



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 08:43 PM BST

PDB ID : 2GMO
Title : NMR-structure of an independently folded C-terminal domain of influenza polymerase subunit PB2
Authors : Boudet, J.; Tarendeau, F.; Guilligay, D.; Mas, P.; Bougault, C.M.; Cusack, S.; Simorre, J.-P.; Hart, D.J.
Deposited on : 2006-04-07

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

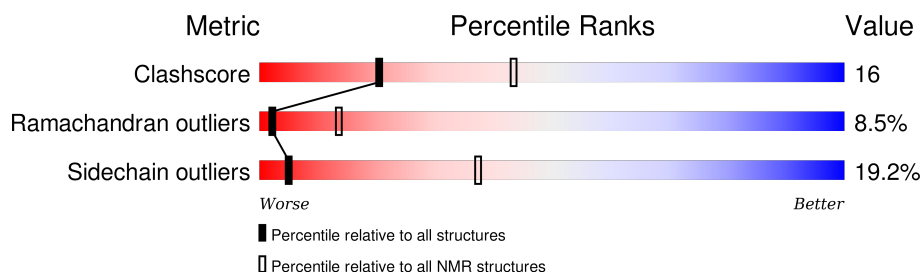
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	83	 55% 28% 6% • 10%

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 8 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:686-A:759 (74)	0.52	8

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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1186 atoms, of which 613 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1186	355	613	108	108	2	

There is a discrepancy between the modelled and reference sequences:

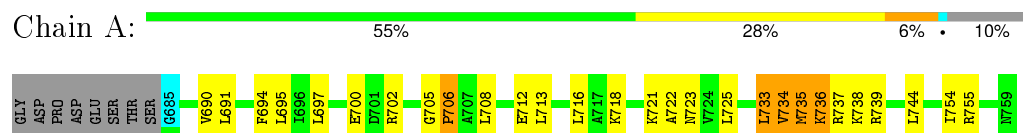
Chain	Residue	Modelled	Actual	Comment	Reference
A	677	GLY	-	CLONING ARTIFACT	UNP P31345

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Polymerase basic protein 2

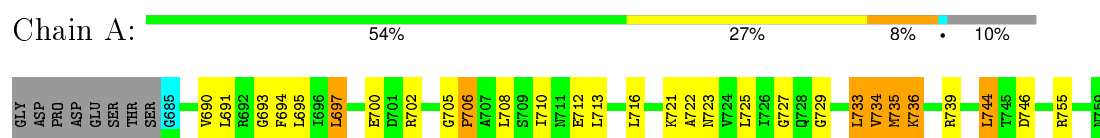


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

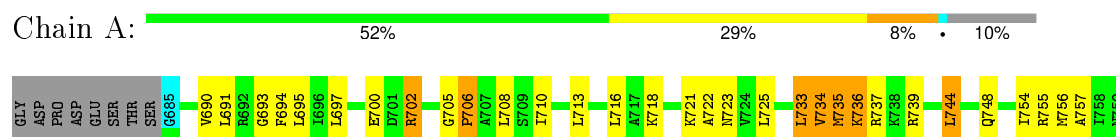
4.2.1 Score per residue for model 1

- Molecule 1: Polymerase basic protein 2



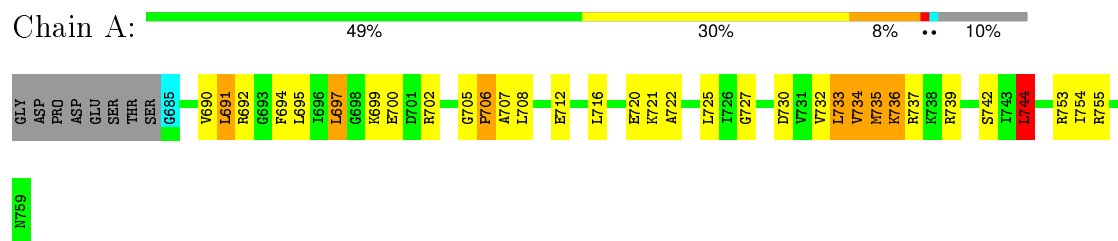
4.2.2 Score per residue for model 2

- Molecule 1: Polymerase basic protein 2



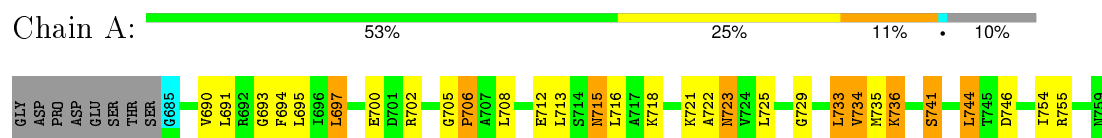
4.2.3 Score per residue for model 3

- Molecule 1: Polymerase basic protein 2



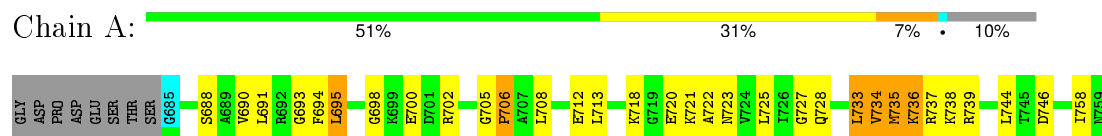
4.2.4 Score per residue for model 4

- Molecule 1: Polymerase basic protein 2



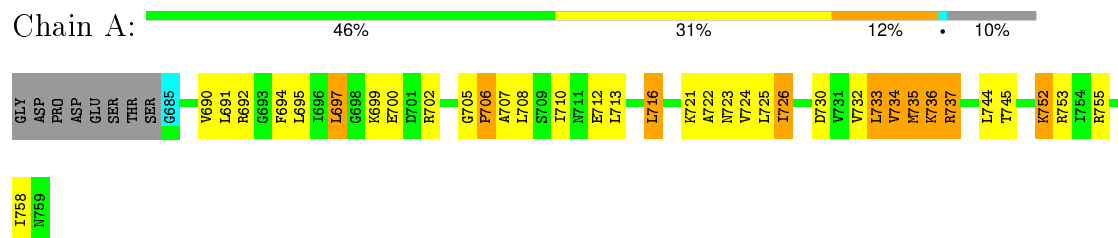
4.2.5 Score per residue for model 5

- Molecule 1: Polymerase basic protein 2



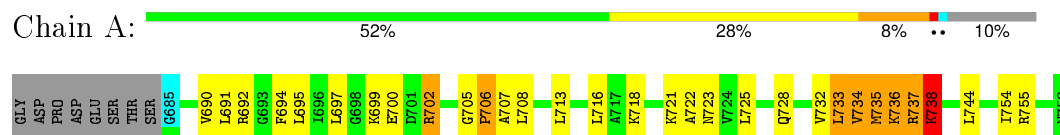
4.2.6 Score per residue for model 6

- Molecule 1: Polymerase basic protein 2



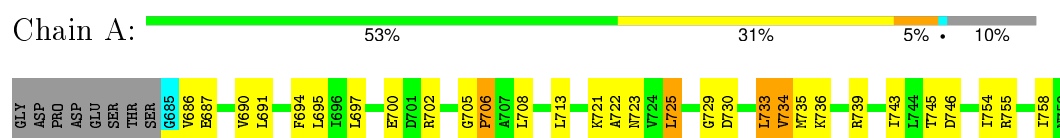
4.2.7 Score per residue for model 7

- Molecule 1: Polymerase basic protein 2



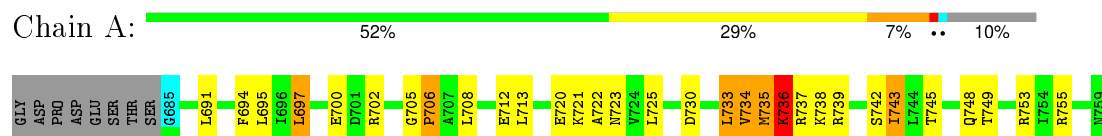
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Polymerase basic protein 2



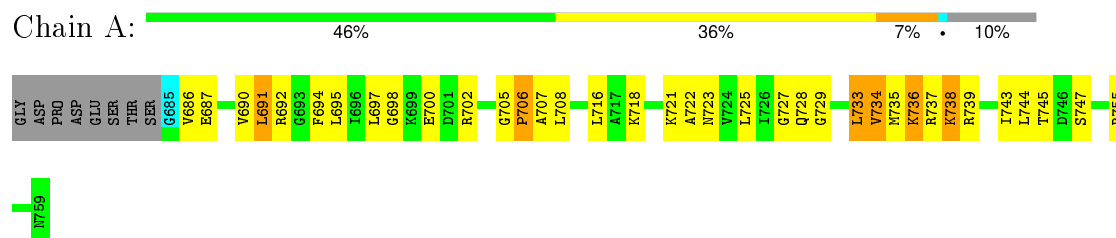
4.2.9 Score per residue for model 9

- Molecule 1: Polymerase basic protein 2



4.2.10 Score per residue for model 10

- Molecule 1: Polymerase basic protein 2



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *10 structures of lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	cns_solve_1.1
CNS	refinement	cns_solve_1.1

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

Chemical shift file(s)	BMRB entry 7056
Number of chemical shift lists	1
Total number of shifts	2043
Number of shifts mapped to atoms	1022
Number of unparsed shifts	1021
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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

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	569	610	610	19±3
All	All	5690	6100	6100	187

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:733:LEU:H	1:A:733:LEU:HD23	0.66	1.50	5	5
1:A:733:LEU:HD23	1:A:733:LEU:H	0.66	1.50	9	5
1:A:700:GLU:O	1:A:733:LEU:HD21	0.64	1.91	4	1
1:A:737:ARG:HA	1:A:744:LEU:HD11	0.62	1.69	5	4
1:A:733:LEU:HD23	1:A:733:LEU:N	0.61	2.10	4	2
1:A:695:LEU:HG	1:A:744:LEU:HD22	0.61	1.71	7	1
1:A:691:LEU:HB3	1:A:694:PHE:CD1	0.58	2.33	10	9
1:A:718:LYS:HG3	1:A:738:LYS:H	0.57	1.59	5	1
1:A:725:LEU:HD13	1:A:725:LEU:H	0.55	1.60	8	1
1:A:697:LEU:HB3	1:A:754:ILE:HG23	0.55	1.78	4	1
1:A:723:ASN:N	1:A:723:ASN:HD22	0.55	1.99	4	1
1:A:722:ALA:O	1:A:733:LEU:HA	0.54	2.01	3	10
1:A:691:LEU:HD21	1:A:710:ILE:HG13	0.54	1.80	1	2
1:A:735:MET:HE2	1:A:736:LYS:O	0.54	2.02	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:743:ILE:HG13	1:A:745:THR:H	0.54	1.63	10	2
1:A:716:LEU:HD13	1:A:736:LYS:HE3	0.53	1.80	2	2
1:A:705:GLY:N	1:A:706:PRO:HD3	0.51	2.20	8	10
1:A:723:ASN:ND2	1:A:733:LEU:HD22	0.50	2.21	4	1
1:A:700:GLU:O	1:A:733:LEU:CD2	0.50	2.60	5	9
1:A:735:MET:HE2	1:A:737:ARG:N	0.50	2.21	7	2
1:A:721:LYS:HA	1:A:734:VAL:O	0.50	2.07	9	10
1:A:737:ARG:HB3	1:A:744:LEU:HD21	0.50	1.83	7	1
1:A:690:VAL:HG23	1:A:691:LEU:N	0.49	2.23	8	9
1:A:723:ASN:HA	1:A:733:LEU:HA	0.49	1.84	6	8
1:A:697:LEU:HB3	1:A:733:LEU:O	0.48	2.08	7	8
1:A:697:LEU:HD11	1:A:733:LEU:HG	0.48	1.85	4	1
1:A:715:ASN:N	1:A:715:ASN:HD22	0.47	2.06	4	1
1:A:758:ILE:HD12	1:A:758:ILE:H	0.47	1.69	5	1
1:A:716:LEU:HB2	1:A:736:LYS:HE2	0.47	1.85	1	1
1:A:736:LYS:HB3	1:A:736:LYS:NZ	0.47	2.25	1	1
1:A:695:LEU:HG	1:A:744:LEU:HD13	0.47	1.86	10	2
1:A:721:LYS:HB3	1:A:733:LEU:HD12	0.46	1.87	10	5
1:A:695:LEU:HB2	1:A:735:MET:HB3	0.46	1.87	6	1
1:A:699:LYS:HB3	1:A:732:VAL:HG12	0.46	1.88	3	3
1:A:716:LEU:HD13	1:A:736:LYS:CE	0.46	2.41	7	2
1:A:720:GLU:O	1:A:736:LYS:HG2	0.46	2.11	9	3
1:A:726:ILE:HD13	1:A:726:ILE:H	0.46	1.70	6	1
1:A:718:LYS:HA	1:A:736:LYS:HB2	0.46	1.88	10	3
1:A:741:SER:HB3	1:A:744:LEU:HA	0.46	1.88	4	1
1:A:718:LYS:HE2	1:A:737:ARG:HE	0.46	1.71	2	1
1:A:695:LEU:O	1:A:734:VAL:HG12	0.46	2.10	2	8
1:A:737:ARG:CA	1:A:744:LEU:HD11	0.46	2.40	5	1
1:A:716:LEU:HD13	1:A:736:LYS:HE2	0.45	1.89	4	2
1:A:687:GLU:O	1:A:691:LEU:HD13	0.45	2.12	10	1
1:A:725:LEU:HA	1:A:730:ASP:O	0.45	2.12	8	1
1:A:697:LEU:HA	1:A:754:ILE:N	0.44	2.26	4	1
1:A:752:LYS:HD2	1:A:752:LYS:N	0.44	2.28	6	1
1:A:738:LYS:HE3	1:A:738:LYS:HA	0.44	1.89	7	1
1:A:691:LEU:HB3	1:A:694:PHE:HD1	0.44	1.72	2	2
1:A:758:ILE:N	1:A:758:ILE:HD12	0.44	2.28	8	1
1:A:713:LEU:HD21	1:A:734:VAL:HG21	0.44	1.90	1	2
1:A:737:ARG:O	1:A:738:LYS:HB3	0.43	2.12	9	2
1:A:695:LEU:HD23	1:A:746:ASP:HB2	0.43	1.90	4	1
1:A:700:GLU:O	1:A:733:LEU:HD22	0.43	2.13	5	2
1:A:716:LEU:HD13	1:A:736:LYS:NZ	0.43	2.27	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:697:LEU:HD23	1:A:735:MET:HG3	0.43	1.91	3	1
1:A:733:LEU:N	1:A:733:LEU:CD2	0.43	2.81	4	1
1:A:695:LEU:HD23	1:A:746:ASP:HB3	0.42	1.92	1	1
1:A:756:MET:HG2	1:A:757:ALA:H	0.42	1.75	2	1
1:A:720:GLU:C	1:A:736:LYS:HZ2	0.42	2.17	5	2
1:A:738:LYS:HD2	1:A:738:LYS:H	0.42	1.74	10	1
1:A:702:ARG:H	1:A:702:ARG:HD3	0.42	1.73	7	1
1:A:710:ILE:HA	1:A:713:LEU:HB2	0.42	1.90	6	1
1:A:721:LYS:HG3	1:A:735:MET:HG2	0.42	1.92	5	1
1:A:688:SER:HB3	1:A:694:PHE:O	0.41	2.15	5	1
1:A:716:LEU:HB2	1:A:736:LYS:HE3	0.41	1.90	6	1
1:A:698:GLY:O	1:A:733:LEU:HD23	0.41	2.16	5	2
1:A:733:LEU:N	1:A:733:LEU:HD23	0.41	2.26	5	1
1:A:737:ARG:HG2	1:A:744:LEU:HG	0.41	1.93	3	1
1:A:702:ARG:HD3	1:A:702:ARG:H	0.41	1.75	2	1
1:A:746:ASP:HB2	1:A:755:ARG:HH21	0.41	1.75	8	1
1:A:702:ARG:HD3	1:A:702:ARG:N	0.41	2.31	7	1
1:A:713:LEU:HD13	1:A:724:VAL:HG11	0.41	1.92	6	1
1:A:695:LEU:N	1:A:735:MET:O	0.40	2.55	5	1
1:A:744:LEU:HA	1:A:744:LEU:HD23	0.40	1.83	7	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	73/83 (88%)	56±2 (76±3%)	11±2 (15±3%)	6±2 (8±3%)	2	13
All	All	730/830 (88%)	556 (76%)	112 (15%)	62 (8%)	2	13

All 24 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	706	PRO	10
1	A	739	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	727	GLY	4
1	A	692	ARG	4
1	A	707	ALA	4
1	A	693	GLY	4
1	A	729	GLY	4
1	A	728	GLN	3
1	A	744	LEU	3
1	A	753	ARG	3
1	A	686	VAL	2
1	A	742	SER	2
1	A	691	LEU	2
1	A	754	ILE	1
1	A	741	SER	1
1	A	746	ASP	1
1	A	738	LYS	1
1	A	749	THR	1
1	A	697	LEU	1
1	A	737	ARG	1
1	A	716	LEU	1
1	A	736	LYS	1
1	A	743	ILE	1
1	A	747	SER	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	62/69 (90%)	50±2 (81±4%)	12±2 (19±4%)	5	37
All	All	620/690 (90%)	501 (81%)	119 (19%)	5	37

All 26 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	733	LEU	10
1	A	734	VAL	10
1	A	702	ARG	10

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Mol	Chain	Res	Type	Models (Total)
1	A	708	LEU	10
1	A	735	MET	10
1	A	725	LEU	10
1	A	736	LYS	10
1	A	755	ARG	8
1	A	713	LEU	6
1	A	712	GLU	6
1	A	697	LEU	4
1	A	744	LEU	4
1	A	754	ILE	3
1	A	730	ASP	3
1	A	748	GLN	2
1	A	738	LYS	2
1	A	745	THR	2
1	A	752	LYS	1
1	A	739	ARG	1
1	A	758	ILE	1
1	A	726	ILE	1
1	A	737	ARG	1
1	A	723	ASN	1
1	A	715	ASN	1
1	A	743	ILE	1
1	A	695	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 7056

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	2043
Number of shifts mapped to atoms	1022
Number of unparsed shifts	1021
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chemical shift has been reported more than once. All 1021 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1023	A	677	GLY	HA2	3.695	0.01	2
1024	A	677	GLY	HA3	3.562	0.01	2
1025	A	677	GLY	CA	43.378	0.15	1
1026	A	678	ASP	HB2	2.623	0.01	2
1027	A	678	ASP	HB3	2.483	0.01	2
1028	A	678	ASP	CA	52.616	0.15	1
1029	A	678	ASP	CB	42.681	0.15	1
1030	A	679	PRO	HB2	2.318	0.01	2
1031	A	679	PRO	HB3	2.083	0.01	2
1032	A	679	PRO	HG2	1.936	0.01	2
1033	A	679	PRO	HG3	1.845	0.01	2
1034	A	679	PRO	HD2	3.561	0.01	2
1035	A	679	PRO	HD3	3.467	0.01	2
1036	A	679	PRO	C	176.188	0.15	1
1037	A	679	PRO	CA	63.096	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1038	A	679	PRO	CB	34.526	0.15	1
1039	A	679	PRO	CG	24.702	0.15	1
1040	A	679	PRO	CD	50.213	0.15	1
1041	A	680	ASP	H	8.774	0.01	1
1042	A	680	ASP	HA	4.731	0.01	1
1043	A	680	ASP	HB2	2.696	0.01	2
1044	A	680	ASP	HB3	2.596	0.01	2
1045	A	680	ASP	C	176.017	0.15	1
1046	A	680	ASP	CA	54.461	0.15	1
1047	A	680	ASP	CB	41.361	0.15	1
1048	A	680	ASP	N	121.088	0.06	1
1049	A	681	GLU	H	8.753	0.01	1
1050	A	681	GLU	HA	4.291	0.01	1
1051	A	681	GLU	HB2	2.106	0.01	2
1052	A	681	GLU	HB3	1.954	0.01	2
1053	A	681	GLU	HG2	2.284	0.01	1
1054	A	681	GLU	HG3	2.284	0.01	1
1055	A	681	GLU	C	176.818	0.15	1
1056	A	681	GLU	CA	56.833	0.15	1
1057	A	681	GLU	CB	30.220	0.15	1
1058	A	681	GLU	CG	36.183	0.15	1
1059	A	681	GLU	N	122.396	0.06	1
1060	A	682	SER	H	8.454	0.01	1
1061	A	682	SER	HA	4.481	0.01	1
1062	A	682	SER	HB2	3.932	0.01	2
1063	A	682	SER	HB3	3.853	0.01	2
1064	A	682	SER	C	175.256	0.15	1
1065	A	682	SER	CA	59.016	0.15	1
1066	A	682	SER	CB	63.810	0.15	1
1067	A	682	SER	N	116.713	0.06	1
1068	A	683	THR	H	8.206	0.01	1
1069	A	683	THR	HA	4.410	0.01	1
1070	A	683	THR	HB	4.325	0.01	1
1071	A	683	THR	HG21	1.225	0.01	1
1072	A	683	THR	HG22	1.225	0.01	1
1073	A	683	THR	HG23	1.225	0.01	1
1074	A	683	THR	C	174.999	0.15	1
1075	A	683	THR	CA	62.191	0.15	1
1076	A	683	THR	CB	69.594	0.15	1
1077	A	683	THR	CG2	21.618	0.15	1
1078	A	683	THR	N	115.459	0.06	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1079	A	684	SER	H	8.348	0.01	1
1080	A	684	SER	HA	4.437	0.01	1
1081	A	684	SER	HB2	3.902	0.01	1
1082	A	684	SER	HB3	3.902	0.01	1
1083	A	684	SER	C	175.231	0.15	1
1084	A	684	SER	CA	58.891	0.15	1
1085	A	684	SER	CB	63.839	0.15	1
1086	A	684	SER	N	117.984	0.06	1
1087	A	685	GLY	H	8.478	0.01	1
1088	A	685	GLY	HA2	4.012	0.01	1
1089	A	685	GLY	HA3	4.012	0.01	1
1090	A	685	GLY	C	174.716	0.15	1
1091	A	685	GLY	CA	45.685	0.15	1
1092	A	685	GLY	N	111.026	0.06	1
1093	A	686	VAL	H	8.118	0.01	1
1094	A	686	VAL	HA	4.077	0.01	1
1095	A	686	VAL	HB	2.113	0.01	1
1096	A	686	VAL	HG11	0.964	0.01	2
1097	A	686	VAL	HG12	0.964	0.01	2
1098	A	686	VAL	HG13	0.964	0.01	2
1099	A	686	VAL	HG21	0.953	0.01	2
1100	A	686	VAL	HG22	0.953	0.01	2
1101	A	686	VAL	HG23	0.953	0.01	2
1102	A	686	VAL	C	176.711	0.15	1
1103	A	686	VAL	CA	63.312	0.15	1
1104	A	686	VAL	CB	32.677	0.15	1
1105	A	686	VAL	CG1	20.918	0.15	1
1106	A	686	VAL	CG2	21.212	0.15	1
1107	A	686	VAL	N	119.913	0.06	1
1108	A	687	GLU	H	8.601	0.01	1
1109	A	687	GLU	HA	4.174	0.01	1
1110	A	687	GLU	HB2	2.023	0.01	1
1111	A	687	GLU	HB3	2.023	0.01	1
1112	A	687	GLU	HG2	2.322	0.01	2
1113	A	687	GLU	HG3	2.254	0.01	2
1114	A	687	GLU	C	177.075	0.15	1
1115	A	687	GLU	CA	57.969	0.15	1
1116	A	687	GLU	CB	29.946	0.15	1
1117	A	687	GLU	CG	36.651	0.15	1
1118	A	687	GLU	N	123.154	0.06	1
1119	A	688	SER	H	8.381	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1120	A	688	SER	HA	4.307	0.01	1
1121	A	688	SER	HB2	3.924	0.01	2
1122	A	688	SER	HB3	3.855	0.01	2
1123	A	688	SER	C	175.690	0.15	1
1124	A	688	SER	CA	59.439	0.15	1
1125	A	688	SER	CB	63.467	0.15	1
1126	A	688	SER	N	115.659	0.06	1
1127	A	689	ALA	H	8.320	0.01	1
1128	A	689	ALA	HA	4.231	0.01	1
1129	A	689	ALA	HB1	1.474	0.01	1
1130	A	689	ALA	HB2	1.474	0.01	1
1131	A	689	ALA	HB3	1.474	0.01	1
1132	A	689	ALA	C	179.340	0.15	1
1133	A	689	ALA	CA	54.181	0.15	1
1134	A	689	ALA	CB	18.717	0.15	1
1135	A	689	ALA	N	126.320	0.06	1
1136	A	690	VAL	H	7.982	0.01	1
1137	A	690	VAL	HA	3.937	0.01	1
1138	A	690	VAL	HB	2.078	0.01	1
1139	A	690	VAL	HG11	1.004	0.01	2
1140	A	690	VAL	HG12	1.004	0.01	2
1141	A	690	VAL	HG13	1.004	0.01	2
1142	A	690	VAL	HG21	0.931	0.01	2
1143	A	690	VAL	HG22	0.931	0.01	2
1144	A	690	VAL	HG23	0.931	0.01	2
1145	A	690	VAL	C	177.472	0.15	1
1146	A	690	VAL	CA	64.559	0.15	1
1147	A	690	VAL	CB	32.429	0.15	1
1148	A	690	VAL	CG1	21.605	0.15	1
1149	A	690	VAL	CG2	21.288	0.15	1
1150	A	690	VAL	N	117.763	0.06	1
1151	A	691	LEU	H	8.039	0.01	1
1152	A	691	LEU	HA	4.404	0.01	1
1153	A	691	LEU	HB2	1.714	0.01	2
1154	A	691	LEU	HB3	1.608	0.01	2
1155	A	691	LEU	HG	1.545	0.01	1
1156	A	691	LEU	HD11	0.733	0.01	2
1157	A	691	LEU	HD12	0.733	0.01	2
1158	A	691	LEU	HD13	0.733	0.01	2
1159	A	691	LEU	HD21	0.544	0.01	2
1160	A	691	LEU	HD22	0.544	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1161	A	691	LEU	HD23	0.544	0.01	2
1162	A	691	LEU	C	176.978	0.15	1
1163	A	691	LEU	CA	54.984	0.15	1
1164	A	691	LEU	CB	41.720	0.15	1
1165	A	691	LEU	CG	27.023	0.15	1
1166	A	691	LEU	CD1	25.446	0.15	1
1167	A	691	LEU	CD2	23.216	0.15	1
1168	A	691	LEU	N	120.198	0.06	1
1169	A	692	ARG	H	7.795	0.01	1
1170	A	692	ARG	HA	4.249	0.01	1
1171	A	692	ARG	HB2	1.922	0.01	1
1172	A	692	ARG	HB3	1.922	0.01	1
1173	A	692	ARG	HG2	1.836	0.01	2
1174	A	692	ARG	HG3	1.699	0.01	2
1175	A	692	ARG	HD2	3.260	0.01	1
1176	A	692	ARG	HD3	3.260	0.01	1
1177	A	692	ARG	C	178.009	0.15	1
1178	A	692	ARG	CA	58.684	0.15	1
1179	A	692	ARG	CB	29.953	0.15	1
1180	A	692	ARG	CG	27.470	0.15	1
1181	A	692	ARG	CD	43.488	0.15	1
1182	A	692	ARG	N	121.039	0.06	1
1183	A	693	GLY	HA2	3.938	0.01	2
1184	A	693	GLY	HA3	3.879	0.01	2
1185	A	693	GLY	C	173.327	0.15	1
1186	A	693	GLY	CA	45.189	0.15	1
1187	A	694	PHE	H	8.198	0.01	1
1188	A	694	PHE	HA	4.949	0.01	1
1189	A	694	PHE	HB2	2.947	0.01	2
1190	A	694	PHE	HB3	2.679	0.01	2
1191	A	694	PHE	HD1	6.948	0.01	1
1192	A	694	PHE	HD2	6.948	0.01	1
1193	A	694	PHE	HE1	7.215	0.01	1
1194	A	694	PHE	HE2	7.215	0.01	1
1195	A	694	PHE	HZ	7.250	0.01	1
1196	A	694	PHE	C	173.802	0.15	1
1197	A	694	PHE	CA	57.510	0.15	1
1198	A	694	PHE	CB	42.048	0.15	1
1199	A	694	PHE	CD1	131.639	0.15	1
1200	A	694	PHE	CD2	131.639	0.15	1
1201	A	694	PHE	N	119.135	0.06	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1202	A	695	LEU	H	9.155	0.01	1
1203	A	695	LEU	HA	4.686	0.01	1
1204	A	695	LEU	HB2	1.538	0.01	2
1205	A	695	LEU	HB3	1.447	0.01	2
1206	A	695	LEU	HG	1.433	0.01	1
1207	A	695	LEU	HD11	0.925	0.01	2
1208	A	695	LEU	HD12	0.925	0.01	2
1209	A	695	LEU	HD13	0.925	0.01	2
1210	A	695	LEU	HD21	0.866	0.01	2
1211	A	695	LEU	HD22	0.866	0.01	2
1212	A	695	LEU	HD23	0.866	0.01	2
1213	A	695	LEU	C	176.188	0.15	1
1214	A	695	LEU	CA	53.512	0.15	1
1215	A	695	LEU	CB	44.675	0.15	1
1216	A	695	LEU	CG	27.296	0.15	1
1217	A	695	LEU	CD1	25.060	0.15	1
1218	A	695	LEU	CD2	24.677	0.15	1
1219	A	695	LEU	N	121.967	0.06	1
1220	A	696	ILE	H	8.900	0.01	1
1221	A	696	ILE	HA	4.328	0.01	1
1222	A	696	ILE	HB	1.914	0.01	1
1223	A	696	ILE	HG12	1.660	0.01	1
1224	A	696	ILE	HG13	1.023	0.01	1
1225	A	696	ILE	HG21	0.872	0.01	1
1226	A	696	ILE	HG22	0.872	0.01	1
1227	A	696	ILE	HG23	0.872	0.01	1
1228	A	696	ILE	HD11	0.822	0.01	1
1229	A	696	ILE	HD12	0.822	0.01	1
1230	A	696	ILE	HD13	0.822	0.01	1
1231	A	696	ILE	C	176.755	0.15	1
1232	A	696	ILE	CA	61.955	0.15	1
1233	A	696	ILE	CB	37.134	0.15	1
1234	A	696	ILE	CG1	27.987	0.15	1
1235	A	696	ILE	CG2	17.467	0.15	1
1236	A	696	ILE	CD1	12.993	0.15	1
1237	A	696	ILE	N	124.104	0.06	1
1238	A	697	LEU	H	9.458	0.01	1
1239	A	697	LEU	HA	4.369	0.01	1
1240	A	697	LEU	HB2	1.514	0.01	2
1241	A	697	LEU	HB3	1.377	0.01	2
1242	A	697	LEU	HG	1.535	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1243	A	697	LEU	HD11	0.732	0.01	2
1244	A	697	LEU	HD12	0.732	0.01	2
1245	A	697	LEU	HD13	0.732	0.01	2
1246	A	697	LEU	HD21	0.773	0.01	2
1247	A	697	LEU	HD22	0.773	0.01	2
1248	A	697	LEU	HD23	0.773	0.01	2
1249	A	697	LEU	C	177.554	0.15	1
1250	A	697	LEU	CA	55.424	0.15	1
1251	A	697	LEU	CB	42.581	0.15	1
1252	A	697	LEU	CG	27.070	0.15	1
1253	A	697	LEU	CD1	25.804	0.15	1
1254	A	697	LEU	CD2	22.797	0.15	1
1255	A	697	LEU	N	129.126	0.06	1
1256	A	698	GLY	H	7.411	0.01	1
1257	A	698	GLY	HA2	4.460	0.01	2
1258	A	698	GLY	HA3	3.905	0.01	2
1259	A	698	GLY	C	172.077	0.15	1
1260	A	698	GLY	CA	44.984	0.15	1
1261	A	698	GLY	N	105.222	0.06	1
1262	A	699	LYS	H	8.278	0.01	1
1263	A	699	LYS	HA	4.404	0.01	1
1264	A	699	LYS	HB2	2.060	0.01	2
1265	A	699	LYS	HB3	1.858	0.01	2
1266	A	699	LYS	HG2	1.585	0.01	1
1267	A	699	LYS	HG3	1.585	0.01	1
1268	A	699	LYS	HD2	1.725	0.01	1
1269	A	699	LYS	HD3	1.725	0.01	1
1270	A	699	LYS	HE2	3.076	0.01	1
1271	A	699	LYS	HE3	3.076	0.01	1
1272	A	699	LYS	C	174.056	0.15	1
1273	A	699	LYS	CA	56.108	0.15	1
1274	A	699	LYS	CB	32.454	0.15	1
1275	A	699	LYS	CG	24.760	0.15	1
1276	A	699	LYS	CD	29.008	0.15	1
1277	A	699	LYS	CE	42.058	0.15	1
1278	A	699	LYS	N	120.181	0.06	1
1279	A	700	GLU	H	7.477	0.01	1
1280	A	700	GLU	HA	3.889	0.01	1
1281	A	700	GLU	HB2	1.731	0.01	2
1282	A	700	GLU	HB3	1.634	0.01	2
1283	A	700	GLU	HG2	1.841	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1284	A	700	GLU	HG3	1.766	0.01	2
1285	A	700	GLU	C	175.644	0.15	1
1286	A	700	GLU	CA	56.735	0.15	1
1287	A	700	GLU	CB	30.856	0.15	1
1288	A	700	GLU	CG	35.501	0.15	1
1289	A	700	GLU	N	117.979	0.06	1
1290	A	701	ASP	H	8.635	0.01	1
1291	A	701	ASP	HA	5.073	0.01	1
1292	A	701	ASP	HB2	3.231	0.01	2
1293	A	701	ASP	HB3	2.638	0.01	2
1294	A	701	ASP	C	178.382	0.15	1
1295	A	701	ASP	CA	52.436	0.15	1
1296	A	701	ASP	CB	43.517	0.15	1
1297	A	701	ASP	N	124.520	0.06	1
1298	A	702	ARG	H	9.430	0.01	1
1299	A	702	ARG	HA	4.249	0.01	1
1300	A	702	ARG	HB2	1.927	0.01	2
1301	A	702	ARG	HB3	1.817	0.01	2
1302	A	702	ARG	HG2	1.666	0.01	2
1303	A	702	ARG	HG3	1.597	0.01	2
1304	A	702	ARG	HD2	3.178	0.01	1
1305	A	702	ARG	HD3	3.178	0.01	1
1306	A	702	ARG	C	177.780	0.15	1
1307	A	702	ARG	CA	58.684	0.15	1
1308	A	702	ARG	CB	29.593	0.15	1
1309	A	702	ARG	CG	27.297	0.15	1
1310	A	702	ARG	CD	43.219	0.15	1
1311	A	702	ARG	N	127.590	0.06	1
1312	A	703	ARG	H	8.506	0.01	1
1313	A	703	ARG	HA	3.961	0.01	1
1314	A	703	ARG	HB2	1.443	0.01	2
1315	A	703	ARG	HB3	1.274	0.01	2
1316	A	703	ARG	HG2	1.436	0.01	2
1317	A	703	ARG	HG3	1.367	0.01	2
1318	A	703	ARG	HD2	3.123	0.01	2
1319	A	703	ARG	HD3	2.981	0.01	2
1320	A	703	ARG	C	177.750	0.15	1
1321	A	703	ARG	CA	58.758	0.15	1
1322	A	703	ARG	CB	29.681	0.15	1
1323	A	703	ARG	CG	26.635	0.15	1
1324	A	703	ARG	CD	43.541	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1325	A	703	ARG	N	121.236	0.06	1
1326	A	704	TYR	H	7.792	0.01	1
1327	A	704	TYR	HA	4.559	0.01	1
1328	A	704	TYR	HB2	3.315	0.01	2
1329	A	704	TYR	HB3	2.553	0.01	2
1330	A	704	TYR	HD1	7.136	0.01	1
1331	A	704	TYR	HD2	7.136	0.01	1
1332	A	704	TYR	HE1	6.757	0.01	1
1333	A	704	TYR	HE2	6.757	0.01	1
1334	A	704	TYR	C	176.267	0.15	1
1335	A	704	TYR	CA	58.380	0.15	1
1336	A	704	TYR	CB	37.346	0.15	1
1337	A	704	TYR	CD1	133.563	0.15	1
1338	A	704	TYR	CD2	133.563	0.15	1
1339	A	704	TYR	CE1	118.063	0.15	1
1340	A	704	TYR	CE2	118.063	0.15	1
1341	A	704	TYR	N	114.288	0.06	1
1342	A	705	GLY	H	7.388	0.01	1
1343	A	705	GLY	HA2	4.475	0.01	2
1344	A	705	GLY	HA3	3.955	0.01	2
1345	A	705	GLY	C	171.500	0.15	1
1346	A	705	GLY	CA	45.477	0.15	1
1347	A	705	GLY	N	107.706	0.06	1
1348	A	706	PRO	HA	4.404	0.01	1
1349	A	706	PRO	HB2	2.335	0.01	2
1350	A	706	PRO	HB3	1.832	0.01	2
1351	A	706	PRO	HG2	2.036	0.01	2
1352	A	706	PRO	HG3	1.969	0.01	2
1353	A	706	PRO	HD2	3.701	0.01	2
1354	A	706	PRO	HD3	3.638	0.01	2
1355	A	706	PRO	C	176.422	0.15	1
1356	A	706	PRO	CA	62.712	0.15	1
1357	A	706	PRO	CB	32.460	0.15	1
1358	A	706	PRO	CG	27.343	0.15	1
1359	A	706	PRO	CD	49.980	0.15	1
1360	A	707	ALA	H	8.640	0.01	1
1361	A	707	ALA	HA	3.952	0.01	1
1362	A	707	ALA	HB1	1.196	0.01	1
1363	A	707	ALA	HB2	1.196	0.01	1
1364	A	707	ALA	HB3	1.196	0.01	1
1365	A	707	ALA	C	177.483	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1366	A	707	ALA	CA	52.485	0.15	1
1367	A	707	ALA	CB	19.294	0.15	1
1368	A	707	ALA	N	123.641	0.06	1
1369	A	708	LEU	H	8.964	0.01	1
1370	A	708	LEU	HA	4.499	0.01	1
1371	A	708	LEU	HB2	1.704	0.01	2
1372	A	708	LEU	HB3	1.589	0.01	2
1373	A	708	LEU	HG	1.980	0.01	1
1374	A	708	LEU	HD11	0.812	0.01	2
1375	A	708	LEU	HD12	0.812	0.01	2
1376	A	708	LEU	HD13	0.812	0.01	2
1377	A	708	LEU	HD21	0.832	0.01	2
1378	A	708	LEU	HD22	0.832	0.01	2
1379	A	708	LEU	HD23	0.832	0.01	2
1380	A	708	LEU	C	176.925	0.15	1
1381	A	708	LEU	CA	53.690	0.15	1
1382	A	708	LEU	CB	43.795	0.15	1
1383	A	708	LEU	CG	27.048	0.15	1
1384	A	708	LEU	CD1	25.930	0.15	1
1385	A	708	LEU	CD2	22.609	0.15	1
1386	A	708	LEU	N	124.931	0.06	1
1387	A	709	SER	H	8.589	0.01	1
1388	A	709	SER	HA	4.796	0.01	1
1389	A	709	SER	HB2	4.179	0.01	2
1390	A	709	SER	HB3	3.941	0.01	2
1391	A	709	SER	C	176.503	0.15	1
1392	A	709	SER	CA	57.216	0.15	1
1393	A	709	SER	CB	65.250	0.15	1
1394	A	709	SER	N	114.628	0.06	1
1395	A	710	ILE	H	8.786	0.01	1
1396	A	710	ILE	HA	3.575	0.01	1
1397	A	710	ILE	HB	1.842	0.01	1
1398	A	710	ILE	HG12	1.559	0.01	1
1399	A	710	ILE	HG13	1.159	0.01	1
1400	A	710	ILE	HG21	0.860	0.01	1
1401	A	710	ILE	HG22	0.860	0.01	1
1402	A	710	ILE	HG23	0.860	0.01	1
1403	A	710	ILE	HD11	0.841	0.01	1
1404	A	710	ILE	HD12	0.841	0.01	1
1405	A	710	ILE	HD13	0.841	0.01	1
1406	A	710	ILE	C	178.089	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1407	A	710	ILE	CA	64.126	0.15	1
1408	A	710	ILE	CB	37.849	0.15	1
1409	A	710	ILE	CG1	28.745	0.15	1
1410	A	710	ILE	CG2	17.678	0.15	1
1411	A	710	ILE	CD1	13.510	0.15	1
1412	A	710	ILE	N	121.501	0.06	1
1413	A	711	ASN	H	8.272	0.01	1
1414	A	711	ASN	HA	4.503	0.01	1
1415	A	711	ASN	HB2	2.801	0.01	2
1416	A	711	ASN	HB3	2.763	0.01	2
1417	A	711	ASN	HD21	7.710	0.01	2
1418	A	711	ASN	HD22	7.033	0.01	2
1419	A	711	ASN	C	177.054	0.15	1
1420	A	711	ASN	CA	55.437	0.15	1
1421	A	711	ASN	CB	38.148	0.15	1
1422	A	711	ASN	CG	176.590	0.15	1
1423	A	711	ASN	N	116.996	0.06	1
1424	A	711	ASN	ND2	113.626	0.06	1
1425	A	712	GLU	H	7.766	0.01	1
1426	A	712	GLU	HA	4.286	0.01	1
1427	A	712	GLU	HB2	2.289	0.01	1
1428	A	712	GLU	HB3	2.289	0.01	1
1429	A	712	GLU	HG2	2.269	0.01	1
1430	A	712	GLU	HG3	2.269	0.01	1
1431	A	712	GLU	C	177.858	0.15	1
1432	A	712	GLU	CA	57.262	0.15	1
1433	A	712	GLU	CB	30.975	0.15	1
1434	A	712	GLU	CG	37.700	0.15	1
1435	A	712	GLU	N	118.618	0.06	1
1436	A	713	LEU	H	7.601	0.01	1
1437	A	713	LEU	HA	3.980	0.01	1
1438	A	713	LEU	HB2	1.625	0.01	2
1439	A	713	LEU	HB3	1.507	0.01	2
1440	A	713	LEU	HG	1.618	0.01	1
1441	A	713	LEU	HD11	0.241	0.01	2
1442	A	713	LEU	HD12	0.241	0.01	2
1443	A	713	LEU	HD13	0.241	0.01	2
1444	A	713	LEU	HD21	0.299	0.01	2
1445	A	713	LEU	HD22	0.299	0.01	2
1446	A	713	LEU	HD23	0.299	0.01	2
1447	A	713	LEU	C	178.910	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1448	A	713	LEU	CA	56.857	0.15	1
1449	A	713	LEU	CB	41.036	0.15	1
1450	A	713	LEU	CG	26.105	0.15	1
1451	A	713	LEU	CD1	25.172	0.15	1
1452	A	713	LEU	CD2	22.687	0.15	1
1453	A	713	LEU	N	119.308	0.06	1
1454	A	714	SER	H	7.773	0.01	1
1455	A	714	SER	HA	4.286	0.01	1
1456	A	714	SER	HB2	3.975	0.01	1
1457	A	714	SER	HB3	3.975	0.01	1
1458	A	714	SER	C	174.981	0.15	1
1459	A	714	SER	CA	61.126	0.15	1
1460	A	714	SER	CB	62.854	0.15	1
1461	A	714	SER	N	112.864	0.06	1
1462	A	715	ASN	H	7.660	0.01	1
1463	A	715	ASN	HA	4.766	0.01	1
1464	A	715	ASN	HB2	2.984	0.01	2
1465	A	715	ASN	HB3	2.788	0.01	2
1466	A	715	ASN	HD21	7.689	0.01	2
1467	A	715	ASN	HD22	7.084	0.01	2
1468	A	715	ASN	C	175.639	0.15	1
1469	A	715	ASN	CA	53.375	0.15	1
1470	A	715	ASN	CB	39.128	0.15	1
1471	A	715	ASN	CG	177.060	0.15	1
1472	A	715	ASN	N	117.096	0.06	1
1473	A	715	ASN	ND2	113.959	0.06	1
1474	A	716	LEU	H	7.387	0.01	1
1475	A	716	LEU	HA	4.240	0.01	1
1476	A	716	LEU	HB2	1.745	0.01	1
1477	A	716	LEU	HB3	1.745	0.01	1
1478	A	716	LEU	HG	1.846	0.01	1
1479	A	716	LEU	HD11	0.902	0.01	2
1480	A	716	LEU	HD12	0.902	0.01	2
1481	A	716	LEU	HD13	0.902	0.01	2
1482	A	716	LEU	HD21	0.837	0.01	2
1483	A	716	LEU	HD22	0.837	0.01	2
1484	A	716	LEU	HD23	0.837	0.01	2
1485	A	716	LEU	C	176.561	0.15	1
1486	A	716	LEU	CA	55.770	0.15	1
1487	A	716	LEU	CB	43.070	0.15	1
1488	A	716	LEU	CG	27.661	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1489	A	716	LEU	CD1	25.431	0.15	1
1490	A	716	LEU	CD2	24.237	0.15	1
1491	A	716	LEU	N	121.348	0.06	1
1492	A	717	ALA	H	9.013	0.01	1
1493	A	717	ALA	HA	4.468	0.01	1
1494	A	717	ALA	HB1	1.446	0.01	1
1495	A	717	ALA	HB2	1.446	0.01	1
1496	A	717	ALA	HB3	1.446	0.01	1
1497	A	717	ALA	C	177.973	0.15	1
1498	A	717	ALA	CA	50.874	0.15	1
1499	A	717	ALA	CB	20.051	0.15	1
1500	A	717	ALA	N	126.924	0.06	1
1501	A	718	LYS	H	8.555	0.01	1
1502	A	718	LYS	HA	3.619	0.01	1
1503	A	718	LYS	HB2	1.782	0.01	2
1504	A	718	LYS	HB3	1.710	0.01	2
1505	A	718	LYS	HG2	1.557	0.01	2
1506	A	718	LYS	HG3	1.410	0.01	2
1507	A	718	LYS	HD2	1.712	0.01	1
1508	A	718	LYS	HD3	1.712	0.01	1
1509	A	718	LYS	HE2	2.980	0.01	1
1510	A	718	LYS	HE3	2.980	0.01	1
1511	A	718	LYS	C	177.880	0.15	1
1512	A	718	LYS	CA	59.031	0.15	1
1513	A	718	LYS	CB	32.395	0.15	1
1514	A	718	LYS	CG	25.270	0.15	1
1515	A	718	LYS	CD	29.601	0.15	1
1516	A	718	LYS	CE	42.096	0.15	1
1517	A	718	LYS	N	120.279	0.06	1
1518	A	719	GLY	H	8.486	0.01	1
1519	A	719	GLY	HA2	4.208	0.01	2
1520	A	719	GLY	HA3	3.700	0.01	2
1521	A	719	GLY	C	172.971	0.15	1
1522	A	719	GLY	CA	45.626	0.15	1
1523	A	719	GLY	N	113.023	0.06	1
1524	A	720	GLU	H	7.877	0.01	1
1525	A	720	GLU	HA	4.348	0.01	1
1526	A	720	GLU	HB2	2.172	0.01	2
1527	A	720	GLU	HB3	2.085	0.01	2
1528	A	720	GLU	HG2	2.430	0.01	2
1529	A	720	GLU	HG3	2.242	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1530	A	720	GLU	C	175.125	0.15	1
1531	A	720	GLU	CA	56.653	0.15	1
1532	A	720	GLU	CB	31.296	0.15	1
1533	A	720	GLU	CG	37.217	0.15	1
1534	A	720	GLU	N	121.135	0.06	1
1535	A	721	LYS	H	8.166	0.01	1
1536	A	721	LYS	HA	5.415	0.01	1
1537	A	721	LYS	HB2	1.067	0.01	2
1538	A	721	LYS	HB3	1.003	0.01	2
1539	A	721	LYS	HG2	1.334	0.01	2
1540	A	721	LYS	HG3	0.958	0.01	2
1541	A	721	LYS	HD2	1.219	0.01	2
1542	A	721	LYS	HD3	1.155	0.01	2
1543	A	721	LYS	HE2	2.795	0.01	2
1544	A	721	LYS	HE3	2.760	0.01	2
1545	A	721	LYS	C	175.830	0.15	1
1546	A	721	LYS	CA	54.736	0.15	1
1547	A	721	LYS	CB	35.430	0.15	1
1548	A	721	LYS	CG	25.849	0.15	1
1549	A	721	LYS	CD	29.967	0.15	1
1550	A	721	LYS	CE	42.341	0.15	1
1551	A	721	LYS	N	121.418	0.06	1
1552	A	722	ALA	H	8.551	0.01	1
1553	A	722	ALA	HA	4.414	0.01	1
1554	A	722	ALA	HB1	1.326	0.01	1
1555	A	722	ALA	HB2	1.326	0.01	1
1556	A	722	ALA	HB3	1.326	0.01	1
1557	A	722	ALA	C	175.137	0.15	1
1558	A	722	ALA	CA	51.703	0.15	1
1559	A	722	ALA	CB	23.796	0.15	1
1560	A	722	ALA	N	120.067	0.06	1
1561	A	723	ASN	H	9.112	0.01	1
1562	A	723	ASN	HA	5.622	0.01	1
1563	A	723	ASN	HB2	2.221	0.01	2
1564	A	723	ASN	HB3	2.015	0.01	2
1565	A	723	ASN	HD21	7.803	0.01	2
1566	A	723	ASN	HD22	7.232	0.01	2
1567	A	723	ASN	C	174.931	0.15	1
1568	A	723	ASN	CA	52.802	0.15	1
1569	A	723	ASN	CB	40.675	0.15	1
1570	A	723	ASN	CG	174.300	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1571	A	723	ASN	N	119.540	0.06	1
1572	A	723	ASN	ND2	115.595	0.06	1
1573	A	724	VAL	H	9.647	0.01	1
1574	A	724	VAL	HA	4.886	0.01	1
1575	A	724	VAL	HB	1.630	0.01	1
1576	A	724	VAL	HG11	0.673	0.01	2
1577	A	724	VAL	HG12	0.673	0.01	2
1578	A	724	VAL	HG13	0.673	0.01	2
1579	A	724	VAL	HG21	0.644	0.01	2
1580	A	724	VAL	HG22	0.644	0.01	2
1581	A	724	VAL	HG23	0.644	0.01	2
1582	A	724	VAL	C	172.724	0.15	1
1583	A	724	VAL	CA	59.579	0.15	1
1584	A	724	VAL	CB	35.724	0.15	1
1585	A	724	VAL	CG1	20.867	0.15	1
1586	A	724	VAL	CG2	22.440	0.15	1
1587	A	724	VAL	N	121.149	0.06	1
1588	A	725	LEU	H	8.201	0.01	1
1589	A	725	LEU	HA	4.681	0.01	1
1590	A	725	LEU	HB2	1.684	0.01	2
1591	A	725	LEU	HB3	1.290	0.01	2
1592	A	725	LEU	HG	1.342	0.01	1
1593	A	725	LEU	HD11	0.780	0.01	2
1594	A	725	LEU	HD12	0.780	0.01	2
1595	A	725	LEU	HD13	0.780	0.01	2
1596	A	725	LEU	HD21	0.779	0.01	2
1597	A	725	LEU	HD22	0.779	0.01	2
1598	A	725	LEU	HD23	0.779	0.01	2
1599	A	725	LEU	C	175.736	0.15	1
1600	A	725	LEU	CA	54.423	0.15	1
1601	A	725	LEU	CB	42.663	0.15	1
1602	A	725	LEU	CG	27.301	0.15	1
1603	A	725	LEU	CD1	25.452	0.15	1
1604	A	725	LEU	CD2	25.016	0.15	1
1605	A	725	LEU	N	129.056	0.06	1
1606	A	726	ILE	H	8.609	0.01	1
1607	A	726	ILE	HA	4.475	0.01	1
1608	A	726	ILE	HB	1.920	0.01	1
1609	A	726	ILE	HG12	1.337	0.01	1
1610	A	726	ILE	HG13	1.037	0.01	1
1611	A	726	ILE	HG21	0.792	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1612	A	726	ILE	HG22	0.792	0.01	1
1613	A	726	ILE	HG23	0.792	0.01	1
1614	A	726	ILE	HD11	0.726	0.01	1
1615	A	726	ILE	HD12	0.726	0.01	1
1616	A	726	ILE	HD13	0.726	0.01	1
1617	A	726	ILE	C	176.176	0.15	1
1618	A	726	ILE	CA	60.536	0.15	1
1619	A	726	ILE	CB	39.839	0.15	1
1620	A	726	ILE	CG1	26.893	0.15	1
1621	A	726	ILE	CG2	18.261	0.15	1
1622	A	726	ILE	CD1	13.851	0.15	1
1623	A	726	ILE	N	123.184	0.06	1
1624	A	727	GLY	H	8.410	0.01	1
1625	A	727	GLY	HA2	4.054	0.01	2
1626	A	727	GLY	HA3	3.891	0.01	2
1627	A	727	GLY	C	173.971	0.15	1
1628	A	727	GLY	CA	45.430	0.15	1
1629	A	727	GLY	N	110.153	0.06	1
1630	A	728	GLN	H	8.844	0.01	1
1631	A	728	GLN	HA	4.183	0.01	1
1632	A	728	GLN	HB2	2.141	0.01	2
1633	A	728	GLN	HB3	2.056	0.01	2
1634	A	728	GLN	HG2	2.354	0.01	1
1635	A	728	GLN	HG3	2.354	0.01	1
1636	A	728	GLN	HE21	7.633	0.01	2
1637	A	728	GLN	HE22	6.900	0.01	2
1638	A	728	GLN	C	176.826	0.15	1
1639	A	728	GLN	CA	56.714	0.15	1
1640	A	728	GLN	CB	27.815	0.15	1
1641	A	728	GLN	CG	33.875	0.15	1
1642	A	728	GLN	CD	180.500	0.15	1
1643	A	728	GLN	N	121.039	0.06	1
1644	A	728	GLN	NE2	112.944	0.06	1
1645	A	729	GLY	H	8.493	0.01	1
1646	A	729	GLY	HA2	4.089	0.01	2
1647	A	729	GLY	HA3	3.716	0.01	2
1648	A	729	GLY	C	173.570	0.15	1
1649	A	729	GLY	CA	45.884	0.15	1
1650	A	729	GLY	N	110.161	0.06	1
1651	A	730	ASP	H	7.877	0.01	1
1652	A	730	ASP	HA	4.803	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1653	A	730	ASP	HB2	2.571	0.01	2
1654	A	730	ASP	HB3	2.359	0.01	2
1655	A	730	ASP	C	173.563	0.15	1
1656	A	730	ASP	CA	53.911	0.15	1
1657	A	730	ASP	CB	41.894	0.15	1
1658	A	730	ASP	N	121.816	0.06	1
1659	A	731	VAL	H	8.290	0.01	1
1660	A	731	VAL	HA	5.003	0.01	1
1661	A	731	VAL	HB	1.852	0.01	1
1662	A	731	VAL	HG11	0.710	0.01	2
1663	A	731	VAL	HG12	0.710	0.01	2
1664	A	731	VAL	HG13	0.710	0.01	2
1665	A	731	VAL	HG21	0.834	0.01	2
1666	A	731	VAL	HG22	0.834	0.01	2
1667	A	731	VAL	HG23	0.834	0.01	2
1668	A	731	VAL	C	176.189	0.15	1
1669	A	731	VAL	CA	61.021	0.15	1
1670	A	731	VAL	CB	33.757	0.15	1
1671	A	731	VAL	CG1	23.196	0.15	1
1672	A	731	VAL	CG2	21.955	0.15	1
1673	A	731	VAL	N	123.045	0.06	1
1674	A	732	VAL	H	8.623	0.01	1
1675	A	732	VAL	HA	4.829	0.01	1
1676	A	732	VAL	HB	2.248	0.01	1
1677	A	732	VAL	HG11	0.809	0.01	2
1678	A	732	VAL	HG12	0.809	0.01	2
1679	A	732	VAL	HG13	0.809	0.01	2
1680	A	732	VAL	HG21	0.709	0.01	2
1681	A	732	VAL	HG22	0.709	0.01	2
1682	A	732	VAL	HG23	0.709	0.01	2
1683	A	732	VAL	C	172.946	0.15	1
1684	A	732	VAL	CA	58.597	0.15	1
1685	A	732	VAL	CB	35.215	0.15	1
1686	A	732	VAL	CG1	22.413	0.15	1
1687	A	732	VAL	CG2	18.586	0.15	1
1688	A	732	VAL	N	119.848	0.06	1
1689	A	733	LEU	H	8.267	0.01	1
1690	A	733	LEU	HA	4.835	0.01	1
1691	A	733	LEU	HB2	1.407	0.01	2
1692	A	733	LEU	HB3	1.361	0.01	2
1693	A	733	LEU	HG	0.790	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1694	A	733	LEU	HD11	0.569	0.01	2
1695	A	733	LEU	HD12	0.569	0.01	2
1696	A	733	LEU	HD13	0.569	0.01	2
1697	A	733	LEU	HD21	0.569	0.01	2
1698	A	733	LEU	HD22	0.569	0.01	2
1699	A	733	LEU	HD23	0.569	0.01	2
1700	A	733	LEU	C	176.447	0.15	1
1701	A	733	LEU	CA	54.289	0.15	1
1702	A	733	LEU	CB	43.416	0.15	1
1703	A	733	LEU	CG	27.186	0.15	1
1704	A	733	LEU	CD1	23.779	0.15	1
1705	A	733	LEU	CD2	23.779	0.15	1
1706	A	733	LEU	N	124.302	0.06	1
1707	A	734	VAL	H	9.233	0.01	1
1708	A	734	VAL	HA	5.626	0.01	1
1709	A	734	VAL	HB	2.145	0.01	1
1710	A	734	VAL	HG11	0.761	0.01	2
1711	A	734	VAL	HG12	0.761	0.01	2
1712	A	734	VAL	HG13	0.761	0.01	2
1713	A	734	VAL	HG21	0.602	0.01	2
1714	A	734	VAL	HG22	0.602	0.01	2
1715	A	734	VAL	HG23	0.602	0.01	2
1716	A	734	VAL	C	174.229	0.15	1
1717	A	734	VAL	CA	58.200	0.15	1
1718	A	734	VAL	CB	36.529	0.15	1
1719	A	734	VAL	CG1	22.470	0.15	1
1720	A	734	VAL	CG2	19.038	0.15	1
1721	A	734	VAL	N	119.408	0.06	1
1722	A	735	MET	H	8.569	0.01	1
1723	A	735	MET	HA	5.160	0.01	1
1724	A	735	MET	HB2	1.878	0.01	1
1725	A	735	MET	HB3	1.878	0.01	1
1726	A	735	MET	HG2	2.291	0.01	2
1727	A	735	MET	HG3	2.164	0.01	2
1728	A	735	MET	HE1	2.050	0.01	1
1729	A	735	MET	HE2	2.050	0.01	1
1730	A	735	MET	HE3	2.050	0.01	1
1731	A	735	MET	C	175.478	0.15	1
1732	A	735	MET	CA	53.890	0.15	1
1733	A	735	MET	CB	38.290	0.15	1
1734	A	735	MET	CG	30.320	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1735	A	735	MET	CE	17.160	0.15	1
1736	A	735	MET	N	115.458	0.06	1
1737	A	736	LYS	H	8.958	0.01	1
1738	A	736	LYS	HA	3.670	0.01	1
1739	A	736	LYS	HB2	1.966	0.01	2
1740	A	736	LYS	HB3	1.409	0.01	2
1741	A	736	LYS	HG2	1.190	0.01	2
1742	A	736	LYS	HG3	0.784	0.01	2
1743	A	736	LYS	HD2	1.367	0.01	2
1744	A	736	LYS	HD3	1.289	0.01	2
1745	A	736	LYS	HE2	2.861	0.01	1
1746	A	736	LYS	HE3	2.861	0.01	1
1747	A	736	LYS	C	176.557	0.15	1
1748	A	736	LYS	CA	57.500	0.15	1
1749	A	736	LYS	CB	32.287	0.15	1
1750	A	736	LYS	CG	25.545	0.15	1
1751	A	736	LYS	CD	29.297	0.15	1
1752	A	736	LYS	CE	42.564	0.15	1
1753	A	736	LYS	N	127.418	0.06	1
1754	A	737	ARG	H	7.942	0.01	1
1755	A	737	ARG	HA	4.045	0.01	1
1756	A	737	ARG	HB2	1.728	0.01	2
1757	A	737	ARG	HB3	1.427	0.01	2
1758	A	737	ARG	HG2	1.534	0.01	2
1759	A	737	ARG	HG3	1.362	0.01	2
1760	A	737	ARG	HD2	3.122	0.01	2
1761	A	737	ARG	HD3	3.008	0.01	2
1762	A	737	ARG	C	176.179	0.15	1
1763	A	737	ARG	CA	57.399	0.15	1
1764	A	737	ARG	CB	31.224	0.15	1
1765	A	737	ARG	CG	28.707	0.15	1
1766	A	737	ARG	CD	43.587	0.15	1
1767	A	737	ARG	N	126.489	0.06	1
1768	A	738	LYS	H	8.586	0.01	1
1769	A	738	LYS	HA	4.151	0.01	1
1770	A	738	LYS	HB2	1.830	0.01	2
1771	A	738	LYS	HB3	1.728	0.01	2
1772	A	738	LYS	HG2	1.435	0.01	2
1773	A	738	LYS	HG3	1.348	0.01	2
1774	A	738	LYS	HD2	1.646	0.01	1
1775	A	738	LYS	HD3	1.646	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1776	A	738	LYS	HE2	2.956	0.01	1
1777	A	738	LYS	HE3	2.956	0.01	1
1778	A	738	LYS	C	176.200	0.15	1
1779	A	738	LYS	CA	56.989	0.15	1
1780	A	738	LYS	CB	33.540	0.15	1
1781	A	738	LYS	CG	25.437	0.15	1
1782	A	738	LYS	CD	29.514	0.15	1
1783	A	738	LYS	CE	42.088	0.15	1
1784	A	738	LYS	N	122.001	0.06	1
1785	A	739	ARG	H	8.200	0.01	1
1786	A	739	ARG	HA	4.317	0.01	1
1787	A	739	ARG	HB2	1.816	0.01	2
1788	A	739	ARG	HB3	1.753	0.01	2
1789	A	739	ARG	HG2	1.596	0.01	1
1790	A	739	ARG	HG3	1.596	0.01	1
1791	A	739	ARG	HD2	3.162	0.01	1
1792	A	739	ARG	HD3	3.162	0.01	1
1793	A	739	ARG	C	175.130	0.15	1
1794	A	739	ARG	CA	55.900	0.15	1
1795	A	739	ARG	CB	31.309	0.15	1
1796	A	739	ARG	CG	27.065	0.15	1
1797	A	739	ARG	CD	43.455	0.15	1
1798	A	739	ARG	N	121.310	0.06	1
1799	A	740	ASP	H	8.136	0.01	1
1800	A	740	ASP	HA	4.276	0.01	1
1801	A	740	ASP	C	180.961	0.15	1
1802	A	740	ASP	CA	56.993	0.15	1
1803	A	740	ASP	N	128.063	0.06	1
1804	A	741	SER	HA	4.435	0.01	1
1805	A	741	SER	HB2	3.945	0.01	1
1806	A	741	SER	HB3	3.945	0.01	1
1807	A	741	SER	C	174.740	0.15	1
1808	A	741	SER	CA	58.597	0.15	1
1809	A	741	SER	CB	63.777	0.15	1
1810	A	742	SER	H	8.550	0.01	1
1811	A	742	SER	HA	4.406	0.01	1
1812	A	742	SER	HB2	3.859	0.01	1
1813	A	742	SER	HB3	3.859	0.01	1
1814	A	742	SER	C	174.480	0.15	1
1815	A	742	SER	CA	58.955	0.15	1
1816	A	742	SER	CB	63.932	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1817	A	742	SER	N	118.440	0.06	1
1818	A	743	ILE	H	8.045	0.01	1
1819	A	743	ILE	HA	4.175	0.01	1
1820	A	743	ILE	HB	1.884	0.01	1
1821	A	743	ILE	HG12	1.450	0.01	1
1822	A	743	ILE	HG13	1.170	0.01	1
1823	A	743	ILE	HG21	0.872	0.01	1
1824	A	743	ILE	HG22	0.872	0.01	1
1825	A	743	ILE	HG23	0.872	0.01	1
1826	A	743	ILE	HD11	0.839	0.01	1
1827	A	743	ILE	HD12	0.839	0.01	1
1828	A	743	ILE	HD13	0.839	0.01	1
1829	A	743	ILE	C	176.401	0.15	1
1830	A	743	ILE	CA	61.444	0.15	1
1831	A	743	ILE	CB	38.800	0.15	1
1832	A	743	ILE	CG1	27.366	0.15	1
1833	A	743	ILE	CG2	17.576	0.15	1
1834	A	743	ILE	CD1	12.954	0.15	1
1835	A	743	ILE	N	122.128	0.06	1
1836	A	744	LEU	H	8.333	0.01	1
1837	A	744	LEU	HA	4.449	0.01	1
1838	A	744	LEU	HB2	1.681	0.01	2
1839	A	744	LEU	HB3	1.590	0.01	2
1840	A	744	LEU	HG	1.638	0.01	1
1841	A	744	LEU	HD11	0.925	0.01	2
1842	A	744	LEU	HD12	0.925	0.01	2
1843	A	744	LEU	HD13	0.925	0.01	2
1844	A	744	LEU	HD21	0.860	0.01	2
1845	A	744	LEU	HD22	0.860	0.01	2
1846	A	744	LEU	HD23	0.860	0.01	2
1847	A	744	LEU	C	177.765	0.15	1
1848	A	744	LEU	CA	55.338	0.15	1
1849	A	744	LEU	CB	42.263	0.15	1
1850	A	744	LEU	CG	27.039	0.15	1
1851	A	744	LEU	CD1	25.060	0.15	1
1852	A	744	LEU	CD2	23.379	0.15	1
1853	A	744	LEU	N	125.944	0.06	1
1854	A	745	THR	H	8.137	0.01	1
1855	A	745	THR	HA	4.301	0.01	1
1856	A	745	THR	HB	4.278	0.01	1
1857	A	745	THR	HG21	1.199	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1858	A	745	THR	HG22	1.199	0.01	1
1859	A	745	THR	HG23	1.199	0.01	1
1860	A	745	THR	C	174.646	0.15	1
1861	A	745	THR	CA	61.979	0.15	1
1862	A	745	THR	CB	69.914	0.15	1
1863	A	745	THR	CG2	21.619	0.15	1
1864	A	745	THR	N	114.474	0.06	1
1865	A	746	ASP	H	8.434	0.01	1
1866	A	746	ASP	HA	4.629	0.01	1
1867	A	746	ASP	HB2	2.732	0.01	2
1868	A	746	ASP	HB3	2.697	0.01	2
1869	A	746	ASP	C	176.804	0.15	1
1870	A	746	ASP	CA	54.788	0.15	1
1871	A	746	ASP	CB	41.104	0.15	1
1872	A	746	ASP	N	122.781	0.06	1
1873	A	747	SER	H	8.363	0.01	1
1874	A	747	SER	HA	4.393	0.01	1
1875	A	747	SER	HB2	3.945	0.01	2
1876	A	747	SER	HB3	3.883	0.01	2
1877	A	747	SER	C	175.292	0.15	1
1878	A	747	SER	CA	59.228	0.15	1
1879	A	747	SER	CB	63.537	0.15	1
1880	A	747	SER	N	116.322	0.06	1
1881	A	748	GLN	H	8.446	0.01	1
1882	A	748	GLN	HA	4.365	0.01	1
1883	A	748	GLN	HB2	2.171	0.01	2
1884	A	748	GLN	HB3	2.093	0.01	2
1885	A	748	GLN	HG2	2.417	0.01	2
1886	A	748	GLN	HG3	2.386	0.01	2
1887	A	748	GLN	HE21	7.646	0.01	2
1888	A	748	GLN	HE22	6.900	0.01	2
1889	A	748	GLN	C	176.773	0.15	1
1890	A	748	GLN	CA	56.552	0.15	1
1891	A	748	GLN	CB	29.295	0.15	1
1892	A	748	GLN	CG	34.092	0.15	1
1893	A	748	GLN	CD	180.630	0.15	1
1894	A	748	GLN	N	121.917	0.06	1
1895	A	748	GLN	NE2	112.886	0.06	1
1896	A	749	THR	H	8.131	0.01	1
1897	A	749	THR	HA	4.234	0.01	1
1898	A	749	THR	HB	4.244	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1899	A	749	THR	HG21	1.225	0.01	1
1900	A	749	THR	HG22	1.225	0.01	1
1901	A	749	THR	HG23	1.225	0.01	1
1902	A	749	THR	C	174.795	0.15	1
1903	A	749	THR	CA	62.727	0.15	1
1904	A	749	THR	CB	69.617	0.15	1
1905	A	749	THR	CG2	21.731	0.15	1
1906	A	749	THR	N	114.835	0.06	1
1907	A	750	ALA	H	8.301	0.01	1
1908	A	750	ALA	HA	4.330	0.01	1
1909	A	750	ALA	HB1	1.427	0.01	1
1910	A	750	ALA	HB2	1.427	0.01	1
1911	A	750	ALA	HB3	1.427	0.01	1
1912	A	750	ALA	C	178.300	0.15	1
1913	A	750	ALA	CA	53.251	0.15	1
1914	A	750	ALA	CB	19.176	0.15	1
1915	A	750	ALA	N	126.111	0.06	1
1916	A	751	THR	H	8.097	0.01	1
1917	A	751	THR	HA	4.238	0.01	1
1918	A	751	THR	HB	4.202	0.01	1
1919	A	751	THR	HG21	1.225	0.01	1
1920	A	751	THR	HG22	1.225	0.01	1
1921	A	751	THR	HG23	1.225	0.01	1
1922	A	751	THR	C	174.787	0.15	1
1923	A	751	THR	CA	62.665	0.15	1
1924	A	751	THR	CB	69.704	0.15	1
1925	A	751	THR	CG2	21.725	0.15	1
1926	A	751	THR	N	113.611	0.06	1
1927	A	752	LYS	H	8.256	0.01	1
1928	A	752	LYS	HA	4.261	0.01	1
1929	A	752	LYS	HB2	1.845	0.01	2
1930	A	752	LYS	HB3	1.785	0.01	2
1931	A	752	LYS	HG2	1.473	0.01	2
1932	A	752	LYS	HG3	1.414	0.01	2
1933	A	752	LYS	HD2	1.673	0.01	1
1934	A	752	LYS	HD3	1.673	0.01	1
1935	A	752	LYS	HE2	2.968	0.01	1
1936	A	752	LYS	HE3	2.968	0.01	1
1937	A	752	LYS	C	176.574	0.15	1
1938	A	752	LYS	CA	56.798	0.15	1
1939	A	752	LYS	CB	32.951	0.15	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1940	A	752	LYS	CG	24.923	0.15	1
1941	A	752	LYS	CD	29.189	0.15	1
1942	A	752	LYS	CE	42.220	0.15	1
1943	A	752	LYS	N	123.922	0.06	1
1944	A	753	ARG	H	8.299	0.01	1
1945	A	753	ARG	HA	4.314	0.01	1
1946	A	753	ARG	HB2	1.814	0.01	2
1947	A	753	ARG	HB3	1.748	0.01	2
1948	A	753	ARG	HG2	1.639	0.01	2
1949	A	753	ARG	HG3	1.572	0.01	2
1950	A	753	ARG	HD2	3.182	0.01	1
1951	A	753	ARG	HD3	3.182	0.01	1
1952	A	753	ARG	C	176.508	0.15	1
1953	A	753	ARG	CA	56.406	0.15	1
1954	A	753	ARG	CB	30.846	0.15	1
1955	A	753	ARG	CG	27.252	0.15	1
1956	A	753	ARG	CD	43.440	0.15	1
1957	A	753	ARG	N	122.358	0.06	1
1958	A	754	ILE	H	8.215	0.01	1
1959	A	754	ILE	HA	4.112	0.01	1
1960	A	754	ILE	HB	1.863	0.01	1
1961	A	754	ILE	HG12	1.501	0.01	1
1962	A	754	ILE	HG13	1.192	0.01	1
1963	A	754	ILE	HG21	0.873	0.01	1
1964	A	754	ILE	HG22	0.873	0.01	1
1965	A	754	ILE	HG23	0.873	0.01	1
1966	A	754	ILE	HD11	0.839	0.01	1
1967	A	754	ILE	HD12	0.839	0.01	1
1968	A	754	ILE	HD13	0.839	0.01	1
1969	A	754	ILE	C	176.290	0.15	1
1970	A	754	ILE	CA	61.409	0.15	1
1971	A	754	ILE	CB	38.678	0.15	1
1972	A	754	ILE	CG1	27.555	0.15	1
1973	A	754	ILE	CG2	17.630	0.15	1
1974	A	754	ILE	CD1	12.954	0.15	1
1975	A	754	ILE	N	122.679	0.06	1
1976	A	755	ARG	H	8.417	0.01	1
1977	A	755	ARG	HA	4.329	0.01	1
1978	A	755	ARG	HB2	1.815	0.01	2
1979	A	755	ARG	HB3	1.766	0.01	2
1980	A	755	ARG	HG2	1.626	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1981	A	755	ARG	HG3	1.580	0.01	2
1982	A	755	ARG	HD2	3.180	0.01	1
1983	A	755	ARG	HD3	3.180	0.01	1
1984	A	755	ARG	C	176.171	0.15	1
1985	A	755	ARG	CA	56.222	0.15	1
1986	A	755	ARG	CB	30.842	0.15	1
1987	A	755	ARG	CG	27.290	0.15	1
1988	A	755	ARG	CD	43.391	0.15	1
1989	A	755	ARG	N	125.176	0.06	1
1990	A	756	MET	H	8.404	0.01	1
1991	A	756	MET	HA	4.429	0.01	1
1992	A	756	MET	HB2	2.084	0.01	2
1993	A	756	MET	HB3	2.003	0.01	2
1994	A	756	MET	HG2	2.626	0.01	2
1995	A	756	MET	HG3	2.550	0.01	2
1996	A	756	MET	HE1	2.097	0.01	1
1997	A	756	MET	HE2	2.097	0.01	1
1998	A	756	MET	HE3	2.097	0.01	1
1999	A	756	MET	C	175.754	0.15	1
2000	A	756	MET	CA	55.338	0.15	1
2001	A	756	MET	CB	33.079	0.15	1
2002	A	756	MET	CG	32.000	0.15	1
2003	A	756	MET	CE	16.968	0.15	1
2004	A	756	MET	N	122.225	0.06	1
2005	A	757	ALA	H	8.313	0.01	1
2006	A	757	ALA	HA	4.346	0.01	1
2007	A	757	ALA	HB1	1.398	0.01	1
2008	A	757	ALA	HB2	1.398	0.01	1
2009	A	757	ALA	HB3	1.398	0.01	1
2010	A	757	ALA	C	177.389	0.15	1
2011	A	757	ALA	CA	52.443	0.15	1
2012	A	757	ALA	CB	19.358	0.15	1
2013	A	757	ALA	N	125.584	0.06	1
2014	A	758	ILE	H	8.170	0.01	1
2015	A	758	ILE	HA	4.183	0.01	1
2016	A	758	ILE	HB	1.888	0.01	1
2017	A	758	ILE	HG12	1.468	0.01	1
2018	A	758	ILE	HG13	1.171	0.01	1
2019	A	758	ILE	HG21	0.898	0.01	1
2020	A	758	ILE	HG22	0.898	0.01	1
2021	A	758	ILE	HG23	0.898	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2022	A	758	ILE	HD11	0.839	0.01	1
2023	A	758	ILE	HD12	0.839	0.01	1
2024	A	758	ILE	HD13	0.839	0.01	1
2025	A	758	ILE	C	175.303	0.15	1
2026	A	758	ILE	CA	61.236	0.15	1
2027	A	758	ILE	CB	38.938	0.15	1
2028	A	758	ILE	CG1	27.052	0.15	1
2029	A	758	ILE	CG2	17.600	0.15	1
2030	A	758	ILE	CD1	13.110	0.15	1
2031	A	758	ILE	N	119.935	0.06	1
2032	A	759	ASN	H	8.038	0.01	1
2033	A	759	ASN	HA	4.465	0.01	1
2034	A	759	ASN	HB2	2.739	0.01	2
2035	A	759	ASN	HB3	2.681	0.01	2
2036	A	759	ASN	HD21	7.570	0.01	2
2037	A	759	ASN	HD22	6.845	0.01	2
2038	A	759	ASN	C	179.478	0.15	1
2039	A	759	ASN	CA	54.765	0.15	1
2040	A	759	ASN	CB	40.495	0.15	1
2041	A	759	ASN	CG	178.220	0.15	1
2042	A	759	ASN	N	127.510	0.06	1
2043	A	759	ASN	ND2	113.178	0.06	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
$^{13}\text{C}_\alpha$	83	-0.29 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	74	0.03 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	81	-0.20 ± 0.15	None needed (< 0.5 ppm)
^{15}N	77	-0.49 ± 0.29	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 90%, i.e. 833 atoms were assigned a chemical shift out of a possible 925. 15 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	364/368 (99%)	145/147 (99%)	148/148 (100%)	71/73 (97%)
Sidechain	454/540 (84%)	274/314 (87%)	174/193 (90%)	6/33 (18%)
Aromatic	15/17 (88%)	9/9 (100%)	6/8 (75%)	0/0 (—%)
Overall	833/925 (90%)	428/470 (91%)	328/349 (94%)	77/106 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 838 atoms were assigned a chemical shift out of a possible 930. 15 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	369/373 (99%)	147/149 (99%)	150/150 (100%)	72/74 (97%)
Sidechain	454/540 (84%)	274/314 (87%)	174/193 (90%)	6/33 (18%)
Aromatic	15/17 (88%)	9/9 (100%)	6/8 (75%)	0/0 (—%)
Overall	838/930 (90%)	430/472 (91%)	330/351 (94%)	78/107 (73%)

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.

Random coil index (RCI) for chain A:

