



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:27 pm GMT

PDB ID : 1ADN
Title : SOLUTION STRUCTURE OF THE DNA METHYLPHOSPHOTRIESTER
REPAIR DOMAIN OF ESCHERICHIA COLI ADA
Authors : Myers, L.C.; Verdine, G.L.; Wagner, G.
Deposited on : 1993-09-30

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

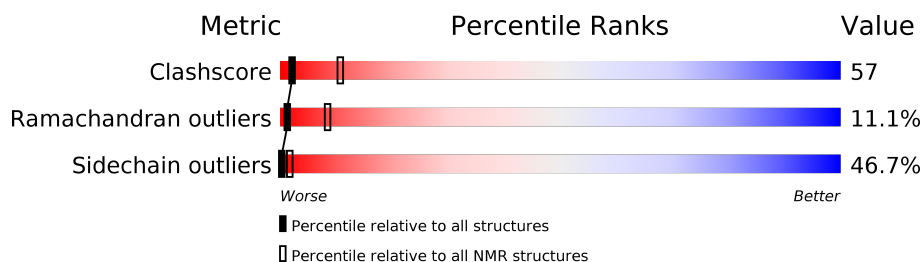
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	92	

2 Ensemble composition and analysis

This entry contains 14 models. Model 11 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:17, A:27-A:72 (56)	0.43	11

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

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

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

Cluster number	Models
1	3, 5, 6, 7, 8, 9, 10, 11, 12, 13
2	1, 2
Single-model clusters	4; 14

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 732 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called N-ADA 10.

Mol	Chain	Residues	Atoms					Trace
1	A	92	Total	C	N	O	S	0
			731	447	148	129	7	

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

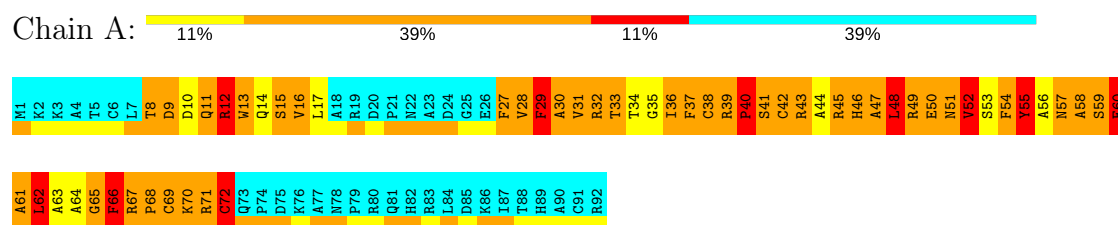
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: N-ADA 10

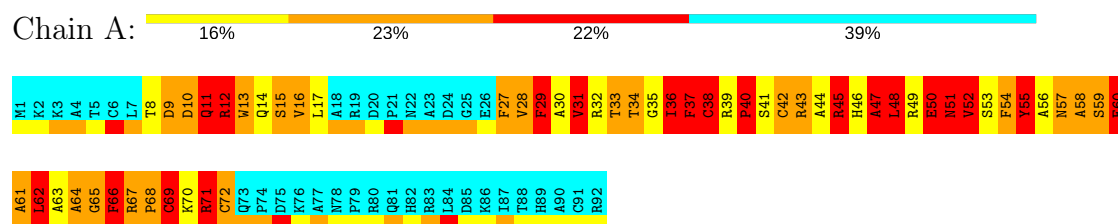


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

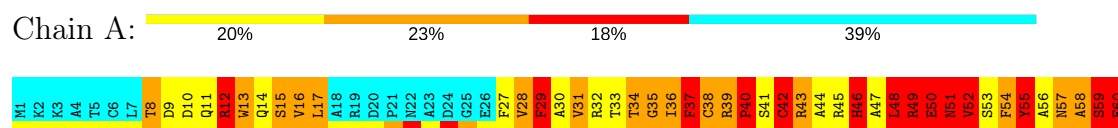
4.2.1 Score per residue for model 1

- Molecule 1: N-ADA 10



4.2.2 Score per residue for model 2

- Molecule 1: N-ADA 10





4.2.3 Score per residue for model 3

- Molecule 1: N-ADA 10

Chain A: 8% 38% 15% 39%



4.2.4 Score per residue for model 4

- Molecule 1: N-ADA 10

Chain A: 15% 27% 18% 39%



4.2.5 Score per residue for model 5

- Molecule 1: N-ADA 10

Chain A: 14% 32% 15% 39%

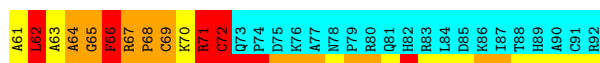


4.2.6 Score per residue for model 6

- Molecule 1: N-ADA 10

Chain A: 22% 22% 17% 39%





4.2.7 Score per residue for model 7

- Molecule 1: N-ADA 10



4.2.8 Score per residue for model 8

- Molecule 1: N-ADA 10



4.2.9 Score per residue for model 9

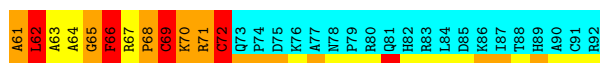
- Molecule 1: N-ADA 10



4.2.10 Score per residue for model 10

- Molecule 1: N-ADA 10





4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: N-ADA 10



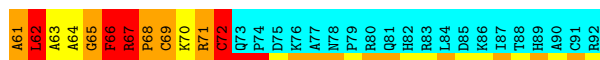
4.2.12 Score per residue for model 12

- Molecule 1: N-ADA 10



4.2.13 Score per residue for model 13

- Molecule 1: N-ADA 10



4.2.14 Score per residue for model 14

- Molecule 1: N-ADA 10



A61	L62	A63	A64	G65	F66	R67	P68	C69	K70	R71	G72	Q73	P74	D75	K76	A77	N78	P79	R80	Q81	H82	R83	L84	D85	K86	I87	T88	H89	A90	C91	R92
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5 Refinement protocol and experimental data overview

The models were refined using the following method: ?.

Of the ? calculated structures, 14 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DGII	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)	BMRB entry 6053, BMRB entry 6054
Number of chemical shift lists	2
Total number of shifts	3396
Number of shifts mapped to atoms	2026
Number of unparsed shifts	0
Number of shifts with mapping errors	1370
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.58±0.01	60±0/458 (13.1±0.0%)	1.71±0.03	22±1/619 (3.6±0.2%)
All	All	2.58	840/6412 (13.1%)	1.71	310/8666 (3.6%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	60	GLU	CD-OE1	10.23	1.36	1.25	6	7
1	A	60	GLU	CD-OE2	10.04	1.36	1.25	13	7
1	A	50	GLU	CD-OE2	10.04	1.36	1.25	13	8
1	A	50	GLU	CD-OE1	10.01	1.36	1.25	11	6
1	A	64	ALA	C-N	8.88	1.49	1.33	6	14
1	A	34	THR	C-N	8.87	1.49	1.33	5	14
1	A	72	CYS	C-N	8.42	1.53	1.34	6	14
1	A	67	ARG	C-N	7.79	1.49	1.34	6	14
1	A	69	CYS	C-N	7.37	1.51	1.34	4	14
1	A	39	ARG	C-N	7.27	1.48	1.34	4	14
1	A	51	ASN	C-N	7.21	1.50	1.34	2	14
1	A	15	SER	C-N	7.13	1.50	1.34	10	14
1	A	12	ARG	C-N	6.88	1.49	1.34	11	14
1	A	41	SER	C-N	6.79	1.49	1.34	1	14
1	A	40	PRO	C-N	6.75	1.49	1.34	2	14
1	A	44	ALA	C-N	6.67	1.49	1.34	4	14
1	A	17	LEU	C-N	6.63	1.49	1.34	13	14
1	A	27	PHE	C-N	6.62	1.49	1.34	11	14
1	A	53	SER	C-N	6.60	1.49	1.34	11	14
1	A	54	PHE	C-N	6.60	1.49	1.34	14	14
1	A	42	CYS	C-N	6.57	1.49	1.34	3	14
1	A	14	GLN	C-N	6.56	1.49	1.34	4	14
1	A	46	HIS	C-N	6.48	1.49	1.34	7	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	71	ARG	C-N	6.43	1.48	1.34	1	14
1	A	66	PHE	C-N	6.43	1.48	1.34	3	14
1	A	55	TYR	C-N	6.42	1.48	1.34	14	14
1	A	45	ARG	C-N	6.41	1.48	1.34	5	14
1	A	28	VAL	C-N	6.41	1.48	1.34	9	14
1	A	13	TRP	C-N	6.41	1.48	1.34	9	14
1	A	49	ARG	C-N	6.40	1.48	1.34	5	14
1	A	57	ASN	C-N	6.40	1.48	1.34	12	14
1	A	31	VAL	C-N	6.39	1.48	1.34	11	14
1	A	68	PRO	C-N	6.39	1.48	1.34	1	14
1	A	63	ALA	C-N	6.39	1.48	1.34	13	14
1	A	35	GLY	C-N	6.39	1.48	1.34	1	14
1	A	43	ARG	C-N	6.38	1.48	1.34	5	14
1	A	48	LEU	C-N	6.37	1.48	1.34	9	14
1	A	70	LYS	C-N	6.36	1.48	1.34	6	14
1	A	10	ASP	C-N	6.36	1.48	1.34	10	14
1	A	59	SER	C-N	6.35	1.48	1.34	8	14
1	A	11	GLN	C-N	6.34	1.48	1.34	14	14
1	A	8	THR	C-N	6.33	1.48	1.34	4	14
1	A	30	ALA	C-N	6.32	1.48	1.34	12	14
1	A	56	ALA	C-N	6.32	1.48	1.34	7	14
1	A	60	GLU	C-N	6.32	1.48	1.34	1	14
1	A	9	ASP	C-N	6.31	1.48	1.34	6	14
1	A	65	GLY	C-N	6.30	1.48	1.34	4	14
1	A	33	THR	C-N	6.30	1.48	1.34	4	14
1	A	29	PHE	C-N	6.30	1.48	1.34	7	14
1	A	47	ALA	C-N	6.29	1.48	1.34	13	14
1	A	62	LEU	C-N	6.27	1.48	1.34	5	14
1	A	58	ALA	C-N	6.26	1.48	1.34	6	14
1	A	36	ILE	C-N	6.25	1.48	1.34	4	14
1	A	38	CYS	C-N	6.23	1.48	1.34	1	14
1	A	32	ARG	C-N	6.21	1.48	1.34	10	14
1	A	52	VAL	C-N	6.21	1.48	1.34	13	14
1	A	61	ALA	C-N	6.21	1.48	1.34	13	14
1	A	37	PHE	C-N	6.20	1.48	1.34	3	14
1	A	16	VAL	C-N	6.13	1.48	1.34	1	14
1	A	50	GLU	C-N	5.88	1.47	1.34	1	14
1	A	9	ASP	CG-OD2	5.17	1.37	1.25	7	9
1	A	10	ASP	CG-OD1	5.17	1.37	1.25	2	6
1	A	10	ASP	CG-OD2	5.16	1.37	1.25	7	8
1	A	9	ASP	CG-OD1	5.16	1.37	1.25	10	5

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	ARG	NE-CZ-NH1	8.38	124.49	120.30	11	14
1	A	12	ARG	NE-CZ-NH1	8.35	124.47	120.30	4	14
1	A	45	ARG	NE-CZ-NH1	8.34	124.47	120.30	14	14
1	A	43	ARG	NE-CZ-NH1	8.32	124.46	120.30	14	14
1	A	39	ARG	NE-CZ-NH1	8.29	124.45	120.30	7	14
1	A	49	ARG	NE-CZ-NH1	8.25	124.43	120.30	9	14
1	A	67	ARG	NE-CZ-NH1	8.19	124.40	120.30	12	14
1	A	71	ARG	NE-CZ-NH1	8.19	124.39	120.30	9	14
1	A	72	CYS	CB-CA-C	7.48	125.35	110.40	6	3
1	A	55	TYR	CB-CG-CD1	-7.03	116.78	121.00	4	2
1	A	69	CYS	CB-CA-C	6.77	123.94	110.40	4	1
1	A	10	ASP	CB-CG-OD2	-6.16	112.76	118.30	1	14
1	A	9	ASP	CB-CG-OD1	-6.15	112.76	118.30	8	14
1	A	10	ASP	CB-CG-OD1	-6.14	112.78	118.30	12	14
1	A	9	ASP	CB-CG-OD2	-6.13	112.78	118.30	7	14
1	A	55	TYR	CB-CG-CD2	-6.12	117.33	121.00	5	5
1	A	45	ARG	NE-CZ-NH2	-5.78	117.41	120.30	2	14
1	A	71	ARG	NE-CZ-NH2	-5.77	117.41	120.30	9	14
1	A	49	ARG	NE-CZ-NH2	-5.76	117.42	120.30	5	14
1	A	67	ARG	NE-CZ-NH2	-5.75	117.42	120.30	6	14
1	A	12	ARG	NE-CZ-NH2	-5.75	117.43	120.30	13	14
1	A	39	ARG	NE-CZ-NH2	-5.73	117.43	120.30	5	14
1	A	43	ARG	NE-CZ-NH2	-5.73	117.43	120.30	8	14
1	A	32	ARG	NE-CZ-NH2	-5.67	117.47	120.30	9	14
1	A	13	TRP	CD1-NE1-CE2	-5.62	103.94	109.00	3	14
1	A	72	CYS	CA-C-O	5.53	131.72	120.10	6	3
1	A	40	PRO	CA-N-CD	-5.15	104.29	111.50	1	2

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	447	0	433	51±8
All	All	6272	0	6062	709

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HG21	1:A:47:ALA:HB1	1.13	1.16	10	7
1:A:31:VAL:HG21	1:A:47:ALA:HB3	1.09	1.16	5	5
1:A:48:LEU:HD22	1:A:50:GLU:HG3	1.06	1.07	13	2
1:A:28:VAL:HG23	1:A:55:TYR:HD1	1.05	1.05	1	4
1:A:37:PHE:HB3	1:A:66:PHE:CD2	1.02	1.90	7	14
1:A:28:VAL:HG23	1:A:55:TYR:CD1	1.02	1.88	1	5
1:A:28:VAL:HG23	1:A:55:TYR:HD2	1.00	1.14	4	1
1:A:13:TRP:HB2	1:A:54:PHE:CZ	0.96	1.95	13	9
1:A:48:LEU:HD22	1:A:50:GLU:CG	0.93	1.93	13	2
1:A:38:CYS:HB2	1:A:69:CYS:O	0.91	1.63	4	1
1:A:29:PHE:HB2	1:A:54:PHE:CE1	0.91	1.98	14	1
1:A:37:PHE:HB3	1:A:66:PHE:HD2	0.91	1.22	11	14
1:A:48:LEU:HD13	1:A:50:GLU:CG	0.90	1.96	4	4
1:A:31:VAL:CG2	1:A:47:ALA:HB1	0.89	1.98	7	6
1:A:31:VAL:HG21	1:A:47:ALA:CB	0.88	1.98	13	10
1:A:38:CYS:HB2	1:A:69:CYS:HB3	0.86	1.47	1	7
1:A:28:VAL:HG23	1:A:55:TYR:CD2	0.84	2.06	4	2
1:A:31:VAL:HG11	1:A:47:ALA:HB2	0.83	1.48	7	5
1:A:55:TYR:CD2	1:A:61:ALA:HB2	0.83	2.09	10	6
1:A:28:VAL:HG22	1:A:55:TYR:HB2	0.82	1.49	6	9
1:A:28:VAL:HG23	1:A:55:TYR:HB2	0.82	1.50	9	4
1:A:48:LEU:HD13	1:A:50:GLU:HG3	0.82	1.52	8	2
1:A:31:VAL:CG2	1:A:47:ALA:HB3	0.81	2.04	5	3
1:A:13:TRP:HB2	1:A:54:PHE:CE2	0.80	2.11	7	2
1:A:55:TYR:CD2	1:A:60:GLU:HG2	0.79	2.11	5	8
1:A:37:PHE:HD2	1:A:61:ALA:CB	0.79	1.90	13	1
1:A:67:ARG:HD3	1:A:68:PRO:HD2	0.78	1.53	6	2
1:A:28:VAL:CG2	1:A:55:TYR:HD2	0.77	1.91	4	2
1:A:55:TYR:CE1	1:A:61:ALA:HB2	0.77	2.14	1	6
1:A:37:PHE:HE1	1:A:58:ALA:HB1	0.76	1.38	5	4
1:A:55:TYR:CE2	1:A:61:ALA:HB2	0.76	2.16	3	7
1:A:29:PHE:HE1	1:A:38:CYS:HB3	0.75	1.39	11	1
1:A:55:TYR:HB3	1:A:60:GLU:HG3	0.75	1.56	6	2
1:A:67:ARG:HD3	1:A:68:PRO:CD	0.75	2.11	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:TRP:HA	1:A:16:VAL:HG23	0.75	1.59	13	9
1:A:28:VAL:HG11	1:A:58:ALA:N	0.75	1.96	5	5
1:A:13:TRP:CZ3	1:A:16:VAL:HG11	0.74	2.16	12	12
1:A:37:PHE:CE2	1:A:68:PRO:HG3	0.74	2.17	1	2
1:A:13:TRP:CE3	1:A:16:VAL:HG21	0.74	2.18	12	13
1:A:48:LEU:CD1	1:A:50:GLU:HG2	0.74	2.11	12	2
1:A:37:PHE:CE2	1:A:62:LEU:HD13	0.73	2.18	14	1
1:A:30:ALA:HB1	1:A:66:PHE:CE2	0.73	2.18	6	4
1:A:38:CYS:HB3	1:A:69:CYS:HB3	0.73	1.58	4	1
1:A:48:LEU:HD22	1:A:50:GLU:HB2	0.73	1.61	2	1
1:A:48:LEU:CD2	1:A:50:GLU:HG3	0.72	2.02	13	2
1:A:11:GLN:HG3	1:A:12:ARG:N	0.72	2.00	14	4
1:A:48:LEU:HD13	1:A:50:GLU:CD	0.72	2.06	4	2
1:A:31:VAL:HG11	1:A:47:ALA:CB	0.71	2.15	12	6
1:A:55:TYR:HD2	1:A:60:GLU:CG	0.71	1.97	13	5
1:A:48:LEU:HB2	1:A:50:GLU:HG3	0.71	1.62	5	1
1:A:38:CYS:HB2	1:A:69:CYS:CB	0.71	2.14	10	3
1:A:55:TYR:HB3	1:A:60:GLU:HG2	0.71	1.62	7	9
1:A:55:TYR:CD1	1:A:60:GLU:HG2	0.71	2.19	4	1
1:A:12:ARG:O	1:A:15:SER:HB2	0.71	1.85	2	5
1:A:12:ARG:O	1:A:15:SER:HB3	0.70	1.86	3	3
1:A:37:PHE:CD1	1:A:61:ALA:HB3	0.70	2.22	4	6
1:A:55:TYR:CD1	1:A:61:ALA:HB2	0.70	2.22	7	6
1:A:31:VAL:HG23	1:A:51:ASN:OD1	0.70	1.85	9	6
1:A:48:LEU:HD13	1:A:50:GLU:HG2	0.69	1.63	1	2
1:A:34:THR:HG22	1:A:36:ILE:HG23	0.69	1.65	1	1
1:A:37:PHE:CE1	1:A:58:ALA:HB1	0.68	2.23	5	4
1:A:57:ASN:OD1	1:A:59:SER:HB3	0.68	1.88	13	3
1:A:27:PHE:CE2	1:A:54:PHE:HE2	0.67	2.07	4	1
1:A:67:ARG:HD3	1:A:68:PRO:N	0.67	2.04	5	3
1:A:52:VAL:HG13	1:A:54:PHE:CE1	0.66	2.25	1	3
1:A:29:PHE:HB3	1:A:54:PHE:CE1	0.66	2.25	11	1
1:A:57:ASN:O	1:A:60:GLU:HG2	0.66	1.90	9	2
1:A:37:PHE:HE1	1:A:58:ALA:CB	0.66	2.03	5	1
1:A:55:TYR:CZ	1:A:61:ALA:HB2	0.66	2.25	13	1
1:A:29:PHE:CE1	1:A:38:CYS:HB3	0.65	2.25	11	2
1:A:48:LEU:HD12	1:A:50:GLU:HG2	0.65	1.67	12	1
1:A:28:VAL:CG2	1:A:55:TYR:CD1	0.65	2.80	6	5
1:A:37:PHE:CE2	1:A:61:ALA:HB3	0.65	2.27	7	1
1:A:45:ARG:O	1:A:46:HIS:HB3	0.65	1.91	4	1
1:A:55:TYR:CD2	1:A:60:GLU:CG	0.64	2.80	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HG23	1:A:51:ASN:HD21	0.64	1.51	4	2
1:A:37:PHE:CD2	1:A:61:ALA:CB	0.64	2.78	13	3
1:A:31:VAL:CG2	1:A:33:THR:HG22	0.64	2.23	4	2
1:A:28:VAL:CG2	1:A:55:TYR:CD2	0.64	2.75	4	2
1:A:27:PHE:CE2	1:A:54:PHE:CE2	0.64	2.86	4	1
1:A:8:THR:OG1	1:A:11:GLN:HG3	0.63	1.91	10	1
1:A:55:TYR:CE2	1:A:61:ALA:CB	0.63	2.81	14	6
1:A:66:PHE:O	1:A:68:PRO:HD3	0.63	1.93	8	3
1:A:48:LEU:HD22	1:A:50:GLU:HG2	0.63	1.71	8	1
1:A:8:THR:O	1:A:12:ARG:HG2	0.62	1.94	6	1
1:A:36:ILE:HD11	1:A:42:CYS:SG	0.62	2.35	14	1
1:A:55:TYR:CD1	1:A:55:TYR:N	0.62	2.68	5	2
1:A:29:PHE:HB3	1:A:54:PHE:HE1	0.62	1.54	11	1
1:A:37:PHE:HE2	1:A:68:PRO:HG3	0.61	1.54	1	2
1:A:38:CYS:HB2	1:A:69:CYS:HB2	0.61	1.72	10	1
1:A:28:VAL:CG2	1:A:55:TYR:CG	0.61	2.83	3	2
1:A:28:VAL:HG22	1:A:55:TYR:CB	0.61	2.23	3	4
1:A:48:LEU:HD22	1:A:50:GLU:CB	0.61	2.25	2	1
1:A:29:PHE:CD2	1:A:52:VAL:CG2	0.60	2.84	14	3
1:A:37:PHE:CZ	1:A:62:LEU:HD13	0.60	2.31	14	1
1:A:29:PHE:HD2	1:A:52:VAL:CG2	0.60	2.08	8	1
1:A:61:ALA:O	1:A:64:ALA:HB3	0.60	1.96	2	4
1:A:55:TYR:HD2	1:A:60:GLU:HG3	0.60	1.53	13	1
1:A:29:PHE:CD2	1:A:52:VAL:HG21	0.59	2.32	14	3
1:A:34:THR:O	1:A:36:ILE:HG23	0.59	1.96	2	1
1:A:31:VAL:CB	1:A:47:ALA:HB1	0.59	2.27	12	4
1:A:31:VAL:HG23	1:A:51:ASN:ND2	0.59	2.12	1	2
1:A:38:CYS:CB	1:A:69:CYS:HB3	0.58	2.28	4	10
1:A:29:PHE:HB2	1:A:54:PHE:HE1	0.58	1.54	14	1
1:A:37:PHE:HD2	1:A:61:ALA:HB3	0.58	1.56	13	1
1:A:38:CYS:CB	1:A:69:CYS:CB	0.58	2.81	10	2
1:A:8:THR:HG22	1:A:9:ASP:N	0.58	2.13	12	1
1:A:31:VAL:HB	1:A:52:VAL:HG23	0.58	1.74	4	4
1:A:37:PHE:HD2	1:A:61:ALA:HB1	0.58	1.58	13	1
1:A:37:PHE:CE2	1:A:68:PRO:CG	0.58	2.87	1	2
1:A:27:PHE:CE1	1:A:40:PRO:CG	0.58	2.86	5	2
1:A:37:PHE:CD1	1:A:61:ALA:CB	0.58	2.86	14	8
1:A:13:TRP:CE3	1:A:16:VAL:CG2	0.58	2.87	14	10
1:A:29:PHE:HD2	1:A:52:VAL:HG21	0.58	1.59	8	1
1:A:8:THR:HG23	1:A:12:ARG:HH11	0.57	1.59	14	1
1:A:55:TYR:N	1:A:55:TYR:CD1	0.57	2.72	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ARG:CZ	1:A:71:ARG:HB3	0.57	2.28	14	1
1:A:48:LEU:HD13	1:A:50:GLU:OE2	0.57	1.99	12	1
1:A:37:PHE:CB	1:A:66:PHE:CD2	0.57	2.87	10	8
1:A:31:VAL:HG23	1:A:33:THR:HG22	0.57	1.76	14	2
1:A:62:LEU:CD2	1:A:68:PRO:HG3	0.56	2.30	1	1
1:A:37:PHE:CD2	1:A:61:ALA:HB3	0.56	2.33	13	2
1:A:48:LEU:HD13	1:A:50:GLU:CB	0.56	2.31	1	1
1:A:48:LEU:HD22	1:A:50:GLU:OE2	0.56	1.99	7	1
1:A:55:TYR:HE2	1:A:61:ALA:HA	0.56	1.61	3	2
1:A:29:PHE:HB2	1:A:54:PHE:CD1	0.56	2.33	14	1
1:A:31:VAL:HG12	1:A:36:ILE:HG13	0.56	1.77	8	1
1:A:55:TYR:HD1	1:A:55:TYR:N	0.56	1.98	5	2
1:A:30:ALA:HB1	1:A:66:PHE:CD2	0.56	2.36	13	3
1:A:27:PHE:HE1	1:A:40:PRO:CG	0.55	2.15	5	1
1:A:8:THR:HG23	1:A:12:ARG:NH1	0.55	2.17	14	1
1:A:52:VAL:CG1	1:A:54:PHE:CE1	0.54	2.89	9	2
1:A:31:VAL:CG1	1:A:47:ALA:HB1	0.54	2.32	12	1
1:A:27:PHE:HE1	1:A:40:PRO:HG3	0.54	1.62	5	1
1:A:67:ARG:HD3	1:A:67:ARG:C	0.54	2.23	5	3
1:A:28:VAL:CG2	1:A:55:TYR:HB2	0.54	2.32	14	10
1:A:55:TYR:CE2	1:A:61:ALA:CA	0.54	2.91	3	4
1:A:62:LEU:HD12	1:A:63:ALA:N	0.54	2.18	3	1
1:A:55:TYR:HD2	1:A:61:ALA:HB2	0.54	1.56	10	1
1:A:29:PHE:HA	1:A:54:PHE:HD1	0.53	1.63	14	1
1:A:16:VAL:HG12	1:A:41:SER:OG	0.53	2.03	14	1
1:A:62:LEU:HD13	1:A:68:PRO:HG3	0.53	1.78	8	1
1:A:52:VAL:CG1	1:A:54:PHE:CZ	0.53	2.92	14	1
1:A:38:CYS:HB2	1:A:69:CYS:SG	0.53	2.43	7	1
1:A:29:PHE:HD1	1:A:29:PHE:O	0.53	1.86	5	1
1:A:36:ILE:N	1:A:66:PHE:CZ	0.53	2.77	4	3
1:A:27:PHE:CD1	1:A:27:PHE:C	0.53	2.81	5	1
1:A:38:CYS:HB2	1:A:69:CYS:C	0.53	2.24	4	1
1:A:16:VAL:HG13	1:A:40:PRO:HB3	0.53	1.81	9	2
1:A:37:PHE:CD1	1:A:61:ALA:HB1	0.53	2.39	8	2
1:A:37:PHE:HB3	1:A:66:PHE:HB3	0.52	1.81	4	1
1:A:37:PHE:CE2	1:A:68:PRO:N	0.52	2.77	8	5
1:A:31:VAL:HG11	1:A:46:HIS:CE1	0.52	2.40	2	1
1:A:31:VAL:CG1	1:A:47:ALA:CB	0.52	2.88	12	2
1:A:55:TYR:HE2	1:A:61:ALA:CB	0.51	2.17	14	2
1:A:28:VAL:HG22	1:A:55:TYR:CG	0.51	2.38	3	1
1:A:48:LEU:HB2	1:A:50:GLU:HG2	0.51	1.81	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:PHE:C	1:A:55:TYR:CD1	0.51	2.84	14	4
1:A:13:TRP:HE1	1:A:17:LEU:HD21	0.51	1.65	12	2
1:A:15:SER:HB3	1:A:27:PHE:CZ	0.51	2.41	8	3
1:A:48:LEU:CB	1:A:50:GLU:HG3	0.51	2.34	5	1
1:A:55:TYR:HE2	1:A:61:ALA:CA	0.51	2.19	3	1
1:A:55:TYR:CZ	1:A:61:ALA:CB	0.51	2.94	13	1
1:A:29:PHE:CD1	1:A:29:PHE:C	0.50	2.84	5	2
1:A:13:TRP:HB2	1:A:54:PHE:HZ	0.50	1.67	10	4
1:A:37:PHE:CE1	1:A:68:PRO:HA	0.50	2.41	13	2
1:A:37:PHE:CD2	1:A:61:ALA:HB1	0.50	2.40	7	1
1:A:31:VAL:HG11	1:A:47:ALA:HB1	0.50	1.83	12	1
1:A:48:LEU:HD13	1:A:50:GLU:HB3	0.50	1.82	1	1
1:A:37:PHE:CE1	1:A:68:PRO:N	0.50	2.80	7	1
1:A:55:TYR:HD2	1:A:60:GLU:HG2	0.49	1.58	5	2
1:A:29:PHE:HD1	1:A:38:CYS:O	0.49	1.89	8	2
1:A:48:LEU:N	1:A:48:LEU:HD12	0.49	2.22	2	1
1:A:13:TRP:CZ3	1:A:16:VAL:HG21	0.49	2.43	2	2
1:A:52:VAL:HG11	1:A:54:PHE:CZ	0.49	2.43	14	1
1:A:29:PHE:HD2	1:A:40:PRO:HD3	0.49	1.66	10	2
1:A:55:TYR:CD1	1:A:60:GLU:CG	0.49	2.94	4	1
1:A:37:PHE:CB	1:A:66:PHE:HD2	0.49	2.15	2	7
1:A:37:PHE:CE2	1:A:61:ALA:CB	0.49	2.96	7	1
1:A:30:ALA:HB2	1:A:55:TYR:OH	0.49	2.08	3	1
1:A:48:LEU:HB3	1:A:50:GLU:HG3	0.49	1.83	6	1
1:A:27:PHE:HD1	1:A:27:PHE:C	0.48	2.11	5	1
1:A:55:TYR:CG	1:A:60:GLU:HG2	0.48	2.42	10	3
1:A:13:TRP:NE1	1:A:17:LEU:HD21	0.48	2.22	12	3
1:A:55:TYR:CE2	1:A:61:ALA:HA	0.48	2.43	5	2
1:A:13:TRP:CZ3	1:A:16:VAL:CG1	0.48	2.94	12	3
1:A:27:PHE:CE1	1:A:40:PRO:HG3	0.48	2.44	3	1
1:A:67:ARG:C	1:A:67:ARG:HD3	0.48	2.29	12	1
1:A:36:ILE:C	1:A:66:PHE:CE2	0.48	2.87	4	7
1:A:54:PHE:C	1:A:55:TYR:HD1	0.47	2.12	5	2
1:A:37:PHE:CG	1:A:61:ALA:HB1	0.47	2.43	3	2
1:A:37:PHE:CE2	1:A:68:PRO:HA	0.47	2.45	12	2
1:A:48:LEU:HD12	1:A:48:LEU:H	0.47	1.70	2	1
1:A:37:PHE:CG	1:A:37:PHE:O	0.47	2.67	14	7
1:A:30:ALA:HB2	1:A:55:TYR:HE1	0.47	1.70	12	1
1:A:46:HIS:CG	1:A:47:ALA:N	0.47	2.82	13	1
1:A:11:GLN:HG3	1:A:12:ARG:H	0.46	1.70	5	1
1:A:59:SER:HA	1:A:62:LEU:HD21	0.46	1.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:PHE:HE2	1:A:68:PRO:CG	0.46	2.21	1	1
1:A:62:LEU:CD2	1:A:68:PRO:CG	0.46	2.93	1	1
1:A:29:PHE:HD1	1:A:29:PHE:C	0.46	2.14	5	1
1:A:34:THR:HG22	1:A:36:ILE:CG2	0.46	2.39	1	1
1:A:55:TYR:CE1	1:A:61:ALA:CB	0.46	2.97	2	2
1:A:67:ARG:NE	1:A:68:PRO:HD2	0.46	2.24	5	1
1:A:29:PHE:HD1	1:A:52:VAL:HG22	0.46	1.70	1	1
1:A:29:PHE:HD1	1:A:52:VAL:CG2	0.46	2.24	1	1
1:A:16:VAL:HG22	1:A:40:PRO:CG	0.46	2.41	9	1
1:A:27:PHE:CE1	1:A:40:PRO:HG2	0.46	2.44	3	2
1:A:60:GLU:O	1:A:64:ALA:N	0.46	2.49	8	5
1:A:29:PHE:CE1	1:A:31:VAL:HG12	0.46	2.46	1	1
1:A:37:PHE:CE2	1:A:68:PRO:CA	0.46	2.99	8	2
1:A:27:PHE:HE2	1:A:54:PHE:CE2	0.45	2.28	4	1
1:A:31:VAL:CG2	1:A:51:ASN:ND2	0.45	2.79	2	2
1:A:33:THR:N	1:A:51:ASN:ND2	0.45	2.64	3	3
1:A:62:LEU:O	1:A:65:GLY:N	0.45	2.50	6	12
1:A:45:ARG:O	1:A:46:HIS:HB2	0.45	2.09	11	1
1:A:29:PHE:CB	1:A:54:PHE:CE1	0.45	2.99	11	1
1:A:29:PHE:HE1	1:A:38:CYS:SG	0.45	2.35	4	1
1:A:37:PHE:HD2	1:A:66:PHE:C	0.45	2.15	10	2
1:A:28:VAL:HG11	1:A:58:ALA:CA	0.45	2.41	13	4
1:A:13:TRP:CE2	1:A:49:ARG:HB2	0.45	2.47	10	1
1:A:28:VAL:HG11	1:A:58:ALA:HB2	0.45	1.88	1	1
1:A:48:LEU:CD1	1:A:50:GLU:CG	0.45	2.91	12	2
1:A:30:ALA:N	1:A:53:SER:O	0.45	2.50	11	4
1:A:49:ARG:HG2	1:A:52:VAL:HG12	0.45	1.88	2	1
1:A:37:PHE:CD2	1:A:66:PHE:HB3	0.45	2.47	4	6
1:A:55:TYR:CB	1:A:60:GLU:HG2	0.45	2.42	14	6
1:A:32:ARG:N	1:A:51:ASN:ND2	0.44	2.65	11	7
1:A:54:PHE:N	1:A:54:PHE:CD1	0.44	2.84	9	1
1:A:37:PHE:CD1	1:A:37:PHE:C	0.44	2.91	2	1
1:A:60:GLU:O	1:A:64:ALA:HB2	0.44	2.11	8	1
1:A:28:VAL:HB	1:A:55:TYR:HD2	0.44	1.72	8	1
1:A:13:TRP:CE2	1:A:49:ARG:HG2	0.44	2.47	9	1
1:A:12:ARG:O	1:A:15:SER:CB	0.44	2.66	10	3
1:A:31:VAL:HB	1:A:47:ALA:HB1	0.44	1.89	12	1
1:A:37:PHE:CZ	1:A:68:PRO:HG3	0.43	2.48	8	2
1:A:37:PHE:CZ	1:A:68:PRO:HB3	0.43	2.48	3	2
1:A:28:VAL:N	1:A:55:TYR:O	0.43	2.51	7	1
1:A:37:PHE:CE1	1:A:61:ALA:HB3	0.43	2.48	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ASN:OD1	1:A:59:SER:HB2	0.43	2.14	3	4
1:A:8:THR:CG2	1:A:9:ASP:N	0.43	2.81	12	1
1:A:55:TYR:CD2	1:A:60:GLU:HG3	0.43	2.41	13	1
1:A:37:PHE:HZ	1:A:62:LEU:HD12	0.43	1.74	13	1
1:A:13:TRP:CD1	1:A:49:ARG:HD2	0.43	2.49	12	1
1:A:48:LEU:H	1:A:48:LEU:HD12	0.43	1.74	13	1
1:A:30:ALA:O	1:A:53:SER:N	0.43	2.52	13	1
1:A:66:PHE:HD1	1:A:67:ARG:NH1	0.42	2.12	3	1
1:A:52:VAL:CG1	1:A:54:PHE:HE1	0.42	2.25	9	1
1:A:67:ARG:CD	1:A:68:PRO:HD2	0.42	2.35	6	1
1:A:67:ARG:C	1:A:67:ARG:HD2	0.42	2.35	13	1
1:A:29:PHE:CD1	1:A:38:CYS:O	0.42	2.72	11	1
1:A:37:PHE:HE1	1:A:68:PRO:HD3	0.42	1.73	7	1
1:A:35:GLY:HA2	1:A:66:PHE:CE1	0.42	2.50	7	1
1:A:13:TRP:CD2	1:A:49:ARG:HB2	0.42	2.49	2	1
1:A:67:ARG:HE	1:A:68:PRO:HD2	0.42	1.75	5	1
1:A:12:ARG:HB3	1:A:54:PHE:CE2	0.42	2.50	4	1
1:A:37:PHE:CZ	1:A:68:PRO:HA	0.42	2.50	5	1
1:A:31:VAL:HG13	1:A:31:VAL:O	0.42	2.15	7	2
1:A:37:PHE:CE1	1:A:68:PRO:CA	0.41	3.03	7	1
1:A:37:PHE:CD1	1:A:66:PHE:HB3	0.41	2.50	7	1
1:A:31:VAL:CB	1:A:47:ALA:CB	0.41	2.99	7	1
1:A:37:PHE:HB3	1:A:66:PHE:CG	0.41	2.49	4	1
1:A:37:PHE:CD2	1:A:67:ARG:C	0.41	2.93	12	2
1:A:13:TRP:CE2	1:A:49:ARG:HB3	0.41	2.51	11	4
1:A:35:GLY:HA2	1:A:66:PHE:CZ	0.41	2.51	2	1
1:A:33:THR:HB	1:A:51:ASN:ND2	0.41	2.31	3	1
1:A:35:GLY:O	1:A:67:ARG:CD	0.41	2.68	3	1
1:A:67:ARG:C	1:A:67:ARG:CD	0.41	2.90	13	1
1:A:28:VAL:HG11	1:A:57:ASN:C	0.41	2.36	5	1
1:A:31:VAL:CG2	1:A:47:ALA:CB	0.41	2.89	9	1
1:A:37:PHE:CD1	1:A:37:PHE:O	0.41	2.73	13	1
1:A:60:GLU:O	1:A:63:ALA:HB3	0.40	2.16	14	1
1:A:37:PHE:HE2	1:A:68:PRO:HD3	0.40	1.77	10	1
1:A:35:GLY:O	1:A:67:ARG:HD3	0.40	2.17	3	1
1:A:44:ALA:C	1:A:46:HIS:N	0.40	2.75	3	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	56/92 (61%)	42±2 (76±4%)	7±2 (13±4%)	6±2 (11±3%)	1	8
All	All	784/1288 (61%)	593 (76%)	104 (13%)	87 (11%)	1	8

All 14 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	72	CYS	14
1	A	40	PRO	14
1	A	45	ARG	11
1	A	41	SER	11
1	A	46	HIS	7
1	A	12	ARG	5
1	A	42	CYS	5
1	A	44	ALA	5
1	A	70	LYS	4
1	A	43	ARG	4
1	A	47	ALA	3
1	A	71	ARG	2
1	A	10	ASP	1
1	A	69	CYS	1

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	46/76 (61%)	25±3 (53±7%)	22±3 (47±7%)	0	2
All	All	644/1064 (61%)	343 (53%)	301 (47%)	0	2

All 43 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	52	VAL	14
1	A	48	LEU	14
1	A	66	PHE	14
1	A	40	PRO	13
1	A	62	LEU	12
1	A	60	GLU	12
1	A	55	TYR	11
1	A	67	ARG	11
1	A	72	CYS	11
1	A	9	ASP	10
1	A	50	GLU	10
1	A	71	ARG	10
1	A	29	PHE	10
1	A	43	ARG	9
1	A	12	ARG	9
1	A	8	THR	9
1	A	11	GLN	9
1	A	27	PHE	8
1	A	36	ILE	8
1	A	45	ARG	8
1	A	39	ARG	7
1	A	49	ARG	7
1	A	46	HIS	7
1	A	37	PHE	6
1	A	10	ASP	6
1	A	51	ASN	6
1	A	32	ARG	5
1	A	41	SER	5
1	A	70	LYS	5
1	A	33	THR	4
1	A	28	VAL	4
1	A	59	SER	4
1	A	31	VAL	3
1	A	38	CYS	3
1	A	15	SER	3
1	A	69	CYS	3
1	A	57	ASN	2
1	A	14	GLN	2
1	A	42	CYS	2
1	A	53	SER	2
1	A	34	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	16	VAL	1
1	A	54	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 87% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6053

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	1679
Number of shifts mapped to atoms	1011
Number of unparsed shifts	0
Number of shifts with mapping errors	668
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

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

- Residue not found in structure. All 668 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	127	THR	CB	68.31	0.05	1
A	121	LYS	N	122.19	0.05	1
A	110	ALA	N	123.33	0.05	1
A	123	THR	C	175.52	0.05	1
A	127	THR	HG22	1.48	0.01	1
A	117	HIS	N	118.69	0.05	1
A	114	PHE	HB2	3.19	0.01	1
A	99	PRO	HB3	1.93	0.01	1
A	123	THR	HG22	1.05	0.01	1
A	102	LEU	HD12	0.96	0.01	1
A	139	ARG	HA	3.84	0.01	1
A	103	GLU	HG2	2.51	0.01	1
A	131	TRP	CH2	125.4	0.05	1
A	113	PRO	HD3	3.95	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	122	ALA	HB3	1.54	0.01	1
A	118	ARG	CG	27.7	0.05	1
A	134	ALA	HB1	1.36	0.01	1
A	107	ASP	HB3	2.76	0.01	1
A	107	ASP	C	179.27	0.05	1
A	127	THR	H	7.92	0.01	1
A	145	ALA	HB3	1.42	0.01	1
A	133	GLN	HG2	2.68	0.01	1
A	124	THR	HG21	0.09	0.01	1
A	98	THR	CA	60.98	0.05	1
A	114	PHE	HD1	6.99	0.01	1
A	93	LEU	HA	3.93	0.01	1
A	116	LEU	HD23	0.8	0.01	1
A	123	THR	HA	4.04	0.01	1
A	110	ALA	CA	52.8	0.05	1
A	144	LEU	HD22	0.89	0.01	1
A	135	TRP	CD1	127.06	0.05	1
A	126	MET	HG3	2.66	0.01	1
A	96	GLN	CA	54.8	0.05	1
A	98	THR	HG21	1.31	0.01	1
A	131	TRP	HH2	7.3	0.01	1
A	102	LEU	CD1	25.71	0.05	1
A	131	TRP	HD1	7.06	0.01	1
A	145	ALA	CA	52.07	0.05	1
A	97	GLU	CA	59.25	0.05	1
A	126	MET	HB3	2.37	0.01	1
A	79	ALA	HB1	1.42	0.01	1
A	132	GLN	HA	4.07	0.01	1
A	112	SER	HB2	4.28	0.01	1
A	141	ARG	CG	27.49	0.05	1
A	142	GLU	HB2	2.07	0.01	1
A	109	VAL	HA	4.44	0.01	1
A	103	GLU	CG	37.81	0.05	1
A	138	ARG	C	177.85	0.05	1
A	119	LEU	CD1	23.68	0.05	1
A	120	PHE	HD1	7.1	0.01	1
A	131	TRP	CZ3	119.95	0.05	1
A	127	THR	N	107.52	0.05	1
A	129	LYS	CB	32.85	0.05	1
A	115	HIS	CA	58.9	0.05	1
A	121	LYS	HG3	1.18	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	117	HIS	CB	31.23	0.05	1
A	103	GLU	HB2	2.1	0.01	1
A	135	TRP	HB2	3.68	0.01	1
A	121	LYS	C	180.12	0.05	1
A	115	HIS	HD2	7.2	0.01	1
A	111	MET	CB	39.77	0.05	1
A	97	GLU	N	119.19	0.05	1
A	80	GLN	N	118.52	0.05	1
A	133	GLN	HB2	2.33	0.01	1
A	140	LEU	CD1	24.13	0.05	1
A	128	PRO	HD3	3.96	0.01	1
A	98	THR	N	116.52	0.05	1
A	142	GLU	CA	57.6	0.05	1
A	132	GLN	HB2	2.07	0.01	1
A	105	LEU	CD1	26.29	0.05	1
A	109	VAL	N	109.53	0.05	1
A	93	LEU	C	177.73	0.05	1
A	108	GLN	HE21	7.09	0.01	1
A	94	LEU	CD1	27.46	0.05	1
A	99	PRO	CB	32.41	0.05	1
A	136	ARG	HA	3.48	0.01	1
A	97	GLU	HB2	2.21	0.01	1
A	102	LEU	CA	58.12	0.05	1
A	116	LEU	CB	40.94	0.05	1
A	96	GLN	HB2	2.01	0.01	1
A	131	TRP	HE3	6.97	0.01	1
A	105	LEU	HA	3.8	0.01	1
A	127	THR	HB	4.83	0.01	1
A	99	PRO	HG2	2.02	0.01	1
A	129	LYS	CE	42.13	0.05	1
A	105	LEU	HB3	1.55	0.01	1
A	119	LEU	HD11	0.9	0.01	1
A	111	MET	CE	17.18	0.05	1
A	144	LEU	CD1	25.37	0.05	1
A	142	GLU	CG	36.72	0.05	1
A	118	ARG	CB	30.73	0.05	1
A	146	LYS	HA	4.16	0.01	1
A	101	THR	H	8.27	0.01	1
A	101	THR	HG23	1.38	0.01	1
A	141	ARG	HA	4.17	0.01	1
A	129	LYS	H	8.19	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	109	VAL	C	174.31	0.05	1
A	75	GLU	HG3	2.15	0.01	1
A	94	LEU	H	7.33	0.01	1
A	110	ALA	HB1	1.4	0.01	1
A	140	LEU	HD23	0.89	0.01	1
A	93	LEU	HB2	1.83	0.01	1
A	104	ALA	HB1	1.46	0.01	1
A	138	ARG	HD2	3.08	0.01	1
A	116	LEU	H	8.73	0.01	1
A	111	MET	HG3	2.61	0.01	1
A	79	ALA	C	178.35	0.05	1
A	117	HIS	HB2	3.28	0.01	1
A	108	GLN	HB2	2.13	0.01	1
A	102	LEU	HD23	1.05	0.01	1
A	144	LEU	HD21	0.89	0.01	1
A	136	ARG	H	8.61	0.01	1
A	135	TRP	CA	62.19	0.05	1
A	96	GLN	CB	30.8	0.05	1
A	125	GLY	HA2	4.38	0.01	1
A	114	PHE	N	116.27	0.05	1
A	108	GLN	H	7.71	0.01	1
A	118	ARG	H	7.53	0.01	1
A	144	LEU	H	7.82	0.01	1
A	140	LEU	HD12	0.86	0.01	1
A	130	ALA	N	122.35	0.05	1
A	96	GLN	HG3	2.12	0.01	1
A	123	THR	CB	69.57	0.05	1
A	110	ALA	HA	4.14	0.01	1
A	108	GLN	CG	35.42	0.05	1
A	126	MET	HE2	2.12	0.01	1
A	121	LYS	HB3	1.59	0.01	1
A	80	GLN	CB	29.39	0.05	1
A	93	LEU	HD13	0.79	0.01	1
A	102	LEU	HB3	1.83	0.01	1
A	120	PHE	CD1	130.51	0.05	1
A	114	PHE	H	8.01	0.01	1
A	134	ALA	CB	17.68	0.05	1
A	114	PHE	CD2	131.63	0.05	1
A	126	MET	HA	5.08	0.01	1
A	126	MET	CA	54.28	0.05	1
A	141	ARG	CB	30.52	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	136	ARG	HB2	2.0	0.01	1
A	103	GLU	HA	3.8	0.01	1
A	105	LEU	HD22	0.83	0.01	1
A	109	VAL	HG23	0.68	0.01	1
A	121	LYS	CE	41.92	0.05	1
A	144	LEU	CB	42.31	0.05	1
A	116	LEU	HD13	0.93	0.01	1
A	99	PRO	C	176.15	0.05	1
A	144	LEU	HD13	0.94	0.01	1
A	102	LEU	CD2	23.27	0.05	1
A	133	GLN	HA	4.15	0.01	1
A	114	PHE	CB	39.23	0.05	1
A	113	PRO	C	177.5	0.05	1
A	120	PHE	N	124.65	0.05	1
A	118	ARG	N	115.83	0.05	1
A	140	LEU	H	7.72	0.01	1
A	93	LEU	N	119.25	0.05	1
A	105	LEU	CD2	24.57	0.05	1
A	99	PRO	CA	63.2	0.05	1
A	105	LEU	HD12	0.68	0.01	1
A	107	ASP	N	116.65	0.05	1
A	114	PHE	HE1	7.33	0.01	1
A	123	THR	CG2	21.38	0.05	1
A	104	ALA	HA	4.23	0.01	1
A	102	LEU	CB	41.33	0.05	1
A	121	LYS	HD3	1.52	0.01	1
A	106	ALA	HB3	1.52	0.01	1
A	130	ALA	HB3	1.69	0.01	1
A	121	LYS	CB	32.43	0.05	1
A	116	LEU	CA	58.26	0.05	1
A	115	HIS	C	178.05	0.05	1
A	141	ARG	HB3	1.9	0.01	1
A	98	THR	CG2	21.7	0.05	1
A	94	LEU	HA	4.09	0.01	1
A	108	GLN	NE2	110.27	0.05	1
A	119	LEU	HA	4.28	0.01	1
A	130	ALA	HB2	1.69	0.01	1
A	103	GLU	CA	61.06	0.05	1
A	119	LEU	HD12	0.9	0.01	1
A	130	ALA	CB	19.26	0.05	1
A	129	LYS	HG3	1.63	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	120	PHE	HB2	3.14	0.01	1
A	131	TRP	HA	4.32	0.01	1
A	120	PHE	HE1	6.91	0.01	1
A	118	ARG	CA	59.33	0.05	1
A	125	GLY	C	173.45	0.05	1
A	114	PHE	CE1	131.51	0.05	1
A	146	LYS	CB	33.76	0.05	1
A	129	LYS	HE3	3.07	0.01	1
A	114	PHE	HA	4.32	0.01	1
A	142	GLU	HA	4.18	0.01	1
A	128	PRO	HB2	1.41	0.01	1
A	144	LEU	N	122.77	0.05	1
A	113	PRO	HD2	4.01	0.01	1
A	125	GLY	CA	45.7	0.05	1
A	127	THR	HG21	1.48	0.01	1
A	114	PHE	HB3	2.9	0.01	1
A	96	GLN	CG	29.37	0.05	1
A	137	ALA	CA	54.56	0.05	1
A	106	ALA	HA	3.81	0.01	1
A	100	VAL	HG11	0.95	0.01	1
A	124	THR	CA	62.82	0.05	1
A	99	PRO	HB2	2.34	0.01	1
A	128	PRO	C	177.47	0.05	1
A	123	THR	HG21	1.05	0.01	1
A	138	ARG	CB	29.82	0.05	1
A	100	VAL	N	125.07	0.05	1
A	103	GLU	HG3	2.18	0.01	1
A	123	THR	CA	65.8	0.05	1
A	94	LEU	HD21	0.78	0.01	1
A	135	TRP	HD1	7.23	0.01	1
A	120	PHE	CD2	130.51	0.05	1
A	139	ARG	CA	57.6	0.05	1
A	107	ASP	HB2	2.84	0.01	1
A	128	PRO	CD	49.62	0.05	1
A	97	GLU	H	8.84	0.01	1
A	145	ALA	HB2	1.42	0.01	1
A	104	ALA	CA	54.79	0.05	1
A	119	LEU	HB2	1.72	0.01	1
A	137	ALA	C	179.9	0.05	1
A	139	ARG	HB2	1.47	0.01	1
A	124	THR	HG22	0.09	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	114	PHE	HD2	6.99	0.01	1
A	109	VAL	H	7.71	0.01	1
A	115	HIS	N	118.93	0.05	1
A	135	TRP	CZ3	121.31	0.05	1
A	129	LYS	HB3	1.8	0.01	1
A	126	MET	HG2	2.66	0.01	1
A	138	ARG	N	118.99	0.05	1
A	137	ALA	N	120.64	0.05	1
A	100	VAL	HG12	0.95	0.01	1
A	146	LYS	HB3	1.72	0.01	1
A	114	PHE	C	177.95	0.05	1
A	139	ARG	CB	29.47	0.05	1
A	124	THR	N	108.85	0.05	1
A	111	MET	HE3	1.93	0.01	1
A	111	MET	N	117.59	0.05	1
A	135	TRP	HZ2	7.4	0.01	1
A	138	ARG	HG2	1.63	0.01	1
A	112	SER	HA	4.84	0.01	1
A	97	GLU	CB	30.77	0.05	1
A	79	ALA	HB2	1.42	0.01	1
A	141	ARG	HG2	1.64	0.01	1
A	113	PRO	HB3	2.05	0.01	1
A	102	LEU	HA	3.95	0.01	1
A	94	LEU	HD13	0.73	0.01	1
A	141	ARG	H	7.79	0.01	1
A	143	SER	HB3	3.95	0.01	1
A	126	MET	CE	17.9	0.05	1
A	142	GLU	HB3	1.99	0.01	1
A	104	ALA	N	122.79	0.05	1
A	142	GLU	C	177.56	0.05	1
A	145	ALA	C	176.56	0.05	1
A	105	LEU	HD11	0.68	0.01	1
A	146	LYS	N	125.78	0.05	1
A	131	TRP	HZ2	7.52	0.01	1
A	96	GLN	NE2	112.52	0.05	1
A	115	HIS	HA	4.41	0.01	1
A	122	ALA	CA	54.56	0.05	1
A	139	ARG	H	7.65	0.01	1
A	131	TRP	CZ2	114.56	0.05	1
A	106	ALA	C	179.52	0.05	1
A	121	LYS	CA	58.72	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	133	GLN	CB	28.28	0.05	1
A	102	LEU	HD11	0.96	0.01	1
A	112	SER	H	8.85	0.01	1
A	135	TRP	HB3	3.68	0.01	1
A	131	TRP	CE3	120.44	0.05	1
A	137	ALA	HB2	1.49	0.01	1
A	110	ALA	H	7.82	0.01	1
A	140	LEU	HB2	1.69	0.01	1
A	119	LEU	CA	57.36	0.05	1
A	100	VAL	CB	34.32	0.05	1
A	121	LYS	HE2	2.94	0.01	1
A	120	PHE	HE2	6.91	0.01	1
A	116	LEU	HA	4.14	0.01	1
A	142	GLU	CB	30.14	0.05	1
A	128	PRO	HD2	3.24	0.01	1
A	132	GLN	HB3	2.07	0.01	1
A	98	THR	HA	4.48	0.01	1
A	94	LEU	CD2	22.97	0.05	1
A	130	ALA	H	7.89	0.01	1
A	112	SER	CB	63.14	0.05	1
A	111	MET	HA	4.78	0.01	1
A	97	GLU	HB3	2.21	0.01	1
A	144	LEU	HD11	0.94	0.01	1
A	79	ALA	CA	53.06	0.05	1
A	97	GLU	HA	4.28	0.01	1
A	126	MET	N	120.23	0.05	1
A	128	PRO	HB3	1.41	0.01	1
A	96	GLN	HB3	2.01	0.01	1
A	101	THR	N	117.45	0.05	1
A	119	LEU	N	121.18	0.05	1
A	99	PRO	HG3	2.17	0.01	1
A	122	ALA	HA	4.13	0.01	1
A	100	VAL	HG23	0.9	0.01	1
A	107	ASP	HA	4.48	0.01	1
A	93	LEU	CD1	22.42	0.05	1
A	122	ALA	HB1	1.54	0.01	1
A	94	LEU	HD22	0.78	0.01	1
A	101	THR	HG22	1.38	0.01	1
A	113	PRO	HA	4.01	0.01	1
A	108	GLN	HG2	2.59	0.01	1
A	103	GLU	H	8.91	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	120	PHE	C	178.99	0.05	1
A	134	ALA	N	122.99	0.05	1
A	106	ALA	H	8.55	0.01	1
A	75	GLU	HG2	2.43	0.01	1
A	141	ARG	N	119.3	0.05	1
A	145	ALA	HB1	1.42	0.01	1
A	118	ARG	HG2	1.72	0.01	1
A	140	LEU	HD22	0.89	0.01	1
A	93	LEU	HB3	1.17	0.01	1
A	104	ALA	CB	18.83	0.05	1
A	104	ALA	HB2	1.46	0.01	1
A	101	THR	CG2	22.35	0.05	1
A	111	MET	HG2	2.61	0.01	1
A	143	SER	H	8.0	0.01	1
A	116	LEU	HD21	0.8	0.01	1
A	100	VAL	CG2	22.0	0.05	1
A	131	TRP	CD1	126.31	0.05	1
A	113	PRO	CB	31.98	0.05	1
A	136	ARG	HG2	2.24	0.01	1
A	106	ALA	HB1	1.52	0.01	1
A	79	ALA	N	124.21	0.05	1
A	124	THR	H	8.2	0.01	1
A	142	GLU	N	119.27	0.05	1
A	102	LEU	HD22	1.05	0.01	1
A	123	THR	HB	3.88	0.01	1
A	135	TRP	CB	28.39	0.05	1
A	125	GLY	HA3	3.92	0.01	1
A	143	SER	C	174.78	0.05	1
A	140	LEU	HD13	0.86	0.01	1
A	99	PRO	HD3	3.74	0.01	1
A	96	GLN	HG2	2.12	0.01	1
A	97	GLU	C	177.61	0.05	1
A	97	GLU	CG	36.87	0.05	1
A	126	MET	HE1	2.12	0.01	1
A	121	LYS	HB2	1.89	0.01	1
A	80	GLN	CA	56.45	0.05	1
A	104	ALA	H	7.77	0.01	1
A	119	LEU	H	8.52	0.01	1
A	134	ALA	CA	54.88	0.05	1
A	145	ALA	HA	4.36	0.01	1
A	113	PRO	CA	66.57	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	120	PHE	HA	3.7	0.01	1
A	126	MET	CB	38.12	0.05	1
A	129	LYS	HA	4.27	0.01	1
A	141	ARG	CA	58.04	0.05	1
A	111	MET	HB2	2.18	0.01	1
A	129	LYS	CA	59.54	0.05	1
A	95	GLU	HB2	1.73	0.01	1
A	107	ASP	CB	41.42	0.05	1
A	124	THR	CG2	19.19	0.05	1
A	112	SER	N	117.95	0.05	1
A	122	ALA	CB	18.93	0.05	1
A	106	ALA	HB2	1.52	0.01	1
A	105	LEU	HD23	0.83	0.01	1
A	121	LYS	CD	29.41	0.05	1
A	102	LEU	N	123.01	0.05	1
A	133	GLN	CA	59.18	0.05	1
A	134	ALA	HA	4.17	0.01	1
A	100	VAL	HB	1.87	0.01	1
A	94	LEU	HB3	1.76	0.01	1
A	116	LEU	HD12	0.93	0.01	1
A	133	GLN	CG	34.19	0.05	1
A	97	GLU	HG3	2.5	0.01	1
A	119	LEU	HG	1.51	0.01	1
A	79	ALA	H	8.28	0.01	1
A	119	LEU	CB	42.12	0.05	1
A	136	ARG	CG	29.04	0.05	1
A	75	GLU	CA	56.98	0.05	1
A	98	THR	CB	69.39	0.05	1
A	140	LEU	C	178.69	0.05	1
A	139	ARG	C	178.43	0.05	1
A	109	VAL	HG13	0.88	0.01	1
A	116	LEU	CD1	23.42	0.05	1
A	118	ARG	C	179.46	0.05	1
A	122	ALA	H	8.04	0.01	1
A	98	THR	HB	4.07	0.01	1
A	95	GLU	CA	54.1	0.05	1
A	125	GLY	H	7.95	0.01	1
A	112	SER	CA	56.47	0.05	1
A	99	PRO	HD2	4.12	0.01	1
A	139	ARG	HD2	2.79	0.01	1
A	105	LEU	C	178.03	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	138	ARG	HA	3.95	0.01	1
A	79	ALA	CB	19.28	0.05	1
A	121	LYS	HD2	1.52	0.01	1
A	135	TRP	HE3	7.5	0.01	1
A	101	THR	C	174.91	0.05	1
A	140	LEU	CA	56.93	0.05	1
A	138	ARG	HB2	1.74	0.01	1
A	135	TRP	N	121.54	0.05	1
A	137	ALA	HB1	1.49	0.01	1
A	124	THR	HB	4.35	0.01	1
A	118	ARG	HD3	3.23	0.01	1
A	119	LEU	HD13	0.9	0.01	1
A	130	ALA	CA	54.97	0.05	1
A	111	MET	CG	32.95	0.05	1
A	117	HIS	H	8.57	0.01	1
A	116	LEU	C	177.59	0.05	1
A	124	THR	C	176.27	0.05	1
A	142	GLU	HG3	2.27	0.01	1
A	137	ALA	H	8.04	0.01	1
A	108	GLN	N	117.3	0.05	1
A	93	LEU	HD23	0.5	0.01	1
A	114	PHE	CE2	131.51	0.05	1
A	110	ALA	HB3	1.4	0.01	1
A	124	THR	CB	71.65	0.05	1
A	139	ARG	CD	42.85	0.05	1
A	140	LEU	HD21	0.89	0.01	1
A	95	GLU	N	120.93	0.05	1
A	121	LYS	HA	4.48	0.01	1
A	129	LYS	N	116.58	0.05	1
A	100	VAL	CG1	21.61	0.05	1
A	115	HIS	HB2	3.2	0.01	1
A	105	LEU	CG	26.38	0.05	1
A	141	ARG	HB2	1.9	0.01	1
A	139	ARG	HG3	1.04	0.01	1
A	96	GLN	HE21	7.47	0.01	1
A	140	LEU	N	120.26	0.05	1
A	120	PHE	H	9.6	0.01	1
A	137	ALA	CB	18.11	0.05	1
A	139	ARG	N	119.13	0.05	1
A	138	ARG	CA	58.77	0.05	1
A	101	THR	HA	4.41	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	117	HIS	HA	3.75	0.01	1
A	93	LEU	HD11	0.79	0.01	1
A	113	PRO	CD	50.52	0.05	1
A	93	LEU	CG	26.69	0.05	1
A	134	ALA	HB3	1.36	0.01	1
A	131	TRP	CA	61.8	0.05	1
A	80	GLN	HB3	2.06	0.01	1
A	75	GLU	CG	36.37	0.05	1
A	119	LEU	HB3	1.72	0.01	1
A	107	ASP	CA	56.39	0.05	1
A	124	THR	HG23	0.09	0.01	1
A	120	PHE	CB	40.25	0.05	1
A	135	TRP	CZ2	114.59	0.05	1
A	109	VAL	HG21	0.68	0.01	1
A	95	GLU	H	6.82	0.01	1
A	111	MET	H	8.17	0.01	1
A	104	ALA	C	170.27	0.05	1
A	116	LEU	HD11	0.93	0.01	1
A	129	LYS	HB2	2.06	0.01	1
A	80	GLN	HE22	6.88	0.01	1
A	100	VAL	HG13	0.95	0.01	1
A	98	THR	HG23	1.31	0.01	1
A	109	VAL	CG1	20.24	0.05	1
A	111	MET	HE2	1.93	0.01	1
A	136	ARG	CB	30.72	0.05	1
A	138	ARG	HG3	1.44	0.01	1
A	108	GLN	CB	29.86	0.05	1
A	79	ALA	HB3	1.42	0.01	1
A	141	ARG	HG3	1.64	0.01	1
A	113	PRO	HB2	2.05	0.01	1
A	94	LEU	HD12	0.73	0.01	1
A	116	LEU	CD2	26.63	0.05	1
A	79	ALA	HA	4.31	0.01	1
A	115	HIS	H	7.51	0.01	1
A	144	LEU	HB2	1.7	0.01	1
A	146	LYS	HB2	1.72	0.01	1
A	98	THR	H	7.93	0.01	1
A	131	TRP	HZ3	7.11	0.01	1
A	130	ALA	HB1	1.69	0.01	1
A	116	LEU	CG	28.21	0.05	1
A	116	LEU	HB3	1.49	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	96	GLN	HA	4.29	0.01	1
A	137	ALA	HB3	1.49	0.01	1
A	145	ALA	CB	19.38	0.05	1
A	103	GLU	C	178.51	0.05	1
A	101	THR	CB	70.7	0.05	1
A	140	LEU	HB3	1.69	0.01	1
A	93	LEU	H	7.75	0.01	1
A	106	ALA	CA	55.44	0.05	1
A	100	VAL	CA	60.93	0.05	1
A	140	LEU	HA	4.15	0.01	1
A	145	ALA	N	124.29	0.05	1
A	94	LEU	CB	44.31	0.05	1
A	121	LYS	HE3	2.94	0.01	1
A	114	PHE	CD1	131.63	0.05	1
A	80	GLN	HG2	2.38	0.01	1
A	118	ARG	HA	4.0	0.01	1
A	143	SER	HB2	3.95	0.01	1
A	75	GLU	HA	4.28	0.01	1
A	99	PRO	CD	51.39	0.05	1
A	136	ARG	HG3	1.83	0.01	1
A	118	ARG	HB3	1.85	0.01	1
A	144	LEU	HD12	0.94	0.01	1
A	100	VAL	C	176.01	0.05	1
A	105	LEU	CB	42.84	0.05	1
A	96	GLN	HE22	6.86	0.01	1
A	127	THR	HG23	1.48	0.01	1
A	129	LYS	C	179.11	0.05	1
A	102	LEU	H	8.71	0.01	1
A	80	GLN	H	8.35	0.01	1
A	94	LEU	C	176.54	0.05	1
A	123	THR	HG23	1.05	0.01	1
A	129	LYS	CG	25.12	0.05	1
A	134	ALA	H	8.44	0.01	1
A	106	ALA	N	119.8	0.05	1
A	136	ARG	N	119.25	0.05	1
A	138	ARG	CD	43.55	0.05	1
A	99	PRO	HA	4.49	0.01	1
A	100	VAL	HG22	0.9	0.01	1
A	122	ALA	HB2	1.54	0.01	1
A	94	LEU	HD23	0.78	0.01	1
A	80	GLN	CG	34.04	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	118	ARG	CD	43.94	0.05	1
A	126	MET	H	8.69	0.01	1
A	101	THR	HG21	1.38	0.01	1
A	108	GLN	HG3	2.39	0.01	1
A	128	PRO	CB	31.44	0.05	1
A	110	ALA	C	175.89	0.05	1
A	143	SER	N	115.27	0.05	1
A	109	VAL	CA	60.84	0.05	1
A	118	ARG	HG3	1.72	0.01	1
A	105	LEU	H	8.29	0.01	1
A	104	ALA	HB3	1.46	0.01	1
A	141	ARG	C	178.02	0.05	1
A	96	GLN	C	174.94	0.05	1
A	127	THR	CA	60.33	0.05	1
A	120	PHE	CA	62.5	0.05	1
A	116	LEU	HD22	0.8	0.01	1
A	122	ALA	N	120.97	0.05	1
A	93	LEU	HG	1.61	0.01	1
A	102	LEU	HD21	1.05	0.01	1
A	144	LEU	HD23	0.89	0.01	1
A	111	MET	HE1	1.93	0.01	1
A	130	ALA	HA	4.3	0.01	1
A	136	ARG	CA	59.88	0.05	1
A	142	GLU	H	8.15	0.01	1
A	135	TRP	HA	3.85	0.01	1
A	143	SER	HA	4.41	0.01	1
A	105	LEU	HB2	1.81	0.01	1
A	126	MET	HB2	2.37	0.01	1
A	141	ARG	HD2	3.21	0.01	1
A	127	THR	CG2	23.33	0.05	1
A	75	GLU	C	176.1	0.05	1
A	138	ARG	H	7.65	0.01	1
A	112	SER	HB3	4.05	0.01	1
A	111	MET	HB3	1.6	0.01	1
A	95	GLU	HB3	1.73	0.01	1
A	108	GLN	HA	4.1	0.01	1
A	133	GLN	HG3	2.54	0.01	1
A	121	LYS	H	8.23	0.01	1
A	109	VAL	HB	2.41	0.01	1
A	80	GLN	C	176.81	0.05	1
A	134	ALA	C	179.73	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	75	GLU	HB3	1.83	0.01	1
A	146	LYS	H	7.76	0.01	1
A	120	PHE	CE2	132.8	0.05	1
A	105	LEU	N	121.03	0.05	1
A	121	LYS	CG	24.86	0.05	1
A	102	LEU	HD13	0.96	0.01	1
A	117	HIS	HD2	6.98	0.01	1
A	121	LYS	HG2	1.34	0.01	1
A	94	LEU	HB2	1.76	0.01	1
A	138	ARG	HB3	1.74	0.01	1
A	103	GLU	HB3	1.99	0.01	1
A	145	ALA	H	7.91	0.01	1
A	119	LEU	C	179.7	0.05	1
A	101	THR	CA	60.91	0.05	1
A	97	GLU	HG2	2.5	0.01	1
A	139	ARG	CG	26.26	0.05	1
A	133	GLN	C	178.82	0.05	1
A	75	GLU	CB	29.04	0.05	1
A	136	ARG	C	176.06	0.05	1
A	133	GLN	HB3	2.18	0.01	1
A	116	LEU	HG	1.41	0.01	1
A	140	LEU	CD2	24.77	0.05	1
A	109	VAL	HG12	0.88	0.01	1
A	119	LEU	CG	27.58	0.05	1
A	108	GLN	HE22	6.78	0.01	1
A	135	TRP	HH2	7.1	0.01	1
A	139	ARG	HD3	2.72	0.01	1
A	105	LEU	CA	57.7	0.05	1
A	106	ALA	CB	17.92	0.05	1
A	80	GLN	HA	4.29	0.01	1
A	140	LEU	CB	42.04	0.05	1
A	127	THR	HA	4.37	0.01	1
A	139	ARG	HB3	1.21	0.01	1
A	124	THR	HA	4.39	0.01	1
A	138	ARG	CG	27.51	0.05	1
A	118	ARG	HD2	3.23	0.01	1
A	135	TRP	HZ3	6.73	0.01	1
A	144	LEU	CD2	23.58	0.05	1
A	100	VAL	HG21	0.9	0.01	1
A	142	GLU	HG2	2.39	0.01	1
A	93	LEU	CA	56.94	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	93	LEU	HD22	0.5	0.01	1
A	128	PRO	CA	66.11	0.05	1
A	100	VAL	H	8.25	0.01	1
A	109	VAL	CB	31.83	0.05	1
A	110	ALA	HB2	1.4	0.01	1
A	135	TRP	C	178.34	0.05	1
A	138	ARG	HD3	3.08	0.01	1
A	102	LEU	C	178.33	0.05	1
A	120	PHE	HD2	7.1	0.01	1
A	108	GLN	HB3	2.13	0.01	1
A	115	HIS	HB3	3.2	0.01	1
A	139	ARG	HG2	1.14	0.01	1
A	116	LEU	N	120.22	0.05	1
A	141	ARG	HD3	3.21	0.01	1
A	105	LEU	HG	1.48	0.01	1
A	100	VAL	HA	4.35	0.01	1
A	103	GLU	N	116.19	0.05	1
A	140	LEU	HD11	0.86	0.01	1
A	101	THR	HB	4.73	0.01	1
A	126	MET	HE3	2.12	0.01	1
A	93	LEU	CB	41.91	0.05	1
A	93	LEU	HD12	0.79	0.01	1
A	102	LEU	HB2	1.78	0.01	1
A	144	LEU	HA	4.37	0.01	1
A	134	ALA	HB2	1.36	0.01	1
A	80	GLN	HB2	2.06	0.01	1
A	136	ARG	HB3	2.0	0.01	1
A	108	GLN	C	178.04	0.05	1
A	117	HIS	HB3	3.28	0.01	1
A	120	PHE	CE1	132.8	0.05	1
A	105	LEU	HD21	0.83	0.01	1
A	109	VAL	HG22	0.68	0.01	1
A	110	ALA	CB	16.61	0.05	1
A	144	LEU	CA	55.37	0.05	1
A	143	SER	CB	63.6	0.05	1
A	125	GLY	N	110.6	0.05	1
A	93	LEU	CD2	26.32	0.05	1
A	137	ALA	HA	4.11	0.01	1
A	80	GLN	HE21	7.49	0.01	1
A	98	THR	HG22	1.31	0.01	1
A	109	VAL	CG2	21.15	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	114	PHE	CA	60.9	0.05	1
A	123	THR	H	7.83	0.01	1
A	123	THR	N	111.11	0.05	1
A	135	TRP	H	8.04	0.01	1
A	94	LEU	N	116.85	0.05	1
A	126	MET	C	173.42	0.05	1
A	108	GLN	CA	58.94	0.05	1
A	143	SER	CA	59.36	0.05	1
A	109	VAL	HG11	0.88	0.01	1
A	94	LEU	HD11	0.73	0.01	1
A	144	LEU	C	177.03	0.05	1
A	126	MET	CG	31.76	0.05	1
A	144	LEU	HB3	1.63	0.01	1
A	111	MET	C	174.71	0.05	1
A	105	LEU	HD13	0.68	0.01	1
A	114	PHE	HE2	7.33	0.01	1
A	128	PRO	HA	3.47	0.01	1
A	122	ALA	C	179.25	0.05	1
A	116	LEU	HB2	1.9	0.01	1
A	107	ASP	H	7.69	0.01	1
A	117	HIS	CA	62.28	0.05	1
A	103	GLU	CB	28.89	0.05	1
A	115	HIS	CB	31.68	0.05	1
A	111	MET	CA	54.91	0.05	1
A	129	LYS	HG2	1.63	0.01	1
A	120	PHE	HB3	3.04	0.01	1
A	94	LEU	CA	55.34	0.05	1
A	135	TRP	CE3	120.78	0.05	1
A	93	LEU	HD21	0.5	0.01	1
A	80	GLN	HG3	2.38	0.01	1
A	75	GLU	HB2	2.2	0.01	1
A	117	HIS	C	176.86	0.05	1
A	146	LYS	CA	57.8	0.05	1
A	129	LYS	HE2	3.07	0.01	1
A	99	PRO	CG	28.04	0.05	1
A	118	ARG	HB2	1.85	0.01	1
A	135	TRP	CH2	123.91	0.05	1
A	141	ARG	CD	43.51	0.05	1
A	80	GLN	NE2	112.15	0.05	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
$^{13}\text{C}_\alpha$	144	-0.36 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	137	-0.03 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	130	-0.35 ± 0.22	None needed (< 0.5 ppm)
^{15}N	130	0.27 ± 0.20	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 87%, i.e. 619 atoms were assigned a chemical shift out of a possible 714. 7 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	274/276 (99%)	110/110 (100%)	110/112 (98%)	54/54 (100%)
Sidechain	286/367 (78%)	178/218 (82%)	101/120 (84%)	7/29 (24%)
Aromatic	59/71 (83%)	34/39 (87%)	24/31 (77%)	1/1 (100%)
Overall	619/714 (87%)	322/367 (88%)	235/263 (89%)	62/84 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 918 atoms were assigned a chemical shift out of a possible 1173. 8 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	419/450 (93%)	169/179 (94%)	169/184 (92%)	81/87 (93%)
Sidechain	438/640 (68%)	275/381 (72%)	152/210 (72%)	11/49 (22%)
Aromatic	61/83 (73%)	36/47 (77%)	24/35 (69%)	1/1 (100%)
Overall	918/1173 (78%)	480/607 (79%)	345/429 (80%)	93/137 (68%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	49	ARG	NE	111.97	92.63 – 76.73	17.2
1	A	39	ARG	NE	111.93	92.63 – 76.73	17.1
1	A	12	ARG	NE	109.99	92.63 – 76.73	15.9

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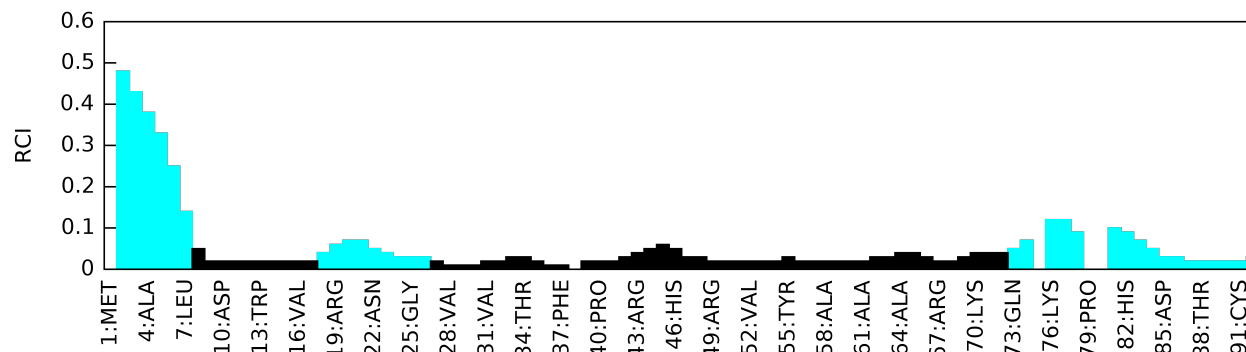
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	12	ARG	HB3	-0.18	3.17 – 0.37	-7.0
1	A	87	ILE	CG2	9.19	24.63 – 10.43	-5.9
1	A	49	ARG	HD3	1.65	4.36 – 1.86	-5.8
1	A	61	ALA	HB1	-0.05	2.61 – 0.11	-5.6
1	A	61	ALA	HB2	-0.05	2.61 – 0.11	-5.6
1	A	61	ALA	HB3	-0.05	2.61 – 0.11	-5.6
1	A	12	ARG	HD3	1.73	4.36 – 1.86	-5.5
1	A	49	ARG	HD2	1.96	4.27 – 1.97	-5.0
1	A	12	ARG	HG3	0.10	3.00 – 0.10	-5.0

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:



7.2 Chemical shift list 2

File name: BMRB entry 6054

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 Bookkeeping [i](#)

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	1717
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Number of shifts mapped to atoms	1015
Number of unparsed shifts	0
Number of shifts with mapping errors	702
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	18

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

- Residue not found in structure. All 702 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	127	THR	CB	68.29	0.05	1
A	121	LYS	N	122.2	0.05	1
A	110	ALA	N	123.4	0.05	1
A	123	THR	C	175.52	0.05	1
A	127	THR	HG22	1.48	0.01	1
A	117	HIS	N	118.67	0.05	1
A	114	PHE	HB2	3.23	0.01	1
A	99	PRO	HB3	1.91	0.01	1
A	123	THR	HG22	1.09	0.01	1
A	102	LEU	HD12	1.05	0.01	1
A	139	ARG	HA	3.88	0.01	1
A	103	GLU	HG2	2.52	0.01	1
A	131	TRP	CH2	125.4	0.05	1
A	113	PRO	HD3	3.95	0.01	1
A	122	ALA	HB3	1.55	0.01	1
A	118	ARG	CG	27.42	0.05	1
A	134	ALA	HB1	1.38	0.01	1
A	107	ASP	HB3	2.77	0.01	1
A	107	ASP	C	179.28	0.05	1
A	127	THR	H	7.93	0.01	1
A	145	ALA	HB3	1.43	0.01	1
A	133	GLN	HG2	2.68	0.01	1
A	124	THR	HG21	0.12	0.01	1
A	98	THR	CA	60.83	0.05	1
A	114	PHE	HD1	7.05	0.01	1
A	93	LEU	HA	3.95	0.01	1
A	116	LEU	HD23	0.81	0.01	1
A	123	THR	HA	4.06	0.01	1
A	110	ALA	CA	52.93	0.05	1
A	144	LEU	HD22	0.9	0.01	1
A	135	TRP	CD1	127.09	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	126	MET	HG3	2.65	0.01	1
A	96	GLN	CA	54.8	0.05	1
A	98	THR	HG21	1.32	0.01	1
A	131	TRP	HH2	7.31	0.01	1
A	102	LEU	CD1	23.32	0.05	1
A	131	TRP	HD1	7.07	0.01	1
A	145	ALA	CA	52.64	0.05	1
A	97	GLU	CA	59.24	0.05	1
A	126	MET	HB3	2.32	0.01	1
A	79	ALA	HB1	1.47	0.01	1
A	132	GLN	HA	4.06	0.01	1
A	112	SER	HB2	4.31	0.01	1
A	141	ARG	CG	27.62	0.05	1
A	142	GLU	HB2	2.08	0.01	1
A	109	VAL	HA	4.47	0.01	1
A	103	GLU	CG	37.64	0.05	1
A	138	ARG	C	177.84	0.05	1
A	119	LEU	CD1	23.5	0.05	1
A	120	PHE	HD1	7.12	0.01	1
A	131	TRP	CZ3	119.97	0.05	1
A	127	THR	N	107.45	0.05	1
A	129	LYS	CB	32.66	0.05	1
A	115	HIS	CA	58.36	0.05	1
A	121	LYS	HG3	1.36	0.01	1
A	117	HIS	CB	30.81	0.05	1
A	103	GLU	HB2	2.1	0.01	1
A	135	TRP	HB2	3.64	0.01	1
A	131	TRP	H	8.09	0.01	1
A	121	LYS	C	179.74	0.05	1
A	115	HIS	HD2	7.26	0.01	1
A	111	MET	CB	39.78	0.05	1
A	140	LEU	HG	1.74	0.01	1
A	97	GLU	N	119.26	0.05	1
A	80	GLN	N	118.46	0.05	1
A	133	GLN	HB2	2.34	0.01	1
A	95	GLU	HA	4.04	0.01	1
A	140	LEU	CD1	24.04	0.05	1
A	128	PRO	HD3	3.97	0.01	1
A	98	THR	N	116.52	0.05	1
A	142	GLU	CA	57.71	0.05	1
A	132	GLN	HB2	2.12	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	105	LEU	CD1	24.48	0.05	1
A	109	VAL	N	109.54	0.05	1
A	93	LEU	C	177.74	0.05	1
A	108	GLN	HE21	6.78	0.01	1
A	94	LEU	CD1	27.45	0.05	1
A	99	PRO	CB	32.46	0.05	1
A	135	TRP	NE1	130.2	0.05	1
A	136	ARG	HA	3.49	0.01	1
A	97	GLU	HB2	2.17	0.01	1
A	102	LEU	CA	57.9	0.05	1
A	113	PRO	HG2	2.02	0.01	1
A	135	TRP	HE1	10.27	0.01	1
A	116	LEU	CB	41.14	0.05	1
A	96	GLN	HB2	2.01	0.01	1
A	131	TRP	HE3	6.99	0.01	1
A	105	LEU	HA	3.81	0.01	1
A	127	THR	HB	4.83	0.01	1
A	99	PRO	HG2	2.18	0.01	1
A	129	LYS	CE	42.01	0.05	1
A	105	LEU	HB3	1.53	0.01	1
A	119	LEU	HD11	0.93	0.01	1
A	111	MET	CE	17.2	0.05	1
A	144	LEU	CD1	25.38	0.05	1
A	142	GLU	CG	36.63	0.05	1
A	118	ARG	CB	30.65	0.05	1
A	146	LYS	HA	4.16	0.01	1
A	101	THR	H	8.28	0.01	1
A	101	THR	HG23	1.39	0.01	1
A	141	ARG	HA	4.16	0.01	1
A	129	LYS	H	8.19	0.01	1
A	109	VAL	C	174.35	0.05	1
A	75	GLU	HG3	2.2	0.01	1
A	94	LEU	H	7.33	0.01	1
A	110	ALA	HB1	1.41	0.01	1
A	140	LEU	HD23	0.9	0.01	1
A	93	LEU	HB2	1.84	0.01	1
A	104	ALA	HB1	1.47	0.01	1
A	138	ARG	HD2	3.09	0.01	1
A	116	LEU	H	8.74	0.01	1
A	111	MET	HG3	2.63	0.01	1
A	79	ALA	C	178.3	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	38	CYM	HD	2.27	0.01	1
A	117	HIS	HB2	3.31	0.01	1
A	108	GLN	HB2	2.14	0.01	1
A	102	LEU	HD23	0.99	0.01	1
A	144	LEU	HD21	0.9	0.01	1
A	136	ARG	H	8.62	0.01	1
A	135	TRP	CA	62.2	0.05	1
A	96	GLN	CB	30.8	0.05	1
A	125	GLY	HA2	4.41	0.01	1
A	114	PHE	N	116.07	0.05	1
A	108	GLN	H	7.73	0.01	1
A	118	ARG	H	7.53	0.01	1
A	144	LEU	H	7.84	0.01	1
A	140	LEU	HD12	0.87	0.01	1
A	130	ALA	N	122.37	0.05	1
A	96	GLN	HG3	2.14	0.01	1
A	123	THR	CB	69.5	0.05	1
A	110	ALA	HA	4.16	0.01	1
A	108	GLN	CG	35.25	0.05	1
A	126	MET	HE2	2.12	0.01	1
A	121	LYS	HB3	1.61	0.01	1
A	80	GLN	CB	29.09	0.05	1
A	93	LEU	HD13	0.81	0.01	1
A	102	LEU	HB3	1.75	0.01	1
A	120	PHE	CD1	130.49	0.05	1
A	114	PHE	H	8.02	0.01	1
A	134	ALA	CB	17.46	0.05	1
A	114	PHE	CD2	131.65	0.05	1
A	126	MET	HA	5.09	0.01	1
A	126	MET	CA	54.35	0.05	1
A	141	ARG	CB	30.52	0.05	1
A	119	LEU	HD22	0.87	0.01	1
A	105	LEU	HD11	0.84	0.01	1
A	136	ARG	HB2	2.01	0.01	1
A	103	GLU	HA	3.8	0.01	1
A	105	LEU	HD22	0.69	0.01	1
A	109	VAL	HG23	0.69	0.01	1
A	121	LYS	CE	41.98	0.05	1
A	144	LEU	CB	42.5	0.05	1
A	116	LEU	HD13	0.94	0.01	1
A	99	PRO	C	176.17	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	144	LEU	HD13	0.95	0.01	1
A	102	LEU	CD2	25.8	0.05	1
A	133	GLN	HA	4.16	0.01	1
A	114	PHE	CB	39.08	0.05	1
A	38	CYM	N	115.71	0.05	1
A	113	PRO	C	177.52	0.05	1
A	120	PHE	N	124.68	0.05	1
A	118	ARG	N	115.82	0.05	1
A	140	LEU	H	7.73	0.01	1
A	93	LEU	N	119.38	0.05	1
A	105	LEU	CD2	26.35	0.05	1
A	99	PRO	CA	63.5	0.05	1
A	105	LEU	HD12	0.84	0.01	1
A	107	ASP	N	116.66	0.05	1
A	114	PHE	HE1	7.35	0.01	1
A	123	THR	CG2	21.36	0.05	1
A	104	ALA	HA	4.24	0.01	1
A	38	CYM	C	173.5	0.05	1
A	102	LEU	CB	41.44	0.05	1
A	121	LYS	HD3	1.52	0.01	1
A	106	ALA	HB3	1.53	0.01	1
A	130	ALA	HB3	1.7	0.01	1
A	121	LYS	CB	32.4	0.05	1
A	116	LEU	CA	58.23	0.05	1
A	115	HIS	C	178.09	0.05	1
A	141	ARG	HB3	1.91	0.01	1
A	98	THR	CG2	21.65	0.05	1
A	94	LEU	HA	4.12	0.01	1
A	108	GLN	NE2	110.18	0.05	1
A	119	LEU	HA	4.3	0.01	1
A	130	ALA	HB2	1.7	0.01	1
A	103	GLU	CA	61.14	0.05	1
A	130	ALA	CB	19.25	0.05	1
A	129	LYS	HG3	1.64	0.01	1
A	120	PHE	HB2	3.15	0.01	1
A	131	TRP	HA	4.35	0.01	1
A	120	PHE	HE1	6.92	0.01	1
A	118	ARG	CA	59.22	0.05	1
A	125	GLY	C	173.47	0.05	1
A	114	PHE	CE1	131.56	0.05	1
A	146	LYS	CB	33.92	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	129	LYS	HE3	3.09	0.01	1
A	114	PHE	HA	4.36	0.01	1
A	142	GLU	HA	4.2	0.01	1
A	128	PRO	HB2	1.47	0.01	1
A	144	LEU	N	122.81	0.05	1
A	113	PRO	HD2	4.04	0.01	1
A	125	GLY	CA	45.7	0.05	1
A	127	THR	HG21	1.48	0.01	1
A	114	PHE	HB3	2.94	0.01	1
A	96	GLN	CG	29.16	0.05	1
A	137	ALA	CA	54.52	0.05	1
A	106	ALA	HA	3.84	0.01	1
A	100	VAL	HG11	0.96	0.01	1
A	124	THR	CA	62.87	0.05	1
A	99	PRO	HB2	2.34	0.01	1
A	128	PRO	C	177.5	0.05	1
A	123	THR	HG21	1.09	0.01	1
A	138	ARG	CB	29.96	0.05	1
A	100	VAL	N	125.06	0.05	1
A	103	GLU	HG3	2.2	0.01	1
A	123	THR	CA	65.8	0.05	1
A	94	LEU	HD21	0.8	0.01	1
A	135	TRP	HD1	7.25	0.01	1
A	120	PHE	CD2	130.49	0.05	1
A	139	ARG	CA	57.5	0.05	1
A	107	ASP	HB2	2.85	0.01	1
A	128	PRO	CD	49.55	0.05	1
A	97	GLU	H	8.84	0.01	1
A	145	ALA	HB2	1.43	0.01	1
A	104	ALA	CA	54.64	0.05	1
A	137	ALA	C	174.31	0.05	1
A	139	ARG	HB2	1.5	0.01	1
A	124	THR	HG22	0.12	0.01	1
A	114	PHE	HD2	7.05	0.01	1
A	109	VAL	H	7.72	0.01	1
A	115	HIS	N	119.04	0.05	1
A	135	TRP	CZ3	121.35	0.05	1
A	129	LYS	HB3	1.81	0.01	1
A	126	MET	HG2	2.65	0.01	1
A	138	ARG	N	118.9	0.05	1
A	137	ALA	N	120.7	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	100	VAL	HG12	0.96	0.01	1
A	146	LYS	HB3	1.73	0.01	1
A	114	PHE	C	177.98	0.05	1
A	139	ARG	CB	29.49	0.05	1
A	124	THR	N	108.9	0.05	1
A	111	MET	HE3	1.95	0.01	1
A	111	MET	N	117.65	0.05	1
A	135	TRP	HZ2	7.41	0.01	1
A	138	ARG	HG2	1.64	0.01	1
A	112	SER	HA	4.86	0.01	1
A	97	GLU	CB	30.96	0.05	1
A	79	ALA	HB2	1.47	0.01	1
A	141	ARG	HG2	1.64	0.01	1
A	113	PRO	HB3	2.06	0.01	1
A	102	LEU	HA	3.96	0.01	1
A	94	LEU	HD13	0.74	0.01	1
A	141	ARG	H	7.8	0.01	1
A	143	SER	HB3	3.96	0.01	1
A	126	MET	CE	17.92	0.05	1
A	142	GLU	HB3	2.03	0.01	1
A	104	ALA	N	122.8	0.05	1
A	142	GLU	C	177.55	0.05	1
A	145	ALA	C	176.57	0.05	1
A	146	LYS	N	125.83	0.05	1
A	131	TRP	HZ2	7.53	0.01	1
A	96	GLN	NE2	112.6	0.05	1
A	115	HIS	HA	4.46	0.01	1
A	122	ALA	CA	54.92	0.05	1
A	139	ARG	H	7.66	0.01	1
A	131	TRP	CZ2	114.54	0.05	1
A	106	ALA	C	179.53	0.05	1
A	121	LYS	CA	58.73	0.05	1
A	133	GLN	CB	28.41	0.05	1
A	102	LEU	HD11	1.05	0.01	1
A	112	SER	H	8.85	0.01	1
A	135	TRP	HB3	3.64	0.01	1
A	131	TRP	CE3	120.46	0.05	1
A	137	ALA	HB2	1.49	0.01	1
A	110	ALA	H	7.84	0.01	1
A	140	LEU	HB2	1.68	0.01	1
A	119	LEU	CA	57.46	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	100	VAL	CB	34.27	0.05	1
A	121	LYS	HE2	2.96	0.01	1
A	120	PHE	HE2	6.92	0.01	1
A	116	LEU	HA	4.15	0.01	1
A	142	GLU	CB	30.16	0.05	1
A	128	PRO	HD2	3.27	0.01	1
A	132	GLN	HB3	2.12	0.01	1
A	98	THR	HA	4.49	0.01	1
A	94	LEU	CD2	22.96	0.05	1
A	130	ALA	H	7.89	0.01	1
A	112	SER	CB	63.05	0.05	1
A	111	MET	HA	4.82	0.01	1
A	97	GLU	HB3	2.17	0.01	1
A	144	LEU	HD11	0.95	0.01	1
A	79	ALA	CA	53.26	0.05	1
A	113	PRO	HG3	2.1	0.01	1
A	97	GLU	HA	4.29	0.01	1
A	126	MET	N	120.25	0.05	1
A	128	PRO	HB3	1.47	0.01	1
A	96	GLN	HB3	2.01	0.01	1
A	101	THR	N	117.47	0.05	1
A	119	LEU	N	121.2	0.05	1
A	99	PRO	HG3	2.02	0.01	1
A	129	LYS	CD	28.77	0.05	1
A	122	ALA	HA	4.15	0.01	1
A	100	VAL	HG23	0.92	0.01	1
A	107	ASP	HA	4.5	0.01	1
A	93	LEU	CD1	22.52	0.05	1
A	122	ALA	HB1	1.55	0.01	1
A	94	LEU	HD22	0.8	0.01	1
A	101	THR	HG22	1.39	0.01	1
A	113	PRO	HA	4.04	0.01	1
A	108	GLN	HG2	2.61	0.01	1
A	103	GLU	H	8.91	0.01	1
A	120	PHE	C	178.99	0.05	1
A	134	ALA	N	123.01	0.05	1
A	106	ALA	H	8.55	0.01	1
A	38	CYM	H	9.04	0.01	1
A	75	GLU	HG2	2.42	0.01	1
A	141	ARG	N	119.37	0.05	1
A	145	ALA	HB1	1.43	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	118	ARG	HG2	1.72	0.01	1
A	140	LEU	HD22	0.9	0.01	1
A	93	LEU	HB3	1.17	0.01	1
A	104	ALA	CB	18.84	0.05	1
A	104	ALA	HB2	1.47	0.01	1
A	101	THR	CG2	22.33	0.05	1
A	111	MET	HG2	2.63	0.01	1
A	143	SER	H	8.0	0.01	1
A	116	LEU	HD21	0.81	0.01	1
A	100	VAL	CG2	21.93	0.05	1
A	131	TRP	CD1	126.34	0.05	1
A	113	PRO	CB	31.95	0.05	1
A	136	ARG	HG2	1.84	0.01	1
A	106	ALA	HB1	1.53	0.01	1
A	79	ALA	N	124.23	0.05	1
A	124	THR	H	8.21	0.01	1
A	142	GLU	N	119.3	0.05	1
A	102	LEU	HD22	0.99	0.01	1
A	123	THR	HB	3.9	0.01	1
A	135	TRP	CB	28.39	0.05	1
A	125	GLY	HA3	3.93	0.01	1
A	143	SER	C	174.78	0.05	1
A	140	LEU	HD13	0.87	0.01	1
A	99	PRO	HD3	3.76	0.01	1
A	96	GLN	HG2	2.14	0.01	1
A	97	GLU	C	177.66	0.05	1
A	97	GLU	CG	36.65	0.05	1
A	126	MET	HE1	2.12	0.01	1
A	121	LYS	HB2	1.89	0.01	1
A	80	GLN	CA	56.84	0.05	1
A	104	ALA	H	7.79	0.01	1
A	119	LEU	H	8.54	0.01	1
A	134	ALA	CA	54.87	0.05	1
A	145	ALA	HA	4.37	0.01	1
A	113	PRO	CA	66.57	0.05	1
A	120	PHE	HA	3.71	0.01	1
A	126	MET	CB	38.26	0.05	1
A	129	LYS	HA	4.28	0.01	1
A	141	ARG	CA	57.98	0.05	1
A	111	MET	HB2	2.18	0.01	1
A	129	LYS	CA	59.49	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	95	GLU	HB2	1.72	0.01	1
A	107	ASP	CB	41.13	0.05	1
A	124	THR	CG2	19.19	0.05	1
A	112	SER	N	117.92	0.05	1
A	132	GLN	CA	58.89	0.05	1
A	122	ALA	CB	18.79	0.05	1
A	106	ALA	HB2	1.53	0.01	1
A	105	LEU	HD23	0.69	0.01	1
A	121	LYS	CD	29.41	0.05	1
A	102	LEU	N	123.04	0.05	1
A	133	GLN	CA	59.15	0.05	1
A	134	ALA	HA	4.18	0.01	1
A	100	VAL	HB	1.88	0.01	1
A	94	LEU	HB3	1.81	0.01	1
A	116	LEU	HD12	0.94	0.01	1
A	133	GLN	CG	34.16	0.05	1
A	97	GLU	HG3	2.51	0.01	1
A	119	LEU	HG	1.53	0.01	1
A	79	ALA	H	8.29	0.01	1
A	119	LEU	CB	42.4	0.05	1
A	136	ARG	CG	28.94	0.05	1
A	75	GLU	CA	56.98	0.05	1
A	98	THR	CB	69.4	0.05	1
A	140	LEU	C	178.69	0.05	1
A	139	ARG	C	178.42	0.05	1
A	109	VAL	HG13	0.9	0.01	1
A	116	LEU	CD1	23.28	0.05	1
A	118	ARG	C	179.46	0.05	1
A	122	ALA	H	8.04	0.01	1
A	98	THR	HB	4.1	0.01	1
A	95	GLU	CA	54.08	0.05	1
A	125	GLY	H	7.96	0.01	1
A	112	SER	CA	56.42	0.05	1
A	99	PRO	HD2	4.13	0.01	1
A	139	ARG	HD2	2.81	0.01	1
A	105	LEU	C	178.06	0.05	1
A	138	ARG	HA	3.96	0.01	1
A	79	ALA	CB	19.32	0.05	1
A	121	LYS	HD2	1.52	0.01	1
A	135	TRP	HE3	7.52	0.01	1
A	101	THR	C	174.91	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	140	LEU	CA	56.84	0.05	1
A	138	ARG	HB2	1.76	0.01	1
A	135	TRP	N	121.57	0.05	1
A	137	ALA	HB1	1.49	0.01	1
A	124	THR	HB	4.36	0.01	1
A	118	ARG	HD3	3.19	0.01	1
A	119	LEU	HD13	0.93	0.01	1
A	130	ALA	CA	54.96	0.05	1
A	111	MET	CG	32.7	0.05	1
A	117	HIS	H	8.57	0.01	1
A	116	LEU	C	177.61	0.05	1
A	124	THR	C	176.28	0.05	1
A	142	GLU	HG3	2.28	0.01	1
A	137	ALA	H	8.04	0.01	1
A	108	GLN	N	117.29	0.05	1
A	93	LEU	HD23	0.5	0.01	1
A	114	PHE	CE2	131.56	0.05	1
A	110	ALA	HB3	1.41	0.01	1
A	124	THR	CB	71.78	0.05	1
A	139	ARG	CD	42.84	0.05	1
A	140	LEU	HD21	0.9	0.01	1
A	95	GLU	N	120.98	0.05	1
A	121	LYS	HA	4.49	0.01	1
A	129	LYS	N	116.6	0.05	1
A	100	VAL	CG1	21.55	0.05	1
A	130	ALA	C	176.27	0.05	1
A	115	HIS	HB2	3.28	0.01	1
A	105	LEU	CG	26.34	0.05	1
A	141	ARG	HB2	1.91	0.01	1
A	139	ARG	HG3	1.08	0.01	1
A	119	LEU	HD12	0.93	0.01	1
A	96	GLN	HE21	7.47	0.01	1
A	140	LEU	N	120.26	0.05	1
A	120	PHE	H	9.62	0.01	1
A	137	ALA	CB	18.15	0.05	1
A	139	ARG	N	119.06	0.05	1
A	138	ARG	CA	58.64	0.05	1
A	101	THR	HA	4.41	0.01	1
A	117	HIS	HA	3.77	0.01	1
A	93	LEU	HD11	0.81	0.01	1
A	113	PRO	CD	50.51	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	93	LEU	CG	26.67	0.05	1
A	134	ALA	HB3	1.38	0.01	1
A	131	TRP	CA	61.79	0.05	1
A	80	GLN	HB3	2.09	0.01	1
A	75	GLU	CG	36.43	0.05	1
A	119	LEU	HB3	1.71	0.01	1
A	146	LYS	HB2	1.73	0.01	1
A	107	ASP	CA	57.12	0.05	1
A	124	THR	HG23	0.12	0.01	1
A	120	PHE	CB	40.21	0.05	1
A	135	TRP	CZ2	114.61	0.05	1
A	109	VAL	HG21	0.69	0.01	1
A	95	GLU	H	6.82	0.01	1
A	111	MET	H	8.17	0.01	1
A	104	ALA	C	170.29	0.05	1
A	116	LEU	HD11	0.94	0.01	1
A	129	LYS	HB2	2.07	0.01	1
A	80	GLN	HE22	7.54	0.01	1
A	100	VAL	HG13	0.96	0.01	1
A	98	THR	HG23	1.32	0.01	1
A	109	VAL	CG1	20.12	0.05	1
A	111	MET	HE2	1.95	0.01	1
A	136	ARG	CB	30.64	0.05	1
A	38	CYM	HB2	3.23	0.01	1
A	138	ARG	HG3	1.45	0.01	1
A	108	GLN	CB	30.0	0.05	1
A	79	ALA	HB3	1.47	0.01	1
A	141	ARG	HG3	1.64	0.01	1
A	113	PRO	HB2	2.06	0.01	1
A	144	LEU	HG	1.68	0.01	1
A	94	LEU	HD12	0.74	0.01	1
A	116	LEU	CD2	26.62	0.05	1
A	79	ALA	HA	4.33	0.01	1
A	115	HIS	H	7.52	0.01	1
A	144	LEU	HB2	1.72	0.01	1
A	95	GLU	CB	26.35	0.05	1
A	98	THR	H	7.93	0.01	1
A	129	LYS	HD3	1.64	0.01	1
A	131	TRP	HZ3	7.12	0.01	1
A	130	ALA	HB1	1.7	0.01	1
A	116	LEU	CG	27.83	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	116	LEU	HB3	1.61	0.01	1
A	144	LEU	CG	27.18	0.05	1
A	96	GLN	HA	4.3	0.01	1
A	137	ALA	HB3	1.49	0.01	1
A	145	ALA	CB	19.35	0.05	1
A	103	GLU	C	178.52	0.05	1
A	101	THR	CB	70.7	0.05	1
A	140	LEU	HB3	1.68	0.01	1
A	93	LEU	H	7.76	0.01	1
A	106	ALA	CA	55.45	0.05	1
A	100	VAL	CA	60.96	0.05	1
A	140	LEU	HA	4.16	0.01	1
A	145	ALA	N	124.38	0.05	1
A	94	LEU	CB	44.08	0.05	1
A	121	LYS	HE3	2.96	0.01	1
A	114	PHE	CD1	131.65	0.05	1
A	80	GLN	HG2	2.43	0.01	1
A	118	ARG	HA	4.03	0.01	1
A	143	SER	HB2	3.96	0.01	1
A	75	GLU	HA	4.32	0.01	1
A	99	PRO	CD	51.51	0.05	1
A	136	ARG	HG3	2.26	0.01	1
A	118	ARG	HB3	1.88	0.01	1
A	144	LEU	HD12	0.95	0.01	1
A	38	CYM	HA	4.44	0.01	1
A	100	VAL	C	176.07	0.05	1
A	105	LEU	CB	42.7	0.05	1
A	102	LEU	CG	27.49	0.05	1
A	96	GLN	HE22	6.86	0.01	1
A	127	THR	HG23	1.48	0.01	1
A	129	LYS	C	179.14	0.05	1
A	102	LEU	H	8.72	0.01	1
A	80	GLN	H	8.36	0.01	1
A	94	LEU	C	176.55	0.05	1
A	123	THR	HG23	1.09	0.01	1
A	129	LYS	CG	25.06	0.05	1
A	134	ALA	H	8.45	0.01	1
A	106	ALA	N	119.86	0.05	1
A	136	ARG	N	119.2	0.05	1
A	138	ARG	CD	43.63	0.05	1
A	99	PRO	HA	4.44	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	100	VAL	HG22	0.92	0.01	1
A	122	ALA	HB2	1.55	0.01	1
A	94	LEU	HD23	0.8	0.01	1
A	80	GLN	CG	34.0	0.05	1
A	118	ARG	CD	43.48	0.05	1
A	126	MET	H	8.7	0.01	1
A	101	THR	HG21	1.39	0.01	1
A	108	GLN	HG3	2.39	0.01	1
A	113	PRO	CG	27.57	0.05	1
A	128	PRO	CB	31.31	0.05	1
A	110	ALA	C	175.92	0.05	1
A	143	SER	N	115.23	0.05	1
A	109	VAL	CA	60.76	0.05	1
A	118	ARG	HG3	1.66	0.01	1
A	105	LEU	H	8.29	0.01	1
A	104	ALA	HB3	1.47	0.01	1
A	141	ARG	C	178.06	0.05	1
A	96	GLN	C	174.94	0.05	1
A	127	THR	CA	60.33	0.05	1
A	120	PHE	CA	62.41	0.05	1
A	116	LEU	HD22	0.81	0.01	1
A	122	ALA	N	120.97	0.05	1
A	93	LEU	HG	1.6	0.01	1
A	102	LEU	HD21	0.99	0.01	1
A	144	LEU	HD23	0.9	0.01	1
A	111	MET	HE1	1.95	0.01	1
A	130	ALA	HA	4.3	0.01	1
A	136	ARG	CA	59.83	0.05	1
A	142	GLU	H	8.16	0.01	1
A	135	TRP	HA	3.89	0.01	1
A	143	SER	HA	4.42	0.01	1
A	105	LEU	HB2	1.82	0.01	1
A	126	MET	HB2	2.32	0.01	1
A	141	ARG	HD2	3.22	0.01	1
A	127	THR	CG2	23.28	0.05	1
A	75	GLU	C	176.09	0.05	1
A	138	ARG	H	7.65	0.01	1
A	112	SER	HB3	4.07	0.01	1
A	111	MET	HB3	1.62	0.01	1
A	95	GLU	HB3	1.72	0.01	1
A	108	GLN	HA	4.13	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	133	GLN	HG3	2.55	0.01	1
A	121	LYS	H	8.24	0.01	1
A	109	VAL	HB	2.46	0.01	1
A	80	GLN	C	176.75	0.05	1
A	134	ALA	C	179.74	0.05	1
A	75	GLU	HB3	1.93	0.01	1
A	132	GLN	CB	29.84	0.05	1
A	146	LYS	H	7.77	0.01	1
A	120	PHE	CE2	132.82	0.05	1
A	105	LEU	N	121.02	0.05	1
A	121	LYS	CG	25.05	0.05	1
A	102	LEU	HD13	1.05	0.01	1
A	117	HIS	HD2	7.07	0.01	1
A	121	LYS	HG2	1.19	0.01	1
A	94	LEU	HB2	1.76	0.01	1
A	138	ARG	HB3	1.76	0.01	1
A	103	GLU	HB3	1.99	0.01	1
A	145	ALA	H	7.93	0.01	1
A	119	LEU	C	179.7	0.05	1
A	101	THR	CA	60.95	0.05	1
A	97	GLU	HG2	2.51	0.01	1
A	139	ARG	CG	26.29	0.05	1
A	133	GLN	C	178.83	0.05	1
A	131	TRP	N	120.74	0.05	1
A	75	GLU	CB	29.53	0.05	1
A	136	ARG	C	178.91	0.05	1
A	133	GLN	HB3	2.18	0.01	1
A	116	LEU	HG	1.41	0.01	1
A	140	LEU	CD2	24.73	0.05	1
A	109	VAL	HG12	0.9	0.01	1
A	119	LEU	CG	27.4	0.05	1
A	108	GLN	HE22	7.08	0.01	1
A	135	TRP	HH2	7.11	0.01	1
A	139	ARG	HD3	2.74	0.01	1
A	105	LEU	CA	57.57	0.05	1
A	106	ALA	CB	17.89	0.05	1
A	80	GLN	HA	4.28	0.01	1
A	140	LEU	CB	42.04	0.05	1
A	127	THR	HA	4.41	0.01	1
A	139	ARG	HB3	1.22	0.01	1
A	124	THR	HA	4.41	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	138	ARG	CG	27.57	0.05	1
A	118	ARG	HD2	3.19	0.01	1
A	135	TRP	HZ3	6.74	0.01	1
A	38	CYM	CA	53.3	0.05	1
A	144	LEU	CD2	23.4	0.05	1
A	100	VAL	HG21	0.92	0.01	1
A	142	GLU	HG2	2.41	0.01	1
A	93	LEU	CA	56.92	0.05	1
A	93	LEU	HD22	0.5	0.01	1
A	128	PRO	CA	66.07	0.05	1
A	100	VAL	H	8.26	0.01	1
A	109	VAL	CB	31.77	0.05	1
A	110	ALA	HB2	1.41	0.01	1
A	135	TRP	C	178.36	0.05	1
A	138	ARG	HD3	3.09	0.01	1
A	102	LEU	C	178.33	0.05	1
A	120	PHE	HD2	7.12	0.01	1
A	108	GLN	HB3	2.1	0.01	1
A	115	HIS	HB3	3.28	0.01	1
A	139	ARG	HG2	1.16	0.01	1
A	116	LEU	N	120.26	0.05	1
A	141	ARG	HD3	3.22	0.01	1
A	105	LEU	HG	1.5	0.01	1
A	100	VAL	HA	4.35	0.01	1
A	103	GLU	N	116.17	0.05	1
A	140	LEU	HD11	0.87	0.01	1
A	101	THR	HB	4.72	0.01	1
A	126	MET	HE3	2.12	0.01	1
A	93	LEU	CB	41.93	0.05	1
A	93	LEU	HD12	0.81	0.01	1
A	102	LEU	HB2	1.83	0.01	1
A	144	LEU	HA	4.38	0.01	1
A	134	ALA	HB2	1.38	0.01	1
A	80	GLN	HB2	2.07	0.01	1
A	119	LEU	HD23	0.87	0.01	1
A	136	ARG	HB3	2.01	0.01	1
A	108	GLN	C	178.06	0.05	1
A	117	HIS	HB3	3.31	0.01	1
A	120	PHE	CE1	132.82	0.05	1
A	105	LEU	HD21	0.69	0.01	1
A	109	VAL	HG22	0.69	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	110	ALA	CB	16.59	0.05	1
A	144	LEU	CA	55.34	0.05	1
A	143	SER	CB	63.6	0.05	1
A	125	GLY	N	110.61	0.05	1
A	93	LEU	CD2	26.32	0.05	1
A	137	ALA	HA	4.12	0.01	1
A	80	GLN	HE21	6.88	0.01	1
A	98	THR	HG22	1.32	0.01	1
A	109	VAL	CG2	21.15	0.05	1
A	114	PHE	CA	60.81	0.05	1
A	123	THR	H	7.84	0.01	1
A	123	THR	N	111.15	0.05	1
A	38	CYM	HB3	1.14	0.01	1
A	135	TRP	H	8.08	0.01	1
A	94	LEU	N	116.87	0.05	1
A	126	MET	C	173.45	0.05	1
A	108	GLN	CA	58.87	0.05	1
A	143	SER	CA	59.34	0.05	1
A	109	VAL	HG11	0.9	0.01	1
A	119	LEU	HD21	0.87	0.01	1
A	102	LEU	HG	1.6	0.01	1
A	94	LEU	HD11	0.74	0.01	1
A	144	LEU	C	177.04	0.05	1
A	126	MET	CG	31.81	0.05	1
A	144	LEU	HB3	1.64	0.01	1
A	111	MET	C	174.71	0.05	1
A	105	LEU	HD13	0.84	0.01	1
A	114	PHE	HE2	7.35	0.01	1
A	119	LEU	HB2	1.71	0.01	1
A	129	LYS	HD2	1.64	0.01	1
A	119	LEU	CD2	25.3	0.05	1
A	128	PRO	HA	3.47	0.01	1
A	122	ALA	C	179.27	0.05	1
A	116	LEU	HB2	1.94	0.01	1
A	107	ASP	H	7.69	0.01	1
A	140	LEU	CG	27.54	0.05	1
A	117	HIS	CA	61.93	0.05	1
A	103	GLU	CB	28.85	0.05	1
A	115	HIS	CB	30.87	0.05	1
A	111	MET	CA	54.84	0.05	1
A	38	CYM	CB	45.23	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	129	LYS	HG2	1.48	0.01	1
A	120	PHE	HB3	3.02	0.01	1
A	94	LEU	CA	55.26	0.05	1
A	135	TRP	CE3	120.76	0.05	1
A	93	LEU	HD21	0.5	0.01	1
A	80	GLN	HG3	2.42	0.01	1
A	75	GLU	HB2	2.19	0.01	1
A	117	HIS	C	176.89	0.05	1
A	146	LYS	CA	57.62	0.05	1
A	129	LYS	HE2	3.09	0.01	1
A	99	PRO	CG	28.04	0.05	1
A	118	ARG	HB2	1.88	0.01	1
A	135	TRP	CH2	123.89	0.05	1
A	141	ARG	CD	43.55	0.05	1
A	80	GLN	NE2	112.17	0.05	1

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	145	-0.37 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	0.04 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	133	-0.26 ± 0.13	None needed (< 0.5 ppm)
^{15}N	131	0.68 ± 0.43	None needed (imprecise)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 613 atoms were assigned a chemical shift out of a possible 714. 7 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	269/276 (97%)	108/110 (98%)	108/112 (96%)	53/54 (98%)
Sidechain	283/367 (77%)	176/218 (81%)	100/120 (83%)	7/29 (24%)
Aromatic	61/71 (86%)	36/39 (92%)	24/31 (77%)	1/1 (100%)
Overall	613/714 (86%)	320/367 (87%)	232/263 (88%)	61/84 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 921 atoms were assigned a chemical shift out of a possible

1173. 8 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	416/450 (92%)	167/179 (93%)	169/184 (92%)	80/87 (92%)
Sidechain	442/640 (69%)	277/381 (73%)	154/210 (73%)	11/49 (22%)
Aromatic	63/83 (76%)	38/47 (81%)	24/35 (69%)	1/1 (100%)
Overall	921/1173 (79%)	482/607 (79%)	347/429 (81%)	92/137 (67%)

7.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	49	ARG	NE	111.74	92.63 – 76.73	17.0
1	A	39	ARG	NE	111.43	92.63 – 76.73	16.8
1	A	12	ARG	NE	109.82	92.63 – 76.73	15.8
1	A	12	ARG	HB3	-0.11	3.17 – 0.37	-6.7
1	A	32	ARG	HG2	3.35	2.92 – 0.22	6.6
1	A	32	ARG	HG3	3.35	3.00 – 0.10	6.2
1	A	49	ARG	HD3	1.58	4.36 – 1.86	-6.1
1	A	87	ILE	CG2	9.21	24.63 – 10.43	-5.9
1	A	32	ARG	HD2	1.78	4.27 – 1.97	-5.8
1	A	65	GLY	N	131.24	129.07 – 90.27	5.6
1	A	12	ARG	HD3	1.74	4.36 – 1.86	-5.5
1	A	32	ARG	HD3	1.78	4.36 – 1.86	-5.3
1	A	61	ALA	HB1	0.03	2.61 – 0.11	-5.3
1	A	61	ALA	HB2	0.03	2.61 – 0.11	-5.3
1	A	61	ALA	HB3	0.03	2.61 – 0.11	-5.3
1	A	49	ARG	HD2	1.92	4.27 – 1.97	-5.2
1	A	68	PRO	HA	2.72	6.05 – 2.75	-5.1
1	A	12	ARG	HG3	0.10	3.00 – 0.10	-5.0

7.2.5 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:

