wwPDB NMR Structure Validation Summary Report

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PDB ID	:	5OVM
BMRB ID	:	34175
Title	:	Solution structure of lipase binding domain LID1 of foldase from Pseudomonas aeruginosa
Authors	:	Viegas, A.; Jaeger, K.-E.; Etzkorn, M.; Gohlke, H.; Verma, N.; Dollinger, P.; Kovacic, F.
Deposited on	:	2017-08-29

This is a wwPDB NMR Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

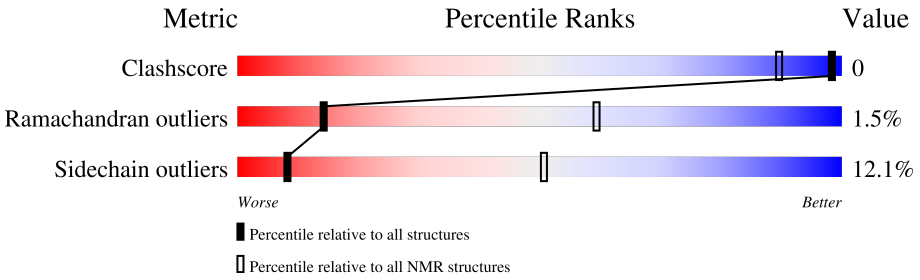
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 was not calculated.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	89	85% . . 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:67-A:146 (80)	1.90	9

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1291 atoms, of which 641 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipase chaperone.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	82	1291	411	641	112	126	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	MET	-	initiating methionine	UNP Q01725
A	59	GLY	-	expression tag	UNP Q01725
A	60	HIS	-	expression tag	UNP Q01725
A	61	HIS	-	expression tag	UNP Q01725
A	62	HIS	-	expression tag	UNP Q01725
A	63	HIS	-	expression tag	UNP Q01725
A	64	HIS	-	expression tag	UNP Q01725
A	65	HIS	-	expression tag	UNP Q01725

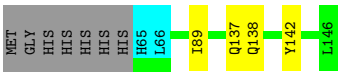
4 Residue-property plots (i)

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: Lipase chaperone

Chain A:

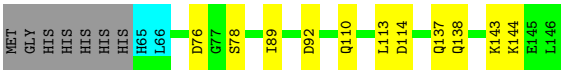


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 9. Colouring as in section 4.1 above.

• Molecule 1: Lipase chaperone

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	
Amber	geometry optimization	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	929
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	929
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

6 Model quality

6.1 Standard geometry

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

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	632	623	623	0±1
All	All	12640	12460	12460	4

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ASP:OD1	1:A:117:ARG:NE	0.59	2.32	12	1
1:A:79:PHE:CE1	1:A:96:LEU:HD13	0.48	2.43	10	1
1:A:93:ILE:HA	1:A:96:LEU:HD12	0.47	1.87	10	1
1:A:93:ILE:HG22	1:A:97:PHE:CE1	0.46	2.45	13	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	79/89 (89%)	72±2 (91±3%)	6±2 (8±2%)	1±1 (2±1%)	14 59
All	All	1580/1780 (89%)	1433 (91%)	123 (8%)	24 (2%)	14 59

5 of 15 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	78	SER	3
1	A	89	ILE	3
1	A	70	PHE	2
1	A	75	VAL	2
1	A	106	GLU	2

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	67/75 (89%)	59±2 (88±3%)	8±2 (12±3%)	8 51
All	All	1340/1500 (89%)	1178 (88%)	162 (12%)	8 51

5 of 35 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	89	ILE	19
1	A	137	GLN	18
1	A	138	GLN	16
1	A	142	TYR	13
1	A	110	GLN	9

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 monosaccharides 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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *MD1_3.1_6.str*

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	929
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	929
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. First 5 (of 929) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	HIS	H	7.809	0.020	1
1	A	8	HIS	CA	56.304	0.300	1
1	A	8	HIS	HA	4.597	0.020	1
1	A	8	HIS	CB	30.891	0.300	1
1	A	8	HIS	HB2	2.977	0.020	2
1	A	8	HIS	HB3	2.977	0.020	2
1	A	8	HIS	C	174.96	0.300	1
1	A	9	LEU	N	124.342	0.300	1
1	A	9	LEU	H	8.154	0.020	1
1	A	9	LEU	CA	52.857	0.300	1
1	A	9	LEU	HA	4.535	0.020	1
1	A	9	LEU	CB	41.855	0.300	1
1	A	9	LEU	HB2	1.444	0.020	2
1	A	9	LEU	HB3	1.535	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	LEU	CG	26.754	0.300	1
1	A	9	LEU	HG	1.479	0.020	1
1	A	9	LEU	HD11	0.796	0.020	2
1	A	9	LEU	HD12	0.796	0.020	2
1	A	9	LEU	HD13	0.796	0.020	2
1	A	9	LEU	HD21	0.784	0.020	2
1	A	9	LEU	HD22	0.784	0.020	2
1	A	9	LEU	HD23	0.784	0.020	2
1	A	9	LEU	CD1	25.047	0.300	1
1	A	9	LEU	CD2	23.42	0.300	1
1	A	9	LEU	C	175.067	0.300	1
1	A	10	PRO	CD	50.507	0.300	1
1	A	10	PRO	CA	63.263	0.300	1
1	A	10	PRO	HA	4.474	0.020	1
1	A	10	PRO	CB	32.041	0.300	1
1	A	10	PRO	HB2	1.918	0.020	2
1	A	10	PRO	HB3	2.3	0.020	2
1	A	10	PRO	CG	27.482	0.300	1
1	A	10	PRO	HG2	1.943	0.020	2
1	A	10	PRO	HG3	1.943	0.020	2
1	A	10	PRO	HD2	3.474	0.020	2
1	A	10	PRO	HD3	3.719	0.020	2
1	A	11	THR	CA	59.639	0.300	1
1	A	11	THR	HA	4.655	0.020	1
1	A	11	THR	CB	71.835	0.300	1
1	A	11	THR	HB	4.582	0.020	1
1	A	11	THR	HG21	1.184	0.020	1
1	A	11	THR	HG22	1.184	0.020	1
1	A	11	THR	HG23	1.184	0.020	1
1	A	11	THR	CG2	21.277	0.300	1
1	A	12	SER	CA	58.415	0.300	1
1	A	12	SER	HA	4.029	0.020	1
1	A	12	SER	CB	64.687	0.300	1
1	A	12	SER	HB2	3.602	0.020	2
1	A	12	SER	HB3	3.602	0.020	2
1	A	12	SER	C	170.821	0.300	1
1	A	13	PHE	N	119.016	0.300	1
1	A	13	PHE	H	8.342	0.020	1
1	A	13	PHE	CA	57.236	0.300	1
1	A	13	PHE	HA	4.759	0.020	1
1	A	13	PHE	CB	40.829	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	PHE	HB2	2.956	0.020	2
1	A	13	PHE	HB3	2.956	0.020	2
1	A	13	PHE	HD1	7.326	0.020	1
1	A	13	PHE	HE1	7.037	0.020	1
1	A	13	PHE	HE2	7.037	0.020	1
1	A	13	PHE	HD2	7.326	0.020	1
1	A	13	PHE	C	175.725	0.300	1
1	A	14	ARG	CA	56.512	0.300	1
1	A	14	ARG	HA	4.6	0.020	1
1	A	14	ARG	CB	30.535	0.300	1
1	A	14	ARG	HB2	1.742	0.020	2
1	A	14	ARG	HB3	1.873	0.020	2
1	A	14	ARG	CG	26.811	0.300	1
1	A	14	ARG	HG2	1.588	0.020	2
1	A	14	ARG	HG3	1.588	0.020	2
1	A	14	ARG	CD	43.418	0.300	1
1	A	14	ARG	HD2	3.151	0.020	2
1	A	14	ARG	HD3	3.151	0.020	2
1	A	18	VAL	H	8.019	0.020	1
1	A	18	VAL	CA	62.3	0.300	1
1	A	18	VAL	HA	3.87	0.020	1
1	A	18	VAL	CB	32.423	0.300	1
1	A	18	VAL	HB	1.849	0.020	1
1	A	18	VAL	HG11	0.719	0.020	2
1	A	18	VAL	HG12	0.719	0.020	2
1	A	18	VAL	HG13	0.719	0.020	2
1	A	18	VAL	HG21	0.641	0.020	2
1	A	18	VAL	HG22	0.641	0.020	2
1	A	18	VAL	HG23	0.641	0.020	2
1	A	18	VAL	CG1	21.225	0.300	1
1	A	18	VAL	CG2	20.916	0.300	1
1	A	19	ASP	CA	54.424	0.300	1
1	A	19	ASP	HA	4.574	0.020	1
1	A	19	ASP	CB	41.267	0.300	1
1	A	19	ASP	HB2	2.562	0.020	2
1	A	19	ASP	HB3	2.627	0.020	2
1	A	19	ASP	C	173.175	0.300	1
1	A	20	GLY	N	109.016	0.300	1
1	A	20	GLY	H	8.056	0.020	1
1	A	20	GLY	CA	45.046	0.300	1
1	A	20	GLY	HA2	3.76	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	GLY	HA3	3.942	0.020	2
1	A	20	GLY	C	173.003	0.300	1
1	A	22	PHE	CA	57.636	0.300	1
1	A	22	PHE	HA	4.451	0.020	1
1	A	22	PHE	CB	39.137	0.300	1
1	A	22	PHE	HB2	2.898	0.020	2
1	A	22	PHE	HB3	2.898	0.020	2
1	A	22	PHE	HD1	6.858	0.020	1
1	A	22	PHE	HE1	7.035	0.020	1
1	A	22	PHE	HE2	7.035	0.020	1
1	A	22	PHE	HD2	6.858	0.020	1
1	A	23	SER	CA	57.876	0.300	1
1	A	23	SER	HA	4.778	0.020	1
1	A	23	SER	CB	65.202	0.300	1
1	A	23	SER	HB2	3.814	0.020	2
1	A	23	SER	HB3	3.878	0.020	2
1	A	23	SER	C	169.734	0.300	1
1	A	24	VAL	N	118.185	0.300	1
1	A	24	VAL	H	8.265	0.020	1
1	A	24	VAL	CA	59.374	0.300	1
1	A	24	VAL	HA	5.118	0.020	1
1	A	24	VAL	CB	35.169	0.300	1
1	A	24	VAL	HB	1.874	0.020	1
1	A	24	VAL	HG11	0.808	0.020	2
1	A	24	VAL	HG12	0.808	0.020	2
1	A	24	VAL	HG13	0.808	0.020	2
1	A	24	VAL	HG21	0.848	0.020	2
1	A	24	VAL	HG22	0.848	0.020	2
1	A	24	VAL	HG23	0.848	0.020	2
1	A	24	VAL	CG1	21.56	0.300	1
1	A	24	VAL	CG2	19.439	0.300	1
1	A	24	VAL	C	176.392	0.300	1
1	A	25	ASP	N	123.462	0.300	1
1	A	25	ASP	H	8.836	0.020	1
1	A	25	ASP	CA	52.547	0.300	1
1	A	25	ASP	HA	4.721	0.020	1
1	A	25	ASP	CB	41.595	0.300	1
1	A	25	ASP	HB2	2.631	0.020	2
1	A	25	ASP	HB3	3.399	0.020	2
1	A	25	ASP	C	178.121	0.300	1
1	A	26	ALA	H	8.319	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	ALA	CA	54.454	0.300	1
1	A	26	ALA	HA	4.186	0.020	1
1	A	26	ALA	HB1	1.492	0.020	1
1	A	26	ALA	HB2	1.492	0.020	1
1	A	26	ALA	HB3	1.492	0.020	1
1	A	26	ALA	CB	18.548	0.300	1
1	A	26	ALA	C	176.246	0.300	1
1	A	27	SER	N	112.974	0.300	1
1	A	27	SER	H	8.194	0.020	1
1	A	27	SER	CA	58.338	0.300	1
1	A	27	SER	HA	4.597	0.020	1
1	A	27	SER	CB	63.812	0.300	1
1	A	27	SER	HB2	3.81	0.020	2
1	A	27	SER	HB3	3.924	0.020	2
1	A	27	SER	C	174.044	0.300	1
1	A	28	GLY	N	109.305	0.300	1
1	A	28	GLY	H	8.169	0.020	1
1	A	28	GLY	CA	45.17	0.300	1
1	A	28	GLY	HA2	3.487	0.020	2
1	A	28	GLY	HA3	4.221	0.020	2
1	A	28	GLY	C	173.914	0.300	1
1	A	29	ASN	N	118.014	0.300	1
1	A	29	ASN	H	8.407	0.020	1
1	A	29	ASN	CA	53.216	0.300	1
1	A	29	ASN	HA	4.749	0.020	1
1	A	29	ASN	CB	39.488	0.300	1
1	A	29	ASN	HB2	2.651	0.020	2
1	A	29	ASN	HB3	2.84	0.020	2
1	A	29	ASN	CG	174.176	0.300	1
1	A	29	ASN	ND2	116.545	0.300	1
1	A	29	ASN	HD21	8.145	0.020	2
1	A	29	ASN	HD22	6.949	0.020	2
1	A	29	ASN	C	175.14	0.300	1
1	A	30	LEU	N	121.788	0.300	1
1	A	30	LEU	H	8.852	0.020	1
1	A	30	LEU	CA	55.454	0.300	1
1	A	30	LEU	HA	4.287	0.020	1
1	A	30	LEU	CB	44.09	0.300	1
1	A	30	LEU	HB2	1.468	0.020	2
1	A	30	LEU	HB3	1.841	0.020	2
1	A	30	LEU	CG	26.119	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	LEU	HG	0.797	0.020	1
1	A	30	LEU	HD11	0.977	0.020	2
1	A	30	LEU	HD12	0.977	0.020	2
1	A	30	LEU	HD13	0.977	0.020	2
1	A	30	LEU	HD21	1.021	0.020	2
1	A	30	LEU	HD22	1.021	0.020	2
1	A	30	LEU	HD23	1.021	0.020	2
1	A	30	LEU	CD1	25.338	0.300	1
1	A	30	LEU	CD2	23.842	0.300	1
1	A	30	LEU	C	176.668	0.300	1
1	A	31	LEU	N	128.473	0.300	1
1	A	31	LEU	H	8.662	0.020	1
1	A	31	LEU	CA	54.139	0.300	1
1	A	31	LEU	HA	4.511	0.020	1
1	A	31	LEU	CB	42.122	0.300	1
1	A	31	LEU	HB2	1.345	0.020	2
1	A	31	LEU	HB3	1.535	0.020	2
1	A	31	LEU	CG	26.981	0.300	1
1	A	31	LEU	HG	1.481	0.020	1
1	A	31	LEU	HD11	0.802	0.020	2
1	A	31	LEU	HD12	0.802	0.020	2
1	A	31	LEU	HD13	0.802	0.020	2
1	A	31	LEU	HD21	0.89	0.020	2
1	A	31	LEU	HD22	0.89	0.020	2
1	A	31	LEU	HD23	0.89	0.020	2
1	A	31	LEU	CD1	25.205	0.300	1
1	A	31	LEU	CD2	23.999	0.300	1
1	A	31	LEU	C	176.127	0.300	1
1	A	32	ILE	N	124.151	0.300	1
1	A	32	ILE	H	8.67	0.020	1
1	A	32	ILE	CA	61.628	0.300	1
1	A	32	ILE	HA	4.036	0.020	1
1	A	32	ILE	CB	36.21	0.300	1
1	A	32	ILE	HB	1.958	0.020	1
1	A	32	ILE	HG21	0.869	0.020	1
1	A	32	ILE	HG22	0.869	0.020	1
1	A	32	ILE	HG23	0.869	0.020	1
1	A	32	ILE	CG2	17.916	0.300	1
1	A	32	ILE	CG1	27.317	0.300	1
1	A	32	ILE	HG12	1.202	0.020	2
1	A	32	ILE	HG13	1.531	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	ILE	HD11	0.843	0.020	1
1	A	32	ILE	HD12	0.843	0.020	1
1	A	32	ILE	HD13	0.843	0.020	1
1	A	32	ILE	CD1	12.08	0.300	1
1	A	32	ILE	C	176.04	0.300	1
1	A	33	THR	CA	62.245	0.300	1
1	A	33	THR	HA	4.245	0.020	1
1	A	33	THR	CB	69.55	0.300	1
1	A	33	THR	HB	4.216	0.020	1
1	A	33	THR	HG21	1.191	0.020	1
1	A	33	THR	HG22	1.191	0.020	1
1	A	33	THR	HG23	1.191	0.020	1
1	A	33	THR	CG2	21.795	0.300	1
1	A	34	ARG	CA	57.272	0.300	1
1	A	34	ARG	HA	4.049	0.020	1
1	A	34	ARG	CB	30.025	0.300	1
1	A	34	ARG	HB2	1.886	0.020	2
1	A	34	ARG	HB3	1.886	0.020	2
1	A	34	ARG	CG	26.885	0.300	1
1	A	34	ARG	HG2	1.692	0.020	2
1	A	34	ARG	HG3	1.692	0.020	2
1	A	34	ARG	CD	43.519	0.300	1
1	A	34	ARG	HD2	3.204	0.020	2
1	A	34	ARG	HD3	3.204	0.020	2
1	A	36	ILE	N	119.324	0.300	1
1	A	36	ILE	H	7.496	0.020	1
1	A	36	ILE	CA	64.262	0.300	1
1	A	36	ILE	HA	3.544	0.020	1
1	A	36	ILE	CB	37.247	0.300	1
1	A	36	ILE	HB	1.843	0.020	1
1	A	36	ILE	HG21	0.601	0.020	1
1	A	36	ILE	HG22	0.601	0.020	1
1	A	36	ILE	HG23	0.601	0.020	1
1	A	36	ILE	CG2	17.734	0.300	1
1	A	36	ILE	CG1	28.871	0.300	1
1	A	36	ILE	HG12	1.099	0.020	2
1	A	36	ILE	HG13	1.64	0.020	2
1	A	36	ILE	HD11	1.091	0.020	1
1	A	36	ILE	HD12	1.091	0.020	1
1	A	36	ILE	HD13	1.091	0.020	1
1	A	36	ILE	CD1	14.137	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	ARG	H	7.379	0.020	1
1	A	37	ARG	CA	59.555	0.300	1
1	A	37	ARG	HA	3.62	0.020	1
1	A	37	ARG	CB	29.416	0.300	1
1	A	37	ARG	HB2	1.826	0.020	2
1	A	37	ARG	HB3	1.826	0.020	2
1	A	37	ARG	CG	27.323	0.300	1
1	A	37	ARG	HG2	1.669	0.020	2
1	A	37	ARG	HG3	1.669	0.020	2
1	A	37	ARG	CD	43.313	0.300	1
1	A	37	ARG	HD2	3.137	0.020	2
1	A	37	ARG	HD3	3.137	0.020	2
1	A	37	ARG	C	175.009	0.300	1
1	A	38	ASN	N	115.866	0.300	1
1	A	38	ASN	H	7.686	0.020	1
1	A	38	ASN	CA	55.869	0.300	1
1	A	38	ASN	HA	4.455	0.020	1
1	A	38	ASN	CB	37.664	0.300	1
1	A	38	ASN	HB2	2.797	0.020	2
1	A	38	ASN	HB3	2.929	0.020	2
1	A	38	ASN	CG	173.099	0.300	1
1	A	38	ASN	ND2	111.77	0.300	1
1	A	38	ASN	HD21	7.936	0.020	2
1	A	38	ASN	HD22	6.83	0.020	2
1	A	38	ASN	C	177.87	0.300	1
1	A	39	LEU	N	122.776	0.300	1
1	A	39	LEU	H	7.714	0.020	1
1	A	39	LEU	CA	58.299	0.300	1
1	A	39	LEU	HA	4.016	0.020	1
1	A	39	LEU	CB	41.68	0.300	1
1	A	39	LEU	HB2	1.421	0.020	2
1	A	39	LEU	HB3	1.711	0.020	2
1	A	39	LEU	CG	26.98	0.300	1
1	A	39	LEU	HG	1.473	0.020	1
1	A	39	LEU	HD11	0.636	0.020	2
1	A	39	LEU	HD12	0.636	0.020	2
1	A	39	LEU	HD13	0.636	0.020	2
1	A	39	LEU	HD21	0.563	0.020	2
1	A	39	LEU	HD22	0.563	0.020	2
1	A	39	LEU	HD23	0.563	0.020	2
1	A	39	LEU	CD1	25.39	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	39	LEU	CD2	24.348	0.300	1
1	A	39	LEU	C	178.767	0.300	1
1	A	40	PHE	N	118.284	0.300	1
1	A	40	PHE	H	8.113	0.020	1
1	A	40	PHE	CA	59.169	0.300	1
1	A	40	PHE	HA	4.453	0.020	1
1	A	40	PHE	CB	36.544	0.300	1
1	A	40	PHE	HB2	2.691	0.020	2
1	A	40	PHE	HB3	2.951	0.020	2
1	A	40	PHE	HD1	6.832	0.020	1
1	A	40	PHE	HE1	6.926	0.020	1
1	A	40	PHE	HZ	7.131	0.020	1
1	A	40	PHE	HE2	6.926	0.020	1
1	A	40	PHE	HD2	6.832	0.020	1
1	A	40	PHE	C	178.024	0.300	1
1	A	41	ASP	N	118.538	0.300	1
1	A	41	ASP	H	8.707	0.020	1
1	A	41	ASP	CA	57.631	0.300	1
1	A	41	ASP	HA	4.495	0.020	1
1	A	41	ASP	CB	40.492	0.300	1
1	A	41	ASP	HB2	2.726	0.020	2
1	A	41	ASP	HB3	2.927	0.020	2
1	A	41	ASP	C	178.967	0.300	1
1	A	42	TYR	N	120.881	0.300	1
1	A	42	TYR	H	8.011	0.020	1
1	A	42	TYR	CA	61.179	0.300	1
1	A	42	TYR	HA	4.293	0.020	1
1	A	42	TYR	CB	38.217	0.300	1
1	A	42	TYR	HB2	3.127	0.020	2
1	A	42	TYR	HB3	3.127	0.020	2
1	A	42	TYR	HD1	6.794	0.020	1
1	A	42	TYR	HE1	7.038	0.020	1
1	A	42	TYR	HE2	7.038	0.020	1
1	A	42	TYR	HD2	6.794	0.020	1
1	A	42	TYR	C	178.143	0.300	1
1	A	43	PHE	N	117.144	0.300	1
1	A	43	PHE	H	8.017	0.020	1
1	A	43	PHE	CA	61.864	0.300	1
1	A	43	PHE	HA	4.039	0.020	1
1	A	43	PHE	CB	40.617	0.300	1
1	A	43	PHE	HB2	3.048	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	PHE	HB3	3.048	0.020	2
1	A	43	PHE	HD1	7.426	0.020	1
1	A	43	PHE	HE1	6.559	0.020	1
1	A	43	PHE	HE2	6.559	0.020	1
1	A	43	PHE	HD2	7.426	0.020	1
1	A	43	PHE	C	177.984	0.300	1
1	A	44	LEU	N	117.048	0.300	1
1	A	44	LEU	H	8.365	0.020	1
1	A	44	LEU	CA	55.856	0.300	1
1	A	44	LEU	HA	4.416	0.020	1
1	A	44	LEU	CB	41.505	0.300	1
1	A	44	LEU	HB2	1.676	0.020	2
1	A	44	LEU	HB3	1.969	0.020	2
1	A	44	LEU	CG	26.743	0.300	1
1	A	44	LEU	HG	1.88	0.020	1
1	A	44	LEU	HD11	0.809	0.020	2
1	A	44	LEU	HD12	0.809	0.020	2
1	A	44	LEU	HD13	0.809	0.020	2
1	A	44	LEU	HD21	0.838	0.020	2
1	A	44	LEU	HD22	0.838	0.020	2
1	A	44	LEU	HD23	0.838	0.020	2
1	A	44	LEU	CD1	25.455	0.300	1
1	A	44	LEU	CD2	23.256	0.300	1
1	A	44	LEU	C	177.783	0.300	1
1	A	45	SER	N	114.293	0.300	1
1	A	45	SER	H	7.722	0.020	1
1	A	45	SER	CA	59.429	0.300	1
1	A	45	SER	HA	4.455	0.020	1
1	A	45	SER	CB	63.835	0.300	1
1	A	45	SER	HB2	3.976	0.020	2
1	A	45	SER	HB3	3.976	0.020	2
1	A	45	SER	C	174.657	0.300	1
1	A	46	ALA	N	125.117	0.300	1
1	A	46	ALA	H	7.76	0.020	1
1	A	46	ALA	CA	52.619	0.300	1
1	A	46	ALA	HA	4.297	0.020	1
1	A	46	ALA	HB1	1.249	0.020	1
1	A	46	ALA	HB2	1.249	0.020	1
1	A	46	ALA	HB3	1.249	0.020	1
1	A	46	ALA	CB	19.095	0.300	1
1	A	46	ALA	C	177.414	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	VAL	N	117.742	0.300	1
1	A	47	VAL	H	7.791	0.020	1
1	A	47	VAL	CA	62.683	0.300	1
1	A	47	VAL	HA	4.116	0.020	1
1	A	47	VAL	CB	32.219	0.300	1
1	A	47	VAL	HB	2.092	0.020	1
1	A	47	VAL	HG11	0.92	0.020	2
1	A	47	VAL	HG12	0.92	0.020	2
1	A	47	VAL	HG13	0.92	0.020	2
1	A	47	VAL	HG21	0.947	0.020	2
1	A	47	VAL	HG22	0.947	0.020	2
1	A	47	VAL	HG23	0.947	0.020	2
1	A	47	VAL	CG1	21.446	0.300	1
1	A	47	VAL	CG2	20.768	0.300	1
1	A	47	VAL	C	176.803	0.300	1
1	A	48	GLY	N	112.824	0.300	1
1	A	48	GLY	H	8.351	0.020	1
1	A	48	GLY	CA	45.429	0.300	1
1	A	48	GLY	HA2	3.857	0.020	2
1	A	48	GLY	HA3	4.091	0.020	2
1	A	48	GLY	C	174.417	0.300	1
1	A	49	GLU	N	121.045	0.300	1
1	A	49	GLU	H	8.454	0.020	1
1	A	49	GLU	CA	57.451	0.300	1
1	A	49	GLU	HA	4.242	0.020	1
1	A	49	GLU	CB	29.885	0.300	1
1	A	49	GLU	HB2	1.983	0.020	2
1	A	49	GLU	HB3	2.131	0.020	2
1	A	49	GLU	CG	36.112	0.300	1
1	A	49	GLU	HG2	2.253	0.020	2
1	A	49	GLU	HG3	2.253	0.020	2
1	A	49	GLU	C	176.539	0.300	1
1	A	50	GLU	H	8.123	0.020	1
1	A	50	GLU	HA	4.604	0.020	1
1	A	51	PRO	CD	50.715	0.300	1
1	A	51	PRO	CA	63.358	0.300	1
1	A	51	PRO	HA	4.475	0.020	1
1	A	51	PRO	CB	32.071	0.300	1
1	A	51	PRO	HB2	1.914	0.020	2
1	A	51	PRO	HB3	2.251	0.020	2
1	A	51	PRO	CG	27.976	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	PRO	HG2	1.96	0.020	2
1	A	51	PRO	HG3	2.039	0.020	2
1	A	51	PRO	HD2	3.594	0.020	2
1	A	51	PRO	HD3	3.936	0.020	2
1	A	52	LEU	CA	58.044	0.300	1
1	A	52	LEU	HA	4.235	0.020	1
1	A	52	LEU	CB	41.846	0.300	1
1	A	52	LEU	HB2	1.993	0.020	2
1	A	52	LEU	HB3	1.854	0.020	2
1	A	52	LEU	CG	26.847	0.300	1
1	A	52	LEU	HG	1.747	0.020	1
1	A	52	LEU	HD11	0.975	0.020	2
1	A	52	LEU	HD12	0.975	0.020	2
1	A	52	LEU	HD13	0.975	0.020	2
1	A	52	LEU	HD21	0.915	0.020	2
1	A	52	LEU	HD22	0.915	0.020	2
1	A	52	LEU	HD23	0.915	0.020	2
1	A	52	LEU	CD1	25.353	0.300	1
1	A	52	LEU	CD2	24.542	0.300	1
1	A	52	LEU	C	175.629	0.300	1
1	A	53	GLN	N	116.27	0.300	1
1	A	53	GLN	H	8.724	0.020	1
1	A	53	GLN	CA	59.031	0.300	1
1	A	53	GLN	HA	3.888	0.020	1
1	A	53	GLN	CB	28.213	0.300	1
1	A	53	GLN	HB2	2.044	0.020	2
1	A	53	GLN	HB3	2.185	0.020	2
1	A	53	GLN	CG	33.29	0.300	1
1	A	53	GLN	HG2	2.455	0.020	2
1	A	53	GLN	HG3	2.455	0.020	2
1	A	53	GLN	CD	177.619	0.300	1
1	A	53	GLN	NE2	114.127	0.300	1
1	A	53	GLN	HE21	7.788	0.020	2
1	A	53	GLN	HE22	6.844	0.020	2
1	A	53	GLN	C	178.083	0.300	1
1	A	54	GLN	N	116.726	0.300	1
1	A	54	GLN	H	7.611	0.020	1
1	A	54	GLN	CA	58.925	0.300	1
1	A	54	GLN	HA	4.244	0.020	1
1	A	54	GLN	CB	28.666	0.300	1
1	A	54	GLN	HB2	2.161	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	GLN	HB3	2.223	0.020	2
1	A	54	GLN	CG	34.51	0.300	1
1	A	54	GLN	HG2	2.448	0.020	2
1	A	54	GLN	HG3	2.448	0.020	2
1	A	54	GLN	CD	177.304	0.300	1
1	A	54	GLN	NE2	111.883	0.300	1
1	A	54	GLN	HE21	7.685	0.020	2
1	A	54	GLN	HE22	6.904	0.020	2
1	A	54	GLN	C	179.05	0.300	1
1	A	55	SER	N	117.585	0.300	1
1	A	55	SER	H	7.984	0.020	1
1	A	55	SER	CA	61.886	0.300	1
1	A	55	SER	HA	4.352	0.020	1
1	A	55	SER	CB	62.885	0.300	1
1	A	55	SER	HB2	4.114	0.020	2
1	A	55	SER	HB3	4.114	0.020	2
1	A	55	SER	C	179.073	0.300	1
1	A	56	LEU	N	121.267	0.300	1
1	A	56	LEU	H	8.545	0.020	1
1	A	56	LEU	CA	58.071	0.300	1
1	A	56	LEU	HA	3.963	0.020	1
1	A	56	LEU	CB	41.522	0.300	1
1	A	56	LEU	HB2	1.681	0.020	2
1	A	56	LEU	HB3	1.858	0.020	2
1	A	56	LEU	CG	26.582	0.300	1
1	A	56	LEU	HG	1.411	0.020	1
1	A	56	LEU	HD11	0.853	0.020	2
1	A	56	LEU	HD12	0.853	0.020	2
1	A	56	LEU	HD13	0.853	0.020	2
1	A	56	LEU	HD21	0.92	0.020	2
1	A	56	LEU	HD22	0.92	0.020	2
1	A	56	LEU	HD23	0.92	0.020	2
1	A	56	LEU	CD1	25.454	0.300	1
1	A	56	LEU	CD2	23.374	0.300	1
1	A	56	LEU	C	179.224	0.300	1
1	A	57	ASP	N	119.862	0.300	1
1	A	57	ASP	H	8.264	0.020	1
1	A	57	ASP	CA	57.878	0.300	1
1	A	57	ASP	HA	4.441	0.020	1
1	A	57	ASP	CB	40.104	0.300	1
1	A	57	ASP	HB2	2.68	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	ASP	HB3	2.866	0.020	2
1	A	57	ASP	C	179.733	0.300	1
1	A	58	ARG	N	121.061	0.300	1
1	A	58	ARG	H	7.94	0.020	1
1	A	58	ARG	CA	59.966	0.300	1
1	A	58	ARG	HA	4.149	0.020	1
1	A	58	ARG	CB	30.381	0.300	1
1	A	58	ARG	HB2	2.003	0.020	2
1	A	58	ARG	HB3	2.203	0.020	2
1	A	58	ARG	CG	28.586	0.300	1
1	A	58	ARG	HG2	1.691	0.020	2
1	A	58	ARG	HG3	1.691	0.020	2
1	A	58	ARG	CD	43.421	0.300	1
1	A	58	ARG	HD2	3.362	0.020	2
1	A	58	ARG	HD3	3.362	0.020	2
1	A	58	ARG	C	179.137	0.300	1
1	A	59	LEU	N	122.565	0.300	1
1	A	59	LEU	H	7.957	0.020	1
1	A	59	LEU	CA	57.658	0.300	1
1	A	59	LEU	HA	3.579	0.020	1
1	A	59	LEU	CB	40.808	0.300	1
1	A	59	LEU	HB2	1.148	0.020	2
1	A	59	LEU	HB3	1.874	0.020	2
1	A	59	LEU	CG	26.674	0.300	1
1	A	59	LEU	HG	1.487	0.020	1
1	A	59	LEU	HD11	0.634	0.020	2
1	A	59	LEU	HD12	0.634	0.020	2
1	A	59	LEU	HD13	0.634	0.020	2
1	A	59	LEU	HD21	0.662	0.020	2
1	A	59	LEU	HD22	0.662	0.020	2
1	A	59	LEU	HD23	0.662	0.020	2
1	A	59	LEU	CD1	25.933	0.300	1
1	A	59	LEU	CD2	21.945	0.300	1
1	A	59	LEU	C	178.126	0.300	1
1	A	60	ARG	N	118.987	0.300	1
1	A	60	ARG	H	8.677	0.020	1
1	A	60	ARG	CA	60.616	0.300	1
1	A	60	ARG	HA	3.728	0.020	1
1	A	60	ARG	CB	30.121	0.300	1
1	A	60	ARG	HB2	1.85	0.020	2
1	A	60	ARG	HB3	1.85	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	ARG	CG	28.87	0.300	1
1	A	60	ARG	HG2	1.481	0.020	2
1	A	60	ARG	HG3	1.481	0.020	2
1	A	60	ARG	CD	43.272	0.300	1
1	A	60	ARG	HD2	3.186	0.020	2
1	A	60	ARG	HD3	3.186	0.020	2
1	A	60	ARG	C	178.704	0.300	1
1	A	61	ALA	N	120.375	0.300	1
1	A	61	ALA	H	7.854	0.020	1
1	A	61	ALA	CA	54.868	0.300	1
1	A	61	ALA	HA	4.134	0.020	1
1	A	61	ALA	HB1	1.545	0.020	1
1	A	61	ALA	HB2	1.545	0.020	1
1	A	61	ALA	HB3	1.545	0.020	1
1	A	61	ALA	CB	18.229	0.300	1
1	A	61	ALA	C	180.187	0.300	1
1	A	62	TYR	N	121.856	0.300	1
1	A	62	TYR	H	8.031	0.020	1
1	A	62	TYR	CA	61.732	0.300	1
1	A	62	TYR	HA	4.256	0.020	1
1	A	62	TYR	CB	38.871	0.300	1
1	A	62	TYR	HB2	3.082	0.020	2
1	A	62	TYR	HB3	3.082	0.020	2
1	A	62	TYR	HD1	7.0	0.020	1
1	A	62	TYR	HE1	6.753	0.020	1
1	A	62	TYR	HE2	6.753	0.020	1
1	A	62	TYR	HD2	7.0	0.020	1
1	A	62	TYR	C	177.197	0.300	1
1	A	63	ILE	N	118.832	0.300	1
1	A	63	ILE	H	8.414	0.020	1
1	A	63	ILE	CA	66.146	0.300	1
1	A	63	ILE	HA	3.232	0.020	1
1	A	63	ILE	CB	38.362	0.300	1
1	A	63	ILE	HB	1.896	0.020	1
1	A	63	ILE	HG21	0.847	0.020	1
1	A	63	ILE	HG22	0.847	0.020	1
1	A	63	ILE	HG23	0.847	0.020	1
1	A	63	ILE	CG2	18.896	0.300	1
1	A	63	ILE	CG1	30.419	0.300	1
1	A	63	ILE	HG12	0.966	0.020	2
1	A	63	ILE	HG13	0.966	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	63	ILE	HD11	0.852	0.020	1
1	A	63	ILE	HD12	0.852	0.020	1
1	A	63	ILE	HD13	0.852	0.020	1
1	A	63	ILE	CD1	14.47	0.300	1
1	A	63	ILE	C	176.896	0.300	1
1	A	64	ALA	N	117.186	0.300	1
1	A	64	ALA	H	7.882	0.020	1
1	A	64	ALA	CA	54.517	0.300	1
1	A	64	ALA	HA	3.879	0.020	1
1	A	64	ALA	HB1	1.42	0.020	1
1	A	64	ALA	HB2	1.42	0.020	1
1	A	64	ALA	HB3	1.42	0.020	1
1	A	64	ALA	CB	18.105	0.300	1
1	A	64	ALA	C	178.403	0.300	1
1	A	65	ALA	N	117.666	0.300	1
1	A	65	ALA	H	7.595	0.020	1
1	A	65	ALA	CA	53.642	0.300	1
1	A	65	ALA	HA	4.205	0.020	1
1	A	65	ALA	HB1	1.485	0.020	1
1	A	65	ALA	HB2	1.485	0.020	1
1	A	65	ALA	HB3	1.485	0.020	1
1	A	65	ALA	CB	19.385	0.300	1
1	A	65	ALA	C	179.883	0.300	1
1	A	66	GLU	N	115.07	0.300	1
1	A	66	GLU	H	7.836	0.020	1
1	A	66	GLU	CA	57.036	0.300	1
1	A	66	GLU	HA	4.175	0.020	1
1	A	66	GLU	CB	31.861	0.300	1
1	A	66	GLU	HB2	1.498	0.020	2
1	A	66	GLU	HB3	2.066	0.020	2
1	A	66	GLU	CG	35.95	0.300	1
1	A	66	GLU	HG2	1.726	0.020	2
1	A	66	GLU	HG3	1.945	0.020	2
1	A	66	GLU	C	176.836	0.300	1
1	A	67	LEU	N	117.679	0.300	1
1	A	67	LEU	H	7.718	0.020	1
1	A	67	LEU	CA	53.441	0.300	1
1	A	67	LEU	HA	4.71	0.020	1
1	A	67	LEU	CB	44.547	0.300	1
1	A	67	LEU	HB2	1.123	0.020	2
1	A	67	LEU	HB3	1.594	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	67	LEU	CG	26.275	0.300	1
1	A	67	LEU	HG	1.161	0.020	1
1	A	67	LEU	HD11	0.189	0.020	2
1	A	67	LEU	HD12	0.189	0.020	2
1	A	67	LEU	HD13	0.189	0.020	2
1	A	67	LEU	HD21	0.633	0.020	2
1	A	67	LEU	HD22	0.633	0.020	2
1	A	67	LEU	HD23	0.633	0.020	2
1	A	67	LEU	CD1	26.132	0.300	1
1	A	67	LEU	CD2	22.699	0.300	1
1	A	67	LEU	C	176.36	0.300	1
1	A	68	GLN	N	119.921	0.300	1
1	A	68	GLN	H	8.887	0.020	1
1	A	68	GLN	CA	53.51	0.300	1
1	A	68	GLN	HA	4.516	0.020	1
1	A	68	GLN	CB	30.437	0.300	1
1	A	68	GLN	HB2	1.891	0.020	2
1	A	68	GLN	HB3	2.319	0.020	2
1	A	68	GLN	CG	33.895	0.300	1
1	A	68	GLN	HG2	2.43	0.020	2
1	A	68	GLN	HG3	2.43	0.020	2
1	A	68	GLN	CD	178.077	0.300	1
1	A	68	GLN	NE2	113.729	0.300	1
1	A	68	GLN	HE21	7.62	0.020	2
1	A	68	GLN	HE22	6.825	0.020	2
1	A	68	GLN	C	177.686	0.300	1
1	A	69	GLU	N	120.81	0.300	1
1	A	69	GLU	H	8.931	0.020	1
1	A	69	GLU	CA	56.023	0.300	1
1	A	69	GLU	HA	4.829	0.020	1
1	A	69	GLU	CB	27.958	0.300	1
1	A	69	GLU	HB2	1.694	0.020	2
1	A	69	GLU	HB3	1.694	0.020	2
1	A	69	GLU	CG	30.76	0.300	1
1	A	69	GLU	HG2	1.98	0.020	2
1	A	69	GLU	HG3	2.225	0.020	2
1	A	69	GLU	C	177.325	0.300	1
1	A	70	PRO	CD	50.326	0.300	1
1	A	70	PRO	CA	63.426	0.300	1
1	A	70	PRO	HA	5.254	0.020	1
1	A	70	PRO	CB	34.072	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	PRO	HB2	2.344	0.020	2
1	A	70	PRO	HB3	2.344	0.020	2
1	A	70	PRO	CG	24.178	0.300	1
1	A	70	PRO	HG2	1.627	0.020	2
1	A	70	PRO	HG3	1.944	0.020	2
1	A	70	PRO	HD2	3.47	0.020	2
1	A	70	PRO	HD3	3.644	0.020	2
1	A	70	PRO	C	173.83	0.300	1
1	A	71	ALA	N	128.529	0.300	1
1	A	71	ALA	H	7.672	0.020	1
1	A	71	ALA	CA	55.668	0.300	1
1	A	71	ALA	HA	4.315	0.020	1
1	A	71	ALA	HB1	1.584	0.020	1
1	A	71	ALA	HB2	1.584	0.020	1
1	A	71	ALA	HB3	1.584	0.020	1
1	A	71	ALA	CB	18.749	0.300	1
1	A	71	ALA	C	178.707	0.300	1
1	A	72	ARG	N	118.361	0.300	1
1	A	72	ARG	H	8.104	0.020	1
1	A	72	ARG	CA	59.88	0.300	1
1	A	72	ARG	HA	3.436	0.020	1
1	A	72	ARG	CB	30.447	0.300	1
1	A	72	ARG	HB2	1.193	0.020	2
1	A	72	ARG	HB3	1.334	0.020	2
1	A	72	ARG	CG	25.139	0.300	1
1	A	72	ARG	HG2	1.389	0.020	2
1	A	72	ARG	HG3	1.389	0.020	2
1	A	72	ARG	CD	44.037	0.300	1
1	A	72	ARG	HD2	3.151	0.020	2
1	A	72	ARG	HD3	3.224	0.020	2
1	A	72	ARG	C	177.061	0.300	1
1	A	73	GLY	N	107.959	0.300	1
1	A	73	GLY	H	8.958	0.020	1
1	A	73	GLY	CA	47.347	0.300	1
1	A	73	GLY	HA2	3.85	0.020	2
1	A	73	GLY	HA3	4.062	0.020	2
1	A	73	GLY	C	178.295	0.300	1
1	A	74	GLN	N	121.981	0.300	1
1	A	74	GLN	H	7.797	0.020	1
1	A	74	GLN	CA	58.783	0.300	1
1	A	74	GLN	HA	4.126	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	GLN	CB	27.393	0.300	1
1	A	74	GLN	HB2	1.912	0.020	2
1	A	74	GLN	HB3	2.495	0.020	2
1	A	74	GLN	CG	34.195	0.300	1
1	A	74	GLN	HG2	2.391	0.020	2
1	A	74	GLN	HG3	2.516	0.020	2
1	A	74	GLN	CD	176.199	0.300	1
1	A	74	GLN	NE2	108.588	0.300	1
1	A	74	GLN	HE21	7.321	0.020	2
1	A	74	GLN	C	179.268	0.300	1
1	A	75	ALA	N	123.845	0.300	1
1	A	75	ALA	H	8.901	0.020	1
1	A	75	ALA	CA	55.437	0.300	1
1	A	75	ALA	HA	4.011	0.020	1
1	A	75	ALA	HB1	1.362	0.020	1
1	A	75	ALA	HB2	1.362	0.020	1
1	A	75	ALA	HB3	1.362	0.020	1
1	A	75	ALA	CB	18.577	0.300	1
1	A	75	ALA	C	179.818	0.300	1
1	A	76	LEU	N	118.341	0.300	1
1	A	76	LEU	H	8.426	0.020	1
1	A	76	LEU	CA	58.195	0.300	1
1	A	76	LEU	HA	4.081	0.020	1
1	A	76	LEU	CB	41.312	0.300	1
1	A	76	LEU	HB2	1.524	0.020	2
1	A	76	LEU	HB3	1.943	0.020	2
1	A	76	LEU	CG	26.784	0.300	1
1	A	76	LEU	HG	1.876	0.020	1
1	A	76	LEU	HD11	0.864	0.020	2
1	A	76	LEU	HD12	0.864	0.020	2
1	A	76	LEU	HD13	0.864	0.020	2
1	A	76	LEU	HD21	0.919	0.020	2
1	A	76	LEU	HD22	0.919	0.020	2
1	A	76	LEU	HD23	0.919	0.020	2
1	A	76	LEU	CD1	25.454	0.300	1
1	A	76	LEU	CD2	23.219	0.300	1
1	A	76	LEU	C	180.098	0.300	1
1	A	77	ALA	N	123.257	0.300	1
1	A	77	ALA	H	8.044	0.020	1
1	A	77	ALA	CA	55.116	0.300	1
1	A	77	ALA	HA	4.275	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	ALA	HB1	1.547	0.020	1
1	A	77	ALA	HB2	1.547	0.020	1
1	A	77	ALA	HB3	1.547	0.020	1
1	A	77	ALA	CB	17.823	0.300	1
1	A	77	ALA	C	180.805	0.300	1
1	A	78	LEU	N	120.311	0.300	1
1	A	78	LEU	H	7.932	0.020	1
1	A	78	LEU	CA	57.846	0.300	1
1	A	78	LEU	HA	4.177	0.020	1
1	A	78	LEU	CB	42.217	0.300	1
1	A	78	LEU	HB2	1.553	0.020	2
1	A	78	LEU	HB3	1.84	0.020	2
1	A	78	LEU	CG	26.85	0.300	1
1	A	78	LEU	HG	1.538	0.020	1
1	A	78	LEU	HD11	0.877	0.020	2
1	A	78	LEU	HD12	0.877	0.020	2
1	A	78	LEU	HD13	0.877	0.020	2
1	A	78	LEU	HD21	0.811	0.020	2
1	A	78	LEU	HD22	0.811	0.020	2
1	A	78	LEU	HD23	0.811	0.020	2
1	A	78	LEU	CD1	25.101	0.300	1
1	A	78	LEU	CD2	23.563	0.300	1
1	A	78	LEU	C	179.267	0.300	1
1	A	79	MET	N	119.919	0.300	1
1	A	79	MET	H	8.484	0.020	1
1	A	79	MET	CA	59.406	0.300	1
1	A	79	MET	HA	3.436	0.020	1
1	A	79	MET	CB	32.803	0.300	1
1	A	79	MET	HB2	1.812	0.020	2
1	A	79	MET	HB3	1.984	0.020	2
1	A	79	MET	CG	31.874	0.300	1
1	A	79	MET	HG2	1.92	0.020	2
1	A	79	MET	HG3	2.266	0.020	2
1	A	79	MET	C	177.262	0.300	1
1	A	80	GLN	N	117.934	0.300	1
1	A	80	GLN	H	7.8	0.020	1
1	A	80	GLN	CA	58.682	0.300	1
1	A	80	GLN	HA	3.895	0.020	1
1	A	80	GLN	CB	28.443	0.300	1
1	A	80	GLN	HB2	2.038	0.020	2
1	A	80	GLN	HB3	2.213	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	GLN	CG	33.549	0.300	1
1	A	80	GLN	HG2	2.455	0.020	2
1	A	80	GLN	HG3	2.455	0.020	2
1	A	80	GLN	CD	177.314	0.300	1
1	A	80	GLN	NE2	114.319	0.300	1
1	A	80	GLN	HE21	7.756	0.020	2
1	A	80	GLN	HE22	6.769	0.020	2
1	A	80	GLN	C	177.682	0.300	1
1	A	81	GLN	N	117.49	0.300	1
1	A	81	GLN	H	7.852	0.020	1
1	A	81	GLN	CA	58.77	0.300	1
1	A	81	GLN	HA	4.152	0.020	1
1	A	81	GLN	CB	28.727	0.300	1
1	A	81	GLN	HB2	2.21	0.020	2
1	A	81	GLN	HB3	2.21	0.020	2
1	A	81	GLN	CG	34.188	0.300	1
1	A	81	GLN	HG2	2.463	0.020	2
1	A	81	GLN	HG3	2.463	0.020	2
1	A	81	GLN	CD	177.301	0.300	1
1	A	81	GLN	NE2	110.704	0.300	1
1	A	81	GLN	HE21	7.368	0.020	2
1	A	81	GLN	HE22	6.769	0.020	2
1	A	81	GLN	C	178.141	0.300	1
1	A	82	TYR	N	120.239	0.300	1
1	A	82	TYR	H	8.244	0.020	1
1	A	82	TYR	CA	61.108	0.300	1
1	A	82	TYR	HA	4.309	0.020	1
1	A	82	TYR	CB	38.889	0.300	1
1	A	82	TYR	HB2	3.117	0.020	2
1	A	82	TYR	HB3	3.117	0.020	2
1	A	82	TYR	HD1	7.049	0.020	1
1	A	82	TYR	HE1	7.001	0.020	1
1	A	82	TYR	HE2	7.001	0.020	1
1	A	82	TYR	HD2	7.049	0.020	1
1	A	82	TYR	C	177.541	0.300	1
1	A	83	ILE	N	118.132	0.300	1
1	A	83	ILE	H	8.039	0.020	1
1	A	83	ILE	CA	63.887	0.300	1
1	A	83	ILE	HA	3.713	0.020	1
1	A	83	ILE	CB	37.952	0.300	1
1	A	83	ILE	HB	1.99	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	83	ILE	HG21	0.94	0.020	1
1	A	83	ILE	HG22	0.94	0.020	1
1	A	83	ILE	HG23	0.94	0.020	1
1	A	83	ILE	CG2	17.64	0.300	1
1	A	83	ILE	CG1	28.268	0.300	1
1	A	83	ILE	HG12	1.662	0.020	2
1	A	83	ILE	HG13	1.297	0.020	2
1	A	83	ILE	HD11	0.846	0.020	1
1	A	83	ILE	HD12	0.846	0.020	1
1	A	83	ILE	HD13	0.846	0.020	1
1	A	83	ILE	CD1	13.811	0.300	1
1	A	83	ILE	C	177.94	0.300	1
1	A	84	ASP	N	120.692	0.300	1
1	A	84	ASP	H	8.146	0.020	1
1	A	84	ASP	CA	56.628	0.300	1
1	A	84	ASP	HA	4.46	0.020	1
1	A	84	ASP	CB	40.487	0.300	1
1	A	84	ASP	HB2	2.655	0.020	2
1	A	84	ASP	HB3	2.655	0.020	2
1	A	84	ASP	C	177.961	0.300	1
1	A	85	TYR	N	119.82	0.300	1
1	A	85	TYR	H	7.868	0.020	1
1	A	85	TYR	CA	59.135	0.300	1
1	A	85	TYR	HA	4.437	0.020	1
1	A	85	TYR	CB	38.241	0.300	1
1	A	85	TYR	HB2	3.125	0.020	2
1	A	85	TYR	HB3	3.125	0.020	2
1	A	85	TYR	HD1	7.074	0.020	1
1	A	85	TYR	HE1	6.729	0.020	1
1	A	85	TYR	HE2	6.729	0.020	1
1	A	85	TYR	HD2	7.074	0.020	1
1	A	85	TYR	C	176.819	0.300	1
1	A	86	LYS	N	120.255	0.300	1
1	A	86	LYS	H	7.887	0.020	1
1	A	86	LYS	CA	56.758	0.300	1
1	A	86	LYS	HA	3.997	0.020	1
1	A	86	LYS	CB	31.969	0.300	1
1	A	86	LYS	HB2	1.738	0.020	2
1	A	86	LYS	HB3	1.738	0.020	2
1	A	86	LYS	CG	24.485	0.300	1
1	A	86	LYS	HG2	1.284	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	LYS	HG3	1.284	0.020	2
1	A	86	LYS	CD	28.792	0.300	1
1	A	86	LYS	HD2	1.561	0.020	2
1	A	86	LYS	HD3	1.561	0.020	2
1	A	86	LYS	CE	42.075	0.300	1
1	A	86	LYS	HE2	2.93	0.020	2
1	A	86	LYS	HE3	2.93	0.020	2
1	A	86	LYS	C	177.016	0.300	1
1	A	87	LYS	N	119.831	0.300	1
1	A	87	LYS	H	7.825	0.020	1
1	A	87	LYS	CA	57.029	0.300	1
1	A	87	LYS	HA	4.157	0.020	1
1	A	87	LYS	CB	32.967	0.300	1
1	A	87	LYS	HB2	1.849	0.020	2
1	A	87	LYS	HB3	1.849	0.020	2
1	A	87	LYS	CG	24.841	0.300	1
1	A	87	LYS	HG2	1.5	0.020	2
1	A	87	LYS	HG3	1.859	0.020	2
1	A	87	LYS	CD	29.251	0.300	1
1	A	87	LYS	HD2	1.7	0.020	2
1	A	87	LYS	HD3	1.7	0.020	2
1	A	87	LYS	CE	42.208	0.300	1
1	A	87	LYS	HE2	2.996	0.020	2
1	A	87	LYS	HE3	2.996	0.020	2
1	A	87	LYS	C	176.548	0.300	1
1	A	88	GLU	N	120.706	0.300	1
1	A	88	GLU	H	8.023	0.020	1
1	A	88	GLU	CA	56.669	0.300	1
1	A	88	GLU	HA	4.297	0.020	1
1	A	88	GLU	CB	30.26	0.300	1
1	A	88	GLU	HB2	1.906	0.020	2
1	A	88	GLU	HB3	2.118	0.020	2
1	A	88	GLU	CG	36.084	0.300	1
1	A	88	GLU	HG2	2.175	0.020	2
1	A	88	GLU	HG3	2.278	0.020	2
1	A	88	GLU	C	175.521	0.300	1
1	A	89	LEU	N	128.156	0.300	1
1	A	89	LEU	H	7.658	0.020	1
1	A	89	LEU	CA	56.726	0.300	1
1	A	89	LEU	HA	4.149	0.020	1
1	A	89	LEU	CB	43.389	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	89	LEU	HB2	1.57	0.020	2
1	A	89	LEU	HB3	1.57	0.020	2
1	A	89	LEU	CG	26.924	0.300	1
1	A	89	LEU	HG	1.592	0.020	1
1	A	89	LEU	HD11	0.869	0.020	2
1	A	89	LEU	HD12	0.869	0.020	2
1	A	89	LEU	HD13	0.869	0.020	2
1	A	89	LEU	HD21	0.824	0.020	2
1	A	89	LEU	HD22	0.824	0.020	2
1	A	89	LEU	HD23	0.824	0.020	2
1	A	89	LEU	CD1	25.462	0.300	1
1	A	89	LEU	CD2	23.502	0.300	1
1	A	89	LEU	C	182.446	0.300	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	76	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	72	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	67	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	60	0.00 ± 0.00	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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1099. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/399 (0%)	0/162 (0%)	0/160 (0%)	0/77 (0%)
Sidechain	0/624 (0%)	0/405 (0%)	0/191 (0%)	0/28 (0%)
Aromatic	0/76 (0%)	0/36 (0%)	0/40 (0%)	0/0 (—%)
Overall	0/1099 (0%)	0/603 (0%)	0/391 (0%)	0/105 (0%)

7.1.4 Statistically unusual chemical shifts

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: