	0.004	1
1	A	70	LEU	HD23	0.657	0.004	1
1	A	70	LEU	C	179.097	0.000	1
1	A	70	LEU	CA	58.086	0.072	1
1	A	70	LEU	CB	41.058	0.055	1
1	A	70	LEU	CD1	25.505	0.015	1
1	A	70	LEU	CD2	23.999	0.327	1
1	A	71	THR	H	7.577	0.029	1
1	A	71	THR	HA	3.774	0.005	1
1	A	71	THR	HB	4.296	0.007	1
1	A	71	THR	HG21	1.201	0.013	1
1	A	71	THR	HG22	1.201	0.013	1
1	A	71	THR	HG23	1.201	0.013	1
1	A	71	THR	CA	66.534	0.000	1
1	A	71	THR	CB	68.507	0.000	1
1	A	71	THR	CG2	21.996	0.023	1
1	A	71	THR	N	115.304	0.360	1
1	A	72	MET	H	7.778	0.009	1
1	A	72	MET	HA	3.769	0.003	1
1	A	72	MET	HB2	2.127	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	MET	HB3	1.965	0.000	2
1	A	72	MET	HG2	2.39	0.000	1
1	A	72	MET	HG3	2.39	0.000	1
1	A	72	MET	C	177.746	0.000	1
1	A	72	MET	CA	58.788	0.000	1
1	A	72	MET	CB	32.976	0.126	1
1	A	72	MET	CG	31.364	0.000	1
1	A	72	MET	N	121.61	0.154	1
1	A	73	MET	H	7.989	0.054	1
1	A	73	MET	CA	55.869	0.000	1
1	A	73	MET	CB	31.344	0.000	1
1	A	73	MET	N	116.573	0.041	1
1	A	77	MET	HA	4.385	0.000	1
1	A	77	MET	HE1	2.154	0.001	1
1	A	77	MET	HE2	2.154	0.001	1
1	A	77	MET	HE3	2.154	0.001	1
1	A	77	MET	CE	17.176	0.000	1
1	A	78	LYS	HA	4.37	0.000	1
1	A	78	LYS	HB2	2.087	0.000	2
1	A	78	LYS	HB3	1.985	0.000	2
1	A	78	LYS	CA	56.29	0.000	1
1	A	78	LYS	CB	33.408	0.000	1
1	A	79	ASP	H	8.273	0.010	1
1	A	79	ASP	HA	4.66	0.000	1
1	A	79	ASP	HB2	2.751	0.000	2
1	A	79	ASP	HB3	2.621	0.000	2
1	A	79	ASP	CA	54.722	0.078	1
1	A	79	ASP	CB	41.084	0.032	1
1	A	79	ASP	N	121.518	0.262	1
1	A	80	THR	H	7.97	0.012	1
1	A	80	THR	HA	4.332	0.008	1
1	A	80	THR	HB	4.212	0.003	1
1	A	80	THR	HG21	1.215	0.011	1
1	A	80	THR	HG22	1.215	0.011	1
1	A	80	THR	HG23	1.215	0.011	1
1	A	80	THR	CA	61.937	0.000	1
1	A	80	THR	CB	69.958	0.014	1
1	A	80	THR	CG2	21.61	0.001	1
1	A	80	THR	N	113.776	0.034	1
1	A	81	ASP	H	8.398	0.009	1
1	A	81	ASP	HA	4.725	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	ASP	HB2	2.676	0.008	1
1	A	81	ASP	HB3	2.676	0.008	1
1	A	81	ASP	C	176.398	0.000	1
1	A	81	ASP	CA	54.534	0.052	1
1	A	81	ASP	CB	41.529	0.037	1
1	A	81	ASP	N	122.88	0.047	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
$^{13}\text{C}_\alpha$	143	-0.41 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	132	0.12 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	123	-0.45 ± 0.14	None needed (< 0.5 ppm)
^{15}N	138	0.01 ± 0.59	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 69%, i.e. 721 atoms were assigned a chemical shift out of a possible 1038. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	330/380 (87%)	137/155 (88%)	127/150 (85%)	66/75 (88%)
Sidechain	373/596 (63%)	254/382 (66%)	119/187 (64%)	0/27 (0%)
Aromatic	18/62 (29%)	18/31 (58%)	0/29 (0%)	0/2 (0%)
Overall	721/1038 (69%)	409/568 (72%)	246/366 (67%)	66/104 (63%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 66%, i.e. 733 atoms were assigned a chemical shift out of a possible 1106. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	338/405 (83%)	140/165 (85%)	130/160 (81%)	68/80 (85%)
Sidechain	377/639 (59%)	256/409 (63%)	121/202 (60%)	0/28 (0%)
Aromatic	18/62 (29%)	18/31 (58%)	0/29 (0%)	0/2 (0%)
Overall	733/1106 (66%)	414/605 (68%)	251/391 (64%)	68/110 (62%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

