Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 11:30 PM BST

PDB ID	:	2KGS
Title	:	Solution structure of the amino-terminal domain of OmpATb, a pore forming protein from Mycobacterium tuberculosis
Authors	:	Yang, Y.; Auguin, D.; Delbecq, S.; Dumas, E.; Molle, V.; Saint, N.
Deposited on	:	2009-03-18

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 (1)) were used in the production of this report:

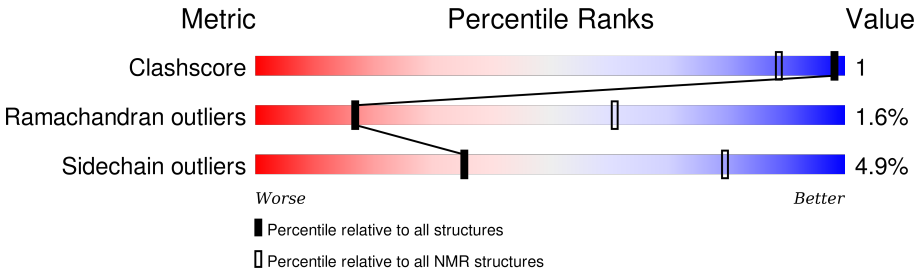
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 71%.

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	132	84% · 13%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:79-A:193 (115)	0.23	4

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 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1927 atoms, of which 970 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein Rv0899/MT0922.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	132	1927	602	970	161	192	2	0

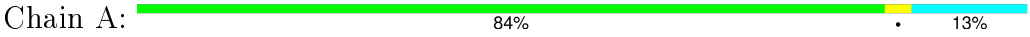
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A:



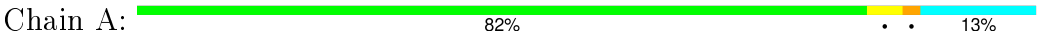
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Uncharacterized protein Rv0899/MT0922

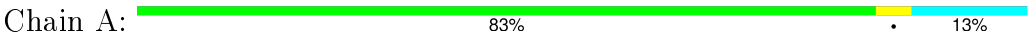
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein Rv0899/MT0922

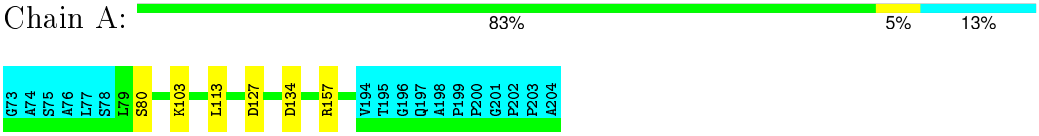
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Uncharacterized protein Rv0899/MT0922

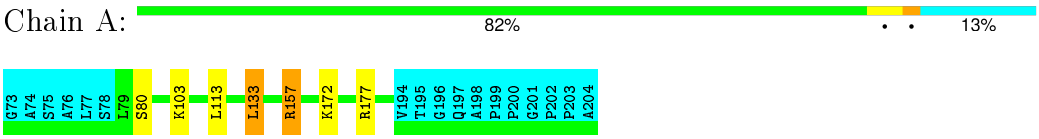
Chain A:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Uncharacterized protein Rv0899/MT0922

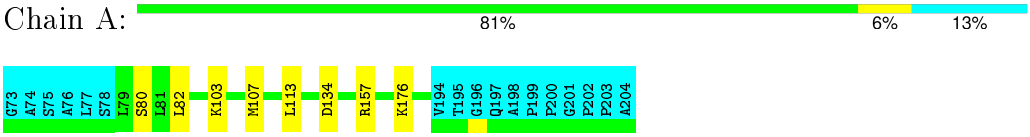
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Uncharacterized protein Rv0899/MT0922

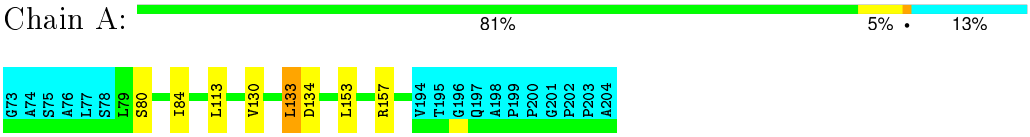
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Uncharacterized protein Rv0899/MT0922

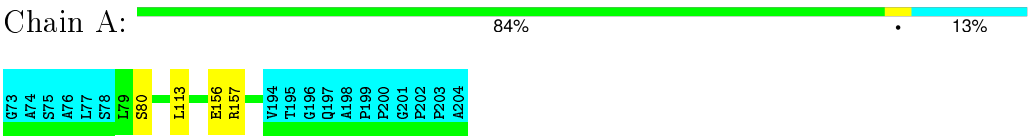
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Uncharacterized protein Rv0899/MT0922

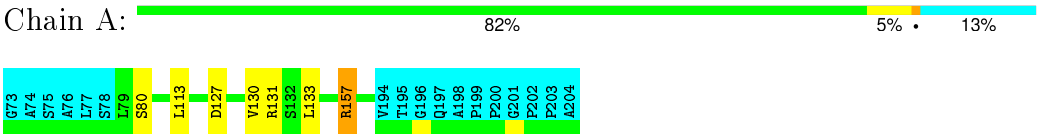
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Uncharacterized protein Rv0899/MT0922

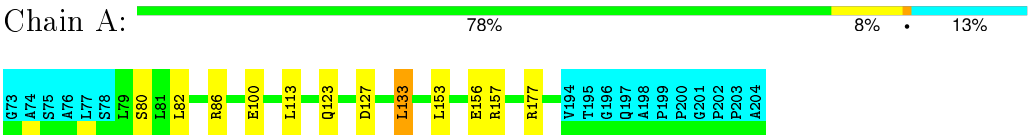
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Uncharacterized protein Rv0899/MT0922

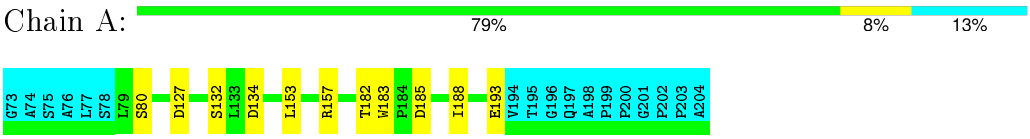
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Uncharacterized protein Rv0899/MT0922

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, minimization.*

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
AMBER	refinement	8
CYANA	structure solution	2.1

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

Chemical shift file(s)	BMRB entry 16237
Number of chemical shift lists	1
Total number of shifts	2296
Number of shifts mapped to atoms	1237
Number of unparsed shifts	54
Number of shifts with mapping errors	1005
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.61±0.02	0±0/869 (0.0±0.0%)	1.13±0.40	2±2/1190 (0.1±0.2%)
All	All	0.61	1/8690 (0.0%)	1.20	15/11900 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	193	GLU	CG-CD	6.67	1.61	1.51	10	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	185	ASP	CB-CG-OD1	-38.90	83.29	118.30	10	1
1	A	193	GLU	OE1-CD-OE2	37.04	167.74	123.30	10	1
1	A	185	ASP	CB-CG-OD2	-36.70	85.27	118.30	10	1
1	A	185	ASP	OD1-CG-OD2	23.82	168.56	123.30	10	1
1	A	193	GLU	CG-CD-OE1	-17.34	83.62	118.30	10	1
1	A	193	GLU	CG-CD-OE2	-17.08	84.13	118.30	10	1
1	A	177	ARG	NE-CZ-NH1	6.39	123.50	120.30	1	3
1	A	157	ARG	NE-CZ-NH1	6.26	123.43	120.30	4	2
1	A	86	ARG	NE-CZ-NH1	5.42	123.01	120.30	9	2
1	A	177	ARG	NE-CZ-NH2	-5.32	117.64	120.30	1	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	853	866	864	1±1
All	All	8530	8660	8640	9

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:H	1:A:133:LEU:HD12	0.64	1.51	9	2
1:A:133:LEU:HD12	1:A:133:LEU:H	0.63	1.54	6	1
1:A:182:THR:HG23	1:A:183:TRP:CD2	0.54	2.37	10	1
1:A:124:ILE:HD12	1:A:124:ILE:H	0.49	1.67	2	1
1:A:133:LEU:H	1:A:133:LEU:CD1	0.45	2.25	4	1
1:A:133:LEU:CD1	1:A:133:LEU:H	0.45	2.23	9	2
1:A:103:LYS:HD2	1:A:124:ILE:HD13	0.43	1.91	2	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	115/132 (87%)	106±1 (92±1%)	7±1 (6±1%)	2±0 (2±0%)	17	61
All	All	1150/1320 (87%)	1063 (92%)	69 (6%)	18 (2%)	17	61

All 2 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	157	ARG	10
1	A	80	SER	8

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	97/107 (91%)	92±2 (95±2%)	5±2 (5±2%)	35 79
All	All	970/1070 (91%)	922 (95%)	48 (5%)	35 79

All 21 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	113	LEU	8
1	A	133	LEU	5
1	A	134	ASP	4
1	A	127	ASP	4
1	A	80	SER	3
1	A	103	LYS	3
1	A	153	LEU	3
1	A	82	LEU	3
1	A	156	GLU	2
1	A	130	VAL	2
1	A	157	ARG	1
1	A	131	ARG	1
1	A	100	GLU	1
1	A	123	GLN	1
1	A	188	ILE	1
1	A	172	LYS	1
1	A	84	ILE	1
1	A	107	MET	1
1	A	154	LYS	1
1	A	132	SER	1
1	A	176	LYS	1

6.3.3 RNA (i)

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 71% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16237

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	2296
Number of shifts mapped to atoms	1237
Number of unparsed shifts	54
Number of shifts with mapping errors	1005
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- Chemical shift has been reported more than once. All 54 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1356	A	146	VAL	H	7.488	.	1
1357	A	146	VAL	HA	3.994	.	1
1358	A	146	VAL	HB	2.355	.	1
1359	A	146	VAL	HG11	1.061	.	2
1360	A	146	VAL	HG12	1.061	.	2
1361	A	146	VAL	HG13	1.061	.	2
1362	A	146	VAL	HG21	0.977	.	2
1363	A	146	VAL	HG22	0.977	.	2
1364	A	146	VAL	HG23	0.977	.	2
1368	A	146	VAL	N	115.4	.	1
1523	A	173	ASP	H	7.690	.	1
1524	A	173	ASP	HA	4.353	.	1
1525	A	173	ASP	HB2	2.791	.	2
1526	A	173	ASP	HB3	2.648	.	2
1527	A	173	ASP	C	177.1	.	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1528	A	173	ASP	CA	55.44	.	1
1529	A	173	ASP	CB	37.90	.	1
1530	A	173	ASP	N	116.0	.	1
1557	A	176	LYS	H	8.588	.	1
1558	A	176	LYS	HA	3.913	.	1
1559	A	176	LYS	HB2	1.786	.	2
1560	A	176	LYS	HB3	1.754	.	2
1561	A	176	LYS	HD2	1.604	.	4
1562	A	176	LYS	HD3	1.604	.	4
1563	A	176	LYS	HG2	1.357	.	4
1564	A	176	LYS	HG3	1.357	.	4
1565	A	176	LYS	C	175.5	.	1
1566	A	176	LYS	CA	56.85	.	1
1567	A	176	LYS	CB	29.65	.	1
1568	A	176	LYS	N	117.7	.	1
1689	A	191	ASN	H	7.000	.	1
1690	A	191	ASN	HA	4.791	.	1
1691	A	191	ASN	HB2	3.183	.	2
1692	A	191	ASN	HB3	2.632	.	2
1693	A	191	ASN	C	174.3	.	1
1694	A	191	ASN	CA	50.06	.	1
1695	A	191	ASN	CB	35.72	.	1
1696	A	191	ASN	N	113.2	.	1
1725	A	196	GLY	H	8.362	.	1
1726	A	196	GLY	HA2	3.878	.	2
1727	A	196	GLY	HA3	3.825	.	2
1728	A	196	GLY	C	173.0	.	1
1729	A	196	GLY	CA	43.87	.	1
1730	A	196	GLY	N	104.5	.	1
1766	A	200	PRO	HA	4.439	.	1
1767	A	200	PRO	HB2	2.261	.	2
1768	A	200	PRO	HB3	1.939	.	2
1769	A	200	PRO	HD2	3.519	.	2
1770	A	200	PRO	HD3	3.519	.	2
1771	A	200	PRO	HG2	2.033	.	2
1772	A	200	PRO	HG3	2.033	.	2
1773	A	200	PRO	C	177.2	.	1
1774	A	200	PRO	CA	63.66	.	1
1775	A	200	PRO	CB	27.92	.	1

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

- Residue not found in structure. All 1005 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	221	ASP	C	174.8	-1.0	1
A	254	ASN	N	131.7	-1.0	1
A	243	ARG	HG3	2.127	-1.0	2
A	139	LEU	HG	1.547	-1.0	1
A	198	ASN	H	8.411	-1.0	1
A	246	ASN	HA	4.559	-1.0	1
A	150	PRO	C	174.0	-1.0	1
A	182	ARG	N	121.4	-1.0	1
A	222	HIS	HB2	4.098	-1.0	2
A	142	ALA	HB1	1.548	-1.0	1
A	144	ASN	CB	34.58	-1.0	1
A	206	ALA	C	176.4	-1.0	1
A	227	GLY	CA	43.34	-1.0	1
A	175	LEU	HD13	0.745	-1.0	2
A	199	ILE	HD11	0.847	-1.0	1
A	136	CYS	HB3	2.895	-1.0	2
A	198	ASN	HB3	2.768	-1.0	2
A	172	ALA	HB3	1.523	-1.0	1
A	245	LYS	HD2	1.377	-1.0	4
A	201	LEU	H	7.66	-1.0	1
A	224	ALA	CB	19.37	-1.0	1
A	204	GLN	HB3	2.247	-1.0	2
A	234	ILE	HD11	0.727	-1.0	1
A	180	ASP	CB	38.79	-1.0	1
A	183	VAL	CA	56.76	-1.0	1
A	230	SER	CA	62.13	-1.0	1
A	189	THR	HB	3.87	-1.0	1
A	207	LYS	CA	57.11	-1.0	1
A	251	ILE	CB	36.3	-1.0	1
A	238	ALA	HA	4.24	-1.0	1
A	217	GLY	C	172.4	-1.0	1
A	244	ALA	CA	52.56	-1.0	1
A	167	ILE	HB	1.679	-1.0	1
A	175	LEU	HD22	0.718	-1.0	2
A	184	THR	HG23	1.008	-1.0	1
A	141	SER	HA	4.186	-1.0	1
A	148	GLY	N	110.6	-1.0	1
A	172	ALA	HA	3.762	-1.0	1
A	224	ALA	HB2	1.417	-1.0	1
A	210	ALA	HB1	1.466	-1.0	1
A	159	SER	N	106.5	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	133	SER	C	172.2	-1.0	1
A	240	PRO	HD3	3.85	-1.0	2
A	197	ILE	HG13	1.24	-1.0	2
A	253	VAL	HG11	1.083	-1.0	2
A	170	ARG	CB	28.85	-1.0	1
A	230	SER	HB2	3.676	-1.0	2
A	214	VAL	HG12	1.038	-1.0	2
A	241	GLU	C	176.7	-1.0	1
A	186	ASN	HA	5.476	-1.0	1
A	223	ILE	N	117.9	-1.0	1
A	185	ILE	HG12	1.401	-1.0	2
A	223	ILE	HG13	1.642	-1.0	2
A	201	LEU	CB	40.06	-1.0	1
A	172	ALA	HB1	1.523	-1.0	1
A	224	ALA	H	8.607	-1.0	1
A	235	ALA	HB1	1.291	-1.0	1
A	174	LYS	HG2	1.518	-1.0	4
A	140	GLN	HG2	2.461	-1.0	2
A	253	VAL	CB	30.33	-1.0	1
A	238	ALA	CA	51.41	-1.0	1
A	212	TYR	N	122.5	-1.0	1
A	222	HIS	CB	25.85	-1.0	1
A	213	LEU	HD12	0.866	-1.0	2
A	172	ALA	N	120.4	-1.0	1
A	197	ILE	HD12	0.837	-1.0	1
A	252	VAL	HG21	0.68	-1.0	2
A	214	VAL	N	120.4	-1.0	1
A	221	ASP	HB3	2.695	-1.0	2
A	249	VAL	HG11	0.948	-1.0	2
A	208	ILE	C	177.3	-1.0	1
A	168	LEU	CA	55.52	-1.0	1
A	209	VAL	HB	2.317	-1.0	1
A	219	ALA	HB3	1.243	-1.0	1
A	185	ILE	HG23	1.229	-1.0	1
A	159	SER	H	8.185	-1.0	1
A	206	ALA	HA	3.926	-1.0	1
A	251	ILE	HD12	0.68	-1.0	1
A	140	GLN	H	9.108	-1.0	1
A	151	ILE	HG21	0.778	-1.0	1
A	175	LEU	CA	55.27	-1.0	1
A	171	VAL	HG13	1.002	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	207	LYS	N	118.9	-1.0	1
A	241	GLU	HG3	2.252	-1.0	2
A	183	VAL	HG13	0.773	-1.0	2
A	192	THR	CA	61.11	-1.0	1
A	190	ASP	HA	4.661	-1.0	1
A	174	LYS	C	176.3	-1.0	1
A	216	ARG	CA	51.46	-1.0	1
A	178	CYS	HA	5.16	-1.0	1
A	197	ILE	HG22	0.909	-1.0	1
A	231	VAL	HG13	1.099	-1.0	2
A	208	ILE	HA	3.97	-1.0	1
A	156	ASP	HA	4.552	-1.0	1
A	189	THR	C	171.3	-1.0	1
A	244	ALA	N	116.2	-1.0	1
A	145	ALA	HA	4.21	-1.0	1
A	247	ARG	H	6.798	-1.0	1
A	134	GLY	HA2	4.284	-1.0	2
A	219	ALA	HA	4.141	-1.0	1
A	199	ILE	H	8.637	-1.0	1
A	133	SER	HB2	3.843	-1.0	2
A	178	CYS	HB3	2.636	-1.0	2
A	204	GLN	HG3	2.359	-1.0	2
A	223	ILE	C	172.1	-1.0	1
A	212	TYR	HA	4.177	-1.0	1
A	135	PRO	C	175.8	-1.0	1
A	229	GLY	HA2	4.076	-1.0	2
A	203	ALA	HB3	1.485	-1.0	1
A	184	THR	CA	59.69	-1.0	1
A	249	VAL	H	8.65	-1.0	1
A	144	ASN	N	120.7	-1.0	1
A	139	LEU	C	176.2	-1.0	1
A	249	VAL	HG23	0.948	-1.0	2
A	250	GLU	H	9.45	-1.0	1
A	239	THR	HB	4.632	-1.0	1
A	213	LEU	HD11	0.866	-1.0	2
A	214	VAL	CB	29.43	-1.0	1
A	226	VAL	HG21	0.749	-1.0	2
A	232	ASN	HB2	2.978	-1.0	2
A	230	SER	H	9.646	-1.0	1
A	140	GLN	HB3	2.153	-1.0	2
A	227	GLY	HA3	3.219	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	221	ASP	CB	36.64	-1.0	1
A	168	LEU	N	117.5	-1.0	1
A	163	ALA	H	8.326	-1.0	1
A	244	ALA	H	7.55	-1.0	1
A	195	GLU	HG2	2.425	-1.0	2
A	158	ALA	N	123.7	-1.0	1
A	190	ASP	CB	39.1	-1.0	1
A	251	ILE	HB	1.787	-1.0	1
A	152	ALA	HB1	1.376	-1.0	1
A	143	ILE	HG21	1.178	-1.0	1
A	179	PRO	HD3	3.406	-1.0	2
A	205	ARG	H	7.58	-1.0	1
A	236	SER	HB3	3.751	-1.0	2
A	254	ASN	H	8.753	-1.0	1
A	177	ALA	CB	16.62	-1.0	1
A	136	CYS	N	115.9	-1.0	1
A	243	ARG	HA	4.048	-1.0	1
A	180	ASP	HB3	2.575	-1.0	2
A	246	ASN	N	113.6	-1.0	1
A	222	HIS	HA	4.665	-1.0	1
A	165	TYR	H	7.293	-1.0	1
A	171	VAL	C	175.2	-1.0	1
A	214	VAL	H	8.423	-1.0	1
A	158	ALA	HB2	1.4	-1.0	1
A	192	THR	HG21	1.192	-1.0	1
A	204	GLN	HA	4.07	-1.0	1
A	210	ALA	HA	3.814	-1.0	1
A	206	ALA	CB	15.98	-1.0	1
A	195	GLU	HB3	2.075	-1.0	2
A	142	ALA	HB2	1.548	-1.0	1
A	231	VAL	HG23	1.099	-1.0	2
A	217	GLY	H	7.843	-1.0	1
A	179	PRO	HB2	1.978	-1.0	2
A	207	LYS	HA	3.964	-1.0	1
A	190	ASP	H	7.855	-1.0	1
A	199	ILE	N	119.8	-1.0	1
A	253	VAL	N	126.7	-1.0	1
A	147	THR	HG23	1.11	-1.0	1
A	167	ILE	HG23	0.946	-1.0	1
A	225	THR	C	171.9	-1.0	1
A	189	THR	H	8.344	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	213	LEU	HD23	0.741	-1.0	2
A	251	ILE	HG22	0.779	-1.0	1
A	220	GLY	HA3	3.674	-1.0	2
A	167	ILE	HD11	0.83	-1.0	1
A	218	VAL	N	123.7	-1.0	1
A	209	VAL	HG13	1.166	-1.0	2
A	184	THR	H	9.584	-1.0	1
A	177	ALA	H	6.896	-1.0	1
A	197	ILE	H	7.195	-1.0	1
A	174	LYS	HD2	1.803	-1.0	4
A	230	SER	CB	55.73	-1.0	1
A	232	ASN	HB3	2.64	-1.0	2
A	151	ILE	HD12	0.692	-1.0	1
A	188	TYR	HB2	3.582	-1.0	2
A	170	ARG	HB2	1.815	-1.0	2
A	252	VAL	HB	2.001	-1.0	1
A	181	ALA	HB2	1.384	-1.0	1
A	139	LEU	H	7.653	-1.0	1
A	224	ALA	HA	4.888	-1.0	1
A	158	ALA	H	8.313	-1.0	1
A	249	VAL	C	172.1	-1.0	1
A	209	VAL	CB	29.02	-1.0	1
A	206	ALA	H	7.293	-1.0	1
A	175	LEU	HD21	0.718	-1.0	2
A	213	LEU	HA	3.813	-1.0	1
A	227	GLY	H	8.564	-1.0	1
A	244	ALA	HB1	1.458	-1.0	1
A	224	ALA	HB1	1.417	-1.0	1
A	199	ILE	HA	3.58	-1.0	1
A	214	VAL	C	178.7	-1.0	1
A	249	VAL	HB	1.962	-1.0	1
A	233	PRO	HA	4.325	-1.0	1
A	164	ASP	N	111.4	-1.0	1
A	215	ALA	C	177.4	-1.0	1
A	220	GLY	CA	45.5	-1.0	1
A	179	PRO	HA	4.337	-1.0	1
A	152	ALA	HB3	1.376	-1.0	1
A	186	ASN	CA	49.33	-1.0	1
A	183	VAL	HG23	0.773	-1.0	2
A	165	TYR	N	119.4	-1.0	1
A	233	PRO	HB3	1.921	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	201	LEU	HD21	0.899	-1.0	2
A	184	THR	CB	68.31	-1.0	1
A	222	HIS	CA	53.25	-1.0	1
A	213	LEU	N	117.5	-1.0	1
A	204	GLN	C	176.3	-1.0	1
A	217	GLY	CA	43.03	-1.0	1
A	249	VAL	HG12	0.948	-1.0	2
A	210	ALA	C	176.3	-1.0	1
A	247	ARG	C	170.1	-1.0	1
A	169	ASN	HB3	3.048	-1.0	2
A	185	ILE	CB	34.38	-1.0	1
A	168	LEU	CB	25.03	-1.0	1
A	143	ILE	N	118.0	-1.0	1
A	188	TYR	H	8.546	-1.0	1
A	145	ALA	HB3	1.535	-1.0	1
A	189	THR	HG21	1.201	-1.0	1
A	178	CYS	N	116.4	-1.0	1
A	182	ARG	HA	5.084	-1.0	1
A	148	GLY	HA3	3.848	-1.0	2
A	209	VAL	H	7.207	-1.0	1
A	229	GLY	C	171.7	-1.0	1
A	205	ARG	HA	3.733	-1.0	1
A	149	GLY	H	7.953	-1.0	1
A	142	ALA	CA	52.86	-1.0	1
A	216	ARG	H	7.372	-1.0	1
A	151	ILE	HG13	1.317	-1.0	2
A	156	ASP	N	119.2	-1.0	1
A	171	VAL	HA	3.359	-1.0	1
A	138	ASP	H	8.405	-1.0	1
A	140	GLN	CB	26.55	-1.0	1
A	177	ALA	N	117.9	-1.0	1
A	228	LEU	CB	39.52	-1.0	1
A	245	LYS	HB2	1.83	-1.0	2
A	167	ILE	HG12	1.679	-1.0	2
A	190	ASP	C	171.7	-1.0	1
A	250	GLU	N	123.1	-1.0	1
A	218	VAL	HG13	0.915	-1.0	2
A	135	PRO	CB	29.68	-1.0	1
A	247	ARG	HG3	1.264	-1.0	2
A	194	SER	N	114.3	-1.0	1
A	138	ASP	HB3	2.5	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	143	ILE	HG13	1.655	-1.0	2
A	154	GLY	N	107.7	-1.0	1
A	219	ALA	C	177.5	-1.0	1
A	226	VAL	N	123.5	-1.0	1
A	204	GLN	CB	25.59	-1.0	1
A	226	VAL	HG22	0.749	-1.0	2
A	142	ALA	C	178.6	-1.0	1
A	180	ASP	HB2	2.781	-1.0	2
A	213	LEU	CA	56.22	-1.0	1
A	199	ILE	HG22	0.873	-1.0	1
A	212	TYR	H	7.733	-1.0	1
A	216	ARG	C	173.8	-1.0	1
A	245	LYS	HG2	1.291	-1.0	4
A	144	ASN	H	8.753	-1.0	1
A	193	GLY	H	8.234	-1.0	1
A	138	ASP	CB	37.5	-1.0	1
A	246	ASN	C	173.8	-1.0	1
A	252	VAL	HG12	0.871	-1.0	2
A	247	ARG	HB3	2.165	-1.0	2
A	142	ALA	N	125.1	-1.0	1
A	183	VAL	HB	1.93	-1.0	1
A	181	ALA	N	123.7	-1.0	1
A	177	ALA	HA	4.274	-1.0	1
A	185	ILE	HA	4.565	-1.0	1
A	215	ALA	HA	4.084	-1.0	1
A	211	ASP	CA	54.78	-1.0	1
A	171	VAL	CB	28.96	-1.0	1
A	214	VAL	HG22	0.953	-1.0	2
A	160	LEU	H	8.485	-1.0	1
A	204	GLN	H	8.069	-1.0	1
A	139	LEU	HA	4.114	-1.0	1
A	239	THR	HG21	1.196	-1.0	1
A	134	GLY	HA3	4.078	-1.0	2
A	205	ARG	HB2	1.517	-1.0	2
A	248	ARG	HB3	1.746	-1.0	2
A	223	ILE	HD13	0.651	-1.0	1
A	225	THR	HG22	0.979	-1.0	1
A	137	ALA	HB1	1.336	-1.0	1
A	209	VAL	C	174.5	-1.0	1
A	228	LEU	HD11	0.669	-1.0	2
A	216	ARG	HG2	1.477	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	194	SER	H	7.806	-1.0	1
A	229	GLY	N	108.6	-1.0	1
A	248	ARG	CB	29.65	-1.0	1
A	138	ASP	C	174.3	-1.0	1
A	205	ARG	C	174.8	-1.0	1
A	243	ARG	HD3	3.04	-1.0	2
A	251	ILE	HG21	0.779	-1.0	1
A	174	LYS	CA	55.42	-1.0	1
A	175	LEU	HB3	1.806	-1.0	2
A	150	PRO	CB	30.4	-1.0	1
A	170	ARG	HG2	2.061	-1.0	2
A	234	ILE	HG23	0.852	-1.0	1
A	216	ARG	HD3	2.84	-1.0	2
A	139	LEU	HD23	0.912	-1.0	2
A	226	VAL	HG13	0.749	-1.0	2
A	246	ASN	HB2	2.546	-1.0	2
A	234	ILE	HG13	1.111	-1.0	2
A	181	ALA	HB1	1.384	-1.0	1
A	251	ILE	N	121.7	-1.0	1
A	153	PHE	CA	54.81	-1.0	1
A	186	ASN	N	125.5	-1.0	1
A	236	SER	HA	4.24	-1.0	1
A	140	GLN	N	118.0	-1.0	1
A	251	ILE	HG13	1.659	-1.0	2
A	228	LEU	N	125.1	-1.0	1
A	207	LYS	HB3	1.872	-1.0	2
A	192	THR	HB	4.08	-1.0	1
A	224	ALA	C	174.0	-1.0	1
A	209	VAL	HG22	0.957	-1.0	2
A	186	ASN	HB2	2.684	-1.0	2
A	250	GLU	C	172.4	-1.0	1
A	212	TYR	CA	60.21	-1.0	1
A	181	ALA	H	8.093	-1.0	1
A	213	LEU	HB2	2.192	-1.0	2
A	170	ARG	N	119.7	-1.0	1
A	186	ASN	CB	39.04	-1.0	1
A	227	GLY	N	113.2	-1.0	1
A	140	GLN	C	176.2	-1.0	1
A	201	LEU	N	119.5	-1.0	1
A	137	ALA	CA	51.08	-1.0	1
A	219	ALA	HB2	1.243	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	199	ILE	HD12	0.847	-1.0	1
A	202	SER	HA	3.746	-1.0	1
A	198	ASN	HB2	2.768	-1.0	2
A	245	LYS	HD3	1.377	-1.0	4
A	216	ARG	N	114.4	-1.0	1
A	207	LYS	HG3	1.483	-1.0	4
A	233	PRO	HB2	1.921	-1.0	2
A	224	ALA	CA	48.05	-1.0	1
A	252	VAL	CB	32.04	-1.0	1
A	234	ILE	HD12	0.727	-1.0	1
A	183	VAL	CB	33.23	-1.0	1
A	175	LEU	HA	3.933	-1.0	1
A	175	LEU	N	117.0	-1.0	1
A	251	ILE	CA	59.03	-1.0	1
A	145	ALA	HB2	1.535	-1.0	1
A	181	ALA	CB	17.26	-1.0	1
A	140	GLN	CA	56.91	-1.0	1
A	218	VAL	HG22	0.915	-1.0	2
A	228	LEU	CA	52.05	-1.0	1
A	155	ASN	HB2	2.838	-1.0	2
A	239	THR	H	7.14	-1.0	1
A	159	SER	HA	4.205	-1.0	1
A	215	ALA	HB3	1.368	-1.0	1
A	199	ILE	HG23	0.873	-1.0	1
A	154	GLY	H	8.417	-1.0	1
A	248	ARG	HA	5.576	-1.0	1
A	205	ARG	N	117.7	-1.0	1
A	219	ALA	CA	50.69	-1.0	1
A	210	ALA	HB2	1.466	-1.0	1
A	197	ILE	HG12	1.481	-1.0	2
A	207	LYS	C	175.1	-1.0	1
A	170	ARG	CA	57.06	-1.0	1
A	203	ALA	CA	52.51	-1.0	1
A	230	SER	HB3	3.598	-1.0	2
A	214	VAL	HG13	1.038	-1.0	2
A	155	ASN	H	8.527	-1.0	1
A	201	LEU	C	176.9	-1.0	1
A	202	SER	CB	59.89	-1.0	1
A	185	ILE	HG13	1.353	-1.0	2
A	223	ILE	HG12	1.642	-1.0	2
A	137	ALA	N	123.8	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	238	ALA	H	8.466	-1.0	1
A	193	GLY	N	108.6	-1.0	1
A	252	VAL	H	9.236	-1.0	1
A	140	GLN	HG3	2.275	-1.0	2
A	215	ALA	HB2	1.368	-1.0	1
A	248	ARG	N	121.2	-1.0	1
A	133	SER	CA	55.47	-1.0	1
A	237	ASN	HB3	2.481	-1.0	2
A	221	ASP	N	115.3	-1.0	1
A	253	VAL	HG21	0.725	-1.0	2
A	147	THR	N	108.5	-1.0	1
A	241	GLU	CA	57.43	-1.0	1
A	251	ILE	HD11	0.68	-1.0	1
A	223	ILE	HG23	0.746	-1.0	1
A	148	GLY	C	171.5	-1.0	1
A	195	GLU	N	126.4	-1.0	1
A	216	ARG	CB	26.76	-1.0	1
A	170	ARG	C	177.8	-1.0	1
A	189	THR	N	111.5	-1.0	1
A	145	ALA	CA	52.21	-1.0	1
A	183	VAL	HG12	0.773	-1.0	2
A	183	VAL	HA	5.238	-1.0	1
A	210	ALA	H	8.613	-1.0	1
A	169	ASN	CB	34.57	-1.0	1
A	228	LEU	HD21	0.555	-1.0	2
A	145	ALA	C	177.4	-1.0	1
A	197	ILE	HG23	0.909	-1.0	1
A	159	SER	HB2	3.772	-1.0	2
A	185	ILE	HB	2.073	-1.0	1
A	208	ILE	HB	2.232	-1.0	1
A	214	VAL	HG21	0.953	-1.0	2
A	253	VAL	HG23	0.725	-1.0	2
A	177	ALA	HB1	1.522	-1.0	1
A	133	SER	HB3	3.843	-1.0	2
A	252	VAL	N	130.5	-1.0	1
A	204	GLN	HG2	2.491	-1.0	2
A	235	ALA	HA	4.532	-1.0	1
A	234	ILE	HB	2.172	-1.0	1
A	226	VAL	H	8.686	-1.0	1
A	206	ALA	N	118.5	-1.0	1
A	212	TYR	HB2	3.288	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	249	VAL	HG22	0.948	-1.0	2
A	137	ALA	HB2	1.336	-1.0	1
A	161	ILE	N	114.8	-1.0	1
A	252	VAL	HG22	0.68	-1.0	2
A	214	VAL	CA	62.84	-1.0	1
A	171	VAL	HG23	0.857	-1.0	2
A	248	ARG	CA	52.23	-1.0	1
A	140	GLN	HB2	2.25	-1.0	2
A	206	ALA	HB3	1.33	-1.0	1
A	150	PRO	HG3	2.11	-1.0	2
A	217	GLY	HA2	4.326	-1.0	2
A	134	GLY	N	110.0	-1.0	1
A	227	GLY	HA2	4.134	-1.0	2
A	164	ASP	H	8.142	-1.0	1
A	241	GLU	N	118.0	-1.0	1
A	223	ILE	HG22	0.746	-1.0	1
A	250	GLU	HB3	2.06	-1.0	2
A	243	ARG	H	8.014	-1.0	1
A	139	LEU	CA	55.48	-1.0	1
A	136	CYS	H	8.54	-1.0	1
A	225	THR	CA	68.53	-1.0	1
A	183	VAL	N	113.6	-1.0	1
A	151	ILE	H	9.157	-1.0	1
A	245	LYS	CA	55.36	-1.0	1
A	185	ILE	C	171.2	-1.0	1
A	147	THR	H	8.533	-1.0	1
A	143	ILE	H	8.643	-1.0	1
A	195	GLU	HA	4.223	-1.0	1
A	198	ASN	HA	4.543	-1.0	1
A	218	VAL	HG12	0.915	-1.0	2
A	226	VAL	HG23	0.749	-1.0	2
A	149	GLY	N	107.5	-1.0	1
A	152	ALA	N	130.3	-1.0	1
A	177	ALA	C	174.5	-1.0	1
A	242	GLY	H	8.106	-1.0	1
A	192	THR	H	8.216	-1.0	1
A	158	ALA	HB1	1.4	-1.0	1
A	171	VAL	HB	2.307	-1.0	1
A	228	LEU	HD12	0.669	-1.0	2
A	190	ASP	CA	51.74	-1.0	1
A	242	GLY	CA	44.64	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	223	ILE	HB	1.71	-1.0	1
A	206	ALA	CA	53.01	-1.0	1
A	189	THR	HA	4.344	-1.0	1
A	158	ALA	HA	4.367	-1.0	1
A	142	ALA	HB3	1.548	-1.0	1
A	148	GLY	H	8.265	-1.0	1
A	175	LEU	HD11	0.745	-1.0	2
A	201	LEU	HD22	0.899	-1.0	2
A	219	ALA	HB1	1.243	-1.0	1
A	218	VAL	H	7.947	-1.0	1
A	151	ILE	HG23	0.778	-1.0	1
A	220	GLY	C	173.4	-1.0	1
A	143	ILE	HD13	0.941	-1.0	1
A	197	ILE	HD13	0.837	-1.0	1
A	147	THR	HG22	1.11	-1.0	1
A	167	ILE	HG22	0.946	-1.0	1
A	144	ASN	HA	4.58	-1.0	1
A	238	ALA	C	175.0	-1.0	1
A	147	THR	CB	66.32	-1.0	1
A	143	ILE	CB	34.76	-1.0	1
A	155	ASN	C	173.2	-1.0	1
A	133	SER	H	8.179	-1.0	1
A	230	SER	HA	4.665	-1.0	1
A	151	ILE	HD13	0.692	-1.0	1
A	177	ALA	CA	50.48	-1.0	1
A	145	ALA	HB1	1.535	-1.0	1
A	245	LYS	CB	29.83	-1.0	1
A	233	PRO	HD2	3.656	-1.0	2
A	182	ARG	H	8.65	-1.0	1
A	188	TYR	HA	5.565	-1.0	1
A	142	ALA	H	7.904	-1.0	1
A	166	GLU	HB2	2.148	-1.0	2
A	202	SER	HB3	3.848	-1.0	2
A	199	ILE	HG13	1.775	-1.0	2
A	184	THR	HB	3.874	-1.0	1
A	253	VAL	HB	1.963	-1.0	1
A	174	LYS	HB3	1.666	-1.0	2
A	152	ALA	H	8.356	-1.0	1
A	138	ASP	HA	4.711	-1.0	1
A	230	SER	N	119.8	-1.0	1
A	220	GLY	H	8.869	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	233	PRO	CA	61.53	-1.0	1
A	235	ALA	HB3	1.291	-1.0	1
A	241	GLU	HB2	2.006	-1.0	2
A	215	ALA	HB1	1.368	-1.0	1
A	133	SER	CB	62.13	-1.0	1
A	232	ASN	H	8.662	-1.0	1
A	141	SER	CB	59.9	-1.0	1
A	253	VAL	H	8.955	-1.0	1
A	253	VAL	HG22	0.725	-1.0	2
A	169	ASN	HB2	3.283	-1.0	2
A	185	ILE	CA	57.04	-1.0	1
A	208	ILE	H	8.173	-1.0	1
A	199	ILE	HG21	0.873	-1.0	1
A	138	ASP	N	119.2	-1.0	1
A	148	GLY	HA2	4.026	-1.0	2
A	243	ARG	CB	28.24	-1.0	1
A	180	ASP	C	174.5	-1.0	1
A	142	ALA	CB	16.27	-1.0	1
A	171	VAL	HG11	1.002	-1.0	2
A	135	PRO	HD3	3.635	-1.0	2
A	197	ILE	HA	4.213	-1.0	1
A	151	ILE	HG12	1.317	-1.0	2
A	156	ASP	HB3	2.714	-1.0	2
A	247	ARG	CA	53.78	-1.0	1
A	223	ILE	HG21	0.746	-1.0	1
A	218	VAL	C	172.7	-1.0	1
A	150	PRO	HA	4.623	-1.0	1
A	245	LYS	HB3	1.596	-1.0	2
A	166	GLU	N	117.2	-1.0	1
A	167	ILE	HG13	1.155	-1.0	2
A	135	PRO	CA	62.09	-1.0	1
A	247	ARG	HG2	1.375	-1.0	2
A	177	ALA	HB2	1.522	-1.0	1
A	175	LEU	H	7.892	-1.0	1
A	211	ASP	C	177.2	-1.0	1
A	138	ASP	HB2	2.861	-1.0	2
A	234	ILE	HA	4.244	-1.0	1
A	203	ALA	HB1	1.485	-1.0	1
A	240	PRO	HA	4.142	-1.0	1
A	139	LEU	HB2	1.691	-1.0	2
A	187	GLY	N	109.5	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	219	ALA	CB	16.19	-1.0	1
A	254	ASN	HA	4.416	-1.0	1
A	170	ARG	H	7.77	-1.0	1
A	161	ILE	H	6.523	-1.0	1
A	199	ILE	HG12	1.775	-1.0	2
A	222	HIS	H	8.21	-1.0	1
A	244	ALA	C	178.1	-1.0	1
A	147	THR	C	175.0	-1.0	1
A	243	ARG	HG2	2.127	-1.0	2
A	237	ASN	C	173.1	-1.0	1
A	138	ASP	CA	51.17	-1.0	1
A	153	PHE	H	8.986	-1.0	1
A	217	GLY	HA3	3.648	-1.0	2
A	182	ARG	HB2	1.838	-1.0	2
A	143	ILE	HG23	1.178	-1.0	1
A	151	ILE	HB	1.546	-1.0	1
A	208	ILE	N	119.3	-1.0	1
A	198	ASN	CB	35.85	-1.0	1
A	211	ASP	HB3	2.597	-1.0	2
A	250	GLU	HG3	2.296	-1.0	2
A	171	VAL	CA	65.1	-1.0	1
A	201	LEU	HB2	1.743	-1.0	2
A	154	GLY	HA3	3.951	-1.0	2
A	192	THR	HG23	1.192	-1.0	1
A	231	VAL	CA	59.19	-1.0	1
A	212	TYR	HB3	3.173	-1.0	2
A	223	ILE	HA	4.835	-1.0	1
A	243	ARG	C	176.7	-1.0	1
A	205	ARG	HB3	1.175	-1.0	2
A	239	THR	N	105.0	-1.0	1
A	218	VAL	HA	3.65	-1.0	1
A	244	ALA	CB	15.71	-1.0	1
A	240	PRO	HD2	4.023	-1.0	2
A	248	ARG	HB2	1.746	-1.0	2
A	225	THR	HG23	0.979	-1.0	1
A	174	LYS	HA	4.101	-1.0	1
A	201	LEU	HD12	0.899	-1.0	2
A	204	GLN	CA	56.59	-1.0	1
A	180	ASP	H	8.399	-1.0	1
A	231	VAL	HB	2.288	-1.0	1
A	197	ILE	CA	59.27	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	147	THR	HG21	1.11	-1.0	1
A	167	ILE	HG21	0.946	-1.0	1
A	160	LEU	N	121.9	-1.0	1
A	237	ASN	N	123.3	-1.0	1
A	141	SER	N	114.2	-1.0	1
A	167	ILE	HD13	0.83	-1.0	1
A	139	LEU	HD12	0.942	-1.0	2
A	251	ILE	H	8.613	-1.0	1
A	137	ALA	H	7.537	-1.0	1
A	143	ILE	CA	62.53	-1.0	1
A	228	LEU	HG	1.104	-1.0	1
A	238	ALA	HB3	1.426	-1.0	1
A	170	ARG	HG3	2.061	-1.0	2
A	184	THR	N	122.6	-1.0	1
A	139	LEU	HD22	0.912	-1.0	2
A	198	ASN	C	176.1	-1.0	1
A	226	VAL	HG12	0.749	-1.0	2
A	188	TYR	N	118.3	-1.0	1
A	212	TYR	C	174.9	-1.0	1
A	231	VAL	HG11	1.099	-1.0	2
A	169	ASN	HA	4.393	-1.0	1
A	243	ARG	HB2	1.951	-1.0	2
A	209	VAL	HG21	0.957	-1.0	2
A	197	ILE	N	118.2	-1.0	1
A	244	ALA	HB3	1.458	-1.0	1
A	186	ASN	HB3	2.074	-1.0	2
A	157	GLY	H	8.106	-1.0	1
A	205	ARG	CB	26.85	-1.0	1
A	231	VAL	N	117.7	-1.0	1
A	184	THR	HA	4.853	-1.0	1
A	186	ASN	C	172.7	-1.0	1
A	187	GLY	HA2	4.89	-1.0	2
A	143	ILE	C	175.8	-1.0	1
A	172	ALA	CA	53.32	-1.0	1
A	153	PHE	C	174.2	-1.0	1
A	232	ASN	HA	4.342	-1.0	1
A	213	LEU	HB3	1.459	-1.0	2
A	202	SER	C	173.6	-1.0	1
A	147	THR	HA	4.153	-1.0	1
A	233	PRO	CB	28.63	-1.0	1
A	137	ALA	CB	16.46	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	222	HIS	C	169.7	-1.0	1
A	199	ILE	HB	2.07	-1.0	1
A	150	PRO	HB2	1.96	-1.0	2
A	199	ILE	HD13	0.847	-1.0	1
A	228	LEU	HB3	1.19	-1.0	2
A	141	SER	CA	59.9	-1.0	1
A	135	PRO	HB2	2.07	-1.0	2
A	207	LYS	HG2	1.483	-1.0	4
A	152	ALA	HA	4.79	-1.0	1
A	189	THR	HG23	1.201	-1.0	1
A	201	LEU	HD11	0.899	-1.0	2
A	234	ILE	HD13	0.727	-1.0	1
A	185	ILE	N	126.7	-1.0	1
A	134	GLY	H	8.332	-1.0	1
A	145	ALA	CB	15.64	-1.0	1
A	231	VAL	H	6.939	-1.0	1
A	225	THR	HB	3.956	-1.0	1
A	247	ARG	CB	26.82	-1.0	1
A	194	SER	HB3	3.886	-1.0	2
A	151	ILE	N	122.7	-1.0	1
A	139	LEU	HD11	0.942	-1.0	2
A	155	ASN	HB3	2.719	-1.0	2
A	250	GLU	HB2	2.135	-1.0	2
A	249	VAL	CB	33.76	-1.0	1
A	184	THR	HG21	1.008	-1.0	1
A	197	ILE	HB	1.964	-1.0	1
A	141	SER	C	174.7	-1.0	1
A	187	GLY	H	9.236	-1.0	1
A	210	ALA	HB3	1.466	-1.0	1
A	182	ARG	CA	52.36	-1.0	1
A	247	ARG	HD2	3.307	-1.0	2
A	246	ASN	CB	35.72	-1.0	1
A	252	VAL	CA	58.88	-1.0	1
A	184	THR	C	169.7	-1.0	1
A	167	ILE	H	7.116	-1.0	1
A	228	LEU	C	176.0	-1.0	1
A	216	ARG	HA	4.175	-1.0	1
A	174	LYS	HG3	1.312	-1.0	4
A	213	LEU	C	177.5	-1.0	1
A	218	VAL	CA	60.93	-1.0	1
A	193	GLY	HA3	3.962	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	178	CYS	H	7.323	-1.0	1
A	241	GLU	HG2	2.4	-1.0	2
A	237	ASN	HB2	3.151	-1.0	2
A	203	ALA	C	177.4	-1.0	1
A	179	PRO	HG2	2.271	-1.0	2
A	136	CYS	HA	4.731	-1.0	1
A	221	ASP	H	8.338	-1.0	1
A	247	ARG	HA	4.153	-1.0	1
A	234	ILE	CA	58.57	-1.0	1
A	168	LEU	H	8.46	-1.0	1
A	151	ILE	HA	3.966	-1.0	1
A	183	VAL	HG11	0.773	-1.0	2
A	188	TYR	CB	42.49	-1.0	1
A	169	ASN	CA	53.89	-1.0	1
A	228	LEU	HD22	0.555	-1.0	2
A	159	SER	HB3	3.772	-1.0	2
A	225	THR	H	8.448	-1.0	1
A	226	VAL	CA	59.42	-1.0	1
A	143	ILE	HA	3.699	-1.0	1
A	166	GLU	H	8.136	-1.0	1
A	193	GLY	C	171.4	-1.0	1
A	148	GLY	CA	43.97	-1.0	1
A	245	LYS	HA	4.016	-1.0	1
A	190	ASP	HB3	3.027	-1.0	2
A	216	ARG	HB2	2.114	-1.0	2
A	223	ILE	CA	58.21	-1.0	1
A	218	VAL	HB	1.452	-1.0	1
A	234	ILE	C	172.7	-1.0	1
A	223	ILE	HD11	0.651	-1.0	1
A	135	PRO	HG2	2.298	-1.0	2
A	149	GLY	HA3	3.629	-1.0	2
A	249	VAL	HG21	0.948	-1.0	2
A	137	ALA	HB3	1.336	-1.0	1
A	245	LYS	N	116.7	-1.0	1
A	174	LYS	H	7.47	-1.0	1
A	179	PRO	CB	29.61	-1.0	1
A	171	VAL	HG22	0.857	-1.0	2
A	231	VAL	HA	4.129	-1.0	1
A	226	VAL	HB	2.282	-1.0	1
A	227	GLY	C	170.4	-1.0	1
A	206	ALA	HB2	1.33	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	197	ILE	CB	36.25	-1.0	1
A	150	PRO	HG2	2.18	-1.0	2
A	141	SER	HB3	3.897	-1.0	2
A	201	LEU	HD13	0.899	-1.0	2
A	145	ALA	N	122.1	-1.0	1
A	166	GLU	HG3	2.333	-1.0	2
A	207	LYS	H	8.173	-1.0	1
A	236	SER	H	8.411	-1.0	1
A	240	PRO	C	177.5	-1.0	1
A	188	TYR	CA	54.89	-1.0	1
A	139	LEU	CB	40.25	-1.0	1
A	234	ILE	N	116.1	-1.0	1
A	225	THR	CB	57.32	-1.0	1
A	202	SER	H	8.35	-1.0	1
A	139	LEU	HD21	0.912	-1.0	2
A	169	ASN	N	120.3	-1.0	1
A	242	GLY	N	111.5	-1.0	1
A	252	VAL	C	173.0	-1.0	1
A	157	GLY	N	106.6	-1.0	1
A	230	SER	C	173.7	-1.0	1
A	209	VAL	CA	64.85	-1.0	1
A	218	VAL	HG11	0.915	-1.0	2
A	249	VAL	N	115.4	-1.0	1
A	142	ALA	HA	4.211	-1.0	1
A	229	GLY	H	8.698	-1.0	1
A	245	LYS	C	175.2	-1.0	1
A	183	VAL	H	8.436	-1.0	1
A	203	ALA	N	126.7	-1.0	1
A	222	HIS	HB3	3.268	-1.0	2
A	144	ASN	CA	53.05	-1.0	1
A	231	VAL	HG21	1.099	-1.0	2
A	185	ILE	H	9.175	-1.0	1
A	147	THR	HB	4.502	-1.0	1
A	136	CYS	C	173.0	-1.0	1
A	175	LEU	HD12	0.745	-1.0	2
A	237	ASN	HA	4.783	-1.0	1
A	235	ALA	N	126.9	-1.0	1
A	143	ILE	HD12	0.941	-1.0	1
A	136	CYS	HB2	3.289	-1.0	2
A	133	SER	N	114.0	-1.0	1
A	201	LEU	HG	1.497	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	155	ASN	HA	4.718	-1.0	1
A	245	LYS	H	7.262	-1.0	1
A	213	LEU	HD21	0.741	-1.0	2
A	147	THR	CA	61.1	-1.0	1
A	204	GLN	HB2	2.247	-1.0	2
A	209	VAL	HG11	1.166	-1.0	2
A	248	ARG	H	7.415	-1.0	1
A	238	ALA	N	121.8	-1.0	1
A	228	LEU	H	8.491	-1.0	1
A	242	GLY	HA2	4.365	-1.0	2
A	226	VAL	HA	4.191	-1.0	1
A	225	THR	HA	5.135	-1.0	1
A	236	SER	N	113.0	-1.0	1
A	180	ASP	HA	4.802	-1.0	1
A	136	CYS	CA	52.67	-1.0	1
A	233	PRO	HD3	3.656	-1.0	2
A	249	VAL	CA	57.12	-1.0	1
A	155	ASN	CA	51.01	-1.0	1
A	175	LEU	HD23	0.718	-1.0	2
A	184	THR	HG22	1.008	-1.0	1
A	166	GLU	HB3	1.916	-1.0	2
A	252	VAL	HG13	0.871	-1.0	2
A	240	PRO	CB	29.2	-1.0	1
A	224	ALA	HB3	1.417	-1.0	1
A	253	VAL	HG12	1.083	-1.0	2
A	214	VAL	HG11	1.038	-1.0	2
A	174	LYS	HB2	2.063	-1.0	2
A	232	ASN	N	114.3	-1.0	1
A	253	VAL	HG13	1.083	-1.0	2
A	253	VAL	C	172.8	-1.0	1
A	212	TYR	CB	36.31	-1.0	1
A	144	ASN	HB2	3.005	-1.0	2
A	172	ALA	HB2	1.523	-1.0	1
A	235	ALA	HB2	1.291	-1.0	1
A	219	ALA	N	130.2	-1.0	1
A	241	GLU	HB3	1.898	-1.0	2
A	179	PRO	HG3	2.271	-1.0	2
A	253	VAL	CA	59.7	-1.0	1
A	228	LEU	HD13	0.669	-1.0	2
A	185	ILE	HG22	1.229	-1.0	1
A	254	ASN	HB3	2.464	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	213	LEU	HD13	0.866	-1.0	2
A	214	VAL	HA	4.404	-1.0	1
A	186	ASN	H	8.802	-1.0	1
A	239	THR	HG22	1.196	-1.0	1
A	183	VAL	C	173.0	-1.0	1
A	203	ALA	CB	15.36	-1.0	1
A	209	VAL	HA	3.627	-1.0	1
A	215	ALA	N	125.2	-1.0	1
A	210	ALA	CA	53.94	-1.0	1
A	251	ILE	HD13	0.68	-1.0	1
A	139	LEU	N	121.0	-1.0	1
A	252	VAL	HG11	0.871	-1.0	2
A	181	ALA	HA	4.268	-1.0	1
A	225	THR	N	112.0	-1.0	1
A	171	VAL	H	8.375	-1.0	1
A	171	VAL	HG12	1.002	-1.0	2
A	201	LEU	HD23	0.899	-1.0	2
A	135	PRO	HD2	3.777	-1.0	2
A	156	ASP	HB2	2.714	-1.0	2
A	197	ILE	HG21	0.909	-1.0	1
A	244	ALA	HA	3.913	-1.0	1
A	223	ILE	CB	38.77	-1.0	1
A	198	ASN	N	119.9	-1.0	1
A	155	ASN	N	118.0	-1.0	1
A	154	GLY	HA2	4.106	-1.0	2
A	177	ALA	HB3	1.522	-1.0	1
A	178	CYS	HB2	3.244	-1.0	2
A	220	GLY	N	111.6	-1.0	1
A	229	GLY	HA3	3.09	-1.0	2
A	234	ILE	HG12	1.792	-1.0	2
A	203	ALA	HB2	1.485	-1.0	1
A	204	GLN	N	120.2	-1.0	1
A	145	ALA	H	7.977	-1.0	1
A	139	LEU	HB3	1.691	-1.0	2
A	248	ARG	C	171.4	-1.0	1
A	225	THR	HG21	0.979	-1.0	1
A	231	VAL	HG12	1.099	-1.0	2
A	206	ALA	HB1	1.33	-1.0	1
A	222	HIS	N	117.5	-1.0	1
A	194	SER	HA	4.63	-1.0	1
A	237	ASN	CB	37.15	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	216	ARG	HG3	1.477	-1.0	2
A	140	GLN	HA	3.807	-1.0	1
A	179	PRO	HD2	3.705	-1.0	2
A	210	ALA	N	122.8	-1.0	1
A	228	LEU	HA	4.321	-1.0	1
A	156	ASP	H	8.356	-1.0	1
A	242	GLY	C	173.6	-1.0	1
A	151	ILE	HG22	0.778	-1.0	1
A	252	VAL	HG23	0.68	-1.0	2
A	192	THR	C	173.0	-1.0	1
A	253	VAL	HA	4.361	-1.0	1
A	246	ASN	CA	52.43	-1.0	1
A	246	ASN	H	7.33	-1.0	1
A	171	VAL	HG21	0.857	-1.0	2
A	175	LEU	CB	39.18	-1.0	1
A	243	ARG	CA	58.34	-1.0	1
A	143	ILE	HG22	1.178	-1.0	1
A	163	ALA	N	118.0	-1.0	1
A	221	ASP	HB2	2.997	-1.0	2
A	215	ALA	H	7.953	-1.0	1
A	236	SER	HB2	4.019	-1.0	2
A	198	ASN	CA	53.47	-1.0	1
A	211	ASP	HB2	2.844	-1.0	2
A	250	GLU	HG2	2.296	-1.0	2
A	250	GLU	CA	52.39	-1.0	1
A	202	SER	N	114.8	-1.0	1
A	254	ASN	HB2	2.771	-1.0	2
A	169	ASN	H	8.662	-1.0	1
A	158	ALA	HB3	1.4	-1.0	1
A	151	ILE	C	172.2	-1.0	1
A	192	THR	HG22	1.192	-1.0	1
A	231	VAL	CB	30.04	-1.0	1
A	239	THR	HG23	1.196	-1.0	1
A	195	GLU	HB2	2.075	-1.0	2
A	201	LEU	HA	4.221	-1.0	1
A	231	VAL	HG22	1.099	-1.0	2
A	195	GLU	H	9.334	-1.0	1
A	237	ASN	H	8.515	-1.0	1
A	172	ALA	C	176.3	-1.0	1
A	144	ASN	HB3	2.871	-1.0	2
A	179	PRO	HB3	1.901	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	243	ARG	N	118.6	-1.0	1
A	143	ILE	HD11	0.941	-1.0	1
A	135	PRO	HA	4.446	-1.0	1
A	202	SER	CA	59.89	-1.0	1
A	231	VAL	C	171.1	-1.0	1
A	183	VAL	HG21	0.773	-1.0	2
A	213	LEU	HD22	0.741	-1.0	2
A	251	ILE	HG23	0.779	-1.0	1
A	167	ILE	N	117.7	-1.0	1
A	220	GLY	HA2	3.916	-1.0	2
A	167	ILE	HD12	0.83	-1.0	1
A	139	LEU	HD13	0.942	-1.0	2
A	190	ASP	N	117.0	-1.0	1
A	215	ALA	CB	14.81	-1.0	1
A	249	VAL	HG13	0.948	-1.0	2
A	209	VAL	HG12	1.166	-1.0	2
A	174	LYS	HD3	1.803	-1.0	4
A	234	ILE	HG21	0.852	-1.0	1
A	187	GLY	C	169.2	-1.0	1
A	151	ILE	HD11	0.692	-1.0	1
A	226	VAL	HG11	0.749	-1.0	2
A	135	PRO	HB3	1.996	-1.0	2
A	188	TYR	HB3	2.715	-1.0	2
A	241	GLU	CB	25.99	-1.0	1
A	170	ARG	HB3	1.815	-1.0	2
A	252	VAL	HA	4.702	-1.0	1
A	181	ALA	HB3	1.384	-1.0	1
A	247	ARG	N	117.7	-1.0	1
A	136	CYS	CB	38.32	-1.0	1
A	241	GLU	HA	4.032	-1.0	1
A	195	GLU	HG3	2.425	-1.0	2
A	211	ASP	N	115.9	-1.0	1
A	155	ASN	CB	36.43	-1.0	1
A	221	ASP	HA	4.675	-1.0	1
A	243	ARG	HB3	1.904	-1.0	2
A	244	ALA	HB2	1.458	-1.0	1
A	215	ALA	CA	52.46	-1.0	1
A	187	GLY	HA3	3.809	-1.0	2
A	218	VAL	HG21	0.915	-1.0	2
A	182	ARG	HB3	1.545	-1.0	2
A	233	PRO	C	176.0	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	208	ILE	CB	35.62	-1.0	1
A	183	VAL	HG22	0.773	-1.0	2
A	187	GLY	CA	41.96	-1.0	1
A	229	GLY	CA	44.06	-1.0	1
A	208	ILE	CA	62.48	-1.0	1
A	185	ILE	HG21	1.229	-1.0	1
A	150	PRO	HB3	1.85	-1.0	2
A	228	LEU	HB2	1.42	-1.0	2
A	214	VAL	HB	2.091	-1.0	1
A	174	LYS	N	118.4	-1.0	1
A	210	ALA	CB	17.44	-1.0	1
A	218	VAL	CB	28.9	-1.0	1
A	238	ALA	HB1	1.426	-1.0	1
A	189	THR	HG22	1.201	-1.0	1
A	203	ALA	HA	3.82	-1.0	1
A	213	LEU	H	8.21	-1.0	1
A	180	ASP	CA	52.25	-1.0	1
A	170	ARG	HA	4.241	-1.0	1
A	249	VAL	HA	5.625	-1.0	1
A	238	ALA	CB	17.1	-1.0	1
A	211	ASP	HA	4.281	-1.0	1
A	153	PHE	N	120.7	-1.0	1
A	209	VAL	N	119.0	-1.0	1
A	194	SER	HB2	4.035	-1.0	2
A	251	ILE	C	172.6	-1.0	1
A	218	VAL	HG23	0.915	-1.0	2
A	234	ILE	H	7.66	-1.0	1
A	238	ALA	HB2	1.426	-1.0	1
A	167	ILE	HA	3.536	-1.0	1
A	240	PRO	CA	62.93	-1.0	1
A	182	ARG	CB	29.78	-1.0	1
A	247	ARG	HD3	3.078	-1.0	2
A	143	ILE	HG12	1.655	-1.0	2
A	137	ALA	HA	4.196	-1.0	1
A	188	TYR	C	174.0	-1.0	1
A	207	LYS	CB	30.08	-1.0	1
A	201	LEU	CA	56.05	-1.0	1
A	242	GLY	HA3	3.534	-1.0	2
A	193	GLY	HA2	3.962	-1.0	2
A	213	LEU	CB	38.29	-1.0	1
A	223	ILE	H	7.342	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	197	ILE	HD11	0.837	-1.0	1
A	237	ASN	CA	52.27	-1.0	1
A	182	ARG	C	173.2	-1.0	1
A	175	LEU	C	177.7	-1.0	1
A	245	LYS	HG3	1.291	-1.0	4
A	224	ALA	N	130.2	-1.0	1
A	217	GLY	N	105.4	-1.0	1
A	202	SER	HB2	3.848	-1.0	2
A	180	ASP	N	115.1	-1.0	1
A	192	THR	N	114.1	-1.0	1
A	235	ALA	H	8.619	-1.0	1
A	234	ILE	CB	36.69	-1.0	1
A	247	ARG	HB2	2.285	-1.0	2
A	172	ALA	H	8.601	-1.0	1
A	141	SER	H	7.861	-1.0	1
A	241	GLU	H	9.041	-1.0	1
A	192	THR	CB	67.49	-1.0	1
A	228	LEU	HD23	0.555	-1.0	2
A	226	VAL	CB	32.97	-1.0	1
A	226	VAL	C	172.0	-1.0	1
A	143	ILE	HB	2.024	-1.0	1
A	211	ASP	CB	37.33	-1.0	1
A	214	VAL	HG23	0.953	-1.0	2
A	203	ALA	H	8.026	-1.0	1
A	137	ALA	C	175.1	-1.0	1
A	190	ASP	HB2	3.151	-1.0	2
A	216	ARG	HB3	1.764	-1.0	2
A	223	ILE	HD12	0.651	-1.0	1
A	135	PRO	HG3	2.298	-1.0	2
A	239	THR	HA	5.023	-1.0	1
A	133	SER	HA	4.502	-1.0	1
A	179	PRO	CA	62.2	-1.0	1
A	193	GLY	CA	42.36	-1.0	1
A	197	ILE	C	175.4	-1.0	1
A	144	ASN	C	176.2	-1.0	1
A	192	THR	HA	4.188	-1.0	1
A	172	ALA	CB	15.78	-1.0	1
A	141	SER	HB2	3.897	-1.0	2
A	221	ASP	CA	51.83	-1.0	1
A	243	ARG	HD2	3.146	-1.0	2
A	166	GLU	HG2	2.333	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	174	LYS	CB	29.21	-1.0	1
A	175	LEU	HB2	1.806	-1.0	2
A	201	LEU	HB3	1.654	-1.0	2
A	219	ALA	H	8.313	-1.0	1
A	150	PRO	CA	60.29	-1.0	1
A	171	VAL	N	121.0	-1.0	1
A	250	GLU	CB	30.76	-1.0	1
A	251	ILE	HA	4.48	-1.0	1
A	211	ASP	H	9.291	-1.0	1
A	234	ILE	HG22	0.852	-1.0	1
A	216	ARG	HD2	2.88	-1.0	2
A	250	GLU	HA	5.032	-1.0	1
A	149	GLY	HA2	4.664	-1.0	2
A	152	ALA	HB2	1.376	-1.0	1
A	153	PHE	CB	39.18	-1.0	1
A	246	ASN	HB3	2.487	-1.0	2
A	179	PRO	C	174.5	-1.0	1
A	251	ILE	HG12	1.659	-1.0	2
A	207	LYS	HB2	2.053	-1.0	2
A	209	VAL	HG23	0.957	-1.0	2
A	169	ASN	C	176.0	-1.0	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	191	2.14 ± 0.10	Should be applied
$^{13}C_{\beta}$	181	2.73 ± 0.13	Should be applied
$^{13}C'$	193	2.43 ± 0.11	Should be applied
^{15}N	230	-0.70 ± 0.65	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 940 atoms were assigned a chemical shift out of a possible 1316. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	519/559 (93%)	222/222 (100%)	190/230 (83%)	107/107 (100%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	421/693 (61%)	329/400 (82%)	92/270 (34%)	0/23 (0%)
Aromatic	0/64 (0%)	0/34 (0%)	0/25 (0%)	0/5 (0%)
Overall	940/1316 (71%)	551/656 (84%)	282/525 (54%)	107/135 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1044 atoms were assigned a chemical shift out of a possible 1472. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	580/636 (91%)	252/252 (100%)	208/264 (79%)	120/120 (100%)
Sidechain	464/772 (60%)	364/448 (81%)	100/300 (33%)	0/24 (0%)
Aromatic	0/64 (0%)	0/34 (0%)	0/25 (0%)	0/5 (0%)
Overall	1044/1472 (71%)	616/734 (84%)	308/589 (52%)	120/149 (81%)

7.1.4 Statistically unusual chemical shifts (i)

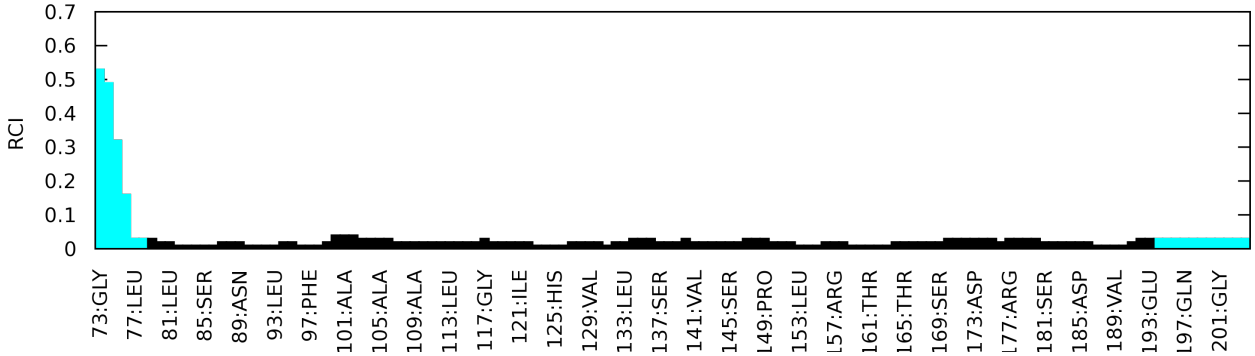
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	168	LEU	CB	25.03	51.69 – 32.89	-9.2
1	A	225	THR	CB	57.32	78.10 – 61.30	-7.4
1	A	83	SER	CB	54.64	71.24 – 56.34	-6.1
1	A	161	THR	CB	59.80	78.10 – 61.30	-5.9
1	A	230	SER	CB	55.73	71.24 – 56.34	-5.4

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
73:GLY
77:LEU
81:LEU
85:SER
89:ASN
93:LEU
97:PHE
101:ALA
105:ALA
109:ALA
113:LEU
117:GLY
121:ILE
125:HIS
129:VAL
133:LEU
137:SER
141:VAL
145:SER
149:PRO
153:LEU
157:ARG
161:THR
165:THR
169:SER
173:ASP
177:ARG
181:SER
185:ASP
189:VAL
193:GLU
197:GLN
201:GLY