Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 11:29 PM BST

PDB ID	:	2KKE
Title	:	Solution NMR Structure of a dimeric protein of unknown function from Methanobacterium thermoautotrophicum, Northeast Structural Genomics Consortium Target TR5
Authors	:	Swapna, G.V.T.; Gunsalus, X.; Huang, L.; Xiao, K.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-06-18

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 (i) symbol.

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

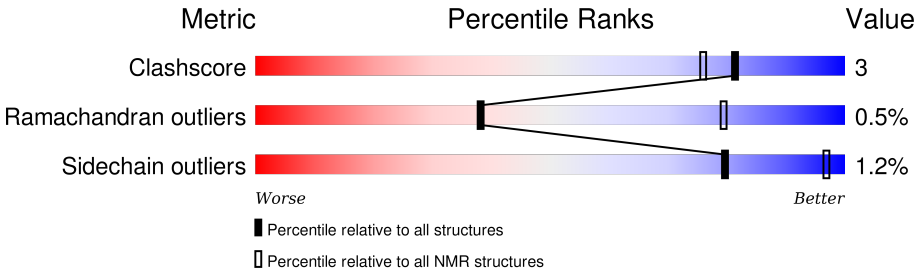
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	53	79% 21%
1	B	53	79% 21%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:11-A:52, B:212-B:253 (84)	0.53	5

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1711 atoms, of which 876 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	53	Total	C	H	N	O	S	0
			856	261	439	78	76	2	
1	B	53	Total	C	H	N	O	S	0
			855	261	437	78	77	2	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	GLU	ASP	SEE REMARK 999	UNP O26567
B	253	GLU	ASP	SEE REMARK 999	UNP O26567

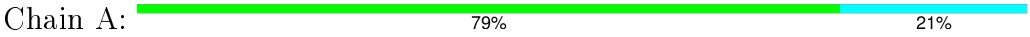
4 Residue-property plots

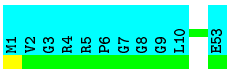
4.1 Average score per residue in the NMR ensemble

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: Uncharacterized protein

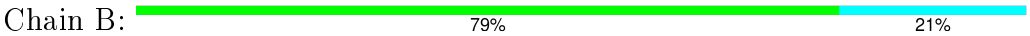
Chain A:

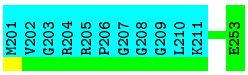




• Molecule 1: Uncharacterized protein

Chain B:





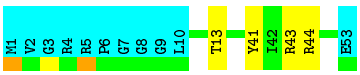
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

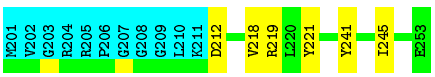
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

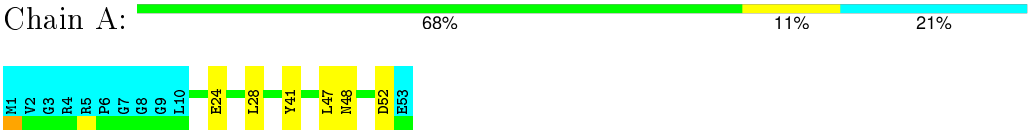
Chain B:



4.2.2 Score per residue for model 2

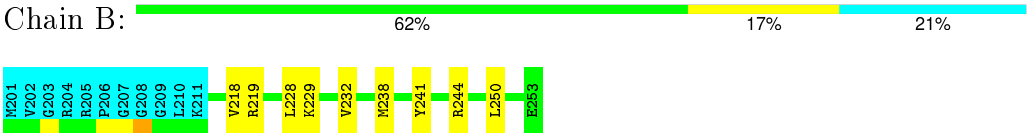
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

Chain B:



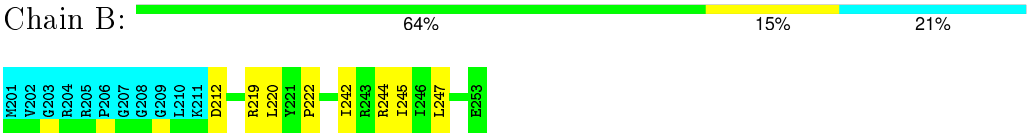
4.2.3 Score per residue for model 3

• Molecule 1: Uncharacterized protein

Chain A:

• Molecule 1: Uncharacterized protein

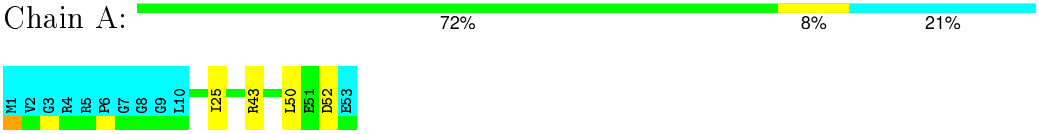
Chain B:



4.2.4 Score per residue for model 4

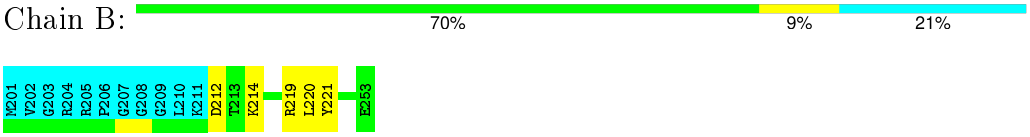
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

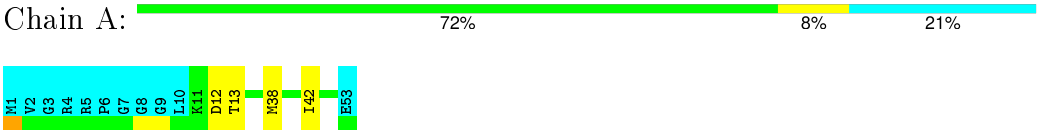
Chain B:



4.2.5 Score per residue for model 5 (medoid)

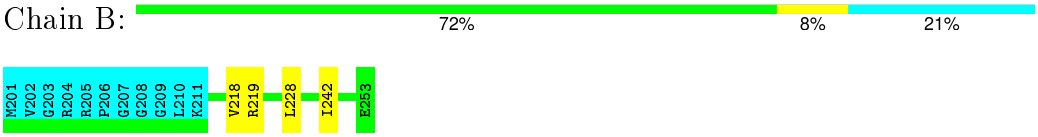
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

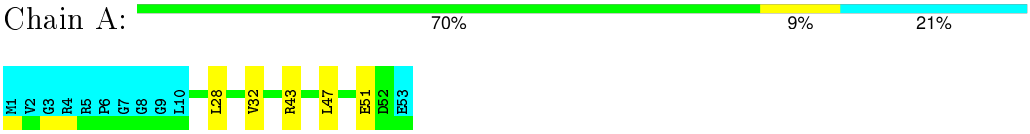
Chain B:



4.2.6 Score per residue for model 6

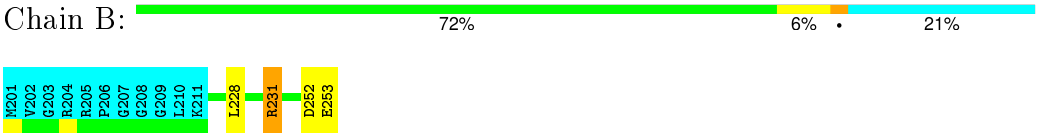
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

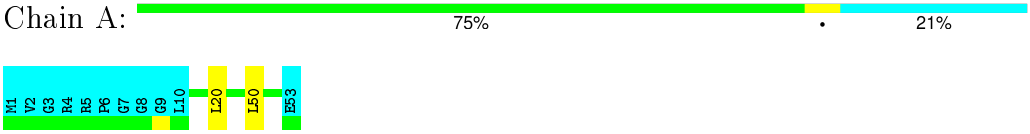
Chain B:



4.2.7 Score per residue for model 7

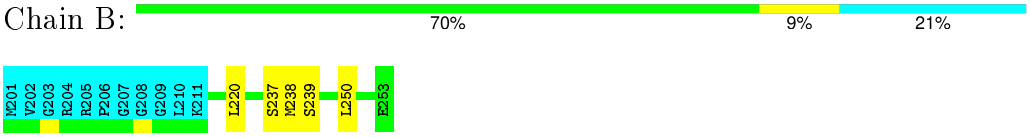
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

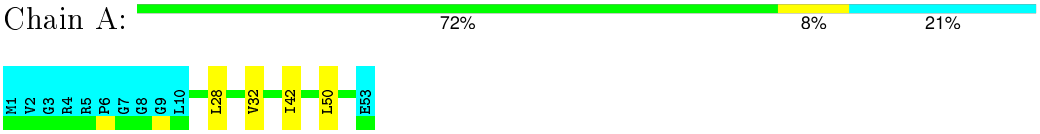
Chain B:



4.2.8 Score per residue for model 8

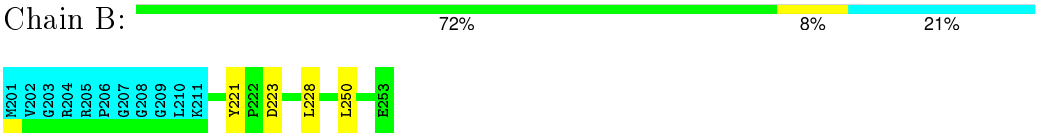
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

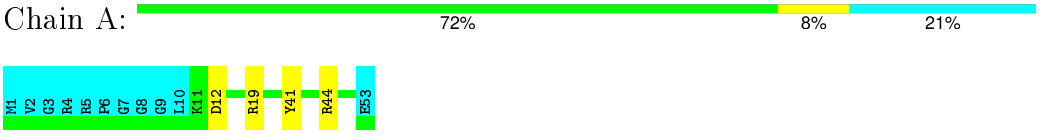
Chain B:



4.2.9 Score per residue for model 9

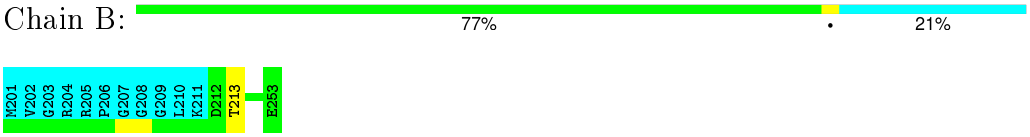
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

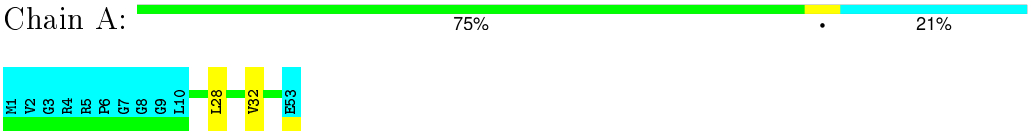
Chain B:



4.2.10 Score per residue for model 10

• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

Chain B:

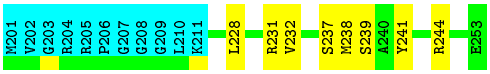
4.2.11 Score per residue for model 11

• Molecule 1: Uncharacterized protein

Chain A:

• Molecule 1: Uncharacterized protein

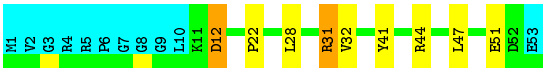
Chain B:



4.2.12 Score per residue for model 12

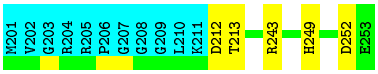
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

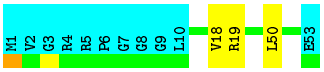
Chain B:



4.2.13 Score per residue for model 13

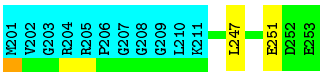
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

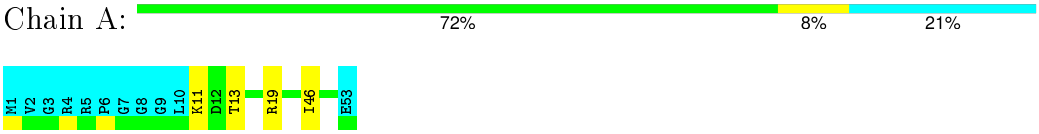
Chain B:



4.2.14 Score per residue for model 14

• Molecule 1: Uncharacterized protein

Chain A:



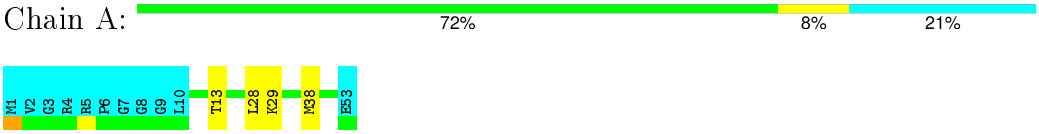
• Molecule 1: Uncharacterized protein

Chain B:

4.2.15 Score per residue for model 15

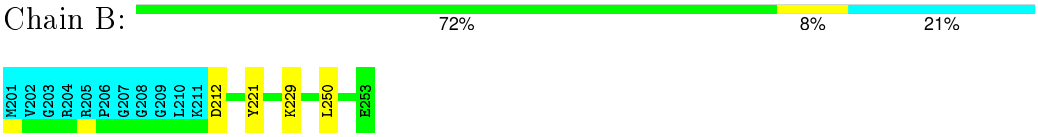
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

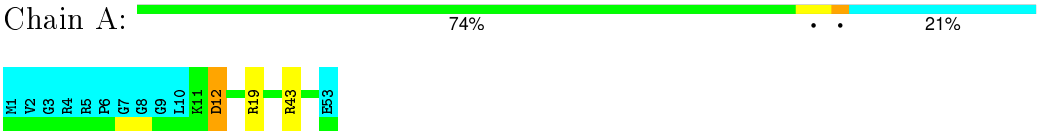
Chain B:



4.2.16 Score per residue for model 16

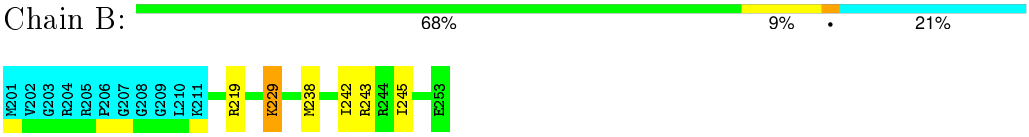
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

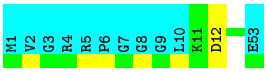
Chain B:



4.2.17 Score per residue for model 17

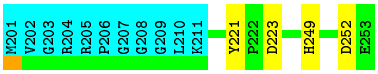
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

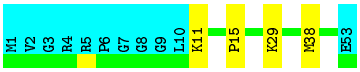
Chain B:



4.2.18 Score per residue for model 18

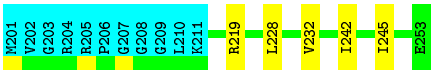
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

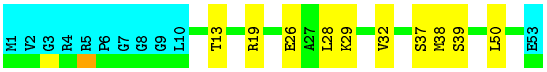
Chain B:



4.2.19 Score per residue for model 19

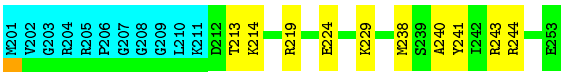
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

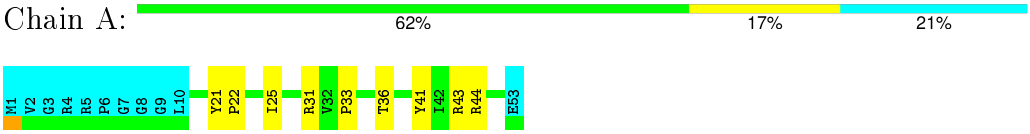
Chain B:



4.2.20 Score per residue for model 20

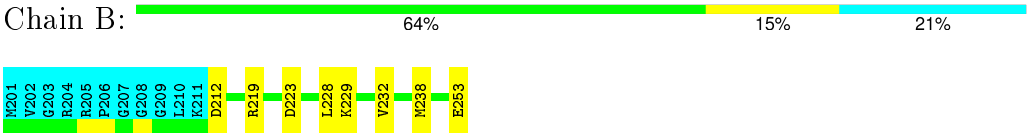
- Molecule 1: Uncharacterized protein

Chain A:



- Molecule 1: Uncharacterized protein

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	geometry optimization	2.1
CNS	geometry optimization	2.0.6
CNS	refinement	2.0.6

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 16357
Number of chemical shift lists	1
Total number of shifts	2568
Number of shifts mapped to atoms	1284
Number of unparsed shifts	0
Number of shifts with mapping errors	1284
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	340	357	356	3±2
1	B	341	350	349	3±2
All	All	13620	14140	14100	88

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLU:HB3	1:B:250:LEU:HG	0.60	1.72	2	1
1:A:13:THR:OG1	1:B:219:ARG:HB3	0.57	2.00	14	3
1:B:244:ARG:HA	1:B:247:LEU:HB3	0.57	1.77	3	1
1:B:228:LEU:HD21	1:B:242:ILE:HD11	0.56	1.77	5	1
1:B:218:VAL:HG22	1:B:219:ARG:H	0.56	1.61	1	2
1:A:50:LEU:HD11	1:B:228:LEU:HB2	0.55	1.78	8	1
1:A:15:PRO:HA	1:B:219:ARG:HG2	0.54	1.80	18	1
1:B:229:LYS:HB3	1:B:238:MET:SD	0.53	2.43	16	3
1:A:13:THR:HG21	1:A:43:ARG:HD2	0.52	1.81	1	1
1:A:37:SER:O	1:A:39:SER:N	0.52	2.43	19	1
1:B:229:LYS:HE2	1:B:238:MET:SD	0.51	2.46	2	1
1:A:33:PRO:HG2	1:A:36:THR:HB	0.51	1.83	20	1
1:B:249:HIS:HA	1:B:252:ASP:HB3	0.51	1.82	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:TYR:O	1:A:44:ARG:HG2	0.49	2.07	3	5
1:B:242:ILE:HD13	1:B:245:ILE:HD12	0.49	1.84	18	3
1:A:50:LEU:HG	1:B:220:LEU:HD11	0.49	1.85	4	2
1:B:213:THR:HG21	1:B:243:ARG:HD2	0.49	1.84	12	1
1:A:19:ARG:HB3	1:B:213:THR:HB	0.48	1.85	19	2
1:A:29:LYS:HB3	1:A:38:MET:SD	0.48	2.48	15	2
1:B:229:LYS:HA	1:B:232:VAL:HG22	0.48	1.85	2	1
1:A:25:ILE:HD12	1:B:214:LYS:HB2	0.48	1.85	4	1
1:A:28:LEU:O	1:A:32:VAL:HG13	0.47	2.09	6	5
1:A:31:ARG:NH2	1:B:253:GLU:HG3	0.47	2.25	20	1
1:B:218:VAL:HG22	1:B:219:ARG:N	0.47	2.25	5	2
1:A:47:LEU:O	1:A:51:GLU:HG2	0.46	2.10	6	2
1:A:19:ARG:HB3	1:B:213:THR:OG1	0.46	2.11	14	1
1:A:11:LYS:O	1:A:11:LYS:HG3	0.45	2.11	3	1
1:A:13:THR:HB	1:B:219:ARG:HB3	0.44	1.90	19	1
1:B:228:LEU:O	1:B:232:VAL:HG13	0.44	2.12	2	5
1:B:241:TYR:O	1:B:244:ARG:HG2	0.44	2.12	19	2
1:B:226:GLU:HG3	1:B:229:LYS:HE2	0.44	1.89	10	1
1:A:13:THR:HG22	1:B:221:TYR:HA	0.44	1.89	15	1
1:A:49:HIS:HD2	1:B:245:ILE:HG23	0.44	1.73	3	1
1:A:28:LEU:HD11	1:A:41:TYR:CE2	0.43	2.49	2	1
1:A:46:ILE:HD12	1:B:220:LEU:HD13	0.43	1.90	14	1
1:A:43:ARG:HG3	1:B:219:ARG:O	0.43	2.14	16	1
1:A:38:MET:O	1:A:42:ILE:HG12	0.43	2.14	5	1
1:B:247:LEU:O	1:B:251:GLU:HG2	0.43	2.13	13	1
1:A:50:LEU:HG	1:B:220:LEU:HD21	0.43	1.91	7	1
1:A:28:LEU:HD21	1:A:42:ILE:HD11	0.42	1.92	8	1
1:A:43:ARG:O	1:A:47:LEU:HD13	0.42	2.15	6	1
1:B:237:SER:O	1:B:239:SER:N	0.42	2.53	11	2
1:A:28:LEU:O	1:A:31:ARG:HG2	0.42	2.13	12	1
1:B:233:PRO:HG2	1:B:236:THR:HB	0.42	1.91	10	1
1:A:21:TYR:O	1:A:25:ILE:HG13	0.42	2.14	20	1
1:A:43:ARG:HD3	1:B:219:ARG:HB2	0.42	1.90	4	2
1:B:228:LEU:HD12	1:B:231:ARG:HH21	0.41	1.75	6	1
1:A:19:ARG:O	1:B:243:ARG:HG3	0.41	2.15	16	1
1:A:48:ASN:O	1:A:52:ASP:HB2	0.41	2.16	2	1
1:A:28:LEU:HD13	1:B:250:LEU:HD11	0.41	1.91	8	1
1:A:18:VAL:HG12	1:A:19:ARG:N	0.41	2.30	13	1
1:A:28:LEU:HB2	1:B:250:LEU:HD11	0.41	1.91	15	1
1:A:20:LEU:HD21	1:B:250:LEU:HG	0.41	1.93	7	1
1:A:50:LEU:HB3	1:B:224:GLU:HB3	0.41	1.93	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:241:TYR:O	1:B:245:ILE:HG13	0.40	2.16	1	1
1:B:252:ASP:O	1:B:253:GLU:HG2	0.40	2.17	6	1
1:B:240:ALA:O	1:B:243:ARG:HB3	0.40	2.17	19	1
1:A:26:GLU:HA	1:A:29:LYS:HG2	0.40	1.94	19	1
1:B:231:ARG:NH2	1:B:241:TYR:OH	0.40	2.53	11	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	42/53 (79%)	39±2 (93±4%)	3±2 (6±4%)	0±0 (0±1%)	38	79
1	B	41/53 (77%)	39±1 (94±3%)	2±1 (5±3%)	0±0 (0±1%)	38	79
All	All	1660/2120 (78%)	1555 (94%)	97 (6%)	8 (0%)	38	79

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	238	MET	2
1	A	12	ASP	1
1	A	52	ASP	1
1	B	231	ARG	1
1	B	212	ASP	1
1	A	22	PRO	1
1	A	38	MET	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	39/46 (85%)	39±1 (99±1%)	0±1 (1±1%)	87 98
1	B	39/46 (85%)	38±1 (98±2%)	1±1 (2±2%)	71 95
All	All	1560/1840 (85%)	1541 (99%)	19 (1%)	79 97

All 12 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	B	212	ASP	5
1	A	12	ASP	2
1	B	223	ASP	2
1	B	229	LYS	2
1	A	14	LYS	1
1	B	244	ARG	1
1	A	11	LYS	1
1	A	50	LEU	1
1	A	31	ARG	1
1	B	214	LYS	1
1	B	253	GLU	1
1	B	231	ARG	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

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16357

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	2568
Number of shifts mapped to atoms	1284
Number of unparsed shifts	0
Number of shifts with mapping errors	1284
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Residue not found in structure. All 1284 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	70	VAL	HA	4.496	0.05	1
A	69	VAL	HG12	0.902	0.05	2
A	95	ILE	HG21	0.875	0.05	1
A	90	SER	HB2	4.476	0.05	2
A	98	ILE	CG2	17.699	0.3	1
B	105	ASP	H	7.827	0.05	1
A	77	GLU	N	123.513	0.3	1
A	100	LEU	HD12	0.937	0.05	2
A	78	ILE	CG2	17.32	0.3	1
B	102	HIS	HB2	3.218	0.05	2
B	70	VAL	CG2	21.976	0.3	2
B	60	GLY	CA	45.26	0.3	1
A	82	LYS	CB	32.712	0.3	1
A	81	LEU	CB	42.454	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	69	VAL	CA	61.845	0.3	1
B	90	SER	HA	4.664	0.05	1
A	67	LYS	HG3	1.465	0.05	2
B	78	ILE	HG23	0.98	0.05	1
A	55	VAL	CG2	21.0	0.3	2
A	54	MET	HE2	2.166	0.05	1
B	104	GLU	H	7.75	0.05	1
B	79	GLU	CG	36.011	0.3	1
A	82	LYS	HB2	1.994	0.05	2
B	87	ALA	HA	4.227	0.05	1
A	69	VAL	HG23	0.865	0.05	2
A	90	SER	CA	56.974	0.3	1
A	89	THR	N	114.49	0.3	1
B	101	ASN	HA	4.524	0.05	1
B	74	TYR	CA	58.93	0.3	1
A	63	LEU	HD11	0.98	0.05	2
A	72	ARG	H	8.173	0.05	1
A	75	PRO	HB2	2.479	0.05	2
A	95	ILE	C	178.148	0.3	1
B	101	ASN	ND2	111.0	0.3	1
B	81	LEU	CB	42.454	0.3	1
A	102	HIS	CD2	123.4	0.3	1
A	93	ALA	CB	18.761	0.3	1
A	57	ARG	CD	43.419	0.3	1
A	106	GLU	N	125.725	0.3	1
B	84	ARG	HG2	1.829	0.05	2
A	60	GLY	HA2	4.09	0.05	2
A	95	ILE	HD12	0.803	0.05	1
B	89	THR	H	7.73	0.05	1
A	75	PRO	CD	51.15	0.3	1
B	63	LEU	CD2	23.3	0.3	2
B	97	ARG	CG	26.53	0.3	1
A	58	ARG	HD2	3.354	0.05	2
B	93	ALA	HB1	1.7	0.05	1
A	66	THR	HA	4.256	0.05	1
A	106	GLU	HB2	1.969	0.05	2
B	92	SER	HA	4.18	0.05	1
A	100	LEU	HB3	1.929	0.05	2
A	89	THR	HG22	1.469	0.05	1
B	94	TYR	H	8.48	0.05	1
A	94	TYR	CD1	132.7	0.3	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	87	ALA	CB	18.533	0.3	1
A	100	LEU	CD1	24.895	0.3	2
B	101	ASN	HB2	2.912	0.05	2
B	77	GLU	CG	36.88	0.3	1
B	84	ARG	HD3	3.301	0.05	2
A	83	SER	HB2	4.11	0.05	2
A	87	ALA	HB3	1.49	0.05	1
A	58	ARG	N	123.728	0.3	1
A	83	SER	CB	63.599	0.3	1
A	88	ASN	ND2	113.1	0.3	1
A	105	ASP	H	7.827	0.05	1
B	73	LEU	HD11	1.01	0.05	2
B	89	THR	HA	4.635	0.05	1
B	55	VAL	HG23	1.037	0.05	2
A	70	VAL	CB	32.841	0.3	1
B	58	ARG	CD	43.676	0.3	1
B	77	GLU	N	123.513	0.3	1
A	86	PRO	HA	4.512	0.05	1
A	94	TYR	HA	4.29	0.05	1
A	86	PRO	HG3	2.228	0.05	2
B	75	PRO	CB	32.334	0.3	1
B	64	LYS	HA	4.415	0.05	1
A	98	ILE	N	118.487	0.3	1
A	97	ARG	CG	26.53	0.3	1
A	73	LEU	HB2	1.629	0.05	2
B	89	THR	CB	71.101	0.3	1
B	78	ILE	HD13	0.85	0.05	1
B	63	LEU	CB	42.353	0.3	1
A	98	ILE	HD13	0.388	0.05	1
B	100	LEU	HB2	1.56	0.05	2
B	68	PRO	HB3	1.932	0.05	2
A	103	LEU	HD21	1.0	0.05	2
A	72	ARG	CA	54.233	0.3	1
A	99	ILE	HD12	0.925	0.05	1
B	94	TYR	HB2	3.251	0.05	2
B	94	TYR	CB	39.893	0.3	1
A	98	ILE	CA	65.095	0.3	1
A	96	ARG	C	177.081	0.3	1
A	63	LEU	HB2	1.762	0.05	2
A	99	ILE	CB	38.012	0.3	1
A	78	ILE	HG12	1.796	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	88	ASN	HB3	3.12	0.05	2
A	98	ILE	CD1	13.836	0.3	1
A	96	ARG	HB3	2.11	0.05	2
A	102	HIS	CB	29.31	0.3	1
B	104	GLU	CB	30.26	0.3	1
B	64	LYS	CE	42.421	0.3	1
B	54	MET	HB3	2.147	0.05	2
A	70	VAL	C	175.975	0.3	1
A	73	LEU	HD21	0.845	0.05	2
A	54	MET	HB3	2.147	0.05	2
A	70	VAL	H	8.338	0.05	1
B	83	SER	CB	63.599	0.3	1
B	76	ASP	HB2	2.86	0.05	2
B	94	TYR	HD2	6.99	0.05	3
B	65	ASP	H	8.187	0.05	1
B	89	THR	HG23	1.469	0.05	1
B	101	ASN	HB3	2.95	0.05	2
A	97	ARG	HA	3.956	0.05	1
A	102	HIS	C	177.294	0.3	1
A	92	SER	N	112.404	0.3	1
B	71	VAL	HG11	0.926	0.05	2
A	83	SER	N	111.985	0.3	1
A	103	LEU	CD1	22.47	0.3	2
A	70	VAL	HG13	0.83	0.05	2
B	64	LYS	HG3	1.55	0.05	2
A	94	TYR	CD2	132.7	0.3	3
A	82	LYS	HA	3.858	0.05	1
B	91	MET	HB3	2.589	0.05	2
B	58	ARG	HB3	2.081	0.05	2
B	85	VAL	CG2	22.01	0.3	2
B	67	LYS	HD3	1.775	0.05	2
B	78	ILE	CB	37.613	0.3	1
B	69	VAL	HG23	0.865	0.05	2
B	86	PRO	CA	62.841	0.3	1
B	71	VAL	HG23	0.985	0.05	2
A	82	LYS	C	179.54	0.3	1
A	69	VAL	CG1	21.088	0.3	2
A	74	TYR	HE1	6.82	0.05	3
B	55	VAL	HB	2.16	0.05	1
A	84	ARG	HG3	1.829	0.05	2
B	106	GLU	HA	4.22	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	102	HIS	HA	4.544	0.05	1
A	94	TYR	HB2	3.251	0.05	2
B	103	LEU	HD11	0.89	0.05	2
A	104	GLU	HB3	2.139	0.05	2
B	89	THR	CG2	20.573	0.3	1
B	88	ASN	CB	37.83	0.3	1
A	104	GLU	CB	30.26	0.3	1
B	106	GLU	HB3	2.118	0.05	2
A	74	TYR	CB	37.2	0.3	1
A	74	TYR	HD2	7.432	0.05	3
A	78	ILE	HG21	0.98	0.05	1
A	85	VAL	HA	3.28	0.05	1
A	84	ARG	CD	43.052	0.3	1
B	100	LEU	HD23	0.948	0.05	2
B	97	ARG	H	7.668	0.05	1
A	61	GLY	C	175.236	0.3	1
B	103	LEU	C	178.471	0.3	1
B	63	LEU	HA	4.312	0.05	1
A	78	ILE	CG1	30.95	0.3	1
B	70	VAL	CG1	22.008	0.3	2
A	67	LYS	N	119.891	0.3	1
B	81	LEU	HB3	1.817	0.05	2
A	81	LEU	CA	58.251	0.3	1
B	80	ALA	HB2	1.656	0.05	1
B	69	VAL	CB	34.265	0.3	1
A	74	TYR	HB2	3.406	0.05	2
B	84	ARG	HB3	2.285	0.05	2
A	72	ARG	CD	43.5	0.3	1
A	86	PRO	HD3	3.346	0.05	2
A	55	VAL	HG21	1.037	0.05	2
A	61	GLY	N	108.964	0.3	1
B	79	GLU	CB	29.411	0.3	1
B	77	GLU	HA	4.11	0.05	1
B	78	ILE	H	7.85	0.05	1
B	87	ALA	H	8.436	0.05	1
B	97	ARG	C	178.607	0.3	1
A	77	GLU	HB2	1.87	0.05	2
B	89	THR	N	114.49	0.3	1
B	101	ASN	CA	56.083	0.3	1
A	80	ALA	N	121.839	0.3	1
B	63	LEU	N	121.467	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	76	ASP	H	9.15	0.05	1
B	65	ASP	CA	54.4	0.3	1
B	102	HIS	CB	29.31	0.3	1
B	100	LEU	N	120.336	0.3	1
A	63	LEU	HD23	0.907	0.05	2
B	88	ASN	H	8.684	0.05	1
A	104	GLU	H	7.75	0.05	1
B	74	TYR	HB3	2.604	0.05	2
B	95	ILE	HG21	0.875	0.05	1
B	82	LYS	CA	60.333	0.3	1
B	103	LEU	CA	56.577	0.3	1
A	74	TYR	H	8.915	0.05	1
A	79	GLU	HB3	2.167	0.05	2
B	94	TYR	N	121.11	0.3	1
B	66	THR	HB	3.681	0.05	1
A	54	MET	HA	4.562	0.05	1
B	105	ASP	HB3	2.88	0.05	2
A	75	PRO	CG	28.589	0.3	1
B	97	ARG	CB	29.76	0.3	1
A	82	LYS	HE2	2.985	0.05	2
B	67	LYS	HE3	3.059	0.05	2
B	68	PRO	CA	62.351	0.3	1
A	75	PRO	C	178.823	0.3	1
A	71	VAL	HG22	0.985	0.05	2
B	55	VAL	H	8.215	0.05	1
A	70	VAL	CG1	22.008	0.3	2
A	68	PRO	HG2	2.325	0.05	2
B	59	PRO	CG	27.751	0.3	1
A	93	ALA	HA	4.289	0.05	1
A	92	SER	C	177.583	0.3	1
B	70	VAL	HG11	0.83	0.05	2
A	60	GLY	CA	45.26	0.3	1
B	63	LEU	HB2	1.762	0.05	2
B	82	LYS	CB	32.712	0.3	1
B	69	VAL	HG21	0.865	0.05	2
B	97	ARG	HD2	3.245	0.05	2
A	79	GLU	CA	59.55	0.3	1
A	64	LYS	HB3	1.99	0.05	2
B	95	ILE	HG13	0.808	0.05	2
A	65	ASP	HB3	3.01	0.05	2
A	67	LYS	CA	52.486	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	57	ARG	CB	31.179	0.3	1
A	78	ILE	HG22	0.98	0.05	1
B	82	LYS	C	179.54	0.3	1
A	104	GLU	N	117.196	0.3	1
A	72	ARG	HB2	1.912	0.05	2
B	102	HIS	H	7.85	0.05	1
A	94	TYR	CA	62.03	0.3	1
A	54	MET	HG3	2.61	0.05	2
A	101	ASN	HA	4.524	0.05	1
A	61	GLY	CA	45.46	0.3	1
B	75	PRO	CG	28.589	0.3	1
B	63	LEU	H	8.328	0.05	1
B	68	PRO	C	177.155	0.3	1
A	71	VAL	HG11	0.926	0.05	2
B	82	LYS	H	8.895	0.05	1
A	81	LEU	HD13	1.031	0.05	2
B	104	GLU	HG3	2.53	0.05	2
A	75	PRO	HD2	3.747	0.05	2
B	97	ARG	HA	3.956	0.05	1
B	102	HIS	CA	59.101	0.3	1
B	81	LEU	HD13	1.031	0.05	2
B	63	LEU	HD12	0.98	0.05	2
A	82	LYS	CA	60.333	0.3	1
B	55	VAL	CB	32.822	0.3	1
A	94	TYR	HE2	6.798	0.05	3
A	70	VAL	HG21	0.99	0.05	2
A	96	ARG	CB	28.36	0.3	1
A	103	LEU	HD22	1.0	0.05	2
B	70	VAL	N	125.65	0.3	1
B	66	THR	HG23	0.317	0.05	1
B	94	TYR	CA	62.03	0.3	1
B	86	PRO	HB3	2.081	0.05	2
B	64	LYS	HE3	3.08	0.05	2
A	67	LYS	HE2	3.119	0.05	2
B	85	VAL	H	7.034	0.05	1
B	54	MET	HG3	2.61	0.05	2
A	87	ALA	N	121.917	0.3	1
A	91	MET	C	178.508	0.3	1
A	93	ALA	HB2	1.7	0.05	1
A	71	VAL	CB	34.369	0.3	1
A	78	ILE	HD11	0.85	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	60	GLY	N	109.847	0.3	1
B	93	ALA	N	122.445	0.3	1
B	94	TYR	HD1	6.99	0.05	3
B	68	PRO	HG3	2.13	0.05	2
A	99	ILE	HG23	0.993	0.05	1
B	99	ILE	C	178.004	0.3	1
A	77	GLU	CG	36.88	0.3	1
B	82	LYS	HG3	1.754	0.05	2
B	73	LEU	HD12	1.01	0.05	2
A	57	ARG	HG3	1.665	0.05	2
A	91	MET	HE3	2.233	0.05	1
B	99	ILE	HG22	0.993	0.05	1
B	79	GLU	N	118.181	0.3	1
A	72	ARG	HG3	1.718	0.05	2
B	64	LYS	N	119.917	0.3	1
B	102	HIS	N	119.315	0.3	1
A	105	ASP	HB2	2.77	0.05	2
A	58	ARG	HA	4.594	0.05	1
B	85	VAL	CG1	21.79	0.3	2
B	66	THR	CA	60.358	0.3	1
A	73	LEU	CA	52.96	0.3	1
A	75	PRO	HG3	2.117	0.05	2
A	97	ARG	HB2	2.06	0.05	2
A	75	PRO	HA	4.295	0.05	1
B	81	LEU	HD22	1.093	0.05	2
A	54	MET	CG	32.138	0.3	1
B	70	VAL	CA	62.616	0.3	1
A	71	VAL	H	9.187	0.05	1
B	87	ALA	HB3	1.49	0.05	1
A	80	ALA	HB3	1.656	0.05	1
B	55	VAL	HA	4.189	0.05	1
B	100	LEU	HG	2.009	0.05	1
A	55	VAL	CB	32.822	0.3	1
A	57	ARG	HB3	1.838	0.05	2
B	78	ILE	C	178.317	0.3	1
A	101	ASN	HB2	2.912	0.05	2
B	103	LEU	HD12	0.89	0.05	2
B	103	LEU	HB3	2.069	0.05	2
B	88	ASN	CA	54.245	0.3	1
A	104	GLU	CG	36.32	0.3	1
B	81	LEU	HD11	1.031	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	98	ILE	HG13	0.398	0.05	2
B	100	LEU	H	8.935	0.05	1
B	64	LYS	HD2	1.778	0.05	2
B	86	PRO	HG3	2.228	0.05	2
B	80	ALA	CA	55.27	0.3	1
A	100	LEU	HD22	0.948	0.05	2
B	97	ARG	HG3	1.762	0.05	2
B	82	LYS	HA	3.858	0.05	1
A	96	ARG	HA	3.77	0.05	1
B	98	ILE	CA	65.095	0.3	1
B	57	ARG	HA	4.44	0.05	1
B	103	LEU	CD2	25.659	0.3	2
A	64	LYS	HG3	1.55	0.05	2
B	67	LYS	HG3	1.465	0.05	2
B	102	HIS	HD2	6.727	0.05	1
B	102	HIS	HB3	3.714	0.05	2
A	73	LEU	C	176.68	0.3	1
B	76	ASP	HB3	2.723	0.05	2
B	74	TYR	HD2	7.432	0.05	3
B	74	TYR	H	8.915	0.05	1
A	85	VAL	HG13	0.867	0.05	2
B	80	ALA	HB1	1.656	0.05	1
A	83	SER	HA	4.383	0.05	1
B	71	VAL	CB	34.369	0.3	1
A	82	LYS	CE	42.05	0.3	1
B	79	GLU	CA	59.55	0.3	1
B	76	ASP	C	179.364	0.3	1
A	56	GLY	HA3	4.05	0.05	2
A	63	LEU	H	8.328	0.05	1
A	89	THR	CB	71.101	0.3	1
A	98	ILE	HG23	0.576	0.05	1
A	69	VAL	H	9.112	0.05	1
B	106	GLU	CG	36.72	0.3	1
B	94	TYR	HA	4.29	0.05	1
A	99	ILE	HB	2.196	0.05	1
B	63	LEU	HD23	0.907	0.05	2
B	55	VAL	N	121.358	0.3	1
A	57	ARG	CB	31.179	0.3	1
B	85	VAL	HG23	0.812	0.05	2
B	82	LYS	CD	29.875	0.3	1
B	103	LEU	CB	42.06	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	93	ALA	N	122.445	0.3	1
A	81	LEU	CD1	25.302	0.3	1
B	77	GLU	HB2	1.87	0.05	2
A	63	LEU	CG	27.117	0.3	1
B	104	GLU	HB2	2.204	0.05	2
B	55	VAL	HG11	1.037	0.05	2
A	75	PRO	CB	32.334	0.3	1
B	76	ASP	H	9.15	0.05	1
A	71	VAL	HG21	0.985	0.05	2
A	77	GLU	H	7.515	0.05	1
B	105	ASP	HA	4.658	0.05	1
B	59	PRO	CD	50.879	0.3	1
B	82	LYS	HB3	1.994	0.05	2
B	56	GLY	H	8.55	0.05	1
B	87	ALA	CA	53.93	0.3	1
A	63	LEU	HA	4.312	0.05	1
B	93	ALA	CB	18.761	0.3	1
A	67	LYS	HD3	1.775	0.05	2
A	69	VAL	HG11	0.902	0.05	2
B	98	ILE	N	118.487	0.3	1
A	86	PRO	CG	27.506	0.3	1
A	54	MET	HE3	2.166	0.05	1
A	82	LYS	HB3	1.994	0.05	2
A	98	ILE	CG1	27.38	0.3	1
A	103	LEU	HD13	0.89	0.05	2
A	100	LEU	HD13	0.937	0.05	2
A	61	GLY	HA2	4.07	0.05	2
A	90	SER	HA	4.664	0.05	1
A	69	VAL	CB	34.265	0.3	1
B	74	TYR	HD1	7.432	0.05	3
A	88	ASN	H	8.684	0.05	1
A	81	LEU	HD21	1.093	0.05	2
A	78	ILE	HG23	0.98	0.05	1
A	55	VAL	CG1	21.0	0.3	2
A	104	GLU	HG3	2.53	0.05	2
B	103	LEU	H	8.196	0.05	1
A	97	ARG	HD2	3.245	0.05	2
A	94	TYR	CE1	119.0	0.3	3
B	94	TYR	CD1	132.7	0.3	3
A	92	SER	H	8.626	0.05	1
B	82	LYS	HD3	1.745	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	100	LEU	CG	26.917	0.3	1
B	96	ARG	HG3	1.716	0.05	2
B	69	VAL	CG2	21.156	0.3	2
A	64	LYS	HA	4.415	0.05	1
A	95	ILE	HD13	0.803	0.05	1
B	72	ARG	HB2	1.912	0.05	2
B	63	LEU	CD1	25.09	0.3	2
A	71	VAL	CG1	20.135	0.3	2
A	103	LEU	CD2	25.659	0.3	2
A	57	ARG	CA	55.82	0.3	1
A	78	ILE	HD12	0.85	0.05	1
A	97	ARG	HG2	1.762	0.05	2
A	87	ALA	HA	4.227	0.05	1
B	58	ARG	H	8.522	0.05	1
A	92	SER	HA	4.18	0.05	1
A	57	ARG	HA	4.44	0.05	1
B	89	THR	HG22	1.469	0.05	1
B	83	SER	N	111.985	0.3	1
B	84	ARG	HD2	3.209	0.05	2
A	59	PRO	HG3	2.05	0.05	2
A	87	ALA	HB2	1.49	0.05	1
A	98	ILE	HG22	0.576	0.05	1
B	81	LEU	HG	1.771	0.05	1
A	89	THR	HA	4.635	0.05	1
A	91	MET	CE	16.866	0.3	1
B	95	ILE	HA	3.501	0.05	1
B	69	VAL	C	174.696	0.3	1
A	67	LYS	CE	42.416	0.3	1
B	64	LYS	HB3	1.99	0.05	2
B	66	THR	HG22	0.317	0.05	1
A	100	LEU	C	180.461	0.3	1
A	92	SER	CB	63.51	0.3	1
B	85	VAL	HG11	0.867	0.05	2
B	75	PRO	HD2	3.747	0.05	2
A	85	VAL	CA	61.133	0.3	1
B	101	ASN	C	178.72	0.3	1
B	79	GLU	HB3	2.167	0.05	2
B	69	VAL	N	124.67	0.3	1
A	83	SER	CA	60.922	0.3	1
A	97	ARG	CD	43.787	0.3	1
A	85	VAL	HG21	0.812	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	70	VAL	HB	1.994	0.05	1
B	98	ILE	CG1	27.38	0.3	1
A	98	ILE	HD12	0.388	0.05	1
B	57	ARG	HB2	1.9	0.05	2
A	73	LEU	CB	46.56	0.3	1
A	61	GLY	H	8.382	0.05	1
B	81	LEU	HD21	1.093	0.05	2
A	54	MET	CB	33.026	0.3	1
A	94	TYR	CE2	119.0	0.3	3
B	104	GLU	CG	36.32	0.3	1
A	99	ILE	HD13	0.925	0.05	1
B	99	ILE	H	8.405	0.05	1
B	78	ILE	N	119.2	0.3	1
A	64	LYS	HD2	1.778	0.05	2
B	62	GLY	HA3	4.03	0.05	2
B	96	ARG	CA	60.97	0.3	1
B	72	ARG	CA	54.233	0.3	1
A	78	ILE	HG13	0.859	0.05	2
B	98	ILE	HG21	0.576	0.05	1
B	88	ASN	ND2	113.1	0.3	1
A	55	VAL	CA	62.709	0.3	1
B	105	ASP	N	120.128	0.3	1
A	55	VAL	HA	4.189	0.05	1
A	96	ARG	HB2	1.746	0.05	2
B	59	PRO	HD2	4.33	0.05	2
A	103	LEU	H	8.196	0.05	1
B	64	LYS	CD	29.35	0.3	1
A	99	ILE	HG13	0.931	0.05	2
A	74	TYR	N	120.637	0.3	1
A	100	LEU	HD21	0.948	0.05	2
B	90	SER	CA	56.974	0.3	1
A	54	MET	HB2	2.06	0.05	2
A	68	PRO	CD	50.446	0.3	1
B	74	TYR	HE1	6.82	0.05	3
B	78	ILE	HG21	0.98	0.05	1
A	82	LYS	HG3	1.754	0.05	2
B	103	LEU	CD1	22.47	0.3	2
B	69	VAL	HB	2.054	0.05	1
B	81	LEU	HD12	1.031	0.05	2
B	67	LYS	HB2	1.909	0.05	2
B	74	TYR	HA	4.65	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	99	ILE	HA	3.625	0.05	1
B	57	ARG	HB3	1.838	0.05	2
A	64	LYS	HE2	3.08	0.05	2
B	91	MET	CB	32.376	0.3	1
A	59	PRO	HB3	2.408	0.05	2
B	84	ARG	CD	43.052	0.3	1
A	59	PRO	CB	32.259	0.3	1
A	85	VAL	N	121.674	0.3	1
B	72	ARG	C	175.687	0.3	1
B	60	GLY	HA2	4.09	0.05	2
A	66	THR	HG21	0.317	0.05	1
B	99	ILE	CB	38.012	0.3	1
B	71	VAL	C	174.24	0.3	1
A	89	THR	CA	61.487	0.3	1
A	73	LEU	HD22	0.845	0.05	2
B	61	GLY	C	175.236	0.3	1
B	62	GLY	CA	45.5	0.3	1
B	106	GLU	CB	31.43	0.3	1
A	99	ILE	HA	3.625	0.05	1
A	76	ASP	HA	4.5	0.05	1
A	100	LEU	HG	2.009	0.05	1
A	79	GLU	HG3	2.457	0.05	2
A	79	GLU	HB2	2.165	0.05	2
B	69	VAL	HG22	0.865	0.05	2
A	97	ARG	H	7.668	0.05	1
B	86	PRO	CB	32.622	0.3	1
A	106	GLU	HA	4.22	0.05	1
A	78	ILE	CA	66.024	0.3	1
B	96	ARG	N	120.141	0.3	1
B	72	ARG	N	125.708	0.3	1
B	91	MET	HE1	2.233	0.05	1
A	91	MET	HB2	2.21	0.05	2
A	82	LYS	HE3	3.073	0.05	2
A	84	ARG	HG2	1.829	0.05	2
B	56	GLY	N	112.524	0.3	1
B	97	ARG	N	118.718	0.3	1
A	94	TYR	HB3	3.25	0.05	2
A	83	SER	H	7.558	0.05	1
B	82	LYS	CG	26.135	0.3	1
B	106	GLU	HB2	1.969	0.05	2
A	79	GLU	C	179.616	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	103	LEU	HA	4.055	0.05	1
A	106	GLU	CG	36.72	0.3	1
B	91	MET	H	9.125	0.05	1
A	64	LYS	CA	57.22	0.3	1
A	81	LEU	CD2	24.676	0.3	1
A	81	LEU	HA	4.126	0.05	1
B	71	VAL	CA	59.832	0.3	1
A	95	ILE	HG23	0.875	0.05	1
A	72	ARG	C	175.687	0.3	1
B	87	ALA	N	121.917	0.3	1
A	80	ALA	H	7.77	0.05	1
A	77	GLU	HA	4.11	0.05	1
A	69	VAL	CG2	21.156	0.3	2
B	75	PRO	C	178.823	0.3	1
A	74	TYR	HB3	2.604	0.05	2
B	106	GLU	H	7.919	0.05	1
A	65	ASP	N	118.931	0.3	1
A	86	PRO	HD2	4.053	0.05	2
A	57	ARG	C	176.599	0.3	1
B	62	GLY	HA2	4.03	0.05	2
B	54	MET	HE3	2.166	0.05	1
A	101	ASN	HD21	6.915	0.05	2
A	76	ASP	CA	56.871	0.3	1
B	101	ASN	H	8.34	0.05	1
B	78	ILE	HG12	1.796	0.05	2
B	59	PRO	C	178.098	0.3	1
A	77	GLU	HB3	1.84	0.05	2
B	87	ALA	C	179.218	0.3	1
B	73	LEU	C	176.68	0.3	1
B	94	TYR	CD2	132.7	0.3	3
A	94	TYR	HD2	6.99	0.05	3
B	77	GLU	HG3	2.42	0.05	2
B	59	PRO	HA	4.55	0.05	1
A	94	TYR	H	8.48	0.05	1
A	73	LEU	HD23	0.845	0.05	2
B	101	ASN	HD22	7.787	0.05	2
B	92	SER	HB3	4.076	0.05	2
B	67	LYS	CA	52.486	0.3	1
A	96	ARG	N	120.141	0.3	1
A	65	ASP	CA	54.4	0.3	1
B	88	ASN	HD21	6.966	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	97	ARG	CA	59.609	0.3	1
A	73	LEU	HD13	1.01	0.05	2
B	90	SER	HB2	4.476	0.05	2
B	67	LYS	HE2	3.119	0.05	2
B	71	VAL	H	9.187	0.05	1
B	68	PRO	CB	33.036	0.3	1
B	75	PRO	HB2	2.479	0.05	2
B	99	ILE	CG2	17.66	0.3	1
A	68	PRO	HG3	2.13	0.05	2
B	98	ILE	H	7.693	0.05	1
B	93	ALA	HB2	1.7	0.05	1
B	70	VAL	HG12	0.83	0.05	2
B	99	ILE	CG1	29.426	0.3	1
B	68	PRO	HD2	3.747	0.05	2
B	91	MET	HA	4.235	0.05	1
A	79	GLU	CB	29.411	0.3	1
A	78	ILE	H	7.85	0.05	1
A	101	ASN	C	178.72	0.3	1
B	55	VAL	CG1	21.0	0.3	2
B	90	SER	H	8.622	0.05	1
A	77	GLU	HG2	2.42	0.05	2
B	59	PRO	CA	63.632	0.3	1
A	99	ILE	HG22	0.993	0.05	1
A	92	SER	CA	62.0	0.3	1
A	94	TYR	CB	39.893	0.3	1
A	65	ASP	C	176.436	0.3	1
B	75	PRO	CD	51.15	0.3	1
B	83	SER	HB2	4.11	0.05	2
B	99	ILE	N	122.0	0.3	1
A	68	PRO	HD3	3.861	0.05	2
A	98	ILE	H	7.693	0.05	1
A	81	LEU	HD12	1.031	0.05	2
B	71	VAL	CG1	20.135	0.3	2
A	68	PRO	HB3	1.932	0.05	2
A	98	ILE	HD11	0.388	0.05	1
B	63	LEU	HD13	0.98	0.05	2
A	57	ARG	HG2	1.665	0.05	2
A	78	ILE	N	119.2	0.3	1
A	88	ASN	CA	54.245	0.3	1
B	81	LEU	CG	27.2	0.3	1
B	67	LYS	N	119.891	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	70	VAL	HG22	0.99	0.05	2
A	103	LEU	HD23	1.0	0.05	2
B	73	LEU	HD21	0.845	0.05	2
B	80	ALA	H	7.77	0.05	1
B	77	GLU	C	176.638	0.3	1
B	96	ARG	CB	28.36	0.3	1
B	96	ARG	HB2	1.746	0.05	2
A	67	LYS	HE3	3.059	0.05	2
B	54	MET	HG2	2.53	0.05	2
B	82	LYS	HE2	2.985	0.05	2
A	64	LYS	CE	42.421	0.3	1
B	98	ILE	HG22	0.576	0.05	1
B	90	SER	N	119.067	0.3	1
B	81	LEU	H	8.39	0.05	1
A	55	VAL	HG11	1.037	0.05	2
A	102	HIS	HD2	6.727	0.05	1
A	93	ALA	HB3	1.7	0.05	1
A	105	ASP	N	120.128	0.3	1
A	71	VAL	CA	59.832	0.3	1
B	90	SER	CB	65.755	0.3	1
A	100	LEU	CG	26.917	0.3	1
B	57	ARG	HD3	3.224	0.05	2
B	68	PRO	HG2	2.325	0.05	2
B	77	GLU	CB	29.4	0.3	1
A	85	VAL	H	7.034	0.05	1
A	92	SER	HB3	4.076	0.05	2
A	97	ARG	C	178.607	0.3	1
A	91	MET	CA	59.967	0.3	1
B	94	TYR	CE1	119.0	0.3	3
B	99	ILE	HG12	1.943	0.05	2
B	95	ILE	N	118.174	0.3	1
B	57	ARG	HG2	1.665	0.05	2
B	84	ARG	CG	27.2	0.3	1
B	99	ILE	HD13	0.925	0.05	1
A	81	LEU	HB3	1.817	0.05	2
A	103	LEU	HA	4.055	0.05	1
A	59	PRO	CA	63.632	0.3	1
A	73	LEU	H	8.255	0.05	1
A	91	MET	HE2	2.233	0.05	1
B	99	ILE	HG21	0.993	0.05	1
A	82	LYS	CD	29.875	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	78	ILE	CD1	13.64	0.3	1
B	100	LEU	CD1	24.895	0.3	2
B	84	ARG	HG3	1.829	0.05	2
B	102	HIS	CD2	123.4	0.3	1
A	66	THR	HG22	0.317	0.05	1
B	99	ILE	CA	66.129	0.3	1
B	74	TYR	CE2	118.3	0.3	3
B	96	ARG	H	8.52	0.05	1
B	101	ASN	N	117.516	0.3	1
A	84	ARG	HB2	1.925	0.05	2
B	63	LEU	CG	27.117	0.3	1
B	83	SER	H	7.558	0.05	1
B	76	ASP	CA	56.871	0.3	1
B	98	ILE	HG13	0.398	0.05	2
A	89	THR	HG23	1.469	0.05	1
B	59	PRO	HB2	2.054	0.05	2
A	65	ASP	HA	4.85	0.05	1
A	57	ARG	N	120.49	0.3	1
B	56	GLY	CA	45.39	0.3	1
B	103	LEU	N	117.173	0.3	1
B	71	VAL	HG21	0.985	0.05	2
B	61	GLY	HA3	4.13	0.05	2
B	75	PRO	HG3	2.117	0.05	2
B	69	VAL	HG11	0.902	0.05	2
B	103	LEU	HD13	0.89	0.05	2
B	69	VAL	HA	4.29	0.05	1
B	98	ILE	HD11	0.388	0.05	1
B	67	LYS	H	9.064	0.05	1
B	78	ILE	HB	2.071	0.05	1
B	54	MET	CE	17.265	0.3	1
B	86	PRO	HG2	2.11	0.05	2
B	65	ASP	HA	4.85	0.05	1
B	100	LEU	HD21	0.948	0.05	2
B	57	ARG	HG3	1.665	0.05	2
A	86	PRO	HB3	2.081	0.05	2
A	67	LYS	HG2	1.563	0.05	2
A	101	ASN	N	117.516	0.3	1
B	98	ILE	CB	37.634	0.3	1
A	76	ASP	HB3	2.723	0.05	2
B	78	ILE	CG1	30.95	0.3	1
A	58	ARG	CD	43.676	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	80	ALA	HA	4.26	0.05	1
A	64	LYS	HG2	1.55	0.05	2
B	67	LYS	HG2	1.563	0.05	2
A	100	LEU	HB2	1.56	0.05	2
A	94	TYR	N	121.11	0.3	1
A	81	LEU	C	179.223	0.3	1
B	70	VAL	HG23	0.99	0.05	2
B	88	ASN	C	174.797	0.3	1
B	66	THR	H	7.615	0.05	1
A	69	VAL	C	174.696	0.3	1
B	58	ARG	N	123.728	0.3	1
A	81	LEU	CG	27.2	0.3	1
B	103	LEU	HD23	1.0	0.05	2
A	72	ARG	CB	30.359	0.3	1
A	55	VAL	HG23	1.037	0.05	2
B	73	LEU	CB	46.56	0.3	1
A	93	ALA	H	8.134	0.05	1
A	74	TYR	HA	4.65	0.05	1
B	79	GLU	HG3	2.457	0.05	2
A	81	LEU	N	120.403	0.3	1
B	76	ASP	N	114.907	0.3	1
B	93	ALA	H	8.134	0.05	1
A	96	ARG	HG2	1.716	0.05	2
B	101	ASN	HD21	6.915	0.05	2
A	63	LEU	HD21	0.907	0.05	2
B	63	LEU	HD22	0.907	0.05	2
B	67	LYS	CB	34.372	0.3	1
B	104	GLU	N	117.196	0.3	1
B	95	ILE	HG23	0.875	0.05	1
A	106	GLU	HG3	2.306	0.05	2
B	57	ARG	N	120.49	0.3	1
A	75	PRO	CA	67.002	0.3	1
B	64	LYS	HE2	3.08	0.05	2
B	94	TYR	C	177.802	0.3	1
B	68	PRO	CG	26.933	0.3	1
A	82	LYS	HD2	1.785	0.05	2
A	72	ARG	CG	26.91	0.3	1
B	81	LEU	CD2	24.676	0.3	1
B	102	HIS	C	177.294	0.3	1
A	97	ARG	HG3	1.762	0.05	2
A	105	ASP	CB	41.57	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	102	HIS	HB2	3.218	0.05	2
B	66	THR	CB	72.453	0.3	1
A	84	ARG	CA	55.41	0.3	1
B	93	ALA	CA	55.24	0.3	1
A	67	LYS	HD2	1.78	0.05	2
B	81	LEU	HA	4.126	0.05	1
A	81	LEU	HD22	1.093	0.05	2
A	79	GLU	CG	36.011	0.3	1
A	77	GLU	HG3	2.42	0.05	2
B	73	LEU	H	8.255	0.05	1
B	55	VAL	CG2	21.0	0.3	2
A	103	LEU	HD12	0.89	0.05	2
B	57	ARG	CD	43.419	0.3	1
A	98	ILE	HA	3.612	0.05	1
A	94	TYR	C	177.802	0.3	1
B	75	PRO	CA	67.002	0.3	1
A	70	VAL	HG11	0.83	0.05	2
B	60	GLY	C	175.353	0.3	1
A	101	ASN	CB	38.129	0.3	1
A	99	ILE	C	178.004	0.3	1
A	91	MET	H	9.125	0.05	1
B	92	SER	CA	62.0	0.3	1
A	101	ASN	HD22	7.787	0.05	2
B	73	LEU	HB3	1.916	0.05	2
A	69	VAL	HG21	0.865	0.05	2
A	103	LEU	HB3	2.069	0.05	2
A	99	ILE	CD1	15.948	0.3	1
A	100	LEU	N	120.336	0.3	1
A	63	LEU	HD13	0.98	0.05	2
A	73	LEU	HD11	1.01	0.05	2
A	67	LYS	HB3	1.657	0.05	2
B	86	PRO	HA	4.512	0.05	1
A	88	ASN	HD21	6.966	0.05	2
A	78	ILE	CD1	13.64	0.3	1
B	96	ARG	HG2	1.716	0.05	2
A	95	ILE	HA	3.501	0.05	1
A	102	HIS	H	7.85	0.05	1
B	79	GLU	H	8.07	0.05	1
A	95	ILE	CA	66.02	0.3	1
A	85	VAL	HG23	0.812	0.05	2
B	72	ARG	HB3	1.797	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	76	ASP	CB	39.34	0.3	1
B	65	ASP	C	176.436	0.3	1
A	81	LEU	HD11	1.031	0.05	2
B	59	PRO	HG3	2.05	0.05	2
A	55	VAL	HG12	1.037	0.05	2
B	62	GLY	H	8.533	0.05	1
A	59	PRO	HD3	4.204	0.05	2
B	101	ASN	CB	38.129	0.3	1
B	69	VAL	CG1	21.088	0.3	2
A	55	VAL	C	177.021	0.3	1
A	84	ARG	N	119.557	0.3	1
B	72	ARG	H	8.173	0.05	1
B	95	ILE	C	178.148	0.3	1
A	57	ARG	HD2	3.224	0.05	2
A	89	THR	HB	4.121	0.05	1
A	91	MET	CB	32.376	0.3	1
A	77	GLU	CA	58.5	0.3	1
A	103	LEU	C	178.471	0.3	1
B	95	ILE	HB	1.95	0.05	1
A	62	GLY	CA	45.5	0.3	1
B	84	ARG	CB	31.352	0.3	1
B	55	VAL	HG21	1.037	0.05	2
A	67	LYS	CD	29.114	0.3	1
B	64	LYS	HB2	1.93	0.05	2
B	66	THR	HG21	0.317	0.05	1
A	59	PRO	CD	50.879	0.3	1
A	63	LEU	CD1	25.09	0.3	2
A	72	ARG	N	125.708	0.3	1
A	55	VAL	H	8.215	0.05	1
B	100	LEU	CD2	21.56	0.3	2
B	85	VAL	HG12	0.867	0.05	2
B	75	PRO	HD3	3.945	0.05	2
B	91	MET	HB2	2.21	0.05	2
B	79	GLU	HB2	2.165	0.05	2
A	71	VAL	HA	4.48	0.05	1
A	73	LEU	N	122.019	0.3	1
A	106	GLU	H	7.919	0.05	1
B	55	VAL	C	177.021	0.3	1
A	85	VAL	HG22	0.812	0.05	2
B	100	LEU	C	180.461	0.3	1
A	90	SER	N	119.067	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	81	LEU	N	120.403	0.3	1
B	82	LYS	HD2	1.785	0.05	2
A	87	ALA	H	8.436	0.05	1
B	106	GLU	N	125.725	0.3	1
A	64	LYS	HE3	3.08	0.05	2
B	65	ASP	CB	41.82	0.3	1
A	100	LEU	HA	4.054	0.05	1
B	73	LEU	CD1	23.286	0.3	2
A	54	MET	CA	55.75	0.3	1
A	72	ARG	HB3	1.797	0.05	2
B	81	LEU	HD23	1.093	0.05	2
B	67	LYS	CE	42.416	0.3	1
B	104	GLU	CA	57.23	0.3	1
A	78	ILE	CB	37.613	0.3	1
B	98	ILE	CD1	13.836	0.3	1
B	100	LEU	CB	40.633	0.3	1
B	72	ARG	CB	30.359	0.3	1
B	95	ILE	CD1	14.07	0.3	1
A	59	PRO	HG2	2.05	0.05	2
B	65	ASP	HB2	2.86	0.05	2
A	98	ILE	C	175.056	0.3	1
B	104	GLU	HA	4.312	0.05	1
A	66	THR	N	107.789	0.3	1
A	55	VAL	HB	2.16	0.05	1
B	69	VAL	HG12	0.902	0.05	2
B	59	PRO	HD3	4.204	0.05	2
A	89	THR	HG21	1.469	0.05	1
B	74	TYR	HB2	3.406	0.05	2
B	64	LYS	CG	24.87	0.3	1
A	99	ILE	HG12	1.943	0.05	2
B	72	ARG	HG3	1.718	0.05	2
B	94	TYR	CE2	119.0	0.3	3
A	99	ILE	H	8.405	0.05	1
B	66	THR	N	107.789	0.3	1
A	88	ASN	HA	4.594	0.05	1
A	68	PRO	CG	26.933	0.3	1
B	85	VAL	CB	32.467	0.3	1
A	101	ASN	H	8.34	0.05	1
A	106	GLU	CB	31.43	0.3	1
B	86	PRO	HD2	4.053	0.05	2
B	74	TYR	HE2	6.82	0.05	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	85	VAL	HG12	0.867	0.05	2
B	78	ILE	HG22	0.98	0.05	1
A	97	ARG	HD3	3.35	0.05	2
B	91	MET	C	178.508	0.3	1
B	67	LYS	HB3	1.657	0.05	2
B	99	ILE	HB	2.196	0.05	1
A	62	GLY	N	109.175	0.3	1
B	91	MET	CA	59.967	0.3	1
A	100	LEU	CB	40.633	0.3	1
A	59	PRO	HB2	2.054	0.05	2
A	84	ARG	HD2	3.209	0.05	2
A	84	ARG	H	7.763	0.05	1
B	83	SER	HA	4.383	0.05	1
B	85	VAL	HA	3.28	0.05	1
A	98	ILE	CB	37.634	0.3	1
A	63	LEU	HB3	1.647	0.05	2
B	71	VAL	HG13	0.926	0.05	2
B	88	ASN	HB3	3.12	0.05	2
B	90	SER	HB3	4.141	0.05	2
A	62	GLY	HA3	4.03	0.05	2
B	60	GLY	HA3	4.09	0.05	2
A	66	THR	CG2	20.656	0.3	1
B	54	MET	HA	4.562	0.05	1
A	87	ALA	CB	18.533	0.3	1
A	102	HIS	HA	4.544	0.05	1
B	71	VAL	HB	1.949	0.05	1
B	106	GLU	CA	58.02	0.3	1
B	92	SER	HB2	4.212	0.05	2
B	63	LEU	HD21	0.907	0.05	2
B	67	LYS	CG	24.732	0.3	1
B	97	ARG	HB3	1.98	0.05	2
B	95	ILE	CG2	18.327	0.3	1
A	88	ASN	HB2	3.005	0.05	2
B	82	LYS	HB2	1.994	0.05	2
A	79	GLU	HG2	2.457	0.05	2
B	56	GLY	HA3	4.05	0.05	2
A	90	SER	H	8.622	0.05	1
B	55	VAL	HG13	1.037	0.05	2
B	91	MET	HE2	2.233	0.05	1
A	76	ASP	N	114.907	0.3	1
B	106	GLU	HG2	2.306	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	68	PRO	CD	50.446	0.3	1
B	61	GLY	CA	45.46	0.3	1
B	59	PRO	CB	32.259	0.3	1
B	79	GLU	HA	4.056	0.05	1
B	93	ALA	HB3	1.7	0.05	1
A	68	PRO	HD2	3.747	0.05	2
B	100	LEU	HD13	0.937	0.05	2
B	54	MET	CA	55.75	0.3	1
A	63	LEU	HG	1.712	0.05	1
B	57	ARG	H	8.159	0.05	1
A	64	LYS	CB	32.929	0.3	1
A	84	ARG	CB	31.352	0.3	1
B	75	PRO	HA	4.295	0.05	1
A	69	VAL	HG13	0.902	0.05	2
A	54	MET	HE1	2.166	0.05	1
B	84	ARG	HA	4.417	0.05	1
B	58	ARG	HA	4.594	0.05	1
A	90	SER	HB3	4.141	0.05	2
A	100	LEU	HD11	0.937	0.05	2
A	94	TYR	HE1	6.798	0.05	3
B	57	ARG	CG	27.15	0.3	1
B	78	ILE	HD12	0.85	0.05	1
B	98	ILE	HD13	0.388	0.05	1
A	102	HIS	HB3	3.714	0.05	2
A	101	ASN	CA	56.083	0.3	1
B	54	MET	HE2	2.166	0.05	1
A	96	ARG	H	8.52	0.05	1
B	57	ARG	C	176.599	0.3	1
A	86	PRO	CB	32.622	0.3	1
A	85	VAL	CG1	21.79	0.3	2
A	69	VAL	HG22	0.865	0.05	2
B	95	ILE	H	8.726	0.05	1
A	90	SER	CB	65.755	0.3	1
B	74	TYR	CB	37.2	0.3	1
A	82	LYS	CG	26.135	0.3	1
B	88	ASN	HA	4.594	0.05	1
B	54	MET	C	176.534	0.3	1
A	73	LEU	HD12	1.01	0.05	2
B	81	LEU	CA	58.251	0.3	1
B	62	GLY	N	109.175	0.3	1
B	94	TYR	HE1	6.798	0.05	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	65	ASP	N	118.931	0.3	1
B	81	LEU	CD1	25.302	0.3	1
A	57	ARG	CG	27.15	0.3	1
A	60	GLY	HA3	4.09	0.05	2
A	95	ILE	HD11	0.803	0.05	1
A	74	TYR	CE1	118.3	0.3	3
A	54	MET	HG2	2.53	0.05	2
A	64	LYS	N	119.917	0.3	1
A	63	LEU	CB	42.353	0.3	1
A	64	LYS	H	8.354	0.05	1
B	88	ASN	HD22	7.685	0.05	2
A	88	ASN	C	174.797	0.3	1
A	89	THR	H	7.73	0.05	1
A	72	ARG	HD2	3.147	0.05	2
A	91	MET	N	122.4	0.3	1
B	100	LEU	HD12	0.937	0.05	2
B	75	PRO	HB3	2.05	0.05	2
B	61	GLY	N	108.964	0.3	1
A	66	THR	CA	60.358	0.3	1
B	67	LYS	HA	4.952	0.05	1
B	70	VAL	HG13	0.83	0.05	2
A	100	LEU	CA	58.596	0.3	1
B	58	ARG	HD2	3.354	0.05	2
B	60	GLY	H	8.615	0.05	1
B	68	PRO	HD3	3.861	0.05	2
A	83	SER	HB3	4.11	0.05	2
B	70	VAL	HB	1.994	0.05	1
B	63	LEU	HB3	1.647	0.05	2
A	60	GLY	C	175.353	0.3	1
A	77	GLU	CB	29.4	0.3	1
B	104	GLU	HB3	2.139	0.05	2
A	103	LEU	N	117.173	0.3	1
B	81	LEU	C	179.223	0.3	1
B	79	GLU	C	179.616	0.3	1
B	55	VAL	HG22	1.037	0.05	2
B	95	ILE	CB	37.624	0.3	1
A	67	LYS	CG	24.732	0.3	1
B	95	ILE	HD12	0.803	0.05	1
B	71	VAL	N	127.579	0.3	1
A	63	LEU	CD2	23.3	0.3	2
A	69	VAL	HB	2.054	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	86	PRO	HG2	2.11	0.05	2
B	89	THR	HG21	1.469	0.05	1
A	71	VAL	HB	1.949	0.05	1
B	83	SER	HB3	4.11	0.05	2
A	71	VAL	HG13	0.926	0.05	2
B	89	THR	CA	61.487	0.3	1
A	80	ALA	CA	55.27	0.3	1
B	63	LEU	CA	56.244	0.3	1
A	95	ILE	HG22	0.875	0.05	1
B	71	VAL	CG2	21.961	0.3	2
A	68	PRO	HB2	1.867	0.05	2
A	106	GLU	HG2	2.306	0.05	2
A	87	ALA	HB1	1.49	0.05	1
B	99	ILE	CD1	15.948	0.3	1
B	100	LEU	HB3	1.929	0.05	2
A	98	ILE	HG21	0.576	0.05	1
A	88	ASN	CB	37.83	0.3	1
B	61	GLY	H	8.382	0.05	1
B	68	PRO	HB2	1.867	0.05	2
A	70	VAL	HG23	0.99	0.05	2
B	82	LYS	N	118.43	0.3	1
A	99	ILE	HD11	0.925	0.05	1
A	58	ARG	HB2	2.007	0.05	2
B	94	TYR	HB3	3.25	0.05	2
B	72	ARG	CG	26.91	0.3	1
A	78	ILE	HB	2.071	0.05	1
B	82	LYS	HE3	3.073	0.05	2
B	78	ILE	HD11	0.85	0.05	1
B	98	ILE	HG23	0.576	0.05	1
A	103	LEU	CA	56.577	0.3	1
A	102	HIS	CA	59.101	0.3	1
B	64	LYS	CB	32.929	0.3	1
B	54	MET	HB2	2.06	0.05	2
A	98	ILE	HB	1.884	0.05	1
A	68	PRO	CB	33.036	0.3	1
A	65	ASP	H	8.187	0.05	1
B	57	ARG	HD2	3.224	0.05	2
A	59	PRO	HA	4.55	0.05	1
A	85	VAL	HG11	0.867	0.05	2
B	77	GLU	CA	58.5	0.3	1
A	99	ILE	HG21	0.993	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	92	SER	HB2	4.212	0.05	2
A	106	GLU	HB3	2.118	0.05	2
B	99	ILE	HG13	0.931	0.05	2
B	99	ILE	HD12	0.925	0.05	1
A	81	LEU	HB2	1.958	0.05	2
A	70	VAL	N	125.65	0.3	1
A	73	LEU	HB3	1.916	0.05	2
B	85	VAL	HB	1.97	0.05	1
A	82	LYS	HG2	1.519	0.05	2
A	95	ILE	CD1	14.07	0.3	1
B	57	ARG	CA	55.82	0.3	1
B	91	MET	N	122.4	0.3	1
B	96	ARG	HA	3.77	0.05	1
B	93	ALA	HA	4.289	0.05	1
B	64	LYS	HG2	1.55	0.05	2
A	66	THR	HG23	0.317	0.05	1
A	70	VAL	HG12	0.83	0.05	2
A	84	ARG	HD3	3.301	0.05	2
B	79	GLU	HG2	2.457	0.05	2
B	73	LEU	N	122.019	0.3	1
A	97	ARG	CA	59.609	0.3	1
B	95	ILE	HD13	0.803	0.05	1
A	84	ARG	HB3	2.285	0.05	2
A	78	ILE	HD13	0.85	0.05	1
B	76	ASP	CB	39.34	0.3	1
B	98	ILE	HG12	1.156	0.05	2
B	58	ARG	CB	29.728	0.3	1
B	58	ARG	HB2	2.007	0.05	2
A	105	ASP	C	175.828	0.3	1
B	59	PRO	HB3	2.408	0.05	2
B	74	TYR	CD1	133.4	0.3	3
B	67	LYS	HD2	1.78	0.05	2
A	84	ARG	HA	4.417	0.05	1
A	100	LEU	H	8.935	0.05	1
A	99	ILE	CG2	17.66	0.3	1
B	73	LEU	HD13	1.01	0.05	2
A	54	MET	CE	17.265	0.3	1
B	103	LEU	HD21	1.0	0.05	2
B	64	LYS	H	8.354	0.05	1
B	87	ALA	HB1	1.49	0.05	1
A	104	GLU	HG2	2.396	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	71	VAL	HG22	0.985	0.05	2
B	70	VAL	C	175.975	0.3	1
A	60	GLY	H	8.615	0.05	1
A	91	MET	HE1	2.233	0.05	1
B	100	LEU	HA	4.054	0.05	1
B	69	VAL	H	9.112	0.05	1
A	101	ASN	ND2	111.0	0.3	1
A	71	VAL	C	174.24	0.3	1
B	105	ASP	C	175.828	0.3	1
B	75	PRO	HG2	2.527	0.05	2
A	87	ALA	C	179.218	0.3	1
A	102	HIS	N	119.315	0.3	1
A	104	GLU	HB2	2.204	0.05	2
B	98	ILE	HD12	0.388	0.05	1
A	104	GLU	CA	57.23	0.3	1
B	78	ILE	HA	3.605	0.05	1
A	85	VAL	CB	32.467	0.3	1
A	89	THR	CG2	20.573	0.3	1
B	54	MET	CB	33.026	0.3	1
A	73	LEU	CD2	26.138	0.3	2
A	85	VAL	HB	1.97	0.05	1
A	84	ARG	CG	27.2	0.3	1
A	79	GLU	N	118.181	0.3	1
B	100	LEU	HD22	0.948	0.05	2
A	81	LEU	HG	1.771	0.05	1
A	86	PRO	HB2	2.488	0.05	2
A	95	ILE	CG1	29.985	0.3	1
A	76	ASP	HB2	2.86	0.05	2
B	78	ILE	CG2	17.32	0.3	1
A	58	ARG	CG	26.489	0.3	1
A	58	ARG	HB3	2.081	0.05	2
B	85	VAL	HG22	0.812	0.05	2
A	103	LEU	CB	42.06	0.3	1
B	98	ILE	C	175.056	0.3	1
A	56	GLY	H	8.55	0.05	1
B	70	VAL	HG22	0.99	0.05	2
A	57	ARG	H	8.159	0.05	1
B	91	MET	CE	16.866	0.3	1
A	86	PRO	CD	51.69	0.3	1
B	81	LEU	HB2	1.958	0.05	2
B	80	ALA	HB3	1.656	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	105	ASP	CB	41.57	0.3	1
B	103	LEU	HD22	1.0	0.05	2
A	99	ILE	CG1	29.426	0.3	1
B	98	ILE	HB	1.884	0.05	1
B	54	MET	HE1	2.166	0.05	1
A	55	VAL	HG22	1.037	0.05	2
A	86	PRO	CA	62.841	0.3	1
B	105	ASP	CA	54.871	0.3	1
B	73	LEU	CA	52.96	0.3	1
A	97	ARG	N	118.718	0.3	1
A	74	TYR	CD1	133.4	0.3	3
B	66	THR	CG2	20.656	0.3	1
A	96	ARG	HG3	1.716	0.05	2
B	94	TYR	HE2	6.798	0.05	3
A	88	ASN	N	114.379	0.3	1
A	63	LEU	HD22	0.907	0.05	2
B	72	ARG	HA	4.703	0.05	1
A	91	MET	HB3	2.589	0.05	2
B	95	ILE	HG22	0.875	0.05	1
A	71	VAL	HG12	0.926	0.05	2
A	74	TYR	CD2	133.4	0.3	3
A	74	TYR	CE2	118.3	0.3	3
B	66	THR	HA	4.256	0.05	1
B	86	PRO	CG	27.506	0.3	1
A	63	LEU	CA	56.244	0.3	1
B	105	ASP	HB2	2.77	0.05	2
B	74	TYR	CE1	118.3	0.3	3
A	70	VAL	HA	4.496	0.05	1
A	82	LYS	H	8.895	0.05	1
B	100	LEU	HD11	0.937	0.05	2
B	74	TYR	N	120.637	0.3	1
B	80	ALA	HA	4.26	0.05	1
A	82	LYS	HD3	1.745	0.05	2
A	71	VAL	HG23	0.985	0.05	2
B	88	ASN	N	114.379	0.3	1
A	79	GLU	HA	4.056	0.05	1
A	95	ILE	H	8.726	0.05	1
B	98	ILE	CG2	17.699	0.3	1
A	105	ASP	CA	54.871	0.3	1
A	91	MET	HA	4.235	0.05	1
B	73	LEU	HD22	0.845	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	80	ALA	N	121.839	0.3	1
A	69	VAL	N	124.67	0.3	1
A	85	VAL	CG2	22.01	0.3	2
A	75	PRO	HB3	2.05	0.05	2
B	97	ARG	HD3	3.35	0.05	2
B	63	LEU	HG	1.712	0.05	1
A	64	LYS	HB2	1.93	0.05	2
B	76	ASP	HA	4.5	0.05	1
B	95	ILE	HG12	2.227	0.05	2
A	103	LEU	HD11	0.89	0.05	2
B	95	ILE	CA	66.02	0.3	1
A	67	LYS	CB	34.372	0.3	1
B	84	ARG	N	119.557	0.3	1
B	95	ILE	HD11	0.803	0.05	1
A	69	VAL	HA	4.29	0.05	1
A	94	TYR	HD1	6.99	0.05	3
B	71	VAL	HA	4.48	0.05	1
B	77	GLU	HG2	2.42	0.05	2
B	84	ARG	HB2	1.925	0.05	2
A	81	LEU	HD23	1.093	0.05	2
B	92	SER	CB	63.51	0.3	1
B	73	LEU	HB2	1.629	0.05	2
A	103	LEU	HB2	1.617	0.05	2
A	80	ALA	CB	18.527	0.3	1
B	104	GLU	HG2	2.396	0.05	2
A	75	PRO	HD3	3.945	0.05	2
B	63	LEU	HD11	0.98	0.05	2
A	63	LEU	HD12	0.98	0.05	2
A	88	ASN	HD22	7.685	0.05	2
A	67	LYS	HB2	1.909	0.05	2
B	55	VAL	CA	62.709	0.3	1
B	100	LEU	CA	58.596	0.3	1
A	95	ILE	CB	37.624	0.3	1
B	96	ARG	HB3	2.11	0.05	2
A	93	ALA	CA	55.24	0.3	1
A	71	VAL	N	127.579	0.3	1
B	86	PRO	HB2	2.488	0.05	2
A	99	ILE	CA	66.129	0.3	1
B	96	ARG	CD	43.059	0.3	1
B	72	ARG	CD	43.5	0.3	1
A	104	GLU	HA	4.312	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	95	ILE	HB	1.95	0.05	1
B	92	SER	C	177.583	0.3	1
A	96	ARG	CA	60.97	0.3	1
B	97	ARG	CD	43.787	0.3	1
B	59	PRO	HG2	2.05	0.05	2
A	55	VAL	HG13	1.037	0.05	2
A	59	PRO	HD2	4.33	0.05	2
A	66	THR	CB	72.453	0.3	1
A	93	ALA	HB1	1.7	0.05	1
A	66	THR	HB	3.681	0.05	1
B	64	LYS	CA	57.22	0.3	1
A	80	ALA	HB1	1.656	0.05	1
A	67	LYS	H	9.064	0.05	1
A	68	PRO	CA	62.351	0.3	1
B	72	ARG	HD2	3.147	0.05	2
B	64	LYS	HD3	1.778	0.05	2
B	85	VAL	N	121.674	0.3	1
A	87	ALA	CA	53.93	0.3	1
A	82	LYS	N	118.43	0.3	1
A	57	ARG	HD3	3.224	0.05	2
A	95	ILE	HG13	0.808	0.05	2
A	65	ASP	HB2	2.86	0.05	2
A	59	PRO	C	178.098	0.3	1
B	82	LYS	HG2	1.519	0.05	2
A	78	ILE	C	178.317	0.3	1
B	77	GLU	HB3	1.84	0.05	2
B	89	THR	HB	4.121	0.05	1
B	84	ARG	CA	55.41	0.3	1
B	99	ILE	HD11	0.925	0.05	1
A	63	LEU	N	121.467	0.3	1
A	70	VAL	CA	62.616	0.3	1
B	58	ARG	CG	26.489	0.3	1
A	59	PRO	CG	27.751	0.3	1
B	74	TYR	CD2	133.4	0.3	3
B	99	ILE	HG23	0.993	0.05	1
A	61	GLY	HA3	4.13	0.05	2
A	71	VAL	CG2	21.961	0.3	2
B	85	VAL	HG13	0.867	0.05	2
B	61	GLY	HA2	4.07	0.05	2
A	64	LYS	HD3	1.778	0.05	2
A	79	GLU	H	8.07	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	72	ARG	HG2	1.718	0.05	2
A	97	ARG	CB	29.76	0.3	1
A	77	GLU	C	176.638	0.3	1
A	65	ASP	CB	41.82	0.3	1
A	100	LEU	CD2	21.56	0.3	2
A	68	PRO	C	177.155	0.3	1
A	105	ASP	HB3	2.88	0.05	2
A	78	ILE	HA	3.605	0.05	1
A	66	THR	H	7.615	0.05	1
A	75	PRO	HG2	2.527	0.05	2
B	73	LEU	CD2	26.138	0.3	2
B	70	VAL	CB	32.841	0.3	1
B	87	ALA	HB2	1.49	0.05	1
A	96	ARG	CD	43.059	0.3	1
A	80	ALA	HB2	1.656	0.05	1
A	99	ILE	N	122.0	0.3	1
B	65	ASP	HB3	3.01	0.05	2
A	105	ASP	HA	4.658	0.05	1
B	96	ARG	C	177.081	0.3	1
A	57	ARG	HB2	1.9	0.05	2
B	69	VAL	HG13	0.902	0.05	2
A	101	ASN	HB3	2.95	0.05	2
B	103	LEU	HB2	1.617	0.05	2
A	98	ILE	HG12	1.156	0.05	2
A	76	ASP	C	179.364	0.3	1
B	54	MET	CG	32.138	0.3	1
A	73	LEU	CD1	23.286	0.3	2
A	56	GLY	N	112.524	0.3	1
A	70	VAL	CG2	21.976	0.3	2
A	62	GLY	H	8.533	0.05	1
B	80	ALA	CB	18.527	0.3	1
B	72	ARG	HG2	1.718	0.05	2
A	54	MET	C	176.534	0.3	1
A	64	LYS	CD	29.35	0.3	1
A	100	LEU	HD23	0.948	0.05	2
B	97	ARG	HG2	1.762	0.05	2
B	85	VAL	CA	61.133	0.3	1
B	83	SER	CA	60.922	0.3	1
B	86	PRO	HD3	3.346	0.05	2
A	95	ILE	HG12	2.227	0.05	2
A	72	ARG	HA	4.703	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	95	ILE	CG2	18.327	0.3	1
A	67	LYS	HA	4.952	0.05	1
A	58	ARG	CB	29.728	0.3	1
B	85	VAL	HG21	0.812	0.05	2
B	70	VAL	HG21	0.99	0.05	2
B	92	SER	H	8.626	0.05	1
B	60	GLY	N	109.847	0.3	1
B	77	GLU	H	7.515	0.05	1
B	98	ILE	HA	3.612	0.05	1
B	71	VAL	HG12	0.926	0.05	2
B	88	ASN	HB2	3.005	0.05	2
B	70	VAL	H	8.338	0.05	1
A	56	GLY	HA2	4.051	0.05	2
A	62	GLY	HA2	4.03	0.05	2
B	92	SER	N	112.404	0.3	1
B	78	ILE	HG13	0.859	0.05	2
A	81	LEU	H	8.39	0.05	1
B	69	VAL	CA	61.845	0.3	1
B	73	LEU	HD23	0.845	0.05	2
B	67	LYS	CD	29.114	0.3	1
B	97	ARG	HB2	2.06	0.05	2
B	95	ILE	CG1	29.985	0.3	1
A	97	ARG	HB3	1.98	0.05	2
B	82	LYS	CE	42.05	0.3	1
A	95	ILE	N	118.174	0.3	1
B	84	ARG	H	7.763	0.05	1
B	56	GLY	HA2	4.051	0.05	2
B	78	ILE	CA	66.024	0.3	1
A	106	GLU	CA	58.02	0.3	1
B	86	PRO	CD	51.69	0.3	1
B	55	VAL	HG12	1.037	0.05	2
B	91	MET	HE3	2.233	0.05	1
A	74	TYR	HE2	6.82	0.05	3
A	55	VAL	N	121.358	0.3	1
B	106	GLU	HG3	2.306	0.05	2
A	64	LYS	CG	24.87	0.3	1
A	58	ARG	H	8.522	0.05	1
A	56	GLY	CA	45.39	0.3	1
A	74	TYR	CA	58.93	0.3	1
A	74	TYR	HD1	7.432	0.05	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	208	-0.52 ± 0.25	Should be applied
$^{13}C_{\beta}$	196	0.15 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	140	-0.64 ± 0.11	Should be applied
^{15}N	192	0.04 ± 0.22	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 928 atoms were assigned a chemical shift out of a possible 1092. 2 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	378/408 (93%)	158/162 (98%)	142/168 (85%)	78/78 (100%)
Sidechain	514/636 (81%)	316/372 (85%)	194/231 (84%)	4/33 (12%)
Aromatic	36/48 (75%)	18/24 (75%)	18/20 (90%)	0/4 (0%)
Overall	928/1092 (85%)	492/558 (88%)	354/419 (84%)	82/115 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1132 atoms were assigned a chemical shift out of a possible 1354. 2 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	468/514 (91%)	198/204 (97%)	174/212 (82%)	96/98 (98%)
Sidechain	628/792 (79%)	386/466 (83%)	238/280 (85%)	4/46 (9%)
Aromatic	36/48 (75%)	18/24 (75%)	18/20 (90%)	0/4 (0%)
Overall	1132/1354 (84%)	602/694 (87%)	430/512 (84%)	100/148 (68%)

7.1.4 Statistically unusual chemical shifts (i)

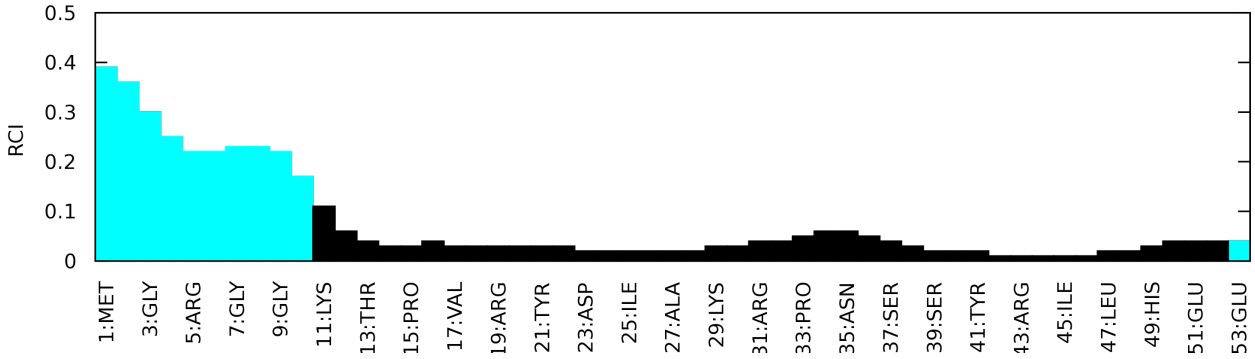
There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The images below report *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:



Random coil index (RCI) for chain B: