



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:29 pm GMT

PDB ID : 1PZQ
Title : Structure of fused docking domains from the erythromycin polyketide synthase (DEBS), a model for the interaction between DEBS 2 and DEBS 3: The A domain
Authors : Broadhurst, R.W.; Nietlispach, D.; Wheatcroft, M.P.; Leadlay, P.F.; Weissman, K.J.
Deposited on : 2003-07-14

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

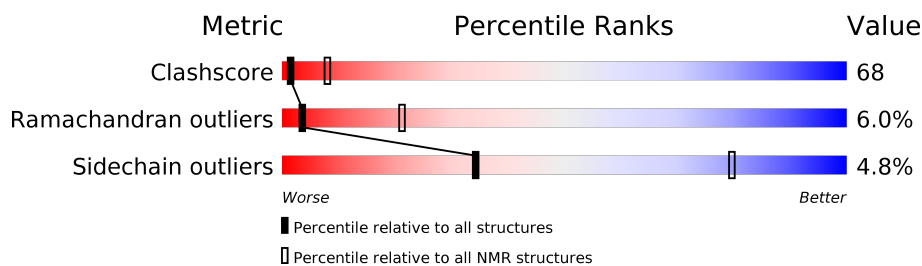
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	60	
1	B	60	

2 Ensemble composition and analysis

This entry contains 8 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:7-A:49, B:7-B:49 (86)	0.14	7

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1758 atoms, of which 856 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Erythronolide synthase.

Mol	Chain	Residues	Atoms					Trace
1	A	60	Total	C	H	N	O	0
			879	267	428	84	100	
1	B	60	Total	C	H	N	O	0
			879	267	428	84	100	

There are 4 discrepancies between the modelled and reference sequences:

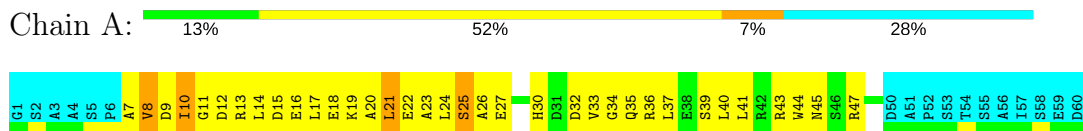
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q03132
A	2	SER	-	CLONING ARTIFACT	UNP Q03132
B	1	GLY	-	CLONING ARTIFACT	UNP Q03132
B	2	SER	-	CLONING ARTIFACT	UNP Q03132

4 Residue-property plots

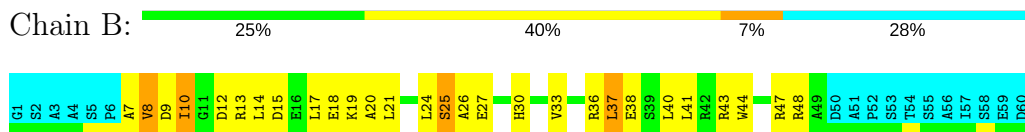
4.1 Average score per residue in the NMR ensemble

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: Erythronolide synthase



- Molecule 1: Erythronolide synthase

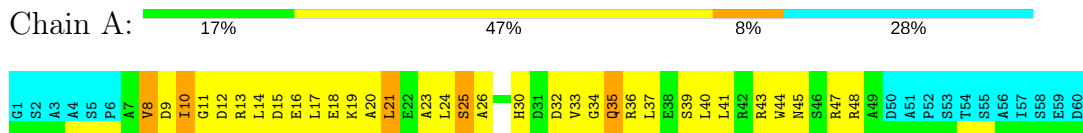


4.2 Scores per residue for each member of the ensemble

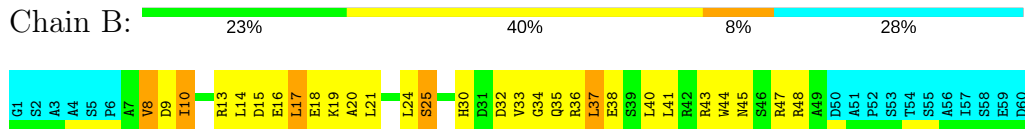
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Erythronolide synthase

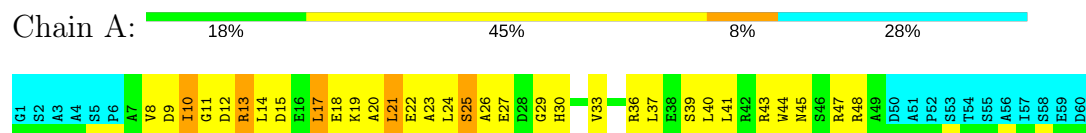


- Molecule 1: Erythronolide synthase

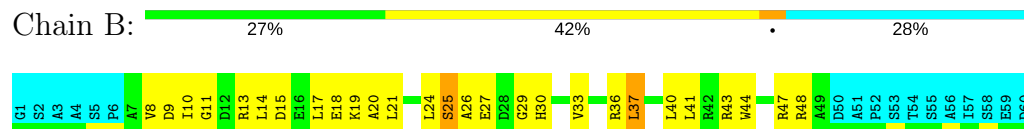


4.2.2 Score per residue for model 2

- Molecule 1: Erythronolide synthase

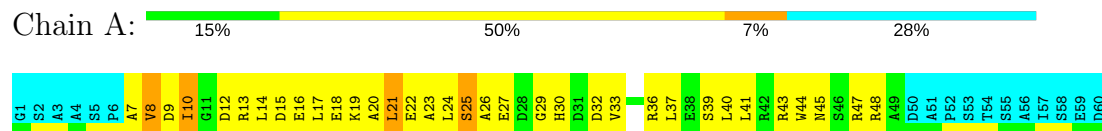


- Molecule 1: Erythronolide synthase

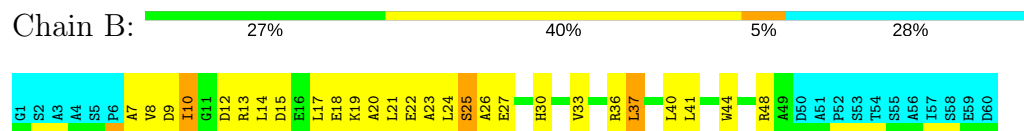


4.2.3 Score per residue for model 3

- Molecule 1: Erythronolide synthase

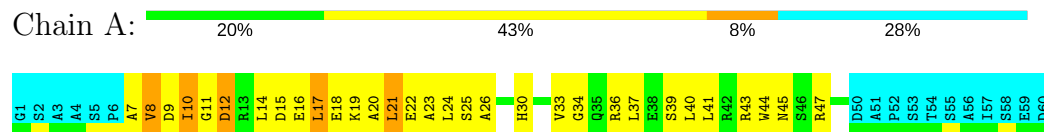


- Molecule 1: Erythronolide synthase

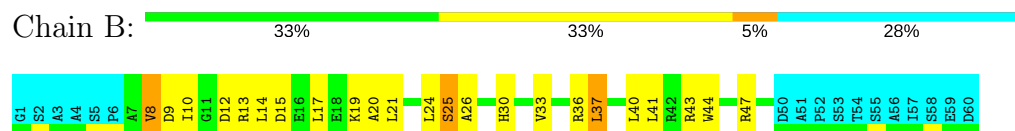


4.2.4 Score per residue for model 4

- Molecule 1: Erythronolide synthase

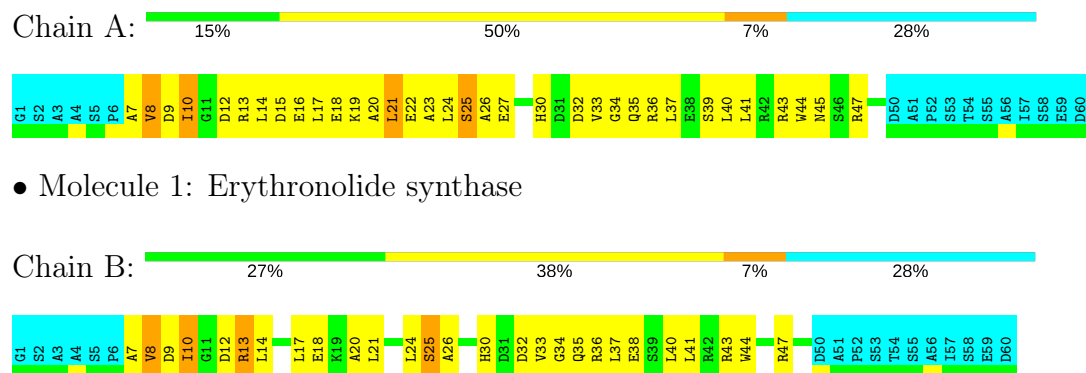


- Molecule 1: Erythronolide synthase



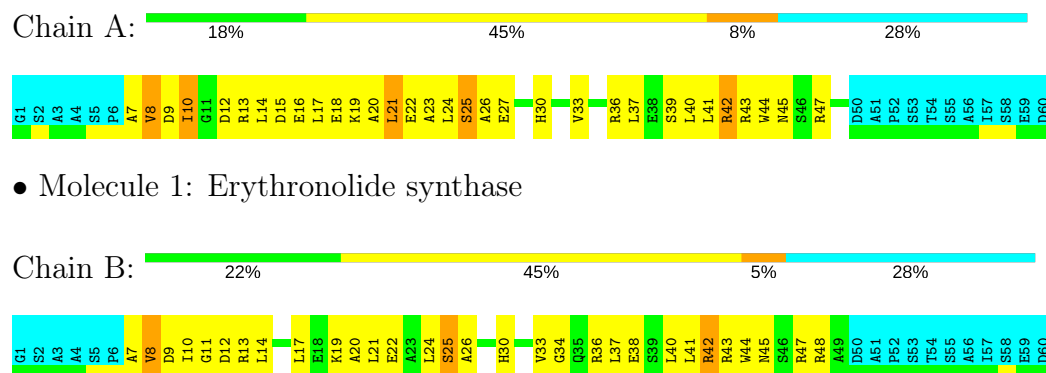
4.2.5 Score per residue for model 5

- Molecule 1: Erythronolide synthase



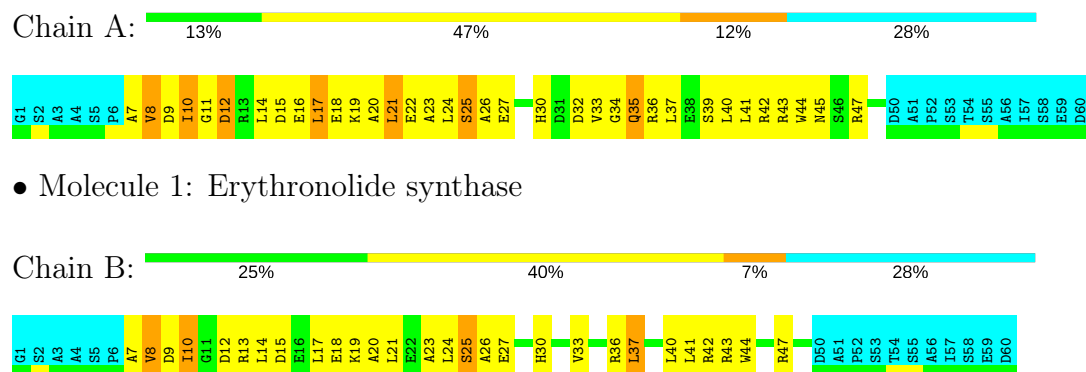
4.2.6 Score per residue for model 6

- Molecule 1: Erythronolide synthase



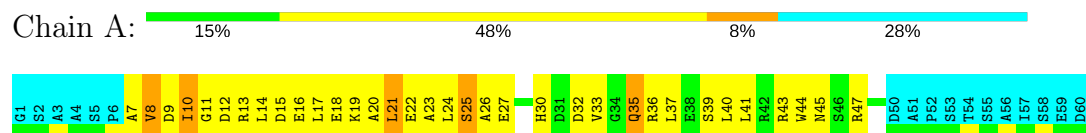
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Erythronolide synthase

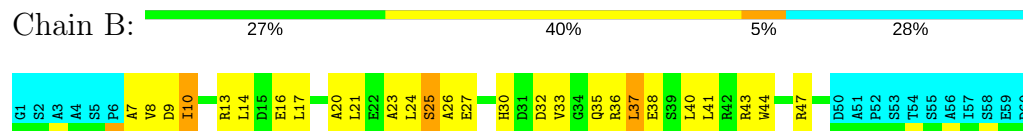


4.2.8 Score per residue for model 8

- Molecule 1: Erythronolide synthase



- Molecule 1: Erythronolide synthase



5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 8 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
CNS	structure solution	1.0
CNS	refinement	1.0

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 5885
Number of chemical shift lists	1
Total number of shifts	2358
Number of shifts mapped to atoms	1136
Number of unparsed shifts	0
Number of shifts with mapping errors	1222
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	342	332	331	75±5
1	B	342	332	331	59±5
All	All	5472	5312	5296	735

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 68.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD11	1:A:33:VAL:HG11	0.93	1.40	5	8
1:A:18:GLU:HB2	1:B:40:LEU:HD22	0.91	1.43	1	2
1:A:17:LEU:HD21	1:B:14:LEU:HD13	0.85	1.46	2	1
1:A:24:LEU:HD13	1:B:10:ILE:HD13	0.84	1.49	3	5
1:A:10:ILE:HG21	1:B:33:VAL:HG22	0.84	1.47	1	8
1:A:41:LEU:HD22	1:A:45:ASN:ND2	0.79	1.92	1	8
1:A:40:LEU:HD13	1:B:17:LEU:HD23	0.79	1.52	2	2
1:B:9:ASP:O	1:B:10:ILE:HG22	0.78	1.79	8	8
1:B:10:ILE:O	1:B:14:LEU:HD23	0.75	1.81	4	2
1:A:14:LEU:HG	1:B:17:LEU:HD11	0.75	1.57	8	7
1:A:15:ASP:O	1:A:19:LYS:HG3	0.72	1.85	3	1
1:A:44:TRP:CZ2	1:B:33:VAL:HB	0.71	2.20	1	8
1:A:13:ARG:NH1	1:B:20:ALA:HB2	0.71	2.00	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ARG:HD3	1:B:25:SER:HB2	0.71	1.61	3	7
1:A:8:VAL:HG13	1:A:12:ASP:HB3	0.71	1.61	6	3
1:A:21:LEU:CD1	1:A:33:VAL:HG11	0.70	2.16	7	8
1:A:17:LEU:HA	1:B:13:ARG:HE	0.70	1.46	2	1
1:A:33:VAL:HG22	1:B:10:ILE:HG21	0.69	1.62	5	8
1:B:10:ILE:HA	1:B:13:ARG:NH1	0.69	2.02	2	1
1:A:13:ARG:HH11	1:B:20:ALA:HB2	0.69	1.47	8	1
1:A:40:LEU:HD11	1:B:14:LEU:HD12	0.69	1.64	2	1
1:A:37:LEU:HA	1:A:40:LEU:HD12	0.69	1.64	2	2
1:A:14:LEU:HD23	1:B:40:LEU:HD11	0.68	1.63	2	5
1:A:24:LEU:HD23	1:B:10:ILE:HD13	0.68	1.65	4	3
1:A:33:VAL:HG13	1:B:14:LEU:HD11	0.68	1.65	8	1
1:A:17:LEU:HD23	1:B:40:LEU:HD13	0.68	1.64	8	1
1:A:17:LEU:HD11	1:B:14:LEU:HG	0.67	1.65	8	3
1:A:8:VAL:HG13	1:A:12:ASP:HB2	0.66	1.66	7	3
1:A:10:ILE:HD12	1:A:13:ARG:HG3	0.66	1.67	3	3
1:A:10:ILE:O	1:A:13:ARG:NH1	0.65	2.29	2	1
1:A:36:ARG:O	1:A:40:LEU:HG	0.65	1.91	1	8
1:A:17:LEU:HD21	1:B:14:LEU:HD22	0.64	1.67	4	1
1:A:17:LEU:HD13	1:B:13:ARG:HB2	0.64	1.69	1	1
1:A:41:LEU:HD22	1:A:45:ASN:HD21	0.63	1.52	1	8
1:A:13:ARG:NH2	1:B:17:LEU:HG	0.63	2.08	2	1
1:A:21:LEU:HD12	1:B:44:TRP:CZ3	0.62	2.29	4	8
1:B:36:ARG:O	1:B:40:LEU:HG	0.62	1.94	1	7
1:A:32:ASP:O	1:A:35:GLN:HG2	0.62	1.94	5	3
1:A:36:ARG:CB	1:B:14:LEU:HG	0.62	2.25	2	2
1:A:36:ARG:HB2	1:B:14:LEU:HD13	0.61	1.72	7	5
1:A:20:ALA:HB2	1:B:13:ARG:HH11	0.61	1.55	8	1
1:A:37:LEU:HG	1:B:14:LEU:HD21	0.61	1.72	3	4
1:A:41:LEU:HG	1:B:37:LEU:HG	0.61	1.71	6	2
1:B:21:LEU:O	1:B:25:SER:N	0.59	2.35	2	8
1:A:39:SER:O	1:A:43:ARG:HG2	0.59	1.97	3	8
1:A:40:LEU:CD2	1:B:18:GLU:HB2	0.59	2.27	1	5
1:A:8:VAL:O	1:A:12:ASP:HB2	0.59	1.98	2	3
1:B:8:VAL:HG13	1:B:12:ASP:HB3	0.59	1.73	3	3
1:A:13:ARG:HB2	1:A:13:ARG:NH1	0.58	2.13	2	1
1:A:13:ARG:HB2	1:A:13:ARG:CZ	0.58	2.27	2	1
1:B:24:LEU:HD22	1:B:24:LEU:N	0.57	2.14	5	2
1:B:32:ASP:O	1:B:35:GLN:HG2	0.57	1.98	1	3
1:A:40:LEU:HB3	1:B:37:LEU:HD21	0.57	1.75	6	2
1:A:17:LEU:HD22	1:B:13:ARG:NH2	0.57	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:LEU:O	1:B:26:ALA:N	0.57	2.37	6	7
1:A:17:LEU:HD22	1:B:13:ARG:CZ	0.57	2.29	2	1
1:A:17:LEU:CD2	1:B:17:LEU:HD12	0.57	2.29	1	1
1:A:42:ARG:HD3	1:A:42:ARG:O	0.57	1.99	7	1
1:A:21:LEU:HD13	1:B:10:ILE:HD11	0.56	1.75	2	8
1:B:24:LEU:N	1:B:24:LEU:HD22	0.56	2.15	6	1
1:B:21:LEU:HD22	1:B:33:VAL:HG11	0.56	1.76	7	6
1:A:24:LEU:CD2	1:B:10:ILE:HD13	0.56	2.31	4	3
1:B:8:VAL:HG13	1:B:12:ASP:HB2	0.56	1.76	7	1
1:A:41:LEU:HA	1:A:44:TRP:HB3	0.56	1.78	4	8
1:B:10:ILE:HA	1:B:13:ARG:HH12	0.56	1.59	2	1
1:A:33:VAL:HG22	1:B:10:ILE:CG2	0.56	2.30	5	7
1:A:40:LEU:HB3	1:B:37:LEU:HD11	0.56	1.76	7	6
1:A:41:LEU:O	1:A:44:TRP:N	0.55	2.40	1	8
1:A:29:GLY:HA2	1:B:48:ARG:HH22	0.55	1.61	3	2
1:A:24:LEU:HD22	1:B:10:ILE:HB	0.55	1.78	6	4
1:A:15:ASP:O	1:A:19:LYS:HG2	0.55	2.02	2	7
1:A:17:LEU:HD21	1:B:14:LEU:HD23	0.55	1.79	8	2
1:A:24:LEU:O	1:A:26:ALA:N	0.54	2.40	1	8
1:A:9:ASP:O	1:A:10:ILE:HG22	0.54	2.02	3	5
1:A:13:ARG:HE	1:B:17:LEU:HA	0.54	1.61	2	1
1:A:17:LEU:HD13	1:B:13:ARG:NH2	0.54	2.18	2	1
1:B:24:LEU:HB3	1:B:30:HIS:CD2	0.54	2.38	7	5
1:A:9:ASP:O	1:A:11:GLY:N	0.54	2.39	2	5
1:B:8:VAL:HG13	1:B:8:VAL:O	0.54	2.02	5	6
1:A:37:LEU:HB3	1:B:41:LEU:HD13	0.54	1.79	1	2
1:A:14:LEU:HG	1:B:17:LEU:HD21	0.54	1.79	1	1
1:A:17:LEU:HD12	1:B:17:LEU:HD23	0.54	1.79	3	1
1:A:10:ILE:CG2	1:A:11:GLY:N	0.54	2.71	2	5
1:A:13:ARG:CB	1:B:17:LEU:HD13	0.54	2.33	3	1
1:A:37:LEU:CB	1:B:41:LEU:HD13	0.53	2.34	3	2
1:A:36:ARG:HB3	1:B:14:LEU:HG	0.53	1.80	2	1
1:A:30:HIS:HB3	1:A:33:VAL:HG23	0.53	1.81	8	8
1:A:11:GLY:HA3	1:B:36:ARG:NH1	0.53	2.19	2	1
1:A:14:LEU:HG	1:B:17:LEU:CD1	0.53	2.31	8	3
1:A:17:LEU:HD22	1:B:13:ARG:HB3	0.53	1.80	4	1
1:B:11:GLY:HA2	1:B:14:LEU:HD23	0.53	1.81	2	1
1:A:12:ASP:O	1:A:16:GLU:HG3	0.52	2.04	5	7
1:B:15:ASP:O	1:B:19:LYS:HD3	0.52	2.04	2	1
1:A:17:LEU:HD11	1:B:14:LEU:CD2	0.52	2.34	6	1
1:B:8:VAL:O	1:B:8:VAL:HG13	0.52	2.04	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LEU:HD13	1:B:13:ARG:HH21	0.52	1.63	2	1
1:A:13:ARG:HB2	1:B:17:LEU:HD13	0.52	1.80	3	1
1:A:23:ALA:O	1:A:27:GLU:HG3	0.52	2.05	6	5
1:A:17:LEU:HD22	1:B:13:ARG:CB	0.52	2.34	4	2
1:A:17:LEU:CD1	1:B:17:LEU:HD23	0.52	2.35	3	1
1:B:10:ILE:O	1:B:14:LEU:HD22	0.52	2.03	2	1
1:A:17:LEU:CD1	1:B:14:LEU:HD22	0.52	2.35	6	1
1:A:24:LEU:N	1:A:24:LEU:HD22	0.51	2.21	8	3
1:B:43:ARG:HB3	1:B:47:ARG:NH1	0.51	2.20	6	2
1:A:13:ARG:HB3	1:B:17:LEU:HG	0.51	1.81	1	1
1:A:10:ILE:HD11	1:B:21:LEU:HD23	0.51	1.81	7	5
1:A:37:LEU:HB3	1:B:41:LEU:CG	0.51	2.35	2	6
1:A:21:LEU:CD1	1:B:44:TRP:CZ3	0.51	2.94	7	8
1:A:10:ILE:HG13	1:A:13:ARG:NH1	0.51	2.21	2	1
1:A:18:GLU:O	1:A:22:GLU:HG3	0.51	2.05	2	7
1:A:37:LEU:HG	1:B:14:LEU:HD11	0.51	1.82	6	2
1:A:42:ARG:O	1:A:42:ARG:HD3	0.51	2.05	6	1
1:B:43:ARG:HB3	1:B:47:ARG:HH12	0.51	1.64	6	1
1:A:40:LEU:HD11	1:B:14:LEU:HD13	0.51	1.81	4	1
1:A:16:GLU:HB3	1:B:13:ARG:NH1	0.50	2.21	5	4
1:B:33:VAL:O	1:B:37:LEU:HB2	0.50	2.05	8	3
1:A:41:LEU:O	1:A:45:ASN:N	0.50	2.44	6	7
1:A:41:LEU:HG	1:B:37:LEU:HD22	0.50	1.83	1	5
1:B:24:LEU:HG	1:B:30:HIS:CD2	0.50	2.41	2	2
1:A:35:GLN:HG2	1:A:36:ARG:NH1	0.50	2.22	7	1
1:A:18:GLU:HB2	1:B:40:LEU:CD2	0.50	2.34	3	6
1:A:17:LEU:HD11	1:B:14:LEU:HD22	0.50	1.82	6	1
1:B:41:LEU:HA	1:B:44:TRP:HB3	0.50	1.83	8	6
1:B:45:ASN:HA	1:B:48:ARG:HD3	0.50	1.83	1	2
1:A:8:VAL:O	1:A:12:ASP:HB3	0.50	2.07	1	1
1:A:20:ALA:HA	1:B:7:ALA:H	0.50	1.67	3	1
1:A:45:ASN:HA	1:A:48:ARG:HD3	0.49	1.82	1	1
1:A:10:ILE:HD11	1:B:21:LEU:HD12	0.49	1.84	1	1
1:A:30:HIS:HB3	1:A:33:VAL:CG2	0.49	2.37	4	8
1:B:36:ARG:O	1:B:40:LEU:HD13	0.49	2.08	5	1
1:A:24:LEU:HD12	1:A:30:HIS:NE2	0.49	2.22	4	1
1:A:20:ALA:O	1:A:23:ALA:HB3	0.49	2.07	2	8
1:A:20:ALA:HB3	1:B:13:ARG:CZ	0.49	2.38	2	1
1:A:40:LEU:HD21	1:B:18:GLU:HB2	0.49	1.83	5	2
1:B:8:VAL:O	1:B:9:ASP:HB3	0.49	2.08	5	2
1:A:20:ALA:CB	1:B:13:ARG:CZ	0.48	2.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HB3	1:B:41:LEU:HG	0.48	1.86	2	6
1:A:44:TRP:CE3	1:B:21:LEU:HD23	0.48	2.43	1	1
1:B:20:ALA:O	1:B:24:LEU:HD12	0.48	2.08	8	1
1:A:11:GLY:O	1:A:15:ASP:HB2	0.48	2.08	8	4
1:B:10:ILE:CG2	1:B:11:GLY:N	0.48	2.76	2	2
1:A:10:ILE:O	1:A:14:LEU:HD12	0.48	2.08	8	2
1:A:9:ASP:HB2	1:A:12:ASP:OD1	0.48	2.09	7	2
1:A:36:ARG:HB2	1:B:14:LEU:HG	0.47	1.86	6	2
1:A:26:ALA:HB2	1:B:48:ARG:HA	0.47	1.86	2	1
1:A:7:ALA:CB	1:B:24:LEU:HD11	0.47	2.39	8	2
1:A:32:ASP:O	1:A:36:ARG:HG2	0.47	2.09	1	5
1:B:8:VAL:O	1:B:9:ASP:HB2	0.47	2.09	7	5
1:B:8:VAL:CG1	1:B:13:ARG:HG3	0.47	2.39	8	2
1:A:41:LEU:HD11	1:B:38:GLU:CA	0.47	2.40	1	4
1:A:41:LEU:HG	1:B:37:LEU:HB3	0.47	1.87	3	1
1:A:21:LEU:HD21	1:A:33:VAL:CG1	0.47	2.39	2	2
1:A:40:LEU:HB2	1:B:37:LEU:HD21	0.47	1.87	4	3
1:A:24:LEU:HD12	1:A:30:HIS:CD2	0.47	2.45	4	2
1:A:36:ARG:CB	1:B:14:LEU:HD13	0.47	2.40	3	3
1:B:10:ILE:O	1:B:13:ARG:NH1	0.47	2.48	2	1
1:A:44:TRP:CE2	1:B:33:VAL:HB	0.46	2.45	5	8
1:A:23:ALA:CB	1:B:7:ALA:HB2	0.46	2.39	6	3
1:A:7:ALA:CB	1:B:24:LEU:HD21	0.46	2.40	5	2
1:B:13:ARG:HB2	1:B:13:ARG:CZ	0.46	2.39	2	1
1:A:37:LEU:O	1:A:40:LEU:HB2	0.46	2.10	6	5
1:A:17:LEU:HD11	1:B:14:LEU:HD23	0.46	1.88	3	1
1:B:34:GLY:O	1:B:38:GLU:HB2	0.46	2.10	6	2
1:B:15:ASP:O	1:B:19:LYS:HG3	0.46	2.10	3	1
1:A:24:LEU:N	1:A:24:LEU:CD2	0.46	2.79	7	2
1:A:21:LEU:HG	1:B:44:TRP:CE3	0.46	2.46	4	8
1:B:42:ARG:HD3	1:B:42:ARG:O	0.46	2.10	7	2
1:A:44:TRP:HZ2	1:B:30:HIS:O	0.46	1.93	8	7
1:B:43:ARG:O	1:B:47:ARG:HG3	0.46	2.11	7	5
1:A:13:ARG:CB	1:A:13:ARG:CZ	0.46	2.93	2	1
1:A:35:GLN:HG2	1:A:36:ARG:HH11	0.46	1.70	7	1
1:A:8:VAL:O	1:A:8:VAL:HG12	0.46	2.11	2	1
1:A:17:LEU:HD12	1:B:17:LEU:CD2	0.46	2.41	3	1
1:A:8:VAL:O	1:A:9:ASP:HB2	0.46	2.10	6	5
1:A:24:LEU:HG	1:B:10:ILE:HB	0.46	1.88	8	3
1:A:17:LEU:CD2	1:B:14:LEU:HD22	0.46	2.38	4	1
1:A:24:LEU:HD21	1:B:7:ALA:HA	0.45	1.86	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HG	1:B:37:LEU:HD13	0.45	1.88	3	6
1:A:37:LEU:HD12	1:B:44:TRP:CD1	0.45	2.46	3	8
1:A:18:GLU:HB2	1:B:40:LEU:HD23	0.45	1.87	2	1
1:A:33:VAL:HB	1:B:44:TRP:CZ2	0.45	2.46	8	8
1:A:41:LEU:HG	1:B:37:LEU:CG	0.45	2.40	5	2
1:A:10:ILE:CD1	1:B:20:ALA:HB1	0.45	2.41	5	3
1:A:10:ILE:CD1	1:A:13:ARG:NH1	0.45	2.80	2	1
1:A:24:LEU:HD23	1:A:30:HIS:CD2	0.45	2.47	2	1
1:B:21:LEU:HD11	1:B:37:LEU:HD22	0.45	1.86	6	1
1:A:17:LEU:HA	1:B:13:ARG:NE	0.45	2.22	2	1
1:B:9:ASP:HB2	1:B:12:ASP:OD1	0.45	2.11	4	2
1:A:14:LEU:HD23	1:B:40:LEU:HD22	0.45	1.89	5	1
1:A:48:ARG:HH22	1:B:29:GLY:HA2	0.45	1.71	2	1
1:B:15:ASP:O	1:B:19:LYS:HG2	0.45	2.12	1	3
1:B:23:ALA:O	1:B:27:GLU:HG3	0.45	2.12	8	3
1:A:17:LEU:HD21	1:B:14:LEU:CD2	0.45	2.42	1	1
1:A:20:ALA:O	1:A:24:LEU:HD23	0.45	2.12	8	2
1:A:17:LEU:HD23	1:B:40:LEU:HD23	0.45	1.88	5	1
1:A:10:ILE:CG1	1:A:13:ARG:NH1	0.44	2.80	2	1
1:A:14:LEU:CG	1:B:17:LEU:HD11	0.44	2.41	4	1
1:A:13:ARG:HD3	1:B:17:LEU:HA	0.44	1.89	1	1
1:A:13:ARG:NE	1:B:17:LEU:HA	0.44	2.28	2	1
1:A:10:ILE:HD13	1:B:24:LEU:HD12	0.44	1.89	4	1
1:A:13:ARG:NH1	1:B:16:GLU:HB3	0.44	2.28	1	1
1:A:17:LEU:HD23	1:B:17:LEU:CD2	0.44	2.43	6	1
1:A:11:GLY:HA2	1:A:14:LEU:HD12	0.43	1.89	7	1
1:A:41:LEU:HD23	1:B:37:LEU:HD23	0.43	1.90	6	1
1:A:33:VAL:CG2	1:B:10:ILE:HG21	0.43	2.41	1	1
1:A:7:ALA:H	1:B:20:ALA:HB1	0.43	1.73	4	1
1:A:20:ALA:HB2	1:B:13:ARG:NH1	0.43	2.25	8	1
1:B:19:LYS:HA	1:B:22:GLU:OE1	0.43	2.13	6	2
1:A:7:ALA:HB2	1:B:24:LEU:HD11	0.43	1.89	8	1
1:A:43:ARG:O	1:A:47:ARG:HG3	0.43	2.14	7	4
1:A:10:ILE:HD12	1:A:13:ARG:NH1	0.43	2.28	2	1
1:A:36:ARG:NH1	1:B:11:GLY:HA3	0.43	2.29	2	1
1:A:21:LEU:O	1:A:24:LEU:N	0.43	2.52	8	3
1:A:21:LEU:O	1:A:25:SER:N	0.43	2.51	6	7
1:A:10:ILE:HD13	1:B:24:LEU:HD13	0.43	1.91	7	1
1:B:10:ILE:HG23	1:B:11:GLY:N	0.43	2.28	2	1
1:B:27:GLU:HB2	1:B:30:HIS:NE2	0.43	2.29	2	1
1:A:17:LEU:HD22	1:B:13:ARG:HB2	0.43	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ARG:HD3	1:B:25:SER:CB	0.43	2.42	7	2
1:A:24:LEU:HD23	1:A:30:HIS:CG	0.43	2.49	1	2
1:A:10:ILE:HG13	1:A:13:ARG:HH12	0.43	1.74	2	1
1:A:17:LEU:HD22	1:B:17:LEU:CD2	0.43	2.44	8	1
1:A:34:GLY:HA2	1:A:37:LEU:HB2	0.43	1.90	1	4
1:B:21:LEU:HD11	1:B:33:VAL:HG11	0.43	1.91	1	2
1:B:10:ILE:HD12	1:B:13:ARG:NH1	0.43	2.29	2	1
1:A:21:LEU:HD21	1:A:37:LEU:HD11	0.43	1.91	5	1
1:A:13:ARG:NH2	1:B:17:LEU:CG	0.43	2.80	2	1
1:A:17:LEU:HD22	1:B:17:LEU:HD12	0.43	1.89	1	1
1:A:13:ARG:NE	1:B:20:ALA:HB2	0.43	2.29	1	1
1:A:40:LEU:HD21	1:B:14:LEU:O	0.43	2.14	4	1
1:B:8:VAL:HG12	1:B:13:ARG:HG2	0.42	1.91	5	2
1:A:44:TRP:CD2	1:B:21:LEU:HD23	0.42	2.49	2	2
1:A:41:LEU:C	1:A:43:ARG:N	0.42	2.72	8	5
1:A:10:ILE:O	1:A:13:ARG:HB2	0.42	2.14	5	2
1:A:16:GLU:O	1:B:13:ARG:NH1	0.42	2.52	8	1
1:A:40:LEU:CB	1:B:37:LEU:HD21	0.42	2.44	4	2
1:A:24:LEU:HD23	1:A:30:HIS:CE1	0.42	2.50	6	3
1:A:13:ARG:NH2	1:B:21:LEU:CD1	0.42	2.82	2	1
1:B:21:LEU:N	1:B:21:LEU:HD23	0.42	2.30	8	2
1:A:13:ARG:HA	1:A:13:ARG:HE	0.42	1.73	5	1
1:A:14:LEU:HD23	1:B:40:LEU:CD1	0.42	2.43	7	2
1:A:24:LEU:HA	1:A:27:GLU:HG3	0.42	1.89	2	1
1:A:17:LEU:HD23	1:B:17:LEU:HD23	0.42	1.90	6	1
1:A:8:VAL:C	1:A:10:ILE:N	0.42	2.74	2	1
1:A:17:LEU:HD23	1:A:17:LEU:O	0.42	2.15	3	1
1:A:19:LYS:HD2	1:A:22:GLU:OE2	0.42	2.15	8	1
1:A:14:LEU:O	1:A:17:LEU:HB3	0.42	2.15	6	1
1:A:8:VAL:HG13	1:A:8:VAL:O	0.42	2.15	4	2
1:A:17:LEU:HG	1:B:17:LEU:HD22	0.42	1.92	2	1
1:B:17:LEU:O	1:B:21:LEU:HD13	0.41	2.15	1	1
1:A:8:VAL:O	1:A:8:VAL:HG13	0.41	2.15	7	1
1:A:14:LEU:HD13	1:B:36:ARG:CB	0.41	2.45	3	1
1:A:13:ARG:HE	1:A:13:ARG:HA	0.41	1.74	6	1
1:A:7:ALA:HA	1:B:24:LEU:HD21	0.41	1.93	6	1
1:B:8:VAL:O	1:B:9:ASP:CB	0.41	2.68	5	1
1:A:40:LEU:CD1	1:B:37:LEU:HD11	0.41	2.45	6	1
1:A:13:ARG:CB	1:B:17:LEU:HG	0.41	2.46	1	1
1:A:44:TRP:HE1	1:B:34:GLY:N	0.41	2.12	1	1
1:B:24:LEU:HD12	1:B:30:HIS:CE1	0.41	2.50	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ASN:O	1:A:48:ARG:HB2	0.41	2.16	3	1
1:B:24:LEU:CD2	1:B:24:LEU:N	0.41	2.83	5	1
1:A:24:LEU:HD12	1:A:30:HIS:CE1	0.41	2.51	4	1
1:A:48:ARG:HH12	1:B:30:HIS:N	0.41	2.14	3	1
1:A:10:ILE:HG23	1:A:11:GLY:N	0.41	2.30	8	1
1:B:24:LEU:N	1:B:24:LEU:CD2	0.41	2.83	6	1
1:A:17:LEU:HD23	1:B:17:LEU:HD12	0.41	1.91	1	1
1:A:41:LEU:CG	1:B:37:LEU:HD13	0.41	2.45	3	1
1:A:24:LEU:HD22	1:B:10:ILE:CB	0.41	2.46	3	2
1:A:8:VAL:O	1:A:9:ASP:HB3	0.41	2.16	5	2
1:A:40:LEU:HD13	1:B:17:LEU:CD2	0.41	2.37	2	1
1:A:17:LEU:HD22	1:B:17:LEU:HD22	0.41	1.92	8	1
1:A:13:ARG:NH1	1:B:16:GLU:O	0.41	2.54	8	1
1:A:10:ILE:HD12	1:A:10:ILE:HA	0.41	1.78	4	1
1:A:20:ALA:CB	1:B:13:ARG:HG3	0.41	2.46	3	1
1:A:14:LEU:CD2	1:B:17:LEU:HD21	0.41	2.46	3	1
1:B:42:ARG:C	1:B:42:ARG:HD3	0.40	2.37	6	1
1:A:7:ALA:HB2	1:B:24:LEU:HD21	0.40	1.93	5	1
1:A:24:LEU:HG	1:B:10:ILE:CG1	0.40	2.46	7	1
1:A:41:LEU:O	1:A:42:ARG:C	0.40	2.60	7	2
1:A:42:ARG:C	1:A:42:ARG:HD3	0.40	2.36	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	43/60 (72%)	36±1 (84±2%)	4±1 (9±2%)	3±0 (7±1%)	3	18
1	B	43/60 (72%)	37±1 (86±1%)	4±0 (8±1%)	2±1 (5±2%)	4	25
All	All	688/960 (72%)	587 (85%)	60 (9%)	41 (6%)	3	21

All 6 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	10	ILE	8
1	A	25	SER	8
1	B	25	SER	8
1	A	8	VAL	7
1	B	10	ILE	5
1	B	8	VAL	5

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	35/47 (74%)	33±1 (94±3%)	2±1 (6±3%)	25	71
1	B	35/47 (74%)	34±0 (97±1%)	1±0 (3±1%)	48	89
All	All	560/752 (74%)	533 (95%)	27 (5%)	34	79

All 10 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	21	LEU	8
1	B	37	LEU	6
1	A	17	LEU	3
1	A	35	GLN	3
1	A	12	ASP	2
1	B	13	ARG	1
1	B	42	ARG	1
1	B	17	LEU	1
1	A	42	ARG	1
1	A	13	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 [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5885

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	2358
Number of shifts mapped to atoms	1136
Number of unparsed shifts	0
Number of shifts with mapping errors	1222
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 1222 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	112	ARG	HB3	1.9968	0.02	1
A	98	LYS	HA	3.8503	0.02	1
A	74	PHE	CA	55.606	0.05	1
A	116	HIS	CA	56.424	0.05	1
A	118	ALA	HB1	1.454	0.02	1
A	72	GLN	CB	28.911	0.05	1
A	84	GLY	H	8.436	0.02	1
B	105	ASP	H	9.0481	0.02	1
B	102	THR	HA	4.041	0.02	1
A	86	ASN	HB2	2.86	0.02	1
A	61	ALA	HB3	1.3784	0.02	1
A	81	LEU	CB	41.926	0.05	1
A	79	ASP	N	120.011	0.05	1
B	110	ARG	HA	4.16	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	91	GLU	HA	4.1593	0.02	1
B	108	THR	C	176.228	0.05	1
A	111	LEU	HD21	1.0021	0.02	1
A	103	GLU	HG2	2.457	0.02	2
B	118	ALA	H	8.2797	0.02	1
A	89	THR	N	118.985	0.05	1
A	118	ALA	H	8.2797	0.02	1
A	96	TYR	CE1	118.4737	0.05	1
A	101	VAL	CA	67.467	0.05	1
B	102	THR	HG23	1.2612	0.02	1
B	81	LEU	CB	41.926	0.05	1
B	62	SER	HB3	3.9317	0.02	2
A	69	MET	C	179.38	0.05	1
B	87	GLY	HA2	4.0	0.02	1
B	62	SER	HA	4.3888	0.02	1
A	74	PHE	C	177.153	0.05	1
B	85	ASP	HB2	2.692	0.02	1
B	70	LEU	CA	57.631	0.05	1
A	99	ARG	HB2	1.699	0.02	1
B	89	THR	H	8.3848	0.02	1
A	67	PHE	CB	36.965	0.05	1
A	75	GLY	CA	45.837	0.05	1
A	74	PHE	HB3	3.1222	0.02	2
B	115	GLU	HA	4.122	0.02	1
A	101	VAL	HG12	1.1774	0.02	2
A	92	LYS	N	120.484	0.05	1
A	109	ALA	N	123.276	0.05	1
A	63	ASP	CA	56.654	0.05	1
B	114	VAL	CB	32.09	0.05	1
A	67	PHE	CZ	128.068	0.05	1
A	94	ARG	C	178.078	0.05	1
B	111	LEU	HD22	1.0021	0.02	1
A	117	ARG	C	176.277	0.05	1
A	88	MET	HB3	2.1355	0.02	2
A	75	GLY	C	174.75	0.05	1
A	85	ASP	H	8.212	0.02	1
A	100	THR	CA	67.753	0.05	1
A	93	LEU	HA	4.1277	0.02	1
A	109	ALA	HB3	1.5713	0.02	1
B	100	THR	HB	3.9695	0.02	1
B	67	PHE	HE1	7.0507	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	83	SER	HB2	3.92	0.02	1
B	66	LEU	HG	1.54	0.02	1
A	73	ARG	CG	27.482	0.05	1
B	74	PHE	HE2	7.3494	0.02	1
B	102	THR	CG2	21.7015	0.05	1
B	68	SER	HA	4.3372	0.02	1
A	105	ASP	H	9.0481	0.02	1
B	117	ARG	N	120.851	0.05	1
A	114	VAL	HG11	1.0836	0.02	2
B	93	LEU	HB2	2.2778	0.02	2
B	66	LEU	HB2	1.521	0.02	1
A	107	VAL	HG22	1.0954	0.02	2
A	74	PHE	CE1	129.082	0.05	1
B	76	GLY	CA	45.48	0.05	1
B	117	ARG	HB3	1.8478	0.02	2
B	104	LEU	CD2	23.058	0.05	2
A	83	SER	CA	58.593	0.05	1
B	73	ARG	HA	4.0762	0.02	1
A	115	GLU	CB	30.154	0.05	1
A	74	PHE	CD1	131.005	0.05	1
B	89	THR	CB	69.004	0.05	1
B	67	PHE	CB	36.965	0.05	1
A	70	LEU	CB	40.583	0.05	1
B	101	VAL	HG12	1.1774	0.02	2
B	104	LEU	HA	4.1554	0.02	1
A	98	LYS	H	8.4272	0.02	1
A	94	ARG	HG2	1.524	0.02	1
A	120	GLU	H	7.868	0.02	1
B	67	PHE	CZ	128.068	0.05	1
A	106	SER	CA	61.691	0.05	1
B	74	PHE	CB	38.827	0.05	1
B	104	LEU	HB3	1.4968	0.02	2
B	115	GLU	HB2	1.985	0.02	1
B	99	ARG	HB2	1.699	0.02	1
B	107	VAL	HA	3.8852	0.02	1
A	82	MET	HB3	2.027	0.02	2
A	75	GLY	N	127.302	0.05	1
B	61	ALA	CB	19.203	0.05	1
B	106	SER	H	8.1317	0.02	1
B	86	ASN	H	8.507	0.02	1
B	110	ARG	HD3	3.2473	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	95	ARG	H	8.3875	0.02	1
A	65	GLU	HA	4.0222	0.02	1
A	96	TYR	CD1	132.505	0.05	1
B	104	LEU	CG	27.402	0.05	1
A	102	THR	CB	68.584	0.05	1
A	91	GLU	H	7.618	0.02	1
B	79	ASP	C	176.446	0.05	1
A	113	GLU	C	178.913	0.05	1
A	83	SER	C	175.04	0.05	1
A	72	GLN	HG3	2.416	0.02	2
A	79	ASP	CB	40.68	0.05	1
A	93	LEU	H	8.6177	0.02	1
B	86	ASN	HB3	2.86	0.02	1
B	61	ALA	HB3	1.3784	0.02	1
B	93	LEU	HA	4.1277	0.02	1
B	78	GLU	CB	30.027	0.05	1
A	103	GLU	HB2	2.024	0.02	1
B	63	ASP	C	176.199	0.05	1
B	73	ARG	CG	27.482	0.05	1
A	102	THR	HG22	1.2612	0.02	1
B	72	GLN	HE21	7.434	0.02	2
B	75	GLY	HA2	4.254	0.02	2
A	79	ASP	HA	4.5162	0.02	1
A	74	PHE	H	8.3558	0.02	1
B	74	PHE	H	8.3558	0.02	1
A	100	THR	HA	4.3533	0.02	1
A	67	PHE	HB3	2.9777	0.02	2
A	62	SER	C	175.38	0.05	1
A	97	LEU	HD13	1.0221	0.02	1
A	88	MET	HG3	2.5652	0.02	2
A	114	VAL	HG23	0.9746	0.02	2
A	116	HIS	HB2	3.3644	0.02	2
B	88	MET	HB3	2.1355	0.02	2
A	97	LEU	CD2	27.251	0.05	1
B	68	SER	C	177.344	0.05	1
B	61	ALA	H	8.278	0.02	1
B	68	SER	CA	61.769	0.05	1
A	62	SER	HB3	3.9317	0.02	2
A	79	ASP	HB3	2.594	0.02	2
A	85	ASP	C	176.308	0.05	1
A	113	GLU	HB3	2.247	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	114	VAL	HG21	0.9746	0.02	2
B	108	THR	HG23	1.3239	0.02	1
B	111	LEU	HD12	1.0021	0.02	1
B	93	LEU	HD23	0.93	0.02	2
A	114	VAL	H	8.033	0.02	1
B	90	GLU	HB3	2.0393	0.02	2
A	89	THR	HG21	1.2918	0.02	1
A	65	GLU	HG3	2.22	0.02	2
A	84	GLY	HA3	3.99	0.02	1
B	67	PHE	HB2	3.1709	0.02	2
B	77	GLY	N	127.741	0.05	1
B	111	LEU	H	8.4697	0.02	1
A	110	ARG	HB3	2.0495	0.02	1
A	94	ARG	H	8.3326	0.02	1
A	111	LEU	HD11	1.0021	0.02	1
B	90	GLU	HG2	2.1665	0.02	1
A	93	LEU	C	178.605	0.05	1
B	63	ASP	CA	56.654	0.05	1
B	67	PHE	CA	58.826	0.05	1
A	104	LEU	C	179.991	0.05	1
A	109	ALA	CB	17.809	0.05	1
B	95	ARG	HG2	1.862	0.02	2
A	104	LEU	H	8.9435	0.02	1
A	84	GLY	N	110.24	0.05	1
B	78	GLU	H	8.504	0.02	1
B	103	GLU	C	178.219	0.05	1
B	101	VAL	HA	3.5666	0.02	1
B	69	MET	HB3	2.2694	0.02	1
B	111	LEU	HB3	1.5034	0.02	2
A	74	PHE	CB	38.827	0.05	1
A	66	LEU	CA	58.092	0.05	1
B	109	ALA	HB3	1.5713	0.02	1
A	72	GLN	CG	34.01	0.05	1
B	84	GLY	C	173.946	0.05	1
A	111	LEU	CA	58.751	0.05	1
B	77	GLY	H	8.415	0.02	1
B	117	ARG	CB	30.615	0.05	1
B	101	VAL	CG1	24.748	0.05	2
B	114	VAL	C	178.062	0.05	1
B	81	LEU	HB3	1.5887	0.02	2
A	81	LEU	CA	55.67	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	86	ASN	N	118.739	0.05	1
A	112	ARG	N	116.931	0.05	1
A	78	GLU	CG	36.283	0.05	1
A	90	GLU	HG3	2.1665	0.02	1
B	78	GLU	HB2	2.059	0.02	2
A	92	LYS	HB2	1.8253	0.02	2
B	86	ASN	HD22	6.965	0.02	1
B	108	THR	HB	4.4064	0.02	1
B	86	ASN	C	175.824	0.05	1
B	80	LEU	HB3	1.525	0.02	2
B	113	GLU	CG	33.981	0.05	1
A	80	LEU	HG	1.562	0.02	1
B	97	LEU	N	124.775	0.05	1
A	102	THR	CG2	21.7015	0.05	1
B	111	LEU	CB	41.5949	0.05	1
B	89	THR	N	118.985	0.05	1
A	117	ARG	HD2	3.244	0.02	1
B	117	ARG	HA	4.2938	0.02	1
A	70	LEU	N	121.809	0.05	1
A	96	TYR	CE2	118.4737	0.05	1
A	72	GLN	C	178.127	0.05	1
A	101	VAL	CB	31.411	0.05	1
A	109	ALA	H	7.9484	0.02	1
A	101	VAL	HG21	0.9529	0.02	2
A	111	LEU	HB3	1.5034	0.02	2
A	104	LEU	HB2	2.4038	0.02	2
A	117	ARG	N	120.851	0.05	1
B	63	ASP	N	122.743	0.05	1
B	105	ASP	HB3	2.6896	0.02	2
B	61	ALA	N	124.679	0.05	1
A	108	THR	CA	67.738	0.05	1
A	93	LEU	HB2	2.2778	0.02	2
B	62	SER	CA	58.466	0.05	1
A	87	GLY	C	177.446	0.05	1
B	114	VAL	CA	64.696	0.05	1
B	88	MET	HG3	2.5652	0.02	2
B	116	HIS	C	175.353	0.05	1
A	119	GLY	C	173.361	0.05	1
A	115	GLU	HG2	2.4338	0.02	2
B	114	VAL	HG22	0.9746	0.02	2
B	87	GLY	CA	45.746	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	65	GLU	CA	59.112	0.05	1
B	73	ARG	HG2	1.809	0.02	1
B	117	ARG	H	8.101	0.02	1
A	101	VAL	HA	3.5666	0.02	1
B	112	ARG	C	178.907	0.05	1
B	74	PHE	CE2	129.082	0.05	1
B	107	VAL	N	120.402	0.05	1
A	111	LEU	HB2	2.141	0.02	2
A	66	LEU	N	122.23	0.05	1
A	113	GLU	HG3	2.4697	0.02	2
A	95	ARG	HB3	1.855	0.02	1
B	104	LEU	HD21	0.9838	0.02	2
A	74	PHE	CE2	129.082	0.05	1
A	112	ARG	CA	59.108	0.05	1
B	113	GLU	HA	4.1707	0.02	1
A	112	ARG	HB2	1.9968	0.02	1
B	110	ARG	CD	43.36	0.05	1
A	93	LEU	CB	44.045	0.05	1
A	111	LEU	HD13	1.0021	0.02	1
A	91	GLU	C	178.68	0.05	1
B	89	THR	HG23	1.2918	0.02	1
B	97	LEU	HD23	1.0221	0.02	1
A	78	GLU	HA	4.2436	0.02	1
B	97	LEU	CA	59.0	0.05	1
A	90	GLU	N	120.081	0.05	1
A	70	LEU	CA	57.631	0.05	1
A	107	VAL	HG12	1.2189	0.02	2
B	67	PHE	CE2	130.187	0.05	1
B	92	LYS	HB3	1.709	0.02	2
A	108	THR	HB	4.4064	0.02	1
B	63	ASP	HB3	2.2455	0.02	2
B	70	LEU	H	8.3178	0.02	1
A	93	LEU	HD13	1.0569	0.02	2
B	64	ASP	N	116.823	0.05	1
A	65	GLU	N	119.941	0.05	1
A	106	SER	CB	62.755	0.05	1
A	120	GLU	N	125.138	0.05	1
A	70	LEU	CD2	21.72	0.05	2
A	107	VAL	CA	66.377	0.05	1
A	113	GLU	H	7.711	0.02	1
B	92	LYS	N	120.484	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	87	GLY	N	127.57	0.05	1
B	104	LEU	CB	41.847	0.05	1
B	85	ASP	CB	41.217	0.05	1
B	96	TYR	CB	38.15	0.05	1
A	118	ALA	C	178.096	0.05	1
A	69	MET	HA	4.1346	0.02	1
A	95	ARG	H	8.3875	0.02	1
B	65	GLU	N	119.941	0.05	1
A	87	GLY	HA3	4.0	0.02	1
B	90	GLU	CA	60.941	0.05	1
B	95	ARG	HB3	1.855	0.02	1
A	103	GLU	HA	4.1932	0.02	1
A	110	ARG	HG2	1.483	0.02	1
B	103	GLU	HB2	2.024	0.02	1
B	72	GLN	CG	34.01	0.05	1
B	109	ALA	N	123.276	0.05	1
A	63	ASP	H	8.5392	0.02	1
B	74	PHE	CE1	129.082	0.05	1
B	78	GLU	CG	36.283	0.05	1
B	63	ASP	HA	4.0461	0.02	1
B	73	ARG	CB	30.439	0.05	1
B	83	SER	C	175.04	0.05	1
B	107	VAL	CG2	22.209	0.05	2
B	67	PHE	HD1	6.6752	0.02	1
B	110	ARG	HB2	2.0495	0.02	1
B	98	LYS	H	8.4272	0.02	1
B	67	PHE	HB3	2.9777	0.02	2
A	80	LEU	HB3	1.525	0.02	2
A	77	GLY	HA2	4.0045	0.02	1
B	103	GLU	HG2	2.457	0.02	2
A	85	ASP	HB2	2.692	0.02	1
A	70	LEU	HD21	0.8188	0.02	2
A	76	GLY	HA3	3.975	0.02	2
B	105	ASP	N	123.415	0.05	1
A	61	ALA	N	124.679	0.05	1
B	107	VAL	HG13	1.2189	0.02	2
A	78	GLU	C	176.451	0.05	1
B	93	LEU	H	8.6177	0.02	1
A	78	GLU	H	8.504	0.02	1
B	107	VAL	HG22	1.0954	0.02	2
A	104	LEU	HD12	1.1055	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	65	GLU	CA	59.112	0.05	1
B	92	LYS	C	178.68	0.05	1
A	80	LEU	C	177.403	0.05	1
B	86	ASN	HD21	7.648	0.02	1
A	86	ASN	HD22	6.965	0.02	1
A	107	VAL	N	120.402	0.05	1
A	88	MET	H	8.2253	0.02	1
A	104	LEU	HD23	0.9838	0.02	2
B	96	TYR	C	179.519	0.05	1
B	96	TYR	HB3	2.9381	0.02	2
A	71	ASP	CA	57.618	0.05	1
B	63	ASP	CB	39.686	0.05	1
B	63	ASP	HB2	2.4453	0.02	2
B	100	THR	C	176.489	0.05	1
A	115	GLU	C	177.308	0.05	1
A	69	MET	N	121.599	0.05	1
B	117	ARG	HG3	1.72	0.02	1
A	116	HIS	H	8.065	0.02	1
A	67	PHE	HA	4.1112	0.02	1
B	71	ASP	HB2	2.945	0.02	2
A	68	SER	HB3	3.9998	0.02	1
A	102	THR	H	7.8492	0.02	1
B	68	SER	HB2	3.9998	0.02	1
B	108	THR	HG22	1.3239	0.02	1
A	103	GLU	N	122.544	0.05	1
B	76	GLY	N	127.652	0.05	1
A	90	GLU	C	176.85	0.05	1
A	80	LEU	CA	55.592	0.05	1
A	97	LEU	C	177.683	0.05	1
B	70	LEU	HD22	0.8188	0.02	2
A	107	VAL	CG1	22.534	0.05	2
A	111	LEU	CD2	26.404	0.05	1
B	111	LEU	HD13	1.0021	0.02	1
B	65	GLU	HB3	2.0165	0.02	2
A	90	GLU	HB2	2.2598	0.02	2
A	83	SER	HA	4.4163	0.02	1
B	88	MET	CG	32.3075	0.05	1
B	96	TYR	CE2	118.4737	0.05	1
A	103	GLU	CA	58.964	0.05	1
B	72	GLN	HB3	2.0145	0.02	2
B	69	MET	HG2	2.7392	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	102	THR	HB	4.2957	0.02	1
B	96	TYR	HD2	7.2139	0.02	1
A	79	ASP	C	176.446	0.05	1
B	110	ARG	HG3	1.483	0.02	1
B	113	GLU	CB	29.797	0.05	1
A	116	HIS	CB	28.596	0.05	1
A	70	LEU	HD13	0.9524	0.02	2
A	90	GLU	CB	29.8281	0.05	1
B	115	GLU	N	119.665	0.05	1
B	97	LEU	HD13	1.0221	0.02	1
A	89	THR	CB	69.004	0.05	1
A	118	ALA	HA	4.347	0.02	1
B	119	GLY	H	8.2435	0.02	1
B	120	GLU	N	125.138	0.05	1
B	68	SER	H	8.0576	0.02	1
B	99	ARG	C	178.589	0.05	1
B	75	GLY	H	7.9742	0.02	1
A	69	MET	CA	59.008	0.05	1
B	62	SER	C	175.38	0.05	1
A	111	LEU	HG	1.717	0.02	1
B	71	ASP	HA	4.4852	0.02	1
B	104	LEU	N	121.08	0.05	1
A	88	MET	HB2	2.2635	0.02	2
B	65	GLU	CB	29.5665	0.05	1
B	113	GLU	HG3	2.4697	0.02	2
B	118	ALA	CB	19.104	0.05	1
B	79	ASP	N	120.011	0.05	1
B	66	LEU	HA	4.0843	0.02	1
A	108	THR	CG2	21.069	0.05	1
B	96	TYR	CD1	132.505	0.05	1
A	95	ARG	HG2	1.862	0.02	2
A	64	ASP	C	179.052	0.05	1
B	89	THR	HA	3.9534	0.02	1
A	61	ALA	C	178.053	0.05	1
A	116	HIS	HA	4.6413	0.02	1
B	100	THR	HG23	1.3291	0.02	1
B	73	ARG	N	119.296	0.05	1
A	91	GLU	N	116.636	0.05	1
B	111	LEU	HA	4.1023	0.02	1
B	93	LEU	CG	27.448	0.05	1
A	92	LYS	C	178.68	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	108	THR	CG2	21.069	0.05	1
A	86	ASN	HB3	2.86	0.02	1
A	61	ALA	HB2	1.3784	0.02	1
B	76	GLY	HA3	3.975	0.02	2
B	67	PHE	CD1	130.7586	0.05	1
A	119	GLY	HA3	3.9922	0.02	1
B	73	ARG	HB3	1.4748	0.02	2
A	73	ARG	HB2	1.6281	0.02	2
A	103	GLU	HG3	2.315	0.02	2
B	85	ASP	HA	4.662	0.02	1
A	115	GLU	N	119.665	0.05	1
B	69	MET	N	121.599	0.05	1
B	76	GLY	C	174.633	0.05	1
A	87	GLY	H	8.562	0.02	1
B	101	VAL	HB	2.2517	0.02	1
B	96	TYR	HA	4.1779	0.02	1
A	108	THR	HA	3.8489	0.02	1
B	67	PHE	N	116.555	0.05	1
A	64	ASP	CA	57.513	0.05	1
B	72	GLN	HG2	2.555	0.02	2
A	72	GLN	HB2	2.1875	0.02	2
A	67	PHE	CD2	130.7586	0.05	1
B	115	GLU	H	8.4233	0.02	1
B	102	THR	HG22	1.2612	0.02	1
A	67	PHE	C	177.788	0.05	1
B	85	ASP	HB3	2.692	0.02	1
B	70	LEU	CB	40.583	0.05	1
B	65	GLU	H	7.8689	0.02	1
B	88	MET	CB	32.3507	0.05	1
A	99	ARG	C	178.589	0.05	1
A	99	ARG	HB3	1.699	0.02	1
B	94	ARG	N	117.978	0.05	1
B	104	LEU	CA	58.168	0.05	1
B	109	ALA	H	7.9484	0.02	1
B	111	LEU	HD23	1.0021	0.02	1
A	101	VAL	C	177.268	0.05	1
B	67	PHE	C	177.788	0.05	1
A	102	THR	N	115.862	0.05	1
A	69	MET	HG2	2.7392	0.02	2
A	62	SER	HA	4.3888	0.02	1
B	80	LEU	HA	4.2365	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	100	THR	CB	67.898	0.05	1
A	109	ALA	HB2	1.5713	0.02	1
B	74	PHE	C	177.153	0.05	1
B	72	GLN	CB	28.911	0.05	1
B	89	THR	HG22	1.2918	0.02	1
B	83	SER	N	115.637	0.05	1
B	98	LYS	N	118.058	0.05	1
B	67	PHE	HE2	7.0507	0.02	1
B	95	ARG	HA	4.0225	0.02	1
A	62	SER	H	8.4597	0.02	1
B	108	THR	H	8.4508	0.02	1
A	89	THR	HA	3.9534	0.02	1
A	99	ARG	H	7.8187	0.02	1
A	112	ARG	HG3	1.685	0.02	2
B	86	ASN	HA	4.6898	0.02	1
B	73	ARG	CA	58.095	0.05	1
A	66	LEU	HG	1.54	0.02	1
A	107	VAL	HG23	1.0954	0.02	2
B	96	TYR	HD1	7.2139	0.02	1
A	78	GLU	N	120.359	0.05	1
A	98	LYS	N	118.058	0.05	1
B	69	MET	CB	31.708	0.05	1
A	114	VAL	N	116.318	0.05	1
B	117	ARG	HB2	1.926	0.02	2
A	114	VAL	CA	64.696	0.05	1
B	104	LEU	C	179.991	0.05	1
B	113	GLU	N	117.678	0.05	1
A	78	GLU	HG2	2.2413	0.02	1
B	115	GLU	CB	30.154	0.05	1
B	101	VAL	HG13	1.1774	0.02	2
A	75	GLY	H	7.9742	0.02	1
B	77	GLY	CA	45.312	0.05	1
A	94	ARG	HG3	1.524	0.02	1
B	97	LEU	CB	41.354	0.05	1
A	120	GLU	HB3	1.926	0.02	2
B	74	PHE	CA	55.606	0.05	1
B	109	ALA	HA	4.1425	0.02	1
B	104	LEU	HB2	2.4038	0.02	2
B	102	THR	N	115.862	0.05	1
B	107	VAL	HB	2.1032	0.02	1
A	71	ASP	CB	40.1067	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	115	GLU	CG	37.2644	0.05	1
B	116	HIS	HB2	3.3644	0.02	2
A	76	GLY	C	174.633	0.05	1
B	61	ALA	C	178.053	0.05	1
A	96	TYR	HE2	6.6582	0.02	1
A	115	GLU	HA	4.122	0.02	1
B	116	HIS	H	8.065	0.02	1
A	104	LEU	HA	4.1554	0.02	1
A	114	VAL	C	178.062	0.05	1
A	110	ARG	H	7.7794	0.02	1
B	79	ASP	CB	40.68	0.05	1
A	72	GLN	HG2	2.555	0.02	2
B	101	VAL	HG23	0.9529	0.02	2
B	111	LEU	CD1	26.404	0.05	1
B	107	VAL	CA	66.377	0.05	1
B	86	ASN	HB2	2.86	0.02	1
A	74	PHE	N	115.746	0.05	1
B	110	ARG	C	178.434	0.05	1
B	70	LEU	HD21	0.8188	0.02	2
A	107	VAL	CG2	22.209	0.05	2
A	111	LEU	CD1	26.404	0.05	1
B	78	GLU	C	176.451	0.05	1
A	102	THR	HG23	1.2612	0.02	1
A	78	GLU	CA	57.064	0.05	1
B	75	GLY	HA3	4.0355	0.02	2
B	108	THR	HA	3.8489	0.02	1
A	97	LEU	HA	4.3064	0.02	1
A	105	ASP	HB2	2.9189	0.02	2
B	84	GLY	N	110.24	0.05	1
A	80	LEU	HA	4.2365	0.02	1
A	93	LEU	CD1	28.096	0.05	2
B	120	GLU	H	7.868	0.02	1
A	88	MET	HG2	2.692	0.02	2
B	88	MET	HB2	2.2635	0.02	2
B	111	LEU	N	120.259	0.05	1
A	89	THR	CA	66.713	0.05	1
B	79	ASP	HB3	2.594	0.02	2
B	118	ALA	HA	4.347	0.02	1
A	72	GLN	NE2	111.83	0.05	1
B	86	ASN	CA	54.282	0.05	1
B	101	VAL	CG2	21.824	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	101	VAL	N	123.121	0.05	1
A	93	LEU	N	118.034	0.05	1
B	74	PHE	HD2	7.1489	0.02	1
A	84	GLY	HA2	3.99	0.02	1
A	106	SER	HA	4.3589	0.02	1
A	110	ARG	CB	29.828	0.05	1
A	107	VAL	HB	2.1032	0.02	1
B	70	LEU	HD11	0.9524	0.02	2
A	109	ALA	CA	55.2767	0.05	1
B	95	ARG	HG3	1.582	0.02	2
A	101	VAL	HG23	0.9529	0.02	2
B	70	LEU	N	121.809	0.05	1
B	65	GLU	CG	36.6105	0.05	1
B	77	GLY	HA2	4.0045	0.02	1
A	114	VAL	CG1	21.731	0.05	2
A	100	THR	N	118.134	0.05	1
B	111	LEU	HB2	2.141	0.02	2
A	108	THR	H	8.4508	0.02	1
B	72	GLN	N	117.125	0.05	1
A	108	THR	HG22	1.3239	0.02	1
B	113	GLU	HB3	2.247	0.02	1
A	118	ALA	HB3	1.454	0.02	1
A	78	GLU	HB3	1.9387	0.02	2
A	66	LEU	CB	41.718	0.05	1
B	87	GLY	C	177.446	0.05	1
B	80	LEU	H	8.0598	0.02	1
A	101	VAL	CG1	24.748	0.05	2
A	92	LYS	CB	33.037	0.05	1
B	110	ARG	H	7.7794	0.02	1
A	73	ARG	HA	4.0762	0.02	1
A	85	ASP	N	119.831	0.05	1
B	114	VAL	HG12	1.0836	0.02	2
A	104	LEU	CD2	23.058	0.05	2
A	94	ARG	N	117.978	0.05	1
B	78	GLU	HB3	1.9387	0.02	2
A	111	LEU	HD12	1.0021	0.02	1
A	110	ARG	HB2	2.0495	0.02	1
A	108	THR	HG23	1.3239	0.02	1
B	80	LEU	HB2	1.553	0.02	2
A	111	LEU	HD23	1.0021	0.02	1
B	114	VAL	CG2	21.77	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	67	PHE	CA	58.826	0.05	1
B	111	LEU	CA	58.751	0.05	1
B	101	VAL	CA	67.467	0.05	1
A	67	PHE	CD1	130.7586	0.05	1
B	116	HIS	CA	56.424	0.05	1
A	84	GLY	C	173.946	0.05	1
A	74	PHE	HB2	3.4556	0.02	2
A	94	ARG	HA	3.828	0.02	1
A	75	GLY	HA3	4.0355	0.02	2
B	64	ASP	CB	40.3157	0.05	1
A	103	GLU	H	7.8134	0.02	1
A	63	ASP	HB2	2.4453	0.02	2
A	96	TYR	HD1	7.2139	0.02	1
B	71	ASP	C	179.685	0.05	1
B	102	THR	CB	68.584	0.05	1
A	104	LEU	HB3	1.4968	0.02	2
B	119	GLY	HA3	3.9922	0.02	1
A	63	ASP	C	176.199	0.05	1
A	115	GLU	HB2	1.985	0.02	1
A	93	LEU	HB3	1.3173	0.02	2
A	102	THR	HA	4.041	0.02	1
B	119	GLY	CA	45.484	0.05	1
B	109	ALA	CB	17.809	0.05	1
A	112	ARG	HD3	3.2367	0.02	1
A	97	LEU	HB2	2.2631	0.02	1
B	84	GLY	H	8.436	0.02	1
A	66	LEU	H	7.7568	0.02	1
B	109	ALA	HB2	1.5713	0.02	1
B	96	TYR	N	118.48	0.05	1
B	74	PHE	HB3	3.1222	0.02	2
B	114	VAL	HG21	0.9746	0.02	2
B	120	GLU	HB3	1.926	0.02	2
B	73	ARG	HG3	1.809	0.02	1
A	70	LEU	HB3	1.3628	0.02	2
A	109	ALA	HB1	1.5713	0.02	1
A	110	ARG	HD3	3.2473	0.02	1
A	69	MET	H	7.926	0.02	1
B	72	GLN	CA	58.266	0.05	1
A	72	GLN	HE22	6.85	0.02	2
B	111	LEU	C	177.945	0.05	1
A	113	GLU	HG2	2.5467	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	74	PHE	CZ	130.6045	0.05	1
A	98	LYS	C	179.251	0.05	1
A	109	ALA	HA	4.1425	0.02	1
B	93	LEU	HD13	1.0569	0.02	2
A	95	ARG	C	180.478	0.05	1
B	111	LEU	HD21	1.0021	0.02	1
A	65	GLU	H	7.8689	0.02	1
B	65	GLU	C	178.519	0.05	1
A	88	MET	CA	55.345	0.05	1
B	83	SER	HB2	3.92	0.02	1
A	71	ASP	HB2	2.945	0.02	2
B	107	VAL	H	8.7596	0.02	1
B	115	GLU	HB3	1.985	0.02	1
B	73	ARG	H	7.776	0.02	1
B	107	VAL	HG12	1.2189	0.02	2
A	61	ALA	CB	19.203	0.05	1
B	67	PHE	CE1	130.187	0.05	1
B	71	ASP	N	120.316	0.05	1
A	87	GLY	HA2	4.0	0.02	1
A	97	LEU	HB3	1.6333	0.02	1
B	79	ASP	HA	4.5162	0.02	1
A	107	VAL	CB	31.72	0.05	1
A	95	ARG	N	118.625	0.05	1
A	78	GLU	HB2	2.059	0.02	2
B	96	TYR	CA	63.042	0.05	1
B	64	ASP	HA	4.3513	0.02	1
A	110	ARG	N	119.071	0.05	1
B	85	ASP	C	176.308	0.05	1
B	97	LEU	C	177.683	0.05	1
B	90	GLU	N	120.081	0.05	1
B	110	ARG	N	119.071	0.05	1
B	81	LEU	H	8.0625	0.02	1
B	99	ARG	N	117.877	0.05	1
B	95	ARG	HB2	1.855	0.02	1
A	100	THR	HG21	1.3291	0.02	1
B	74	PHE	CD1	131.005	0.05	1
A	105	ASP	N	123.415	0.05	1
A	96	TYR	HE1	6.6582	0.02	1
B	93	LEU	CD1	28.096	0.05	2
A	110	ARG	HG3	1.483	0.02	1
A	67	PHE	H	8.455	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	103	GLU	HB3	2.024	0.02	1
B	80	LEU	C	177.403	0.05	1
A	65	GLU	HB3	2.0165	0.02	2
B	67	PHE	HZ	6.9597	0.02	1
A	77	GLY	CA	45.312	0.05	1
B	93	LEU	HG	2.0344	0.02	1
A	81	LEU	HA	4.2574	0.02	1
A	73	ARG	HG3	1.809	0.02	1
A	85	ASP	CB	41.217	0.05	1
A	67	PHE	CE1	130.187	0.05	1
B	93	LEU	N	118.034	0.05	1
A	81	LEU	HB3	1.5887	0.02	2
A	113	GLU	CA	58.842	0.05	1
B	110	ARG	HB3	2.0495	0.02	1
B	88	MET	CA	55.345	0.05	1
B	94	ARG	HG3	1.524	0.02	1
A	62	SER	CA	58.466	0.05	1
A	88	MET	N	119.486	0.05	1
A	119	GLY	N	127.342	0.05	1
A	97	LEU	CA	59.0	0.05	1
B	65	GLU	HG3	2.22	0.02	2
A	70	LEU	HD22	0.8188	0.02	2
A	97	LEU	HD11	1.0221	0.02	1
B	80	LEU	N	121.42	0.05	1
A	68	SER	HA	4.3372	0.02	1
B	81	LEU	HA	4.2574	0.02	1
A	115	GLU	CG	37.2644	0.05	1
B	69	MET	CG	31.678	0.05	1
A	72	GLN	N	117.125	0.05	1
A	85	ASP	HA	4.662	0.02	1
B	112	ARG	CA	59.108	0.05	1
B	107	VAL	HG21	1.0954	0.02	2
A	104	LEU	HD13	1.1055	0.02	2
A	86	ASN	HD21	7.648	0.02	1
A	104	LEU	HD22	0.9838	0.02	2
B	93	LEU	HD21	0.93	0.02	2
B	112	ARG	HD2	3.2367	0.02	1
A	89	THR	HG23	1.2918	0.02	1
A	110	ARG	CA	58.628	0.05	1
B	96	TYR	HB2	3.2251	0.02	2
A	104	LEU	CA	58.168	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	97	LEU	HD23	1.0221	0.02	1
A	107	VAL	HA	3.8852	0.02	1
A	108	THR	N	116.699	0.05	1
B	103	GLU	CA	58.964	0.05	1
A	72	GLN	H	7.6168	0.02	1
A	65	GLU	C	178.519	0.05	1
A	68	SER	CA	61.769	0.05	1
A	114	VAL	CG2	21.77	0.05	2
B	87	GLY	N	127.57	0.05	1
B	94	ARG	C	178.078	0.05	1
B	106	SER	CB	62.755	0.05	1
B	108	THR	HG21	1.3239	0.02	1
A	77	GLY	N	127.741	0.05	1
B	97	LEU	H	9.2677	0.02	1
B	70	LEU	HB2	2.021	0.02	2
A	80	LEU	CB	41.854	0.05	1
B	66	LEU	C	178.453	0.05	1
B	69	MET	HA	4.1346	0.02	1
A	113	GLU	N	117.678	0.05	1
B	117	ARG	CA	56.541	0.05	1
B	106	SER	HA	4.3589	0.02	1
A	67	PHE	HE2	7.0507	0.02	1
B	96	TYR	HE1	6.6582	0.02	1
A	97	LEU	N	124.775	0.05	1
B	104	LEU	HD23	0.9838	0.02	2
B	72	GLN	HB2	2.1875	0.02	2
B	110	ARG	HG2	1.483	0.02	1
A	70	LEU	HD12	0.9524	0.02	2
A	81	LEU	N	120.607	0.05	1
A	90	GLU	CA	60.941	0.05	1
B	97	LEU	HD12	1.0221	0.02	1
A	68	SER	C	177.344	0.05	1
A	111	LEU	N	120.259	0.05	1
B	105	ASP	C	179.011	0.05	1
A	78	GLU	CB	30.027	0.05	1
B	71	ASP	CB	40.1067	0.05	1
B	64	ASP	CA	57.513	0.05	1
A	96	TYR	HD2	7.2139	0.02	1
B	114	VAL	H	8.033	0.02	1
A	93	LEU	HD23	0.93	0.02	2
B	111	LEU	HD11	1.0021	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	97	LEU	CD2	27.251	0.05	1
A	104	LEU	N	121.08	0.05	1
B	76	GLY	HA2	4.129	0.02	2
A	87	GLY	CA	45.746	0.05	1
A	118	ALA	N	123.787	0.05	1
A	71	ASP	HA	4.4852	0.02	1
A	110	ARG	C	178.434	0.05	1
A	105	ASP	CB	39.5007	0.05	1
A	80	LEU	H	8.0598	0.02	1
B	97	LEU	HD21	1.0221	0.02	1
A	117	ARG	HB3	1.8478	0.02	2
B	84	GLY	HA2	3.99	0.02	1
B	96	TYR	CD2	132.505	0.05	1
A	86	ASN	HA	4.6898	0.02	1
B	101	VAL	N	123.121	0.05	1
B	100	THR	HG22	1.3291	0.02	1
A	112	ARG	C	178.907	0.05	1
A	115	GLU	H	8.4233	0.02	1
A	116	HIS	CD2	120.098	0.05	1
B	67	PHE	H	8.455	0.02	1
A	70	LEU	H	8.3178	0.02	1
A	98	LYS	HB3	1.8925	0.02	1
A	61	ALA	HB1	1.3784	0.02	1
B	67	PHE	CD2	130.7586	0.05	1
B	71	ASP	H	8.9831	0.02	1
A	76	GLY	HA2	4.129	0.02	2
A	119	GLY	HA2	3.9922	0.02	1
B	73	ARG	HB2	1.6281	0.02	2
B	104	LEU	CD1	26.18	0.05	2
A	66	LEU	HB3	1.521	0.02	1
A	73	ARG	HB3	1.4748	0.02	2
A	61	ALA	CA	52.678	0.05	1
A	73	ARG	C	178.187	0.05	1
A	93	LEU	HD11	1.0569	0.02	2
A	100	THR	CG2	22.547	0.05	1
B	94	ARG	H	8.3326	0.02	1
B	100	THR	N	118.134	0.05	1
A	110	ARG	HA	4.16	0.02	1
A	93	LEU	CG	27.448	0.05	1
A	117	ARG	H	8.101	0.02	1
A	69	MET	HB2	2.2694	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	71	ASP	N	120.316	0.05	1
B	91	GLU	H	7.618	0.02	1
B	83	SER	H	8.231	0.02	1
A	79	ASP	H	8.5087	0.02	1
B	108	THR	N	116.699	0.05	1
A	118	ALA	CA	52.761	0.05	1
A	100	THR	HG22	1.3291	0.02	1
A	67	PHE	HZ	6.9597	0.02	1
A	102	THR	HG21	1.2612	0.02	1
A	111	LEU	HA	4.1023	0.02	1
B	69	MET	CA	59.008	0.05	1
B	115	GLU	C	177.308	0.05	1
A	69	MET	HG3	2.5146	0.02	2
B	63	ASP	H	8.5392	0.02	1
A	72	GLN	HE21	7.434	0.02	2
B	70	LEU	CD2	21.72	0.05	2
A	66	LEU	C	178.453	0.05	1
B	106	SER	HB2	4.0969	0.02	2
A	100	THR	C	176.489	0.05	1
A	92	LYS	HA	3.9304	0.02	1
B	86	ASN	CB	38.802	0.05	1
A	73	ARG	CA	58.095	0.05	1
A	120	GLU	HA	4.171	0.02	1
B	62	SER	HB2	4.087	0.02	2
B	112	ARG	HG3	1.685	0.02	2
A	89	THR	HB	4.222	0.02	1
A	76	GLY	H	8.4573	0.02	1
A	68	SER	H	8.0576	0.02	1
A	80	LEU	N	121.42	0.05	1
A	67	PHE	CE2	130.187	0.05	1
A	117	ARG	HD3	3.244	0.02	1
A	70	LEU	CD1	26.747	0.05	2
B	102	THR	HG21	1.2612	0.02	1
A	112	ARG	CD	43.449	0.05	1
B	88	MET	HA	4.6645	0.02	1
B	110	ARG	CA	58.628	0.05	1
A	106	SER	N	117.055	0.05	1
A	102	THR	HB	4.2957	0.02	1
A	78	GLU	HG3	2.2413	0.02	1
B	97	LEU	CD1	27.251	0.05	1
B	81	LEU	N	120.607	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	114	VAL	HA	3.9892	0.02	1
B	115	GLU	CA	58.678	0.05	1
A	111	LEU	CB	41.5949	0.05	1
A	102	THR	C	177.031	0.05	1
A	106	SER	HB2	4.0969	0.02	2
B	85	ASP	H	8.212	0.02	1
A	117	ARG	HG2	1.72	0.02	1
A	97	LEU	H	9.2677	0.02	1
B	62	SER	N	116.091	0.05	1
A	71	ASP	C	179.685	0.05	1
B	98	LYS	C	179.251	0.05	1
B	116	HIS	HB3	3.2742	0.02	2
B	107	VAL	CG1	22.534	0.05	2
B	101	VAL	C	177.268	0.05	1
A	77	GLY	H	8.415	0.02	1
A	106	SER	H	8.1317	0.02	1
A	90	GLU	HA	3.8232	0.02	1
B	119	GLY	N	127.342	0.05	1
A	101	VAL	HG22	0.9529	0.02	2
A	68	SER	CB	62.758	0.05	1
B	118	ALA	HB3	1.454	0.02	1
A	64	ASP	HB2	2.668	0.02	2
A	105	ASP	C	179.011	0.05	1
B	79	ASP	CA	54.726	0.05	1
B	116	HIS	CD2	120.098	0.05	1
B	101	VAL	HG22	0.9529	0.02	2
A	63	ASP	HB3	2.2455	0.02	2
B	78	GLU	HG3	2.2413	0.02	1
B	111	LEU	CD2	26.404	0.05	1
B	104	LEU	H	8.9435	0.02	1
A	73	ARG	N	119.296	0.05	1
A	96	TYR	HB2	3.2251	0.02	2
B	61	ALA	HB1	1.3784	0.02	1
A	82	MET	HB2	2.111	0.02	2
B	96	TYR	H	8.8287	0.02	1
B	70	LEU	HA	3.7548	0.02	1
B	101	VAL	CB	31.411	0.05	1
B	90	GLU	H	9.0826	0.02	1
A	74	PHE	HE2	7.3494	0.02	1
B	116	HIS	HD2	7.2787	0.02	1
B	83	SER	HA	4.4163	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	72	GLN	HG3	2.416	0.02	2
A	103	GLU	C	178.219	0.05	1
A	111	LEU	H	8.4697	0.02	1
A	104	LEU	CG	27.402	0.05	1
A	97	LEU	HD21	1.0221	0.02	1
A	61	ALA	H	8.278	0.02	1
A	83	SER	N	115.637	0.05	1
B	82	MET	HB3	2.027	0.02	2
A	70	LEU	HD11	0.9524	0.02	2
B	99	ARG	HA	4.1907	0.02	1
A	74	PHE	HZ	7.19	0.02	1
B	97	LEU	HD11	1.0221	0.02	1
B	79	ASP	HB2	2.7017	0.02	2
B	103	GLU	H	7.8134	0.02	1
B	70	LEU	C	178.045	0.05	1
A	108	THR	CB	68.701	0.05	1
B	104	LEU	HD13	1.1055	0.02	2
B	70	LEU	HD12	0.9524	0.02	2
B	74	PHE	HD1	7.1489	0.02	1
B	118	ALA	HB1	1.454	0.02	1
B	90	GLU	C	176.85	0.05	1
B	98	LYS	HB2	1.8925	0.02	1
B	77	GLY	C	174.525	0.05	1
B	66	LEU	H	7.7568	0.02	1
B	94	ARG	HA	3.828	0.02	1
A	61	ALA	HA	4.336	0.02	1
B	117	ARG	HD3	3.244	0.02	1
A	70	LEU	HG	1.96	0.02	1
A	97	LEU	CD1	27.251	0.05	1
B	77	GLY	HA3	4.0045	0.02	1
A	108	THR	HG21	1.3239	0.02	1
A	101	VAL	H	8.6682	0.02	1
B	76	GLY	H	8.4573	0.02	1
B	112	ARG	HB2	1.9968	0.02	1
B	85	ASP	N	119.831	0.05	1
A	118	ALA	HB2	1.454	0.02	1
B	99	ARG	H	7.8187	0.02	1
A	72	GLN	CA	58.266	0.05	1
A	113	GLU	HA	4.1707	0.02	1
B	67	PHE	HA	4.1112	0.02	1
A	101	VAL	CG2	21.824	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	96	TYR	CA	63.042	0.05	1
A	92	LYS	CA	60.59	0.05	1
B	72	GLN	C	178.127	0.05	1
B	89	THR	CG2	22.326	0.05	1
B	105	ASP	HA	4.5076	0.02	1
A	112	ARG	HD2	3.2367	0.02	1
A	104	LEU	CD1	26.18	0.05	2
A	98	LYS	CA	60.696	0.05	1
A	112	ARG	HA	4.1704	0.02	1
A	111	LEU	HD22	1.0021	0.02	1
B	114	VAL	CG1	21.731	0.05	2
B	65	GLU	HA	4.0222	0.02	1
B	68	SER	N	132.064	0.05	1
B	119	GLY	C	173.361	0.05	1
B	66	LEU	CB	41.718	0.05	1
B	64	ASP	HB2	2.668	0.02	2
A	119	GLY	H	8.2435	0.02	1
B	117	ARG	C	176.277	0.05	1
B	74	PHE	CZ	130.6045	0.05	1
B	81	LEU	CA	55.67	0.05	1
A	75	GLY	HA2	4.254	0.02	2
A	86	ASN	CA	54.282	0.05	1
A	116	HIS	HE1	8.422	0.02	1
B	87	GLY	HA3	4.0	0.02	1
A	83	SER	H	8.231	0.02	1
B	102	THR	CA	66.896	0.05	1
A	90	GLU	H	9.0826	0.02	1
B	109	ALA	C	180.452	0.05	1
A	96	TYR	C	179.519	0.05	1
A	89	THR	H	8.3848	0.02	1
A	115	GLU	HB3	1.985	0.02	1
A	101	VAL	HG13	1.1774	0.02	2
A	63	ASP	CB	39.686	0.05	1
A	84	GLY	CA	45.312	0.05	1
B	74	PHE	HB2	3.4556	0.02	2
B	80	LEU	HG	1.562	0.02	1
B	117	ARG	HG2	1.72	0.02	1
A	70	LEU	HB2	2.021	0.02	2
A	67	PHE	HD1	6.6752	0.02	1
A	110	ARG	HD2	3.2473	0.02	1
B	100	THR	HA	4.3533	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	83	SER	HB3	3.92	0.02	1
B	74	PHE	HE1	7.3494	0.02	1
A	96	TYR	N	118.48	0.05	1
B	118	ALA	CA	52.761	0.05	1
A	86	ASN	C	175.824	0.05	1
B	100	THR	CG2	22.547	0.05	1
A	114	VAL	HG12	1.0836	0.02	2
B	93	LEU	HB3	1.3173	0.02	2
B	93	LEU	HD12	1.0569	0.02	2
B	114	VAL	HG11	1.0836	0.02	2
B	66	LEU	HB3	1.521	0.02	1
A	79	ASP	CA	54.726	0.05	1
B	72	GLN	HA	4.0676	0.02	1
B	93	LEU	CB	44.045	0.05	1
B	102	THR	C	177.031	0.05	1
A	112	ARG	CG	27.5807	0.05	1
A	117	ARG	HB2	1.926	0.02	2
A	88	MET	CB	32.3507	0.05	1
B	89	THR	HG21	1.2918	0.02	1
B	83	SER	HB3	3.92	0.02	1
A	64	ASP	HA	4.3513	0.02	1
B	69	MET	C	179.38	0.05	1
A	71	ASP	HB3	2.6608	0.02	2
B	88	MET	C	176.89	0.05	1
B	80	LEU	CB	41.854	0.05	1
B	89	THR	CA	66.713	0.05	1
B	91	GLU	C	178.68	0.05	1
B	84	GLY	CA	45.312	0.05	1
B	101	VAL	HG11	1.1774	0.02	2
A	72	GLN	HA	4.0676	0.02	1
B	114	VAL	HG13	1.0836	0.02	2
A	70	LEU	C	178.045	0.05	1
A	86	ASN	N	118.739	0.05	1
A	107	VAL	HG13	1.2189	0.02	2
B	99	ARG	HB3	1.699	0.02	1
A	117	ARG	CA	56.541	0.05	1
B	90	GLU	HA	3.8232	0.02	1
B	116	HIS	N	117.217	0.05	1
B	61	ALA	CA	52.678	0.05	1
B	118	ALA	C	178.096	0.05	1
B	97	LEU	HB2	2.2631	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	110	ARG	HD2	3.2473	0.02	1
B	82	MET	C	176.221	0.05	1
B	114	VAL	N	116.318	0.05	1
B	118	ALA	N	123.787	0.05	1
B	96	TYR	CE1	118.4737	0.05	1
B	74	PHE	CD2	131.005	0.05	1
A	104	LEU	HG	1.6745	0.02	1
B	90	GLU	CG	37.062	0.05	1
A	93	LEU	HG	2.0344	0.02	1
B	95	ARG	N	118.625	0.05	1
B	101	VAL	HG21	0.9529	0.02	2
A	74	PHE	HD1	7.1489	0.02	1
B	89	THR	C	175.73	0.05	1
A	65	GLU	HB2	2.093	0.02	2
B	112	ARG	N	116.931	0.05	1
B	61	ALA	HB2	1.3784	0.02	1
A	97	LEU	HG	1.639	0.02	1
A	114	VAL	HG13	1.0836	0.02	2
B	78	GLU	CA	57.064	0.05	1
B	113	GLU	H	7.711	0.02	1
A	103	GLU	HB3	2.024	0.02	1
A	73	ARG	HG2	1.809	0.02	1
A	74	PHE	HE1	7.3494	0.02	1
A	81	LEU	HB2	1.6756	0.02	2
A	113	GLU	CB	29.797	0.05	1
B	94	ARG	HG2	1.524	0.02	1
A	62	SER	CB	63.972	0.05	1
B	115	GLU	HG2	2.4338	0.02	2
A	97	LEU	CB	41.354	0.05	1
A	96	TYR	H	8.8287	0.02	1
A	67	PHE	HB2	3.1709	0.02	2
A	66	LEU	HB2	1.521	0.02	1
A	70	LEU	HD23	0.8188	0.02	2
A	97	LEU	HD12	1.0221	0.02	1
A	89	THR	C	175.73	0.05	1
B	106	SER	C	177.693	0.05	1
A	114	VAL	HG22	0.9746	0.02	2
A	116	HIS	HB3	3.2742	0.02	2
A	90	GLU	CG	37.062	0.05	1
A	69	MET	HB3	2.2694	0.02	1
A	99	ARG	HA	4.1907	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	68	SER	CB	62.758	0.05	1
A	62	SER	HB2	4.087	0.02	2
A	79	ASP	HB2	2.7017	0.02	2
B	66	LEU	N	122.23	0.05	1
A	65	GLU	CG	36.6105	0.05	1
A	113	GLU	HB2	2.247	0.02	1
B	104	LEU	HG	1.6745	0.02	1
B	72	GLN	NE2	111.83	0.05	1
B	92	LYS	HA	3.9304	0.02	1
B	112	ARG	HD3	3.2367	0.02	1
B	90	GLU	HB2	2.2598	0.02	2
A	89	THR	HG22	1.2918	0.02	1
A	65	GLU	HG2	2.308	0.02	2
B	92	LYS	CA	60.59	0.05	1
B	118	ALA	HB2	1.454	0.02	1
B	87	GLY	H	8.562	0.02	1
A	104	LEU	CB	41.847	0.05	1
B	90	GLU	HG3	2.1665	0.02	1
B	88	MET	N	119.486	0.05	1
A	86	ASN	H	8.507	0.02	1
A	119	GLY	CA	45.484	0.05	1
A	111	LEU	C	177.945	0.05	1
B	82	MET	HA	4.486	0.02	1
A	89	THR	CG2	22.326	0.05	1
A	88	MET	HA	4.6645	0.02	1
B	106	SER	N	117.055	0.05	1
A	71	ASP	H	8.9831	0.02	1
B	106	SER	CA	61.691	0.05	1
B	75	GLY	N	127.302	0.05	1
A	112	ARG	HG2	1.8422	0.02	2
A	96	TYR	CB	38.15	0.05	1
B	78	GLU	N	120.359	0.05	1
B	70	LEU	HB3	1.3628	0.02	2
B	101	VAL	H	8.6682	0.02	1
B	79	ASP	H	8.5087	0.02	1
B	81	LEU	HB2	1.6756	0.02	2
A	64	ASP	CB	40.3157	0.05	1
A	72	GLN	HB3	2.0145	0.02	2
B	105	ASP	CB	39.5007	0.05	1
A	114	VAL	CB	32.09	0.05	1
A	114	VAL	HB	2.2135	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	90	GLU	HG2	2.1665	0.02	1
A	92	LYS	HB3	1.709	0.02	2
B	96	TYR	HE2	6.6582	0.02	1
B	112	ARG	H	8.1463	0.02	1
B	65	GLU	HG2	2.308	0.02	2
A	77	GLY	C	174.525	0.05	1
B	105	ASP	CA	57.826	0.05	1
B	75	GLY	C	174.75	0.05	1
A	91	GLU	HA	4.1593	0.02	1
A	108	THR	C	176.228	0.05	1
A	63	ASP	HA	4.0461	0.02	1
A	112	ARG	H	8.1463	0.02	1
B	66	LEU	CA	58.092	0.05	1
B	78	GLU	HA	4.2436	0.02	1
B	97	LEU	HA	4.3064	0.02	1
A	117	ARG	HA	4.2938	0.02	1
B	95	ARG	C	180.478	0.05	1
B	71	ASP	CA	57.618	0.05	1
A	86	ASN	CB	38.802	0.05	1
B	61	ALA	HA	4.336	0.02	1
A	93	LEU	HD22	0.93	0.02	2
B	82	MET	HB2	2.111	0.02	2
B	86	ASN	ND2	112.62	0.05	1
B	100	THR	CB	67.898	0.05	1
A	117	ARG	HG3	1.72	0.02	1
B	70	LEU	HG	1.96	0.02	1
B	74	PHE	HA	5.0077	0.02	1
B	69	MET	H	7.926	0.02	1
A	100	THR	H	8.5228	0.02	1
B	105	ASP	HB2	2.9189	0.02	2
B	116	HIS	CB	28.596	0.05	1
A	67	PHE	HE1	7.0507	0.02	1
A	69	MET	CG	31.678	0.05	1
B	72	GLN	H	7.6168	0.02	1
B	108	THR	CB	68.701	0.05	1
B	88	MET	HG2	2.692	0.02	2
A	105	ASP	CA	57.826	0.05	1
A	115	GLU	HG3	2.1355	0.02	2
B	116	HIS	HE1	8.422	0.02	1
B	114	VAL	HG23	0.9746	0.02	2
A	67	PHE	HD2	6.6752	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	106	SER	C	177.693	0.05	1
A	64	ASP	H	8.028	0.02	1
B	84	GLY	HA3	3.99	0.02	1
B	112	ARG	CB	30.017	0.05	1
B	112	ARG	CG	27.5807	0.05	1
A	95	ARG	HB2	1.855	0.02	1
B	100	THR	HG21	1.3291	0.02	1
B	93	LEU	HD11	1.0569	0.02	2
B	111	LEU	HG	1.717	0.02	1
B	75	GLY	CA	45.837	0.05	1
A	112	ARG	CB	30.017	0.05	1
A	112	ARG	HB3	1.9968	0.02	1
A	88	MET	C	176.89	0.05	1
A	98	LYS	HB2	1.8925	0.02	1
A	62	SER	N	116.091	0.05	1
A	88	MET	CG	32.3075	0.05	1
B	73	ARG	C	178.187	0.05	1
B	97	LEU	HD22	1.0221	0.02	1
B	100	THR	H	8.5228	0.02	1
B	80	LEU	CA	55.592	0.05	1
B	92	LYS	HB2	1.8253	0.02	2
B	112	ARG	HG2	1.8422	0.02	2
A	93	LEU	HD12	1.0569	0.02	2
A	104	LEU	HD21	0.9838	0.02	2
B	113	GLU	CA	58.842	0.05	1
B	104	LEU	HD12	1.1055	0.02	2
B	62	SER	CB	63.972	0.05	1
A	117	ARG	CB	30.615	0.05	1
B	115	GLU	HG3	2.1355	0.02	2
B	93	LEU	HD22	0.93	0.02	2
B	93	LEU	C	178.605	0.05	1
A	100	THR	HG23	1.3291	0.02	1
B	64	ASP	H	8.028	0.02	1
B	103	GLU	N	122.544	0.05	1
A	82	MET	C	176.221	0.05	1
B	92	LYS	H	8.098	0.02	1
B	102	THR	H	7.8492	0.02	1
A	76	GLY	N	127.652	0.05	1
A	68	SER	N	132.064	0.05	1
B	109	ALA	HB1	1.5713	0.02	1
A	74	PHE	HD2	7.1489	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	70	LEU	CD1	26.747	0.05	2
B	88	MET	H	8.2253	0.02	1
A	73	ARG	CB	30.439	0.05	1
A	95	ARG	HG3	1.582	0.02	2
A	66	LEU	HA	4.0843	0.02	1
B	89	THR	HB	4.222	0.02	1
A	107	VAL	HG21	1.0954	0.02	2
B	67	PHE	HD2	6.6752	0.02	1
A	113	GLU	CG	33.981	0.05	1
A	96	TYR	HA	4.1779	0.02	1
A	64	ASP	N	116.823	0.05	1
B	110	ARG	CB	29.828	0.05	1
B	119	GLY	HA2	3.9922	0.02	1
A	80	LEU	HB2	1.553	0.02	2
A	77	GLY	HA3	4.0045	0.02	1
B	103	GLU	HG3	2.315	0.02	2
A	85	ASP	HB3	2.692	0.02	1
B	62	SER	H	8.4597	0.02	1
A	97	LEU	HD22	1.0221	0.02	1
B	107	VAL	C	177.9	0.05	1
B	113	GLU	HB2	2.247	0.02	1
A	115	GLU	CA	58.678	0.05	1
A	74	PHE	CD2	131.005	0.05	1
A	107	VAL	C	177.9	0.05	1
A	118	ALA	CB	19.104	0.05	1
B	114	VAL	HB	2.2135	0.02	1
A	107	VAL	HG11	1.2189	0.02	2
B	107	VAL	HG23	1.0954	0.02	2
A	104	LEU	HD11	1.1055	0.02	2
A	65	GLU	CB	29.5665	0.05	1
B	98	LYS	HA	3.8503	0.02	1
A	106	SER	HB3	4.0958	0.02	2
A	105	ASP	HB3	2.6896	0.02	2
B	97	LEU	HB3	1.6333	0.02	1
B	92	LYS	CB	33.037	0.05	1
B	107	VAL	CB	31.72	0.05	1
A	101	VAL	HG11	1.1774	0.02	2
A	67	PHE	N	116.555	0.05	1
A	82	MET	HA	4.486	0.02	1
A	105	ASP	HA	4.5076	0.02	1
A	86	ASN	ND2	112.62	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	96	TYR	CD2	132.505	0.05	1
B	103	GLU	HA	4.1932	0.02	1
A	73	ARG	H	7.776	0.02	1
A	70	LEU	HA	3.7548	0.02	1
B	108	THR	CA	67.738	0.05	1
A	107	VAL	H	8.7596	0.02	1
A	99	ARG	N	117.877	0.05	1
A	102	THR	CA	66.896	0.05	1
B	71	ASP	HB3	2.6608	0.02	2
A	92	LYS	H	8.098	0.02	1
A	76	GLY	CA	45.48	0.05	1
A	68	SER	HB2	3.9998	0.02	1
B	107	VAL	HG11	1.2189	0.02	2
B	97	LEU	HG	1.639	0.02	1
A	64	ASP	HB3	2.5973	0.02	2
A	116	HIS	HD2	7.2787	0.02	1
B	109	ALA	CA	55.2767	0.05	1
B	68	SER	HB3	3.9998	0.02	1
B	112	ARG	CD	43.449	0.05	1
A	95	ARG	HA	4.0225	0.02	1
B	83	SER	CA	58.593	0.05	1
B	98	LYS	CA	60.696	0.05	1
B	78	GLU	HG2	2.2413	0.02	1
A	96	TYR	HB3	2.9381	0.02	2
A	116	HIS	N	117.217	0.05	1
B	116	HIS	HA	4.6413	0.02	1
B	70	LEU	HD23	0.8188	0.02	2
B	117	ARG	HD2	3.244	0.02	1
B	112	ARG	HA	4.1704	0.02	1
B	72	GLN	HE22	6.85	0.02	2
B	65	GLU	HB2	2.093	0.02	2
A	114	VAL	HA	3.9892	0.02	1
A	90	GLU	HB3	2.0393	0.02	2
B	69	MET	HG3	2.5146	0.02	2
A	100	THR	HB	3.9695	0.02	1
B	104	LEU	HD22	0.9838	0.02	2
B	113	GLU	C	178.913	0.05	1
B	64	ASP	C	179.052	0.05	1
A	116	HIS	C	175.353	0.05	1
B	106	SER	HB3	4.0958	0.02	2
A	81	LEU	H	8.0625	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	93	LEU	HD21	0.93	0.02	2
B	74	PHE	N	115.746	0.05	1
A	74	PHE	HA	5.0077	0.02	1
B	90	GLU	CB	29.8281	0.05	1
B	100	THR	CA	67.753	0.05	1
B	70	LEU	HD13	0.9524	0.02	2
B	120	GLU	HA	4.171	0.02	1
B	104	LEU	HD11	1.1055	0.02	2
B	98	LYS	HB3	1.8925	0.02	1
A	110	ARG	CD	43.36	0.05	1
A	69	MET	CB	31.708	0.05	1
A	101	VAL	HB	2.2517	0.02	1
B	74	PHE	HZ	7.19	0.02	1
B	64	ASP	HB3	2.5973	0.02	2
B	69	MET	HB2	2.2694	0.02	1
A	63	ASP	N	122.743	0.05	1
A	109	ALA	C	180.452	0.05	1
B	113	GLU	HG2	2.5467	0.02	2
B	91	GLU	N	116.636	0.05	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	194	-0.48 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	178	0.25 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}'$	222	-0.55 ± 0.12	Should be applied
^{15}N	222	-0.00 ± 0.14	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 80%, i.e. 870 atoms were assigned a chemical shift out of a possible 1082. 10 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	416/430 (97%)	170/172 (99%)	162/172 (94%)	84/86 (98%)
Sidechain	426/612 (70%)	270/354 (76%)	152/216 (70%)	4/42 (10%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	28/40 (70%)	12/20 (60%)	14/14 (100%)	2/6 (33%)
Overall	870/1082 (80%)	452/546 (83%)	328/402 (82%)	90/134 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1020 atoms were assigned a chemical shift out of a possible 1382. 10 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	510/592 (86%)	210/236 (89%)	196/240 (82%)	104/116 (90%)
Sidechain	482/750 (64%)	312/436 (72%)	166/272 (61%)	4/42 (10%)
Aromatic	28/40 (70%)	12/20 (60%)	14/14 (100%)	2/6 (33%)
Overall	1020/1382 (74%)	534/692 (77%)	376/526 (71%)	110/164 (67%)

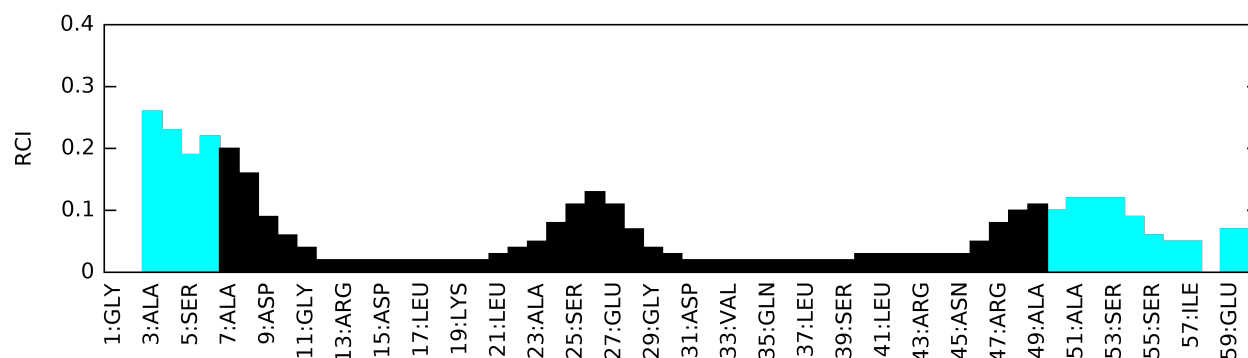
7.1.4 Statistically unusual chemical shifts [i](#)

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:

