



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2ADN
Title : Solution structure of the bacterial antitoxin CcdA: Implications for DNA and toxin binding
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Deposited on : 2005-07-20

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

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

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

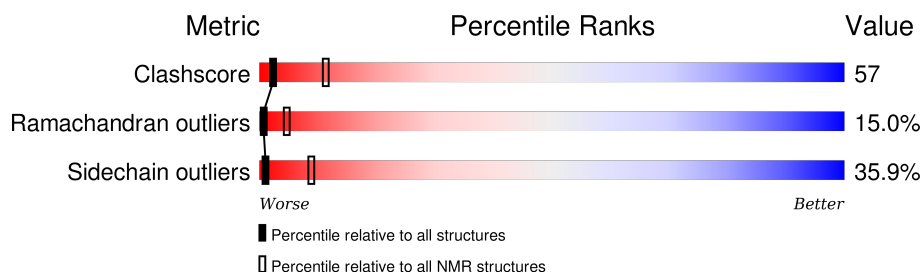
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	72	<div> <div>36%</div> <div>36%</div> <div>24%</div> <div>.</div> </div>
1	B	72	<div> <div>32%</div> <div>40%</div> <div>25%</div> <div>.</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2326 atoms, of which 1150 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CcdA.

Mol	Chain	Residues	Atoms						Trace
1	A	72	Total	C	H	N	O	S	0
			1163	362	575	105	117	4	
1	B	72	Total	C	H	N	O	S	0
			1163	362	575	105	117	4	

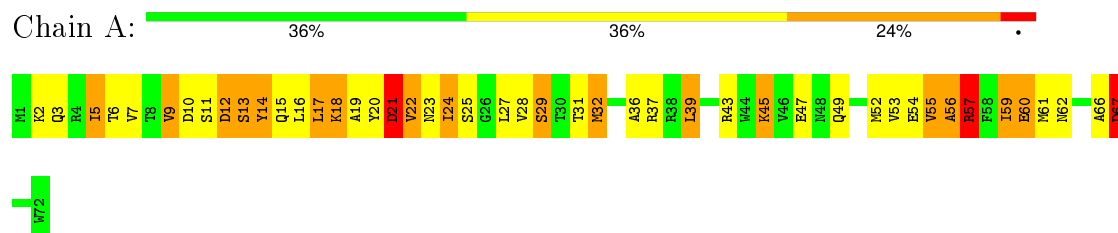
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	LYS	ARG	ENGINEERED	UNP Q9S0Z5
B	170	LYS	ARG	ENGINEERED	UNP Q9S0Z5

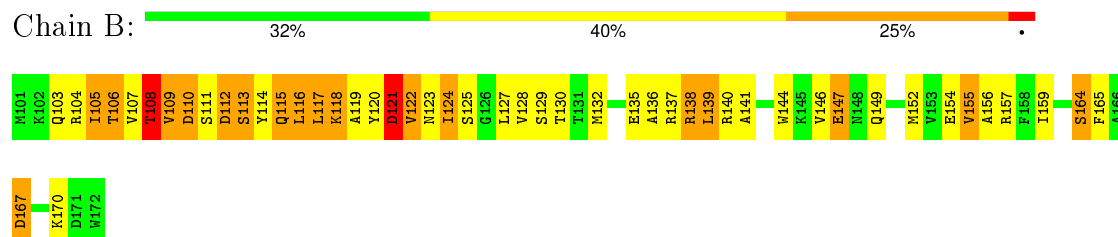
4 Residue-property plots [i](#)

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: CcdA



• Molecule 1: CcdA



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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

Chemical shift file(s)	BMRB entry 6743
Number of chemical shift lists	1
Total number of shifts	3758
Number of shifts mapped to atoms	1558
Number of unparsed shifts	2200
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	588	575	575	85
1	B	588	575	572	88
All	All	1176	1150	1147	132

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:9:VAL:HG21	1:A:14:TYR:CB	0.90	1.96
1:B:109:VAL:HG21	1:B:114:TYR:HB3	0.88	1.44
1:B:109:VAL:HG21	1:B:114:TYR:CB	0.85	2.02
1:B:132:MET:O	1:B:136:ALA:N	0.81	2.14
1:A:9:VAL:HG11	1:A:14:TYR:HB3	0.80	1.54
1:B:124:ILE:HD12	1:B:124:ILE:H	0.80	1.37
1:A:24:ILE:H	1:A:24:ILE:HD13	0.78	1.38
1:B:124:ILE:N	1:B:124:ILE:HD12	0.77	1.95
1:A:14:TYR:HA	1:B:132:MET:HG3	0.76	1.57
1:A:32:MET:HG3	1:B:114:TYR:HA	0.76	1.57
1:A:9:VAL:HG21	1:A:14:TYR:HB3	0.74	1.57
1:A:32:MET:O	1:A:36:ALA:N	0.74	2.20
1:B:154:GLU:O	1:B:155:VAL:HG23	0.73	1.84
1:A:9:VAL:HG21	1:A:14:TYR:CG	0.71	2.21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:9:VAL:HG13	1:A:12:ASP:HB2	0.71	1.61
1:A:5:ILE:HG21	1:B:114:TYR:CD2	0.69	2.22
1:B:128:VAL:O	1:B:132:MET:HG2	0.68	1.87
1:B:109:VAL:HG12	1:B:110:ASP:N	0.68	2.04
1:A:20:TYR:CD2	1:B:139:LEU:HD11	0.68	2.24
1:A:17:LEU:HD21	1:B:135:GLU:HB3	0.65	1.68
1:A:32:MET:CE	1:B:124:ILE:HG21	0.64	2.22
1:A:9:VAL:CG1	1:A:14:TYR:HB3	0.64	2.21
1:B:109:VAL:HG11	1:B:114:TYR:HB3	0.64	1.69
1:A:14:TYR:CD1	1:B:105:ILE:HD13	0.63	2.29
1:A:9:VAL:CG2	1:A:14:TYR:HB3	0.63	2.24
1:A:21:ASP:O	1:A:23:ASN:N	0.63	2.32
1:B:109:VAL:HG13	1:B:112:ASP:HB2	0.63	1.69
1:A:17:LEU:HD21	1:B:135:GLU:CB	0.63	2.22
1:A:32:MET:SD	1:B:124:ILE:HG21	0.62	2.34
1:A:24:ILE:HD13	1:A:24:ILE:N	0.62	2.09
1:A:28:VAL:O	1:A:31:THR:HG22	0.62	1.94
1:B:109:VAL:CG2	1:B:114:TYR:HB3	0.61	2.21
1:A:28:VAL:O	1:A:32:MET:HG2	0.60	1.94
1:B:121:ASP:O	1:B:123:ASN:N	0.59	2.35
1:B:107:VAL:O	1:B:109:VAL:HG23	0.58	1.98
1:B:154:GLU:O	1:B:155:VAL:CG2	0.58	2.51
1:A:5:ILE:HG21	1:B:114:TYR:CG	0.57	2.34
1:A:9:VAL:HG13	1:A:12:ASP:CB	0.57	2.29
1:A:28:VAL:HG13	1:B:128:VAL:CG2	0.57	2.29
1:A:20:TYR:CD2	1:B:139:LEU:CD1	0.56	2.89
1:A:24:ILE:O	1:A:27:LEU:HB3	0.56	2.00
1:B:109:VAL:HG13	1:B:112:ASP:CB	0.56	2.30
1:A:36:ALA:HB1	1:B:116:LEU:HD13	0.55	1.77
1:B:124:ILE:N	1:B:124:ILE:CD1	0.55	2.64
1:B:108:THR:HG22	1:B:108:THR:O	0.54	2.01
1:A:7:VAL:CG2	1:A:7:VAL:O	0.54	2.56
1:B:110:ASP:HA	1:B:115:GLN:CD	0.53	2.23
1:A:19:ALA:O	1:A:67:ASP:HB2	0.53	2.04
1:B:155:VAL:HG12	1:B:155:VAL:O	0.52	2.03
1:A:14:TYR:CD2	1:A:15:GLN:N	0.52	2.78
1:A:24:ILE:O	1:A:27:LEU:N	0.52	2.43
1:B:105:ILE:O	1:B:105:ILE:CG1	0.52	2.58
1:A:7:VAL:HG22	1:A:7:VAL:O	0.51	2.05
1:B:154:GLU:O	1:B:155:VAL:CB	0.51	2.57
1:A:14:TYR:CD1	1:B:105:ILE:CD1	0.51	2.94
1:A:6:THR:HB	1:B:106:THR:HB	0.51	1.82

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:28:VAL:HG13	1:B:128:VAL:HG22	0.51	1.83
1:A:29:SER:O	1:B:113:SER:HB2	0.50	2.06
1:A:2:LYS:HB3	1:B:108:THR:HG23	0.50	1.84
1:B:105:ILE:HD11	1:B:128:VAL:HG11	0.50	1.83
1:B:109:VAL:O	1:B:110:ASP:HB3	0.50	2.06
1:A:5:ILE:HG23	1:B:107:VAL:O	0.50	2.07
1:A:24:ILE:CD1	1:A:24:ILE:N	0.50	2.75
1:B:109:VAL:HG13	1:B:112:ASP:CA	0.49	2.37
1:B:114:TYR:CD2	1:B:115:GLN:N	0.49	2.80
1:B:115:GLN:HA	1:B:118:LYS:CG	0.49	2.37
1:A:3:GLN:N	1:B:110:ASP:HB2	0.49	2.22
1:A:9:VAL:O	1:A:10:ASP:HB3	0.49	2.08
1:A:13:SER:CB	1:B:129:SER:O	0.49	2.61
1:B:124:ILE:O	1:B:128:VAL:N	0.48	2.38
1:B:119:ALA:O	1:B:167:ASP:HB3	0.48	2.08
1:A:39:LEU:HD21	1:B:120:TYR:CE2	0.48	2.44
1:B:109:VAL:CG1	1:B:114:TYR:HB3	0.48	2.38
1:A:24:ILE:O	1:A:28:VAL:N	0.47	2.46
1:A:20:TYR:CG	1:B:139:LEU:HD11	0.47	2.43
1:B:109:VAL:HG12	1:B:110:ASP:H	0.47	1.69
1:A:18:LYS:HA	1:A:22:VAL:HA	0.47	1.86
1:A:15:GLN:O	1:A:19:ALA:N	0.47	2.47
1:A:12:ASP:CB	1:B:129:SER:CB	0.47	2.93
1:A:9:VAL:C	1:A:11:SER:H	0.47	2.13
1:A:9:VAL:N	1:B:103:GLN:O	0.47	2.48
1:B:129:SER:HA	1:B:132:MET:CG	0.47	2.40
1:A:9:VAL:HG12	1:A:10:ASP:N	0.46	2.25
1:A:39:LEU:HD11	1:B:120:TYR:CD2	0.46	2.45
1:A:29:SER:CB	1:B:112:ASP:HB3	0.46	2.40
1:A:15:GLN:O	1:A:19:ALA:HB2	0.46	2.11
1:B:107:VAL:O	1:B:109:VAL:N	0.45	2.49
1:B:109:VAL:C	1:B:111:SER:H	0.45	2.15
1:A:5:ILE:HB	1:B:114:TYR:CZ	0.45	2.47
1:A:17:LEU:HB3	1:A:24:ILE:HG21	0.45	1.88
1:B:128:VAL:O	1:B:132:MET:CG	0.45	2.62
1:A:7:VAL:O	1:A:9:VAL:HG23	0.45	2.12
1:A:15:GLN:O	1:A:19:ALA:CB	0.45	2.64
1:B:118:LYS:HA	1:B:122:VAL:HA	0.45	1.89
1:A:10:ASP:HB2	1:B:103:GLN:N	0.45	2.26
1:A:24:ILE:HG13	1:B:132:MET:CE	0.45	2.42
1:B:135:GLU:O	1:B:139:LEU:HA	0.45	2.12
1:A:29:SER:O	1:B:113:SER:CB	0.44	2.64

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:127:LEU:O	1:B:130:THR:N	0.44	2.51
1:A:22:VAL:O	1:A:22:VAL:HG22	0.44	2.13
1:B:108:THR:CG2	1:B:108:THR:O	0.44	2.64
1:A:5:ILE:HG13	1:A:5:ILE:O	0.44	2.12
1:B:132:MET:O	1:B:136:ALA:CB	0.44	2.65
1:A:56:ALA:O	1:A:57:ARG:CB	0.44	2.64
1:A:24:ILE:O	1:A:25:SER:C	0.43	2.57
1:A:53:VAL:HG13	1:A:54:GLU:N	0.43	2.28
1:B:124:ILE:HA	1:B:127:LEU:CB	0.43	2.44
1:A:24:ILE:HA	1:A:27:LEU:CB	0.43	2.44
1:A:7:VAL:CG2	1:A:9:VAL:HG22	0.43	2.44
1:A:36:ALA:O	1:A:39:LEU:HD23	0.43	2.14
1:A:28:VAL:O	1:A:32:MET:CG	0.42	2.64
1:B:146:VAL:HG12	1:B:147:GLU:N	0.42	2.29
1:A:59:ILE:HG22	1:A:60:GLU:N	0.42	2.28
1:A:6:THR:OG1	1:B:104:ARG:HG2	0.42	2.13
1:A:32:MET:HB3	1:B:117:LEU:HD23	0.42	1.91
1:A:39:LEU:CD1	1:B:120:TYR:CD2	0.42	3.03
1:A:5:ILE:HD13	1:B:114:TYR:CE1	0.42	2.49
1:A:16:LEU:HB3	1:B:136:ALA:HB1	0.42	1.92
1:B:138:ARG:O	1:B:139:LEU:C	0.42	2.58
1:A:32:MET:CE	1:B:124:ILE:CG2	0.41	2.96
1:A:32:MET:O	1:A:36:ALA:CB	0.41	2.68
1:A:39:LEU:HD21	1:B:120:TYR:HE2	0.41	1.75
1:B:113:SER:O	1:B:114:TYR:C	0.41	2.58
1:B:105:ILE:O	1:B:105:ILE:HG13	0.41	2.16
1:A:3:GLN:O	1:B:108:THR:HA	0.41	2.16
1:A:3:GLN:O	1:B:109:VAL:N	0.41	2.54
1:B:119:ALA:C	1:B:120:TYR:CD1	0.41	2.94
1:A:5:ILE:HG12	1:B:114:TYR:CD1	0.40	2.51
1:B:117:LEU:O	1:B:121:ASP:N	0.40	2.54
1:A:18:LYS:HA	1:A:22:VAL:CA	0.40	2.46
1:A:20:TYR:O	1:A:21:ASP:CB	0.40	2.69
1:B:144:TRP:O	1:B:144:TRP:CG	0.40	2.74

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	70/72 (97%)	44 (63%)	14 (20%)	12 (17%)	0	3
1	B	70/72 (97%)	42 (60%)	19 (27%)	9 (13%)	1	6
All	All	140/144 (97%)	86 (61%)	33 (24%)	21 (15%)	1	5

All 21 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	164	SER
1	A	67	ASP
1	A	56	ALA
1	A	49	GLN
1	A	22	VAL
1	B	155	VAL
1	A	55	VAL
1	B	167	ASP
1	B	156	ALA
1	A	21	ASP
1	A	45	LYS
1	A	57	ARG
1	A	52	MET
1	B	108	THR
1	A	66	ALA
1	B	121	ASP
1	A	59	ILE
1	A	9	VAL
1	B	122	VAL
1	B	141	ALA
1	B	109	VAL

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	64/64 (100%)	43 (67%)	21 (33%)	1	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	64/64 (100%)	39 (61%)	25 (39%)	1	6
All	All	128/128 (100%)	82 (64%)	46 (36%)	1	9

All 46 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	164	SER
1	B	112	ASP
1	B	124	ILE
1	A	5	ILE
1	A	55	VAL
1	A	29	SER
1	A	57	ARG
1	B	115	GLN
1	B	157	ARG
1	B	125	SER
1	B	159	ILE
1	A	39	LEU
1	B	105	ILE
1	B	113	SER
1	B	117	LEU
1	B	152	MET
1	B	138	ARG
1	B	139	LEU
1	B	118	LYS
1	A	12	ASP
1	B	137	ARG
1	A	32	MET
1	B	106	THR
1	B	116	LEU
1	A	67	ASP
1	A	17	LEU
1	A	21	ASP
1	A	62	ASN
1	B	149	GLN
1	A	47	GLU
1	B	110	ASP
1	A	24	ILE
1	B	140	ARG
1	A	61	MET
1	A	60	GLU

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Mol	Chain	Res	Type
1	A	37	ARG
1	A	18	LYS
1	B	170	LYS
1	A	14	TYR
1	B	147	GLU
1	B	165	PHE
1	A	45	LYS
1	B	121	ASP
1	A	43	ARG
1	A	13	SER
1	B	108	THR

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

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 76% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6743

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	3758
Number of shifts mapped to atoms	1558
Number of unparsed shifts	2200
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- Chemical shift has been reported more than once. All 2200 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1517	A	2	LYS	HA	4.14	0.02	1
1518	B	102	LYS	HA	4.14	0.02	1
1519	A	2	LYS	HB2	1.41	0.02	2
1520	B	102	LYS	HB2	1.41	0.02	2
1521	A	2	LYS	HB3	1.61	0.02	2
1522	B	102	LYS	HB3	1.61	0.02	2
1523	A	2	LYS	HG2	1.41	0.02	2
1524	B	102	LYS	HG2	1.41	0.02	2
1525	A	2	LYS	HG3	1.51	0.02	2
1526	B	102	LYS	HG3	1.51	0.02	2
1527	A	2	LYS	HD2	1.74	0.02	1
1528	B	102	LYS	HD2	1.74	0.02	1
1529	A	2	LYS	HD3	1.74	0.02	1
1530	B	102	LYS	HD3	1.74	0.02	1
1531	A	2	LYS	HE2	3.01	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1532	B	102	LYS	HE2	3.01	0.02	1
1533	A	2	LYS	HE3	3.01	0.02	1
1534	B	102	LYS	HE3	3.01	0.02	1
1535	A	2	LYS	C	175.74	0.2	1
1536	B	102	LYS	C	175.74	0.2	1
1537	A	2	LYS	CA	55.51	0.2	1
1538	B	102	LYS	CA	55.51	0.2	1
1539	A	2	LYS	CB	34.54	0.2	1
1540	B	102	LYS	CB	34.54	0.2	1
1541	A	2	LYS	CG	24.78	0.2	1
1542	B	102	LYS	CG	24.78	0.2	1
1543	A	2	LYS	CD	29.52	0.2	1
1544	B	102	LYS	CD	29.52	0.2	1
1545	A	3	GLN	H	9.10	0.02	1
1546	B	103	GLN	H	9.10	0.02	1
1547	A	3	GLN	HA	4.70	0.02	1
1548	B	103	GLN	HA	4.70	0.02	1
1549	A	3	GLN	HB2	1.53	0.02	1
1550	B	103	GLN	HB2	1.53	0.02	1
1551	A	3	GLN	HB3	1.53	0.02	1
1552	B	103	GLN	HB3	1.53	0.02	1
1553	A	3	GLN	HG2	1.80	0.02	2
1554	B	103	GLN	HG2	1.80	0.02	2
1555	A	3	GLN	HG3	1.96	0.02	2
1556	B	103	GLN	HG3	1.96	0.02	2
1557	A	3	GLN	HE21	6.81	0.02	2
1558	B	103	GLN	HE21	6.81	0.02	2
1559	A	3	GLN	HE22	7.34	0.02	2
1560	B	103	GLN	HE22	7.34	0.02	2
1561	A	3	GLN	C	173.53	0.2	1
1562	B	103	GLN	C	173.53	0.2	1
1563	A	3	GLN	CA	54.26	0.2	1
1564	B	103	GLN	CA	54.26	0.2	1
1565	A	3	GLN	CG	32.76	0.2	1
1566	B	103	GLN	CG	32.76	0.2	1
1567	A	3	GLN	N	120.19	0.1	1
1568	B	103	GLN	N	120.19	0.1	1
1569	A	3	GLN	NE2	110.67	0.1	1
1570	B	103	GLN	NE2	110.67	0.1	1
1571	A	4	ARG	H	8.69	0.02	1
1572	B	104	ARG	H	8.69	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1573	A	4	ARG	HA	5.08	0.02	1
1574	B	104	ARG	HA	5.08	0.02	1
1575	A	4	ARG	HB2	1.73	0.02	2
1576	B	104	ARG	HB2	1.73	0.02	2
1577	A	4	ARG	HB3	1.61	0.02	2
1578	B	104	ARG	HB3	1.61	0.02	2
1579	A	4	ARG	HG2	1.56	0.02	1
1580	B	104	ARG	HG2	1.56	0.02	1
1581	A	4	ARG	HG3	1.56	0.02	1
1582	B	104	ARG	HG3	1.56	0.02	1
1583	A	4	ARG	HD2	3.15	0.02	1
1584	B	104	ARG	HD2	3.15	0.02	1
1585	A	4	ARG	HD3	3.15	0.02	1
1586	B	104	ARG	HD3	3.15	0.02	1
1587	A	4	ARG	C	176.44	0.2	1
1588	B	104	ARG	C	176.44	0.2	1
1589	A	4	ARG	CA	55.63	0.2	1
1590	B	104	ARG	CA	55.63	0.2	1
1591	A	4	ARG	CB	30.98	0.2	1
1592	B	104	ARG	CB	30.98	0.2	1
1593	A	4	ARG	CG	27.33	0.2	1
1594	B	104	ARG	CG	27.33	0.2	1
1595	A	4	ARG	CD	43.72	0.2	1
1596	B	104	ARG	CD	43.72	0.2	1
1597	A	4	ARG	N	124.82	0.1	1
1598	B	104	ARG	N	124.82	0.1	1
1599	A	5	ILE	H	9.01	0.02	1
1600	B	105	ILE	H	9.01	0.02	1
1601	A	5	ILE	HA	4.78	0.02	1
1602	B	105	ILE	HA	4.78	0.02	1
1603	A	5	ILE	HB	1.75	0.02	1
1604	B	105	ILE	HB	1.75	0.02	1
1605	A	5	ILE	HG12	0.85	0.02	2
1606	B	105	ILE	HG12	0.85	0.02	2
1607	A	5	ILE	HG13	1.19	0.02	2
1608	B	105	ILE	HG13	1.19	0.02	2
1609	A	5	ILE	HG21	0.25	0.02	1
1610	B	105	ILE	HG21	0.25	0.02	1
1611	A	5	ILE	HG22	0.25	0.02	1
1612	B	105	ILE	HG22	0.25	0.02	1
1613	A	5	ILE	HG23	0.25	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1614	B	105	ILE	HG23	0.25	0.02	1
1615	A	5	ILE	HD11	0.54	0.02	1
1616	B	105	ILE	HD11	0.54	0.02	1
1617	A	5	ILE	HD12	0.54	0.02	1
1618	B	105	ILE	HD12	0.54	0.02	1
1619	A	5	ILE	HD13	0.54	0.02	1
1620	B	105	ILE	HD13	0.54	0.02	1
1621	A	5	ILE	C	173.94	0.2	1
1622	B	105	ILE	C	173.94	0.2	1
1623	A	5	ILE	CA	59.26	0.2	1
1624	B	105	ILE	CA	59.26	0.2	1
1625	A	5	ILE	CB	41.97	0.2	1
1626	B	105	ILE	CB	41.97	0.2	1
1627	A	5	ILE	CG1	26.24	0.2	1
1628	B	105	ILE	CG1	26.24	0.2	1
1629	A	5	ILE	CG2	17.05	0.2	1
1630	B	105	ILE	CG2	17.05	0.2	1
1631	A	5	ILE	CD1	14.88	0.2	1
1632	B	105	ILE	CD1	14.88	0.2	1
1633	A	5	ILE	N	119.88	0.1	1
1634	B	105	ILE	N	119.88	0.1	1
1635	A	6	THR	H	8.31	0.02	1
1636	B	106	THR	H	8.31	0.02	1
1637	A	6	THR	HA	5.47	0.02	1
1638	B	106	THR	HA	5.47	0.02	1
1639	A	6	THR	HB	3.91	0.02	1
1640	B	106	THR	HB	3.91	0.02	1
1641	A	6	THR	HG21	1.14	0.02	1
1642	B	106	THR	HG21	1.14	0.02	1
1643	A	6	THR	HG22	1.14	0.02	1
1644	B	106	THR	HG22	1.14	0.02	1
1645	A	6	THR	HG23	1.14	0.02	1
1646	B	106	THR	HG23	1.14	0.02	1
1647	A	6	THR	C	174.55	0.2	1
1648	B	106	THR	C	174.55	0.2	1
1649	A	6	THR	CA	60.79	0.2	1
1650	B	106	THR	CA	60.79	0.2	1
1651	A	6	THR	CB	69.51	0.2	1
1652	B	106	THR	CB	69.51	0.2	1
1653	A	6	THR	CG2	21.90	0.2	1
1654	B	106	THR	CG2	21.90	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1655	A	6	THR	N	116.80	0.1	1
1656	B	106	THR	N	116.80	0.1	1
1657	A	7	VAL	H	8.90	0.02	1
1658	B	107	VAL	H	8.90	0.02	1
1659	A	7	VAL	HA	4.93	0.02	1
1660	B	107	VAL	HA	4.93	0.02	1
1661	A	7	VAL	HB	2.33	0.02	1
1662	B	107	VAL	HB	2.33	0.02	1
1663	A	7	VAL	HG11	0.64	0.02	2
1664	B	107	VAL	HG11	0.64	0.02	2
1665	A	7	VAL	HG12	0.64	0.02	2
1666	B	107	VAL	HG12	0.64	0.02	2
1667	A	7	VAL	HG13	0.64	0.02	2
1668	B	107	VAL	HG13	0.64	0.02	2
1669	A	7	VAL	HG21	0.84	0.02	2
1670	B	107	VAL	HG21	0.84	0.02	2
1671	A	7	VAL	HG22	0.84	0.02	2
1672	B	107	VAL	HG22	0.84	0.02	2
1673	A	7	VAL	HG23	0.84	0.02	2
1674	B	107	VAL	HG23	0.84	0.02	2
1675	A	7	VAL	C	173.61	0.2	1
1676	B	107	VAL	C	173.61	0.2	1
1677	A	7	VAL	CA	58.97	0.2	1
1678	B	107	VAL	CA	58.97	0.2	1
1679	A	7	VAL	CB	36.43	0.2	1
1680	B	107	VAL	CB	36.43	0.2	1
1681	A	7	VAL	CG1	19.07	0.2	2
1682	B	107	VAL	CG1	19.07	0.2	2
1683	A	7	VAL	CG2	21.87	0.2	2
1684	B	107	VAL	CG2	21.87	0.2	2
1685	A	7	VAL	N	119.27	0.1	1
1686	B	107	VAL	N	119.27	0.1	1
1687	A	8	THR	H	8.38	0.02	1
1688	B	108	THR	H	8.38	0.02	1
1689	A	8	THR	HA	4.93	0.02	1
1690	B	108	THR	HA	4.93	0.02	1
1691	A	8	THR	HB	3.99	0.02	1
1692	B	108	THR	HB	3.99	0.02	1
1693	A	8	THR	HG21	1.13	0.02	1
1694	B	108	THR	HG21	1.13	0.02	1
1695	A	8	THR	HG22	1.13	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1696	B	108	THR	HG22	1.13	0.02	1
1697	A	8	THR	HG23	1.13	0.02	1
1698	B	108	THR	HG23	1.13	0.02	1
1699	A	8	THR	C	174.47	0.2	1
1700	B	108	THR	C	174.47	0.2	1
1701	A	8	THR	CA	62.09	0.2	1
1702	B	108	THR	CA	62.09	0.2	1
1703	A	8	THR	CB	69.47	0.2	1
1704	B	108	THR	CB	69.47	0.2	1
1705	A	8	THR	CG2	22.59	0.2	1
1706	B	108	THR	CG2	22.59	0.2	1
1707	A	8	THR	N	119.27	0.1	1
1708	B	108	THR	N	119.27	0.1	1
1709	A	9	VAL	H	8.91	0.02	1
1710	B	109	VAL	H	8.91	0.02	1
1711	A	9	VAL	HA	4.70	0.02	1
1712	B	109	VAL	HA	4.70	0.02	1
1713	A	9	VAL	HB	2.08	0.02	1
1714	B	109	VAL	HB	2.08	0.02	1
1715	A	9	VAL	HG11	0.78	0.02	2
1716	B	109	VAL	HG11	0.78	0.02	2
1717	A	9	VAL	HG12	0.78	0.02	2
1718	B	109	VAL	HG12	0.78	0.02	2
1719	A	9	VAL	HG13	0.78	0.02	2
1720	B	109	VAL	HG13	0.78	0.02	2
1721	A	9	VAL	HG21	0.87	0.02	2
1722	B	109	VAL	HG21	0.87	0.02	2
1723	A	9	VAL	HG22	0.87	0.02	2
1724	B	109	VAL	HG22	0.87	0.02	2
1725	A	9	VAL	HG23	0.87	0.02	2
1726	B	109	VAL	HG23	0.87	0.02	2
1727	A	9	VAL	C	179.13	0.2	1
1728	B	109	VAL	C	179.13	0.2	1
1729	A	9	VAL	CA	58.29	0.2	1
1730	B	109	VAL	CA	58.29	0.2	1
1731	A	9	VAL	CB	36.05	0.2	1
1732	B	109	VAL	CB	36.05	0.2	1
1733	A	9	VAL	CG1	19.68	0.2	2
1734	B	109	VAL	CG1	19.68	0.2	2
1735	A	9	VAL	CG2	22.96	0.2	2
1736	B	109	VAL	CG2	22.96	0.2	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1737	A	9	VAL	N	117.42	0.1	1
1738	B	109	VAL	N	117.42	0.1	1
1739	A	10	ASP	H	8.16	0.02	1
1740	B	110	ASP	H	8.16	0.02	1
1741	A	10	ASP	HA	4.37	0.02	1
1742	B	110	ASP	HA	4.37	0.02	1
1743	A	10	ASP	HB2	2.76	0.02	2
1744	B	110	ASP	HB2	2.76	0.02	2
1745	A	10	ASP	HB3	2.87	0.02	2
1746	B	110	ASP	HB3	2.87	0.02	2
1747	A	10	ASP	C	176.22	0.2	1
1748	B	110	ASP	C	176.22	0.2	1
1749	A	10	ASP	CA	62.33	0.2	1
1750	B	110	ASP	CA	62.33	0.2	1
1751	A	10	ASP	CB	40.76	0.2	1
1752	B	110	ASP	CB	40.76	0.2	1
1753	A	10	ASP	N	115.55	0.1	1
1754	B	110	ASP	N	115.55	0.1	1
1755	A	11	SER	H	8.50	0.02	1
1756	B	111	SER	H	8.50	0.02	1
1757	A	11	SER	HA	4.46	0.02	1
1758	B	111	SER	HA	4.46	0.02	1
1759	A	11	SER	HB2	3.92	0.02	2
1760	B	111	SER	HB2	3.92	0.02	2
1761	A	11	SER	HB3	3.98	0.02	2
1762	B	111	SER	HB3	3.98	0.02	2
1763	A	11	SER	C	174.32	0.2	1
1764	B	111	SER	C	174.32	0.2	1
1765	A	11	SER	CA	58.29	0.2	1
1766	B	111	SER	CA	58.29	0.2	1
1767	A	11	SER	CB	67.88	0.2	1
1768	B	111	SER	CB	67.88	0.2	1
1769	A	11	SER	N	121.10	0.1	1
1770	B	111	SER	N	121.10	0.1	1
1771	A	12	ASP	H	7.91	0.02	1
1772	B	112	ASP	H	7.91	0.02	1
1773	A	12	ASP	HB2	2.72	0.02	2
1774	B	112	ASP	HB2	2.72	0.02	2
1775	A	12	ASP	HB3	2.77	0.02	2
1776	B	112	ASP	HB3	2.77	0.02	2
1777	A	12	ASP	C	176.55	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1778	B	112	ASP	C	176.55	0.2	1
1779	A	12	ASP	CA	55.02	0.2	1
1780	B	112	ASP	CA	55.02	0.2	1
1781	A	12	ASP	CB	43.09	0.2	1
1782	B	112	ASP	CB	43.09	0.2	1
1783	A	12	ASP	N	119.88	0.1	1
1784	B	112	ASP	N	119.88	0.1	1
1785	A	13	SER	H	9.07	0.02	1
1786	B	113	SER	H	9.07	0.02	1
1787	A	13	SER	HA	4.23	0.02	1
1788	B	113	SER	HA	4.23	0.02	1
1789	A	13	SER	HB2	3.90	0.02	2
1790	B	113	SER	HB2	3.90	0.02	2
1791	A	13	SER	HB3	3.98	0.02	2
1792	B	113	SER	HB3	3.98	0.02	2
1793	A	13	SER	C	175.25	0.2	1
1794	B	113	SER	C	175.25	0.2	1
1795	A	13	SER	CA	62.29	0.2	1
1796	B	113	SER	CA	62.29	0.2	1
1797	A	13	SER	CB	63.16	0.2	1
1798	B	113	SER	CB	63.16	0.2	1
1799	A	13	SER	N	122.97	0.1	1
1800	B	113	SER	N	122.97	0.1	1
1801	A	14	TYR	H	7.80	0.02	1
1802	B	114	TYR	H	7.80	0.02	1
1803	A	14	TYR	HA	4.14	0.02	1
1804	B	114	TYR	HA	4.14	0.02	1
1805	A	14	TYR	HB2	3.07	0.02	2
1806	B	114	TYR	HB2	3.07	0.02	2
1807	A	14	TYR	HB3	3.14	0.02	2
1808	B	114	TYR	HB3	3.14	0.02	2
1809	A	14	TYR	HD1	7.00	0.02	1
1810	B	114	TYR	HD1	7.00	0.02	1
1811	A	14	TYR	HD2	7.00	0.02	1
1812	B	114	TYR	HD2	7.00	0.02	1
1813	A	14	TYR	HE1	6.83	0.02	1
1814	B	114	TYR	HE1	6.83	0.02	1
1815	A	14	TYR	HE2	6.83	0.02	1
1816	B	114	TYR	HE2	6.83	0.02	1
1817	A	14	TYR	C	176.03	0.2	1
1818	B	114	TYR	C	176.03	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1819	A	14	TYR	CA	61.60	0.2	1
1820	B	114	TYR	CA	61.60	0.2	1
1821	A	14	TYR	CB	39.03	0.2	1
1822	B	114	TYR	CB	39.03	0.2	1
1823	A	14	TYR	CD1	132.61	0.2	1
1824	B	114	TYR	CD1	132.61	0.2	1
1825	A	14	TYR	CD2	132.61	0.2	1
1826	B	114	TYR	CD2	132.61	0.2	1
1827	A	14	TYR	CE1	118.40	0.2	1
1828	B	114	TYR	CE1	118.40	0.2	1
1829	A	14	TYR	CE2	118.40	0.2	1
1830	B	114	TYR	CE2	118.40	0.2	1
1831	A	14	TYR	N	121.73	0.1	1
1832	B	114	TYR	N	121.73	0.1	1
1833	A	15	GLN	H	8.57	0.02	1
1834	B	115	GLN	H	8.57	0.02	1
1835	A	15	GLN	HA	3.70	0.02	1
1836	B	115	GLN	HA	3.70	0.02	1
1837	A	15	GLN	HB2	2.17	0.02	2
1838	B	115	GLN	HB2	2.17	0.02	2
1839	A	15	GLN	HB3	2.21	0.02	2
1840	B	115	GLN	HB3	2.21	0.02	2
1841	A	15	GLN	HG2	2.61	0.02	2
1842	B	115	GLN	HG2	2.61	0.02	2
1843	A	15	GLN	HG3	2.76	0.02	2
1844	B	115	GLN	HG3	2.76	0.02	2
1845	A	15	GLN	HE21	6.98	0.02	2
1846	B	115	GLN	HE21	6.98	0.02	2
1847	A	15	GLN	HE22	7.58	0.02	2
1848	B	115	GLN	HE22	7.58	0.02	2
1849	A	15	GLN	C	179.13	0.2	1
1850	B	115	GLN	C	179.13	0.2	1
1851	A	15	GLN	CA	58.66	0.2	1
1852	B	115	GLN	CA	58.66	0.2	1
1853	A	15	GLN	CB	28.11	0.2	1
1854	B	115	GLN	CB	28.11	0.2	1
1855	A	15	GLN	CG	34.25	0.2	1
1856	B	115	GLN	CG	34.25	0.2	1
1857	A	15	GLN	N	115.26	0.1	1
1858	B	115	GLN	N	115.26	0.1	1
1859	A	15	GLN	NE2	111.46	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1860	B	115	GLN	NE2	111.46	0.1	1
1861	A	16	LEU	H	7.64	0.02	1
1862	B	116	LEU	H	7.64	0.02	1
1863	A	16	LEU	HA	4.15	0.02	1
1864	B	116	LEU	HA	4.15	0.02	1
1865	A	16	LEU	HB2	1.79	0.02	2
1866	B	116	LEU	HB2	1.79	0.02	2
1867	A	16	LEU	HB3	1.85	0.02	2
1868	B	116	LEU	HB3	1.85	0.02	2
1869	A	16	LEU	HG	1.69	0.02	1
1870	B	116	LEU	HG	1.69	0.02	1
1871	A	16	LEU	HD11	0.93	0.02	2
1872	B	116	LEU	HD11	0.93	0.02	2
1873	A	16	LEU	HD12	0.93	0.02	2
1874	B	116	LEU	HD12	0.93	0.02	2
1875	A	16	LEU	HD13	0.93	0.02	2
1876	B	116	LEU	HD13	0.93	0.02	2
1877	A	16	LEU	HD21	0.95	0.02	2
1878	B	116	LEU	HD21	0.95	0.02	2
1879	A	16	LEU	HD22	0.95	0.02	2
1880	B	116	LEU	HD22	0.95	0.02	2
1881	A	16	LEU	HD23	0.95	0.02	2
1882	B	116	LEU	HD23	0.95	0.02	2
1883	A	16	LEU	C	178.10	0.2	1
1884	B	116	LEU	C	178.10	0.2	1
1885	A	16	LEU	CA	58.22	0.2	1
1886	B	116	LEU	CA	58.22	0.2	1
1887	A	16	LEU	CB	42.09	0.2	1
1888	B	116	LEU	CB	42.09	0.2	1
1889	A	16	LEU	CG	28.06	0.2	1
1890	B	116	LEU	CG	28.06	0.2	1
1891	A	16	LEU	CD1	25.51	0.2	2
1892	B	116	LEU	CD1	25.51	0.2	2
1893	A	16	LEU	CD2	24.78	0.2	2
1894	B	116	LEU	CD2	24.78	0.2	2
1895	A	16	LEU	N	121.73	0.1	1
1896	B	116	LEU	N	121.73	0.1	1
1897	A	17	LEU	H	7.92	0.02	1
1898	B	117	LEU	H	7.92	0.02	1
1899	A	17	LEU	HA	3.91	0.02	1
1900	B	117	LEU	HA	3.91	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1901	A	17	LEU	HB2	1.27	0.02	2
1902	B	117	LEU	HB2	1.27	0.02	2
1903	A	17	LEU	HB3	1.96	0.02	2
1904	B	117	LEU	HB3	1.96	0.02	2
1905	A	17	LEU	HD11	0.88	0.02	2
1906	B	117	LEU	HD11	0.88	0.02	2
1907	A	17	LEU	HD12	0.88	0.02	2
1908	B	117	LEU	HD12	0.88	0.02	2
1909	A	17	LEU	HD13	0.88	0.02	2
1910	B	117	LEU	HD13	0.88	0.02	2
1911	A	17	LEU	HD21	1.02	0.02	2
1912	B	117	LEU	HD21	1.02	0.02	2
1913	A	17	LEU	HD22	1.02	0.02	2
1914	B	117	LEU	HD22	1.02	0.02	2
1915	A	17	LEU	HD23	1.02	0.02	2
1916	B	117	LEU	HD23	1.02	0.02	2
1917	A	17	LEU	C	179.68	0.2	1
1918	B	117	LEU	C	179.68	0.2	1
1919	A	17	LEU	CA	58.23	0.2	1
1920	B	117	LEU	CA	58.23	0.2	1
1921	A	17	LEU	CB	41.90	0.2	1
1922	B	117	LEU	CB	41.90	0.2	1
1923	A	17	LEU	CD1	23.33	0.2	2
1924	B	117	LEU	CD1	23.33	0.2	2
1925	A	17	LEU	CD2	25.88	0.2	2
1926	B	117	LEU	CD2	25.88	0.2	2
1927	A	17	LEU	N	117.42	0.1	1
1928	B	117	LEU	N	117.42	0.1	1
1929	A	18	LYS	H	8.24	0.02	1
1930	B	118	LYS	H	8.24	0.02	1
1931	A	18	LYS	HA	4.11	0.02	1
1932	B	118	LYS	HA	4.11	0.02	1
1933	A	18	LYS	HB2	1.87	0.02	2
1934	B	118	LYS	HB2	1.87	0.02	2
1935	A	18	LYS	HB3	1.97	0.02	2
1936	B	118	LYS	HB3	1.97	0.02	2
1937	A	18	LYS	HG2	1.21	0.02	1
1938	B	118	LYS	HG2	1.21	0.02	1
1939	A	18	LYS	HG3	1.21	0.02	1
1940	B	118	LYS	HG3	1.21	0.02	1
1941	A	18	LYS	HD2	1.53	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1942	B	118	LYS	HD2	1.53	0.02	1
1943	A	18	LYS	HD3	1.53	0.02	1
1944	B	118	LYS	HD3	1.53	0.02	1
1945	A	18	LYS	HE2	2.88	0.02	2
1946	B	118	LYS	HE2	2.88	0.02	2
1947	A	18	LYS	HE3	3.01	0.02	2
1948	B	118	LYS	HE3	3.01	0.02	2
1949	A	18	LYS	C	178.43	0.2	1
1950	B	118	LYS	C	178.43	0.2	1
1951	A	18	LYS	CA	59.54	0.2	1
1952	B	118	LYS	CA	59.54	0.2	1
1953	A	18	LYS	CB	30.54	0.2	1
1954	B	118	LYS	CB	30.54	0.2	1
1955	A	18	LYS	CG	24.44	0.2	1
1956	B	118	LYS	CG	24.44	0.2	1
1957	A	18	LYS	CD	28.79	0.2	1
1958	B	118	LYS	CD	28.79	0.2	1
1959	A	18	LYS	CE	41.54	0.2	1
1960	B	118	LYS	CE	41.54	0.2	1
1961	A	18	LYS	N	118.96	0.1	1
1962	B	118	LYS	N	118.96	0.1	1
1963	A	19	ALA	H	7.76	0.02	1
1964	B	119	ALA	H	7.76	0.02	1
1965	A	19	ALA	HA	4.30	0.02	1
1966	B	119	ALA	HA	4.30	0.02	1
1967	A	19	ALA	HB1	1.61	0.02	1
1968	B	119	ALA	HB1	1.61	0.02	1
1969	A	19	ALA	HB2	1.61	0.02	1
1970	B	119	ALA	HB2	1.61	0.02	1
1971	A	19	ALA	HB3	1.61	0.02	1
1972	B	119	ALA	HB3	1.61	0.02	1
1973	A	19	ALA	C	179.83	0.2	1
1974	B	119	ALA	C	179.83	0.2	1
1975	A	19	ALA	CA	54.79	0.2	1
1976	B	119	ALA	CA	54.79	0.2	1
1977	A	19	ALA	CB	18.22	0.2	1
1978	B	119	ALA	CB	18.22	0.2	1
1979	A	19	ALA	N	120.81	0.1	1
1980	B	119	ALA	N	120.81	0.1	1
1981	A	20	TYR	H	8.07	0.02	1
1982	B	120	TYR	H	8.07	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1983	A	20	TYR	HA	4.20	0.02	1
1984	B	120	TYR	HA	4.20	0.02	1
1985	A	20	TYR	HD1	7.23	0.02	1
1986	B	120	TYR	HD1	7.23	0.02	1
1987	A	20	TYR	HD2	7.23	0.02	1
1988	B	120	TYR	HD2	7.23	0.02	1
1989	A	20	TYR	HE1	6.77	0.02	1
1990	B	120	TYR	HE1	6.77	0.02	1
1991	A	20	TYR	HE2	6.77	0.02	1
1992	B	120	TYR	HE2	6.77	0.02	1
1993	A	20	TYR	CA	58.22	0.2	1
1994	B	120	TYR	CA	58.22	0.2	1
1995	A	20	TYR	CB	39.16	0.2	1
1996	B	120	TYR	CB	39.16	0.2	1
1997	A	20	TYR	CD1	132.59	0.2	1
1998	B	120	TYR	CD1	132.59	0.2	1
1999	A	20	TYR	CD2	132.59	0.2	1
2000	B	120	TYR	CD2	132.59	0.2	1
2001	A	20	TYR	CE1	117.86	0.2	1
2002	B	120	TYR	CE1	117.86	0.2	1
2003	A	20	TYR	CE2	117.86	0.2	1
2004	B	120	TYR	CE2	117.86	0.2	1
2005	A	20	TYR	N	117.73	0.1	1
2006	B	120	TYR	N	117.73	0.1	1
2007	A	21	ASP	H	8.16	0.02	1
2008	B	121	ASP	H	8.16	0.02	1
2009	A	21	ASP	HA	4.48	0.02	1
2010	B	121	ASP	HA	4.48	0.02	1
2011	A	21	ASP	HB2	2.63	0.02	2
2012	B	121	ASP	HB2	2.63	0.02	2
2013	A	21	ASP	HB3	3.18	0.02	2
2014	B	121	ASP	HB3	3.18	0.02	2
2015	A	21	ASP	C	175.27	0.2	1
2016	B	121	ASP	C	175.27	0.2	1
2017	A	21	ASP	CA	55.38	0.2	1
2018	B	121	ASP	CA	55.38	0.2	1
2019	A	21	ASP	CB	39.43	0.2	1
2020	B	121	ASP	CB	39.43	0.2	1
2021	A	21	ASP	N	118.03	0.1	1
2022	B	121	ASP	N	118.03	0.1	1
2023	A	22	VAL	H	7.85	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2024	B	122	VAL	H	7.85	0.02	1
2025	A	22	VAL	HA	3.86	0.02	1
2026	B	122	VAL	HA	3.86	0.02	1
2027	A	22	VAL	HB	1.84	0.02	1
2028	B	122	VAL	HB	1.84	0.02	1
2029	A	22	VAL	HG11	0.90	0.02	2
2030	B	122	VAL	HG11	0.90	0.02	2
2031	A	22	VAL	HG12	0.90	0.02	2
2032	B	122	VAL	HG12	0.90	0.02	2
2033	A	22	VAL	HG13	0.90	0.02	2
2034	B	122	VAL	HG13	0.90	0.02	2
2035	A	22	VAL	HG21	1.13	0.02	2
2036	B	122	VAL	HG21	1.13	0.02	2
2037	A	22	VAL	HG22	1.13	0.02	2
2038	B	122	VAL	HG22	1.13	0.02	2
2039	A	22	VAL	HG23	1.13	0.02	2
2040	B	122	VAL	HG23	1.13	0.02	2
2041	A	22	VAL	C	176.16	0.2	1
2042	B	122	VAL	C	176.16	0.2	1
2043	A	22	VAL	CA	63.03	0.2	1
2044	B	122	VAL	CA	63.03	0.2	1
2045	A	22	VAL	CB	32.80	0.2	1
2046	B	122	VAL	CB	32.80	0.2	1
2047	A	22	VAL	CG1	21.14	0.2	2
2048	B	122	VAL	CG1	21.14	0.2	2
2049	A	22	VAL	CG2	23.33	0.2	2
2050	B	122	VAL	CG2	23.33	0.2	2
2051	A	22	VAL	N	118.96	0.1	1
2052	B	122	VAL	N	118.96	0.1	1
2053	A	23	ASN	H	8.77	0.02	1
2054	B	123	ASN	H	8.77	0.02	1
2055	A	23	ASN	HA	4.83	0.02	1
2056	B	123	ASN	HA	4.83	0.02	1
2057	A	23	ASN	HB2	2.98	0.02	2
2058	B	123	ASN	HB2	2.98	0.02	2
2059	A	23	ASN	HB3	3.25	0.02	2
2060	B	123	ASN	HB3	3.25	0.02	2
2061	A	23	ASN	HD21	7.19	0.02	2
2062	B	123	ASN	HD21	7.19	0.02	2
2063	A	23	ASN	HD22	7.89	0.02	2
2064	B	123	ASN	HD22	7.89	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2065	A	23	ASN	C	175.60	0.2	1
2066	B	123	ASN	C	175.60	0.2	1
2067	A	23	ASN	CA	52.41	0.2	1
2068	B	123	ASN	CA	52.41	0.2	1
2069	A	23	ASN	CB	37.05	0.2	1
2070	B	123	ASN	CB	37.05	0.2	1
2071	A	23	ASN	N	124.51	0.1	1
2072	B	123	ASN	N	124.51	0.1	1
2073	A	23	ASN	ND2	112.29	0.1	1
2074	B	123	ASN	ND2	112.29	0.1	1
2075	A	24	ILE	H	8.38	0.02	1
2076	B	124	ILE	H	8.38	0.02	1
2077	A	24	ILE	HA	3.63	0.02	1
2078	B	124	ILE	HA	3.63	0.02	1
2079	A	24	ILE	HB	2.22	0.02	1
2080	B	124	ILE	HB	2.22	0.02	1
2081	A	24	ILE	HG12	1.38	0.02	2
2082	B	124	ILE	HG12	1.38	0.02	2
2083	A	24	ILE	HG13	1.84	0.02	2
2084	B	124	ILE	HG13	1.84	0.02	2
2085	A	24	ILE	HG21	1.02	0.02	1
2086	B	124	ILE	HG21	1.02	0.02	1
2087	A	24	ILE	HG22	1.02	0.02	1
2088	B	124	ILE	HG22	1.02	0.02	1
2089	A	24	ILE	HG23	1.02	0.02	1
2090	B	124	ILE	HG23	1.02	0.02	1
2091	A	24	ILE	HD11	0.90	0.02	1
2092	B	124	ILE	HD11	0.90	0.02	1
2093	A	24	ILE	HD12	0.90	0.02	1
2094	B	124	ILE	HD12	0.90	0.02	1
2095	A	24	ILE	HD13	0.90	0.02	1
2096	B	124	ILE	HD13	0.90	0.02	1
2097	A	24	ILE	C	177.57	0.2	1
2098	B	124	ILE	C	177.57	0.2	1
2099	A	24	ILE	CA	64.85	0.2	1
2100	B	124	ILE	CA	64.85	0.2	1
2101	A	24	ILE	CB	37.17	0.2	1
2102	B	124	ILE	CB	37.17	0.2	1
2103	A	24	ILE	CG1	28.79	0.2	1
2104	B	124	ILE	CG1	28.79	0.2	1
2105	A	24	ILE	CG2	17.87	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2106	B	124	ILE	CG2	17.87	0.2	1
2107	A	24	ILE	CD1	12.00	0.2	1
2108	B	124	ILE	CD1	12.00	0.2	1
2109	A	24	ILE	N	130.68	0.1	1
2110	B	124	ILE	N	130.68	0.1	1
2111	A	25	SER	H	8.72	0.02	1
2112	B	125	SER	H	8.72	0.02	1
2113	A	25	SER	HA	4.37	0.02	1
2114	B	125	SER	HA	4.37	0.02	1
2115	A	25	SER	HB2	4.15	0.02	2
2116	B	125	SER	HB2	4.15	0.02	2
2117	A	25	SER	HB3	4.22	0.02	2
2118	B	125	SER	HB3	4.22	0.02	2
2119	A	25	SER	C	176.50	0.2	1
2120	B	125	SER	C	176.50	0.2	1
2121	A	25	SER	CA	63.64	0.2	1
2122	B	125	SER	CA	63.64	0.2	1
2123	A	25	SER	CB	68.58	0.2	1
2124	B	125	SER	CB	68.58	0.2	1
2125	A	25	SER	N	116.80	0.1	1
2126	B	125	SER	N	116.80	0.1	1
2127	A	26	GLY	H	8.06	0.02	1
2128	B	126	GLY	H	8.06	0.02	1
2129	A	26	GLY	HA2	3.82	0.02	2
2130	B	126	GLY	HA2	3.82	0.02	2
2131	A	26	GLY	HA3	3.96	0.02	2
2132	B	126	GLY	HA3	3.96	0.02	2
2133	A	26	GLY	C	175.95	0.2	1
2134	B	126	GLY	C	175.95	0.2	1
2135	A	26	GLY	CA	47.53	0.2	1
2136	B	126	GLY	CA	47.53	0.2	1
2137	A	26	GLY	N	109.71	0.1	1
2138	B	126	GLY	N	109.71	0.1	1
2139	A	27	LEU	H	8.01	0.02	1
2140	B	127	LEU	H	8.01	0.02	1
2141	A	27	LEU	HA	4.29	0.02	1
2142	B	127	LEU	HA	4.29	0.02	1
2143	A	27	LEU	HB2	1.75	0.02	2
2144	B	127	LEU	HB2	1.75	0.02	2
2145	A	27	LEU	HB3	2.06	0.02	2
2146	B	127	LEU	HB3	2.06	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2147	A	27	LEU	HD11	0.90	0.02	2
2148	B	127	LEU	HD11	0.90	0.02	2
2149	A	27	LEU	HD12	0.90	0.02	2
2150	B	127	LEU	HD12	0.90	0.02	2
2151	A	27	LEU	HD13	0.90	0.02	2
2152	B	127	LEU	HD13	0.90	0.02	2
2153	A	27	LEU	HD21	0.95	0.02	2
2154	B	127	LEU	HD21	0.95	0.02	2
2155	A	27	LEU	HD22	0.95	0.02	2
2156	B	127	LEU	HD22	0.95	0.02	2
2157	A	27	LEU	HD23	0.95	0.02	2
2158	B	127	LEU	HD23	0.95	0.02	2
2159	A	27	LEU	C	180.07	0.2	1
2160	B	127	LEU	C	180.07	0.2	1
2161	A	27	LEU	CA	58.29	0.2	1
2162	B	127	LEU	CA	58.29	0.2	1
2163	A	27	LEU	CB	42.28	0.2	1
2164	B	127	LEU	CB	42.28	0.2	1
2165	A	27	LEU	CD1	26.60	0.2	2
2166	B	127	LEU	CD1	26.60	0.2	2
2167	A	27	LEU	CD2	23.69	0.2	2
2168	B	127	LEU	CD2	23.69	0.2	2
2169	A	27	LEU	N	124.51	0.1	1
2170	B	127	LEU	N	124.51	0.1	1
2171	A	28	VAL	H	8.77	0.02	1
2172	B	128	VAL	H	8.77	0.02	1
2173	A	28	VAL	HA	3.57	0.02	1
2174	B	128	VAL	HA	3.57	0.02	1
2175	A	28	VAL	HB	2.23	0.02	1
2176	B	128	VAL	HB	2.23	0.02	1
2177	A	28	VAL	HG11	1.05	0.02	2
2178	B	128	VAL	HG11	1.05	0.02	2
2179	A	28	VAL	HG12	1.05	0.02	2
2180	B	128	VAL	HG12	1.05	0.02	2
2181	A	28	VAL	HG13	1.05	0.02	2
2182	B	128	VAL	HG13	1.05	0.02	2
2183	A	28	VAL	HG21	1.14	0.02	2
2184	B	128	VAL	HG21	1.14	0.02	2
2185	A	28	VAL	HG22	1.14	0.02	2
2186	B	128	VAL	HG22	1.14	0.02	2
2187	A	28	VAL	HG23	1.14	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2188	B	128	VAL	HG23	1.14	0.02	2
2189	A	28	VAL	C	177.48	0.2	1
2190	B	128	VAL	C	177.48	0.2	1
2191	A	28	VAL	CA	67.40	0.2	1
2192	B	128	VAL	CA	67.40	0.2	1
2193	A	28	VAL	CB	31.70	0.2	1
2194	B	128	VAL	CB	31.70	0.2	1
2195	A	28	VAL	CG1	23.20	0.2	2
2196	B	128	VAL	CG1	23.20	0.2	2
2197	A	28	VAL	CG2	23.69	0.2	2
2198	B	128	VAL	CG2	23.69	0.2	2
2199	A	28	VAL	N	119.88	0.1	1
2200	B	128	VAL	N	119.88	0.1	1
2201	A	29	SER	H	9.03	0.02	1
2202	B	129	SER	H	9.03	0.02	1
2203	A	29	SER	HA	4.34	0.02	1
2204	B	129	SER	HA	4.34	0.02	1
2205	A	29	SER	HB2	4.27	0.02	1
2206	B	129	SER	HB2	4.27	0.02	1
2207	A	29	SER	HB3	4.27	0.02	1
2208	B	129	SER	HB3	4.27	0.02	1
2209	A	29	SER	C	177.86	0.2	1
2210	B	129	SER	C	177.86	0.2	1
2211	A	29	SER	CA	63.32	0.2	1
2212	B	129	SER	CA	63.32	0.2	1
2213	A	29	SER	CB	65.99	0.2	1
2214	B	129	SER	CB	65.99	0.2	1
2215	A	29	SER	N	115.57	0.1	1
2216	B	129	SER	N	115.57	0.1	1
2217	A	30	THR	H	8.52	0.02	1
2218	B	130	THR	H	8.52	0.02	1
2219	A	30	THR	HA	4.09	0.02	1
2220	B	130	THR	HA	4.09	0.02	1
2221	A	30	THR	HB	4.38	0.02	1
2222	B	130	THR	HB	4.38	0.02	1
2223	A	30	THR	HG21	1.38	0.02	1
2224	B	130	THR	HG21	1.38	0.02	1
2225	A	30	THR	HG22	1.38	0.02	1
2226	B	130	THR	HG22	1.38	0.02	1
2227	A	30	THR	HG23	1.38	0.02	1
2228	B	130	THR	HG23	1.38	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2229	A	30	THR	C	176.26	0.2	1
2230	B	130	THR	C	176.26	0.2	1
2231	A	30	THR	CA	67.00	0.2	1
2232	B	130	THR	CA	67.00	0.2	1
2233	A	30	THR	CB	68.86	0.2	1
2234	B	130	THR	CB	68.86	0.2	1
2235	A	30	THR	CG2	21.56	0.2	1
2236	B	130	THR	CG2	21.56	0.2	1
2237	A	30	THR	N	117.11	0.1	1
2238	B	130	THR	N	117.11	0.1	1
2239	A	31	THR	H	7.89	0.02	1
2240	B	131	THR	H	7.89	0.02	1
2241	A	31	THR	HA	4.16	0.02	1
2242	B	131	THR	HA	4.16	0.02	1
2243	A	31	THR	HB	4.49	0.02	1
2244	B	131	THR	HB	4.49	0.02	1
2245	A	31	THR	HG21	1.39	0.02	1
2246	B	131	THR	HG21	1.39	0.02	1
2247	A	31	THR	HG22	1.39	0.02	1
2248	B	131	THR	HG22	1.39	0.02	1
2249	A	31	THR	HG23	1.39	0.02	1
2250	B	131	THR	HG23	1.39	0.02	1
2251	A	31	THR	C	176.96	0.2	1
2252	B	131	THR	C	176.96	0.2	1
2253	A	31	THR	CA	66.00	0.2	1
2254	B	131	THR	CA	66.00	0.2	1
2255	A	31	THR	CB	67.77	0.2	1
2256	B	131	THR	CB	67.77	0.2	1
2257	A	31	THR	CG2	21.14	0.2	1
2258	B	131	THR	CG2	21.14	0.2	1
2259	A	31	THR	N	118.65	0.1	1
2260	B	131	THR	N	118.65	0.1	1
2261	A	32	MET	H	8.53	0.02	1
2262	B	132	MET	H	8.53	0.02	1
2263	A	32	MET	HA	3.98	0.02	1
2264	B	132	MET	HA	3.98	0.02	1
2265	A	32	MET	HB2	2.40	0.02	2
2266	B	132	MET	HB2	2.40	0.02	2
2267	A	32	MET	HB3	2.48	0.02	2
2268	B	132	MET	HB3	2.48	0.02	2
2269	A	32	MET	HG2	2.99	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2270	B	132	MET	HG2	2.99	0.02	2
2271	A	32	MET	HG3	3.16	0.02	2
2272	B	132	MET	HG3	3.16	0.02	2
2273	A	32	MET	HE1	2.10	0.02	1
2274	B	132	MET	HE1	2.10	0.02	1
2275	A	32	MET	HE2	2.10	0.02	1
2276	B	132	MET	HE2	2.10	0.02	1
2277	A	32	MET	HE3	2.10	0.02	1
2278	B	132	MET	HE3	2.10	0.02	1
2279	A	32	MET	C	177.57	0.2	1
2280	B	132	MET	C	177.57	0.2	1
2281	A	32	MET	CA	60.72	0.2	1
2282	B	132	MET	CA	60.72	0.2	1
2283	A	32	MET	CB	33.53	0.2	1
2284	B	132	MET	CB	33.53	0.2	1
2285	A	32	MET	CG	31.34	0.2	1
2286	B	132	MET	CG	31.34	0.2	1
2287	A	32	MET	CE	17.86	0.2	1
2288	B	132	MET	CE	17.86	0.2	1
2289	A	32	MET	N	120.19	0.1	1
2290	B	132	MET	N	120.19	0.1	1
2291	A	33	GLN	H	8.64	0.02	1
2292	B	133	GLN	H	8.64	0.02	1
2293	A	33	GLN	HA	4.30	0.02	1
2294	B	133	GLN	HA	4.30	0.02	1
2295	A	33	GLN	HB2	2.04	0.02	2
2296	B	133	GLN	HB2	2.04	0.02	2
2297	A	33	GLN	HB3	2.26	0.02	2
2298	B	133	GLN	HB3	2.26	0.02	2
2299	A	33	GLN	HG2	2.48	0.02	2
2300	B	133	GLN	HG2	2.48	0.02	2
2301	A	33	GLN	HG3	2.66	0.02	2
2302	B	133	GLN	HG3	2.66	0.02	2
2303	A	33	GLN	HE21	7.01	0.02	2
2304	B	133	GLN	HE21	7.01	0.02	2
2305	A	33	GLN	HE22	7.40	0.02	2
2306	B	133	GLN	HE22	7.40	0.02	2
2307	A	33	GLN	C	179.07	0.2	1
2308	B	133	GLN	C	179.07	0.2	1
2309	A	33	GLN	CA	59.16	0.2	1
2310	B	133	GLN	CA	59.16	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2311	A	33	GLN	CB	29.23	0.2	1
2312	B	133	GLN	CB	29.23	0.2	1
2313	A	33	GLN	N	119.58	0.1	1
2314	B	133	GLN	N	119.58	0.1	1
2315	A	33	GLN	NE2	111.69	0.1	1
2316	B	133	GLN	NE2	111.69	0.1	1
2317	A	34	ASN	H	8.55	0.02	1
2318	B	134	ASN	H	8.55	0.02	1
2319	A	34	ASN	HA	4.59	0.02	1
2320	B	134	ASN	HA	4.59	0.02	1
2321	A	34	ASN	HB2	2.99	0.02	2
2322	B	134	ASN	HB2	2.99	0.02	2
2323	A	34	ASN	HB3	3.16	0.02	2
2324	B	134	ASN	HB3	3.16	0.02	2
2325	A	34	ASN	HD21	7.06	0.02	2
2326	B	134	ASN	HD21	7.06	0.02	2
2327	A	34	ASN	HD22	7.85	0.02	2
2328	B	134	ASN	HD22	7.85	0.02	2
2329	A	34	ASN	C	178.31	0.2	1
2330	B	134	ASN	C	178.31	0.2	1
2331	A	34	ASN	CA	56.97	0.2	1
2332	B	134	ASN	CA	56.97	0.2	1
2333	A	34	ASN	CB	37.90	0.2	1
2334	B	134	ASN	CB	37.90	0.2	1
2335	A	34	ASN	N	118.96	0.1	1
2336	B	134	ASN	N	118.96	0.1	1
2337	A	34	ASN	ND2	112.22	0.1	1
2338	B	134	ASN	ND2	112.22	0.1	1
2339	A	35	GLU	H	8.34	0.02	1
2340	B	135	GLU	H	8.34	0.02	1
2341	A	35	GLU	HA	4.60	0.02	1
2342	B	135	GLU	HA	4.60	0.02	1
2343	A	35	GLU	C	177.99	0.2	1
2344	B	135	GLU	C	177.99	0.2	1
2345	A	35	GLU	CA	58.31	0.2	1
2346	B	135	GLU	CA	58.31	0.2	1
2347	A	35	GLU	CB	30.21	0.2	1
2348	B	135	GLU	CB	30.21	0.2	1
2349	A	35	GLU	N	122.66	0.1	1
2350	B	135	GLU	N	122.66	0.1	1
2351	A	36	ALA	H	8.63	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2352	B	136	ALA	H	8.63	0.02	1
2353	A	36	ALA	HA	4.03	0.02	1
2354	B	136	ALA	HA	4.03	0.02	1
2355	A	36	ALA	HB1	1.62	0.02	1
2356	B	136	ALA	HB1	1.62	0.02	1
2357	A	36	ALA	HB2	1.62	0.02	1
2358	B	136	ALA	HB2	1.62	0.02	1
2359	A	36	ALA	HB3	1.62	0.02	1
2360	B	136	ALA	HB3	1.62	0.02	1
2361	A	36	ALA	C	179.00	0.2	1
2362	B	136	ALA	C	179.00	0.2	1
2363	A	36	ALA	CA	55.38	0.2	1
2364	B	136	ALA	CA	55.38	0.2	1
2365	A	36	ALA	CB	17.87	0.2	1
2366	B	136	ALA	CB	17.87	0.2	1
2367	A	36	ALA	N	121.73	0.1	1
2368	B	136	ALA	N	121.73	0.1	1
2369	A	37	ARG	H	7.92	0.02	1
2370	B	137	ARG	H	7.92	0.02	1
2371	A	37	ARG	HA	4.01	0.02	1
2372	B	137	ARG	HA	4.01	0.02	1
2373	A	37	ARG	HB2	2.05	0.02	1
2374	B	137	ARG	HB2	2.05	0.02	1
2375	A	37	ARG	HB3	2.05	0.02	1
2376	B	137	ARG	HB3	2.05	0.02	1
2377	A	37	ARG	HG2	1.70	0.02	2
2378	B	137	ARG	HG2	1.70	0.02	2
2379	A	37	ARG	HG3	1.93	0.02	2
2380	B	137	ARG	HG3	1.93	0.02	2
2381	A	37	ARG	HD2	2.98	0.02	2
2382	B	137	ARG	HD2	2.98	0.02	2
2383	A	37	ARG	HD3	3.31	0.02	2
2384	B	137	ARG	HD3	3.31	0.02	2
2385	A	37	ARG	C	179.02	0.2	1
2386	B	137	ARG	C	179.02	0.2	1
2387	A	37	ARG	CA	59.39	0.2	1
2388	B	137	ARG	CA	59.39	0.2	1
2389	A	37	ARG	CB	30.25	0.2	1
2390	B	137	ARG	CB	30.25	0.2	1
2391	A	37	ARG	CG	27.85	0.2	1
2392	B	137	ARG	CG	27.85	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2393	A	37	ARG	CD	43.00	0.2	1
2394	B	137	ARG	CD	43.00	0.2	1
2395	A	37	ARG	N	116.80	0.1	1
2396	B	137	ARG	N	116.80	0.1	1
2397	A	38	ARG	H	7.83	0.02	1
2398	B	138	ARG	H	7.83	0.02	1
2399	A	38	ARG	HA	4.10	0.02	1
2400	B	138	ARG	HA	4.10	0.02	1
2401	A	38	ARG	HB2	2.14	0.02	1
2402	B	138	ARG	HB2	2.14	0.02	1
2403	A	38	ARG	HB3	2.14	0.02	1
2404	B	138	ARG	HB3	2.14	0.02	1
2405	A	38	ARG	HD2	3.31	0.02	1
2406	B	138	ARG	HD2	3.31	0.02	1
2407	A	38	ARG	HD3	3.31	0.02	1
2408	B	138	ARG	HD3	3.31	0.02	1
2409	A	38	ARG	C	178.90	0.2	1
2410	B	138	ARG	C	178.90	0.2	1
2411	A	38	ARG	CA	59.79	0.2	1
2412	B	138	ARG	CA	59.79	0.2	1
2413	A	38	ARG	CB	30.32	0.2	1
2414	B	138	ARG	CB	30.32	0.2	1
2415	A	38	ARG	CD	43.85	0.2	1
2416	B	138	ARG	CD	43.85	0.2	1
2417	A	38	ARG	N	121.12	0.1	1
2418	B	138	ARG	N	121.12	0.1	1
2419	A	39	LEU	H	8.41	0.02	1
2420	B	139	LEU	H	8.41	0.02	1
2421	A	39	LEU	HA	3.96	0.02	1
2422	B	139	LEU	HA	3.96	0.02	1
2423	A	39	LEU	HB2	1.11	0.02	2
2424	B	139	LEU	HB2	1.11	0.02	2
2425	A	39	LEU	HB3	1.76	0.02	2
2426	B	139	LEU	HB3	1.76	0.02	2
2427	A	39	LEU	HG	1.69	0.02	1
2428	B	139	LEU	HG	1.69	0.02	1
2429	A	39	LEU	HD11	0.68	0.02	2
2430	B	139	LEU	HD11	0.68	0.02	2
2431	A	39	LEU	HD12	0.68	0.02	2
2432	B	139	LEU	HD12	0.68	0.02	2
2433	A	39	LEU	HD13	0.68	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2434	B	139	LEU	HD13	0.68	0.02	2
2435	A	39	LEU	HD21	0.76	0.02	2
2436	B	139	LEU	HD21	0.76	0.02	2
2437	A	39	LEU	HD22	0.76	0.02	2
2438	B	139	LEU	HD22	0.76	0.02	2
2439	A	39	LEU	HD23	0.76	0.02	2
2440	B	139	LEU	HD23	0.76	0.02	2
2441	A	39	LEU	C	176.81	0.2	1
2442	B	139	LEU	C	176.81	0.2	1
2443	A	39	LEU	CA	57.57	0.2	1
2444	B	139	LEU	CA	57.57	0.2	1
2445	A	39	LEU	CB	41.90	0.2	1
2446	B	139	LEU	CB	41.90	0.2	1
2447	A	39	LEU	CG	27.28	0.2	1
2448	B	139	LEU	CG	27.28	0.2	1
2449	A	39	LEU	CD1	22.60	0.2	2
2450	B	139	LEU	CD1	22.60	0.2	2
2451	A	39	LEU	CD2	25.88	0.2	2
2452	B	139	LEU	CD2	25.88	0.2	2
2453	A	39	LEU	N	119.27	0.1	1
2454	B	139	LEU	N	119.27	0.1	1
2455	A	40	ARG	H	8.29	0.02	1
2456	B	140	ARG	H	8.29	0.02	1
2457	A	40	ARG	HA	4.51	0.02	1
2458	B	140	ARG	HA	4.51	0.02	1
2459	A	40	ARG	HB2	1.88	0.02	1
2460	B	140	ARG	HB2	1.88	0.02	1
2461	A	40	ARG	HB3	1.88	0.02	1
2462	B	140	ARG	HB3	1.88	0.02	1
2463	A	40	ARG	HG2	1.58	0.02	1
2464	B	140	ARG	HG2	1.58	0.02	1
2465	A	40	ARG	HG3	1.58	0.02	1
2466	B	140	ARG	HG3	1.58	0.02	1
2467	A	40	ARG	C	176.46	0.2	1
2468	B	140	ARG	C	176.46	0.2	1
2469	A	40	ARG	CA	55.75	0.2	1
2470	B	140	ARG	CA	55.75	0.2	1
2471	A	40	ARG	CB	33.07	0.2	1
2472	B	140	ARG	CB	33.07	0.2	1
2473	A	40	ARG	N	120.50	0.1	1
2474	B	140	ARG	N	120.50	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2475	A	41	ALA	H	8.30	0.02	1
2476	B	141	ALA	H	8.30	0.02	1
2477	A	41	ALA	HA	4.34	0.02	1
2478	B	141	ALA	HA	4.34	0.02	1
2479	A	41	ALA	HB1	1.48	0.02	1
2480	B	141	ALA	HB1	1.48	0.02	1
2481	A	41	ALA	HB2	1.48	0.02	1
2482	B	141	ALA	HB2	1.48	0.02	1
2483	A	41	ALA	HB3	1.48	0.02	1
2484	B	141	ALA	HB3	1.48	0.02	1
2485	A	41	ALA	C	178.11	0.2	1
2486	B	141	ALA	C	178.11	0.2	1
2487	A	41	ALA	CA	53.56	0.2	1
2488	B	141	ALA	CA	53.56	0.2	1
2489	A	41	ALA	CB	19.78	0.2	1
2490	B	141	ALA	CB	19.78	0.2	1
2491	A	41	ALA	N	124.82	0.1	1
2492	B	141	ALA	N	124.82	0.1	1
2493	A	42	GLU	H	8.34	0.02	1
2494	B	142	GLU	H	8.34	0.02	1
2495	A	42	GLU	HA	4.33	0.02	1
2496	B	142	GLU	HA	4.33	0.02	1
2497	A	42	GLU	HB2	2.05	0.02	2
2498	B	142	GLU	HB2	2.05	0.02	2
2499	A	42	GLU	HB3	2.13	0.02	2
2500	B	142	GLU	HB3	2.13	0.02	2
2501	A	42	GLU	HG2	2.34	0.02	1
2502	B	142	GLU	HG2	2.34	0.02	1
2503	A	42	GLU	HG3	2.34	0.02	1
2504	B	142	GLU	HG3	2.34	0.02	1
2505	A	42	GLU	CA	57.20	0.2	1
2506	B	142	GLU	CA	57.20	0.2	1
2507	A	42	GLU	CB	30.17	0.2	1
2508	B	142	GLU	CB	30.17	0.2	1
2509	A	42	GLU	CG	36.44	0.2	1
2510	B	142	GLU	CG	36.44	0.2	1
2511	A	42	GLU	N	119.64	0.1	1
2512	B	142	GLU	N	119.64	0.1	1
2513	A	44	TRP	HD1	7.34	0.02	1
2514	B	144	TRP	HD1	7.34	0.02	1
2515	A	44	TRP	HE1	10.19	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2516	B	144	TRP	HE1	10.19	0.02	1
2517	A	44	TRP	HE3	7.65	0.02	1
2518	B	144	TRP	HE3	7.65	0.02	1
2519	A	44	TRP	HZ2	7.51	0.02	1
2520	B	144	TRP	HZ2	7.51	0.02	1
2521	A	44	TRP	HZ3	7.18	0.02	1
2522	B	144	TRP	HZ3	7.18	0.02	1
2523	A	44	TRP	HH2	7.26	0.02	1
2524	B	144	TRP	HH2	7.26	0.02	1
2525	A	44	TRP	CD1	127.10	0.2	1
2526	B	144	TRP	CD1	127.10	0.2	1
2527	A	44	TRP	CE3	121.00	0.2	1
2528	B	144	TRP	CE3	121.00	0.2	1
2529	A	44	TRP	CZ2	114.58	0.2	1
2530	B	144	TRP	CZ2	114.58	0.2	1
2531	A	44	TRP	CZ3	121.93	0.2	1
2532	B	144	TRP	CZ3	121.93	0.2	1
2533	A	44	TRP	CH2	124.59	0.2	1
2534	B	144	TRP	CH2	124.59	0.2	1
2535	A	44	TRP	NE1	129.20	0.2	1
2536	B	144	TRP	NE1	129.20	0.2	1
2577	A	54	GLU	C	177.34	0.2	1
2578	B	154	GLU	C	177.34	0.2	1
2579	A	54	GLU	CA	59.08	0.2	1
2580	B	154	GLU	CA	59.08	0.2	1
2581	A	54	GLU	CB	29.23	0.2	1
2582	B	154	GLU	CB	29.23	0.2	1
2585	A	55	VAL	H	7.87	0.02	1
2586	B	155	VAL	H	7.87	0.02	1
2587	A	55	VAL	HA	4.11	0.02	1
2588	B	155	VAL	HA	4.11	0.02	1
2589	A	55	VAL	HB	1.88	0.02	1
2590	B	155	VAL	HB	1.88	0.02	1
2591	A	55	VAL	HG11	1.42	0.02	2
2592	B	155	VAL	HG11	1.42	0.02	2
2593	A	55	VAL	HG12	1.42	0.02	2
2594	B	155	VAL	HG12	1.42	0.02	2
2595	A	55	VAL	HG13	1.42	0.02	2
2596	B	155	VAL	HG13	1.42	0.02	2
2597	A	55	VAL	HG21	1.42	0.02	2
2598	B	155	VAL	HG21	1.42	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2599	A	55	VAL	HG22	1.42	0.02	2
2600	B	155	VAL	HG22	1.42	0.02	2
2601	A	55	VAL	HG23	1.42	0.02	2
2602	B	155	VAL	HG23	1.42	0.02	2
2603	A	55	VAL	C	176.98	0.2	1
2604	B	155	VAL	C	176.98	0.2	1
2605	A	55	VAL	CA	57.71	0.2	1
2606	B	155	VAL	CA	57.71	0.2	1
2607	A	55	VAL	CB	32.94	0.2	1
2608	B	155	VAL	CB	32.94	0.2	1
2609	A	55	VAL	N	120.51	0.1	1
2610	B	155	VAL	N	120.51	0.1	1
2611	A	56	ALA	H	7.92	0.02	1
2612	B	156	ALA	H	7.92	0.02	1
2613	A	56	ALA	HA	4.24	0.02	1
2614	B	156	ALA	HA	4.24	0.02	1
2615	A	56	ALA	HB1	1.52	0.02	1
2616	B	156	ALA	HB1	1.52	0.02	1
2617	A	56	ALA	HB2	1.52	0.02	1
2618	B	156	ALA	HB2	1.52	0.02	1
2619	A	56	ALA	HB3	1.52	0.02	1
2620	B	156	ALA	HB3	1.52	0.02	1
2621	A	56	ALA	C	178.62	0.2	1
2622	B	156	ALA	C	178.62	0.2	1
2623	A	56	ALA	CA	53.54	0.2	1
2624	B	156	ALA	CA	53.54	0.2	1
2625	A	56	ALA	CB	19.27	0.2	1
2626	B	156	ALA	CB	19.27	0.2	1
2627	A	56	ALA	N	122.98	0.1	1
2628	B	156	ALA	N	122.98	0.1	1
2629	A	57	ARG	H	8.21	0.02	1
2630	B	157	ARG	H	8.21	0.02	1
2631	A	57	ARG	HA	4.29	0.02	1
2632	B	157	ARG	HA	4.29	0.02	1
2633	A	57	ARG	CA	57.13	0.2	1
2634	B	157	ARG	CA	57.13	0.2	1
2635	A	57	ARG	CB	30.27	0.2	1
2636	B	157	ARG	CB	30.27	0.2	1
2637	A	57	ARG	N	118.04	0.1	1
2638	B	157	ARG	N	118.04	0.1	1
2639	A	58	PHE	HD1	7.34	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2640	B	158	PHE	HD1	7.34	0.02	1
2641	A	58	PHE	HD2	7.34	0.02	1
2642	B	158	PHE	HD2	7.34	0.02	1
2643	A	58	PHE	HE1	7.64	0.02	1
2644	B	158	PHE	HE1	7.64	0.02	1
2645	A	58	PHE	HE2	7.64	0.02	1
2646	B	158	PHE	HE2	7.64	0.02	1
2647	A	65	PHE	C	180.67	0.2	1
2648	B	165	PHE	C	180.67	0.2	1
2649	A	65	PHE	CA	58.50	0.2	1
2650	B	165	PHE	CA	58.50	0.2	1
2651	A	65	PHE	CB	42.45	0.2	1
2652	B	165	PHE	CB	42.45	0.2	1
2653	A	66	ALA	H	8.01	0.02	1
2654	B	166	ALA	H	8.01	0.02	1
2655	A	66	ALA	HA	4.17	0.02	1
2656	B	166	ALA	HA	4.17	0.02	1
2657	A	66	ALA	HB1	1.54	0.02	1
2658	B	166	ALA	HB1	1.54	0.02	1
2659	A	66	ALA	HB2	1.54	0.02	1
2660	B	166	ALA	HB2	1.54	0.02	1
2661	A	66	ALA	HB3	1.54	0.02	1
2662	B	166	ALA	HB3	1.54	0.02	1
2663	A	66	ALA	C	179.12	0.2	1
2664	B	166	ALA	C	179.12	0.2	1
2665	A	66	ALA	CA	54.85	0.2	1
2666	B	166	ALA	CA	54.85	0.2	1
2667	A	66	ALA	CB	17.77	0.2	1
2668	B	166	ALA	CB	17.77	0.2	1
2669	A	66	ALA	N	124.52	0.1	1
2670	B	166	ALA	N	124.52	0.1	1
2671	A	67	ASP	H	7.68	0.02	1
2672	B	167	ASP	H	7.68	0.02	1
2673	A	67	ASP	HA	4.62	0.02	1
2674	B	167	ASP	HA	4.62	0.02	1
2675	A	67	ASP	HB2	2.84	0.02	1
2676	B	167	ASP	HB2	2.84	0.02	1
2677	A	67	ASP	HB3	2.84	0.02	1
2678	B	167	ASP	HB3	2.84	0.02	1
2679	A	67	ASP	CA	57.48	0.2	1
2680	B	167	ASP	CA	57.48	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2681	A	67	ASP	CB	38.14	0.2	1
2682	B	167	ASP	CB	38.14	0.2	1
2683	A	67	ASP	N	116.50	0.1	1
2684	B	167	ASP	N	116.50	0.1	1
2685	A	2	LYS	HA	4.14	0.02	1
2686	B	102	LYS	HA	4.14	0.02	1
2687	A	2	LYS	HB2	1.41	0.02	2
2688	B	102	LYS	HB2	1.41	0.02	2
2689	A	2	LYS	HB3	1.61	0.02	2
2690	B	102	LYS	HB3	1.61	0.02	2
2691	A	2	LYS	HG2	1.41	0.02	2
2692	B	102	LYS	HG2	1.41	0.02	2
2693	A	2	LYS	HG3	1.51	0.02	2
2694	B	102	LYS	HG3	1.51	0.02	2
2695	A	2	LYS	HD2	1.74	0.02	1
2696	B	102	LYS	HD2	1.74	0.02	1
2697	A	2	LYS	HD3	1.74	0.02	1
2698	B	102	LYS	HD3	1.74	0.02	1
2699	A	2	LYS	HE2	3.01	0.02	1
2700	B	102	LYS	HE2	3.01	0.02	1
2701	A	2	LYS	HE3	3.01	0.02	1
2702	B	102	LYS	HE3	3.01	0.02	1
2703	A	2	LYS	C	175.74	0.2	1
2704	B	102	LYS	C	175.74	0.2	1
2705	A	2	LYS	CA	55.51	0.2	1
2706	B	102	LYS	CA	55.51	0.2	1
2707	A	2	LYS	CB	34.54	0.2	1
2708	B	102	LYS	CB	34.54	0.2	1
2709	A	2	LYS	CG	24.78	0.2	1
2710	B	102	LYS	CG	24.78	0.2	1
2711	A	2	LYS	CD	29.52	0.2	1
2712	B	102	LYS	CD	29.52	0.2	1
2713	A	3	GLN	H	9.10	0.02	1
2714	B	103	GLN	H	9.10	0.02	1
2715	A	3	GLN	HA	4.70	0.02	1
2716	B	103	GLN	HA	4.70	0.02	1
2717	A	3	GLN	HB2	1.53	0.02	1
2718	B	103	GLN	HB2	1.53	0.02	1
2719	A	3	GLN	HB3	1.53	0.02	1
2720	B	103	GLN	HB3	1.53	0.02	1
2721	A	3	GLN	HG2	1.80	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2722	B	103	GLN	HG2	1.80	0.02	2
2723	A	3	GLN	HG3	1.96	0.02	2
2724	B	103	GLN	HG3	1.96	0.02	2
2725	A	3	GLN	HE21	6.81	0.02	2
2726	B	103	GLN	HE21	6.81	0.02	2
2727	A	3	GLN	HE22	7.34	0.02	2
2728	B	103	GLN	HE22	7.34	0.02	2
2729	A	3	GLN	C	173.53	0.2	1
2730	B	103	GLN	C	173.53	0.2	1
2731	A	3	GLN	CA	54.26	0.2	1
2732	B	103	GLN	CA	54.26	0.2	1
2733	A	3	GLN	CG	32.76	0.2	1
2734	B	103	GLN	CG	32.76	0.2	1
2735	A	3	GLN	N	120.19	0.1	1
2736	B	103	GLN	N	120.19	0.1	1
2737	A	3	GLN	NE2	110.67	0.1	1
2738	B	103	GLN	NE2	110.67	0.1	1
2739	A	4	ARG	H	8.69	0.02	1
2740	B	104	ARG	H	8.69	0.02	1
2741	A	4	ARG	HA	5.08	0.02	1
2742	B	104	ARG	HA	5.08	0.02	1
2743	A	4	ARG	HB2	1.73	0.02	2
2744	B	104	ARG	HB2	1.73	0.02	2
2745	A	4	ARG	HB3	1.61	0.02	2
2746	B	104	ARG	HB3	1.61	0.02	2
2747	A	4	ARG	HG2	1.56	0.02	1
2748	B	104	ARG	HG2	1.56	0.02	1
2749	A	4	ARG	HG3	1.56	0.02	1
2750	B	104	ARG	HG3	1.56	0.02	1
2751	A	4	ARG	HD2	3.15	0.02	1
2752	B	104	ARG	HD2	3.15	0.02	1
2753	A	4	ARG	HD3	3.15	0.02	1
2754	B	104	ARG	HD3	3.15	0.02	1
2755	A	4	ARG	C	176.44	0.2	1
2756	B	104	ARG	C	176.44	0.2	1
2757	A	4	ARG	CA	55.63	0.2	1
2758	B	104	ARG	CA	55.63	0.2	1
2759	A	4	ARG	CB	30.98	0.2	1
2760	B	104	ARG	CB	30.98	0.2	1
2761	A	4	ARG	CG	27.33	0.2	1
2762	B	104	ARG	CG	27.33	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2763	A	4	ARG	CD	43.72	0.2	1
2764	B	104	ARG	CD	43.72	0.2	1
2765	A	4	ARG	N	124.82	0.1	1
2766	B	104	ARG	N	124.82	0.1	1
2767	A	5	ILE	H	9.01	0.02	1
2768	B	105	ILE	H	9.01	0.02	1
2769	A	5	ILE	HA	4.78	0.02	1
2770	B	105	ILE	HA	4.78	0.02	1
2771	A	5	ILE	HB	1.75	0.02	1
2772	B	105	ILE	HB	1.75	0.02	1
2773	A	5	ILE	HG12	0.85	0.02	2
2774	B	105	ILE	HG12	0.85	0.02	2
2775	A	5	ILE	HG13	1.19	0.02	2
2776	B	105	ILE	HG13	1.19	0.02	2
2777	A	5	ILE	HG21	0.25	0.02	1
2778	B	105	ILE	HG21	0.25	0.02	1
2779	A	5	ILE	HG22	0.25	0.02	1
2780	B	105	ILE	HG22	0.25	0.02	1
2781	A	5	ILE	HG23	0.25	0.02	1
2782	B	105	ILE	HG23	0.25	0.02	1
2783	A	5	ILE	HD11	0.54	0.02	1
2784	B	105	ILE	HD11	0.54	0.02	1
2785	A	5	ILE	HD12	0.54	0.02	1
2786	B	105	ILE	HD12	0.54	0.02	1
2787	A	5	ILE	HD13	0.54	0.02	1
2788	B	105	ILE	HD13	0.54	0.02	1
2789	A	5	ILE	C	173.94	0.2	1
2790	B	105	ILE	C	173.94	0.2	1
2791	A	5	ILE	CA	59.26	0.2	1
2792	B	105	ILE	CA	59.26	0.2	1
2793	A	5	ILE	CB	41.97	0.2	1
2794	B	105	ILE	CB	41.97	0.2	1
2795	A	5	ILE	CG1	26.24	0.2	1
2796	B	105	ILE	CG1	26.24	0.2	1
2797	A	5	ILE	CG2	17.05	0.2	1
2798	B	105	ILE	CG2	17.05	0.2	1
2799	A	5	ILE	CD1	14.88	0.2	1
2800	B	105	ILE	CD1	14.88	0.2	1
2801	A	5	ILE	N	119.88	0.1	1
2802	B	105	ILE	N	119.88	0.1	1
2803	A	6	THR	H	8.31	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2804	B	106	THR	H	8.31	0.02	1
2805	A	6	THR	HA	5.47	0.02	1
2806	B	106	THR	HA	5.47	0.02	1
2807	A	6	THR	HB	3.91	0.02	1
2808	B	106	THR	HB	3.91	0.02	1
2809	A	6	THR	HG21	1.14	0.02	1
2810	B	106	THR	HG21	1.14	0.02	1
2811	A	6	THR	HG22	1.14	0.02	1
2812	B	106	THR	HG22	1.14	0.02	1
2813	A	6	THR	HG23	1.14	0.02	1
2814	B	106	THR	HG23	1.14	0.02	1
2815	A	6	THR	C	174.55	0.2	1
2816	B	106	THR	C	174.55	0.2	1
2817	A	6	THR	CA	60.79	0.2	1
2818	B	106	THR	CA	60.79	0.2	1
2819	A	6	THR	CB	69.51	0.2	1
2820	B	106	THR	CB	69.51	0.2	1
2821	A	6	THR	CG2	21.90	0.2	1
2822	B	106	THR	CG2	21.90	0.2	1
2823	A	6	THR	N	116.80	0.1	1
2824	B	106	THR	N	116.80	0.1	1
2825	A	7	VAL	H	8.90	0.02	1
2826	B	107	VAL	H	8.90	0.02	1
2827	A	7	VAL	HA	4.93	0.02	1
2828	B	107	VAL	HA	4.93	0.02	1
2829	A	7	VAL	HB	2.33	0.02	1
2830	B	107	VAL	HB	2.33	0.02	1
2831	A	7	VAL	HG11	0.64	0.02	2
2832	B	107	VAL	HG11	0.64	0.02	2
2833	A	7	VAL	HG12	0.64	0.02	2
2834	B	107	VAL	HG12	0.64	0.02	2
2835	A	7	VAL	HG13	0.64	0.02	2
2836	B	107	VAL	HG13	0.64	0.02	2
2837	A	7	VAL	HG21	0.84	0.02	2
2838	B	107	VAL	HG21	0.84	0.02	2
2839	A	7	VAL	HG22	0.84	0.02	2
2840	B	107	VAL	HG22	0.84	0.02	2
2841	A	7	VAL	HG23	0.84	0.02	2
2842	B	107	VAL	HG23	0.84	0.02	2
2843	A	7	VAL	C	173.61	0.2	1
2844	B	107	VAL	C	173.61	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2845	A	7	VAL	CA	58.97	0.2	1
2846	B	107	VAL	CA	58.97	0.2	1
2847	A	7	VAL	CB	36.43	0.2	1
2848	B	107	VAL	CB	36.43	0.2	1
2849	A	7	VAL	CG1	19.07	0.2	2
2850	B	107	VAL	CG1	19.07	0.2	2
2851	A	7	VAL	CG2	21.87	0.2	2
2852	B	107	VAL	CG2	21.87	0.2	2
2853	A	7	VAL	N	119.27	0.1	1
2854	B	107	VAL	N	119.27	0.1	1
2855	A	8	THR	H	8.38	0.02	1
2856	B	108	THR	H	8.38	0.02	1
2857	A	8	THR	HA	4.93	0.02	1
2858	B	108	THR	HA	4.93	0.02	1
2859	A	8	THR	HB	3.99	0.02	1
2860	B	108	THR	HB	3.99	0.02	1
2861	A	8	THR	HG21	1.13	0.02	1
2862	B	108	THR	HG21	1.13	0.02	1
2863	A	8	THR	HG22	1.13	0.02	1
2864	B	108	THR	HG22	1.13	0.02	1
2865	A	8	THR	HG23	1.13	0.02	1
2866	B	108	THR	HG23	1.13	0.02	1
2867	A	8	THR	C	174.47	0.2	1
2868	B	108	THR	C	174.47	0.2	1
2869	A	8	THR	CA	62.09	0.2	1
2870	B	108	THR	CA	62.09	0.2	1
2871	A	8	THR	CB	69.47	0.2	1
2872	B	108	THR	CB	69.47	0.2	1
2873	A	8	THR	CG2	22.59	0.2	1
2874	B	108	THR	CG2	22.59	0.2	1
2875	A	8	THR	N	119.27	0.1	1
2876	B	108	THR	N	119.27	0.1	1
2877	A	9	VAL	H	8.91	0.02	1
2878	B	109	VAL	H	8.91	0.02	1
2879	A	9	VAL	HA	4.70	0.02	1
2880	B	109	VAL	HA	4.70	0.02	1
2881	A	9	VAL	HB	2.08	0.02	1
2882	B	109	VAL	HB	2.08	0.02	1
2883	A	9	VAL	HG11	0.78	0.02	2
2884	B	109	VAL	HG11	0.78	0.02	2
2885	A	9	VAL	HG12	0.78	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2886	B	109	VAL	HG12	0.78	0.02	2
2887	A	9	VAL	HG13	0.78	0.02	2
2888	B	109	VAL	HG13	0.78	0.02	2
2889	A	9	VAL	HG21	0.87	0.02	2
2890	B	109	VAL	HG21	0.87	0.02	2
2891	A	9	VAL	HG22	0.87	0.02	2
2892	B	109	VAL	HG22	0.87	0.02	2
2893	A	9	VAL	HG23	0.87	0.02	2
2894	B	109	VAL	HG23	0.87	0.02	2
2895	A	9	VAL	C	179.13	0.2	1
2896	B	109	VAL	C	179.13	0.2	1
2897	A	9	VAL	CA	58.29	0.2	1
2898	B	109	VAL	CA	58.29	0.2	1
2899	A	9	VAL	CB	36.05	0.2	1
2900	B	109	VAL	CB	36.05	0.2	1
2901	A	9	VAL	CG1	19.68	0.2	2
2902	B	109	VAL	CG1	19.68	0.2	2
2903	A	9	VAL	CG2	22.96	0.2	2
2904	B	109	VAL	CG2	22.96	0.2	2
2905	A	9	VAL	N	117.42	0.1	1
2906	B	109	VAL	N	117.42	0.1	1
2907	A	10	ASP	H	8.16	0.02	1
2908	B	110	ASP	H	8.16	0.02	1
2909	A	10	ASP	HA	4.37	0.02	1
2910	B	110	ASP	HA	4.37	0.02	1
2911	A	10	ASP	HB2	2.76	0.02	2
2912	B	110	ASP	HB2	2.76	0.02	2
2913	A	10	ASP	HB3	2.87	0.02	2
2914	B	110	ASP	HB3	2.87	0.02	2
2915	A	10	ASP	C	176.22	0.2	1
2916	B	110	ASP	C	176.22	0.2	1
2917	A	10	ASP	CA	62.33	0.2	1
2918	B	110	ASP	CA	62.33	0.2	1
2919	A	10	ASP	CB	40.76	0.2	1
2920	B	110	ASP	CB	40.76	0.2	1
2921	A	10	ASP	N	115.55	0.1	1
2922	B	110	ASP	N	115.55	0.1	1
2923	A	11	SER	H	8.50	0.02	1
2924	B	111	SER	H	8.50	0.02	1
2925	A	11	SER	HA	4.46	0.02	1
2926	B	111	SER	HA	4.46	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2927	A	11	SER	HB2	3.92	0.02	2
2928	B	111	SER	HB2	3.92	0.02	2
2929	A	11	SER	HB3	3.98	0.02	2
2930	B	111	SER	HB3	3.98	0.02	2
2931	A	11	SER	C	174.32	0.2	1
2932	B	111	SER	C	174.32	0.2	1
2933	A	11	SER	CA	58.29	0.2	1
2934	B	111	SER	CA	58.29	0.2	1
2935	A	11	SER	CB	67.88	0.2	1
2936	B	111	SER	CB	67.88	0.2	1
2937	A	11	SER	N	121.10	0.1	1
2938	B	111	SER	N	121.10	0.1	1
2939	A	12	ASP	H	7.91	0.02	1
2940	B	112	ASP	H	7.91	0.02	1
2941	A	12	ASP	HB2	2.72	0.02	2
2942	B	112	ASP	HB2	2.72	0.02	2
2943	A	12	ASP	HB3	2.77	0.02	2
2944	B	112	ASP	HB3	2.77	0.02	2
2945	A	12	ASP	C	176.55	0.2	1
2946	B	112	ASP	C	176.55	0.2	1
2947	A	12	ASP	CA	55.02	0.2	1
2948	B	112	ASP	CA	55.02	0.2	1
2949	A	12	ASP	CB	43.09	0.2	1
2950	B	112	ASP	CB	43.09	0.2	1
2951	A	12	ASP	N	119.88	0.1	1
2952	B	112	ASP	N	119.88	0.1	1
2953	A	13	SER	H	9.07	0.02	1
2954	B	113	SER	H	9.07	0.02	1
2955	A	13	SER	HA	4.23	0.02	1
2956	B	113	SER	HA	4.23	0.02	1
2957	A	13	SER	HB2	3.90	0.02	2
2958	B	113	SER	HB2	3.90	0.02	2
2959	A	13	SER	HB3	3.98	0.02	2
2960	B	113	SER	HB3	3.98	0.02	2
2961	A	13	SER	C	175.25	0.2	1
2962	B	113	SER	C	175.25	0.2	1
2963	A	13	SER	CA	62.29	0.2	1
2964	B	113	SER	CA	62.29	0.2	1
2965	A	13	SER	CB	63.16	0.2	1
2966	B	113	SER	CB	63.16	0.2	1
2967	A	13	SER	N	122.97	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2968	B	113	SER	N	122.97	0.1	1
2969	A	14	TYR	H	7.80	0.02	1
2970	B	114	TYR	H	7.80	0.02	1
2971	A	14	TYR	HA	4.14	0.02	1
2972	B	114	TYR	HA	4.14	0.02	1
2973	A	14	TYR	HB2	3.07	0.02	2
2974	B	114	TYR	HB2	3.07	0.02	2
2975	A	14	TYR	HB3	3.14	0.02	2
2976	B	114	TYR	HB3	3.14	0.02	2
2977	A	14	TYR	HD1	7.00	0.02	1
2978	B	114	TYR	HD1	7.00	0.02	1
2979	A	14	TYR	HD2	7.00	0.02	1
2980	B	114	TYR	HD2	7.00	0.02	1
2981	A	14	TYR	HE1	6.83	0.02	1
2982	B	114	TYR	HE1	6.83	0.02	1
2983	A	14	TYR	HE2	6.83	0.02	1
2984	B	114	TYR	HE2	6.83	0.02	1
2985	A	14	TYR	C	176.03	0.2	1
2986	B	114	TYR	C	176.03	0.2	1
2987	A	14	TYR	CA	61.60	0.2	1
2988	B	114	TYR	CA	61.60	0.2	1
2989	A	14	TYR	CB	39.03	0.2	1
2990	B	114	TYR	CB	39.03	0.2	1
2991	A	14	TYR	CD1	132.61	0.2	1
2992	B	114	TYR	CD1	132.61	0.2	1
2993	A	14	TYR	CD2	132.61	0.2	1
2994	B	114	TYR	CD2	132.61	0.2	1
2995	A	14	TYR	CE1	118.40	0.2	1
2996	B	114	TYR	CE1	118.40	0.2	1
2997	A	14	TYR	CE2	118.40	0.2	1
2998	B	114	TYR	CE2	118.40	0.2	1
2999	A	14	TYR	N	121.73	0.1	1
3000	B	114	TYR	N	121.73	0.1	1
3001	A	15	GLN	H	8.57	0.02	1
3002	B	115	GLN	H	8.57	0.02	1
3003	A	15	GLN	HA	3.70	0.02	1
3004	B	115	GLN	HA	3.70	0.02	1
3005	A	15	GLN	HB2	2.17	0.02	2
3006	B	115	GLN	HB2	2.17	0.02	2
3007	A	15	GLN	HB3	2.21	0.02	2
3008	B	115	GLN	HB3	2.21	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3009	A	15	GLN	HG2	2.61	0.02	2
3010	B	115	GLN	HG2	2.61	0.02	2
3011	A	15	GLN	HG3	2.76	0.02	2
3012	B	115	GLN	HG3	2.76	0.02	2
3013	A	15	GLN	HE21	6.98	0.02	2
3014	B	115	GLN	HE21	6.98	0.02	2
3015	A	15	GLN	HE22	7.58	0.02	2
3016	B	115	GLN	HE22	7.58	0.02	2
3017	A	15	GLN	C	179.13	0.2	1
3018	B	115	GLN	C	179.13	0.2	1
3019	A	15	GLN	CA	58.66	0.2	1
3020	B	115	GLN	CA	58.66	0.2	1
3021	A	15	GLN	CB	28.11	0.2	1
3022	B	115	GLN	CB	28.11	0.2	1
3023	A	15	GLN	CG	34.25	0.2	1
3024	B	115	GLN	CG	34.25	0.2	1
3025	A	15	GLN	N	115.26	0.1	1
3026	B	115	GLN	N	115.26	0.1	1
3027	A	15	GLN	NE2	111.46	0.1	1
3028	B	115	GLN	NE2	111.46	0.1	1
3029	A	16	LEU	H	7.64	0.02	1
3030	B	116	LEU	H	7.64	0.02	1
3031	A	16	LEU	HA	4.15	0.02	1
3032	B	116	LEU	HA	4.15	0.02	1
3033	A	16	LEU	HB2	1.79	0.02	2
3034	B	116	LEU	HB2	1.79	0.02	2
3035	A	16	LEU	HB3	1.85	0.02	2
3036	B	116	LEU	HB3	1.85	0.02	2
3037	A	16	LEU	HG	1.69	0.02	1
3038	B	116	LEU	HG	1.69	0.02	1
3039	A	16	LEU	HD11	0.93	0.02	2
3040	B	116	LEU	HD11	0.93	0.02	2
3041	A	16	LEU	HD12	0.93	0.02	2
3042	B	116	LEU	HD12	0.93	0.02	2
3043	A	16	LEU	HD13	0.93	0.02	2
3044	B	116	LEU	HD13	0.93	0.02	2
3045	A	16	LEU	HD21	0.95	0.02	2
3046	B	116	LEU	HD21	0.95	0.02	2
3047	A	16	LEU	HD22	0.95	0.02	2
3048	B	116	LEU	HD22	0.95	0.02	2
3049	A	16	LEU	HD23	0.95	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3050	B	116	LEU	HD23	0.95	0.02	2
3051	A	16	LEU	C	178.10	0.2	1
3052	B	116	LEU	C	178.10	0.2	1
3053	A	16	LEU	CA	58.22	0.2	1
3054	B	116	LEU	CA	58.22	0.2	1
3055	A	16	LEU	CB	42.09	0.2	1
3056	B	116	LEU	CB	42.09	0.2	1
3057	A	16	LEU	CG	28.06	0.2	1
3058	B	116	LEU	CG	28.06	0.2	1
3059	A	16	LEU	CD1	25.51	0.2	2
3060	B	116	LEU	CD1	25.51	0.2	2
3061	A	16	LEU	CD2	24.78	0.2	2
3062	B	116	LEU	CD2	24.78	0.2	2
3063	A	16	LEU	N	121.73	0.1	1
3064	B	116	LEU	N	121.73	0.1	1
3065	A	17	LEU	H	7.92	0.02	1
3066	B	117	LEU	H	7.92	0.02	1
3067	A	17	LEU	HA	3.91	0.02	1
3068	B	117	LEU	HA	3.91	0.02	1
3069	A	17	LEU	HB2	1.27	0.02	2
3070	B	117	LEU	HB2	1.27	0.02	2
3071	A	17	LEU	HB3	1.96	0.02	2
3072	B	117	LEU	HB3	1.96	0.02	2
3073	A	17	LEU	HD11	0.88	0.02	2
3074	B	117	LEU	HD11	0.88	0.02	2
3075	A	17	LEU	HD12	0.88	0.02	2
3076	B	117	LEU	HD12	0.88	0.02	2
3077	A	17	LEU	HD13	0.88	0.02	2
3078	B	117	LEU	HD13	0.88	0.02	2
3079	A	17	LEU	HD21	1.02	0.02	2
3080	B	117	LEU	HD21	1.02	0.02	2
3081	A	17	LEU	HD22	1.02	0.02	2
3082	B	117	LEU	HD22	1.02	0.02	2
3083	A	17	LEU	HD23	1.02	0.02	2
3084	B	117	LEU	HD23	1.02	0.02	2
3085	A	17	LEU	C	179.68	0.2	1
3086	B	117	LEU	C	179.68	0.2	1
3087	A	17	LEU	CA	58.23	0.2	1
3088	B	117	LEU	CA	58.23	0.2	1
3089	A	17	LEU	CB	41.90	0.2	1
3090	B	117	LEU	CB	41.90	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3091	A	17	LEU	CD1	23.33	0.2	2
3092	B	117	LEU	CD1	23.33	0.2	2
3093	A	17	LEU	CD2	25.88	0.2	2
3094	B	117	LEU	CD2	25.88	0.2	2
3095	A	17	LEU	N	117.42	0.1	1
3096	B	117	LEU	N	117.42	0.1	1
3097	A	18	LYS	H	8.24	0.02	1
3098	B	118	LYS	H	8.24	0.02	1
3099	A	18	LYS	HA	4.11	0.02	1
3100	B	118	LYS	HA	4.11	0.02	1
3101	A	18	LYS	HB2	1.87	0.02	2
3102	B	118	LYS	HB2	1.87	0.02	2
3103	A	18	LYS	HB3	1.97	0.02	2
3104	B	118	LYS	HB3	1.97	0.02	2
3105	A	18	LYS	HG2	1.21	0.02	1
3106	B	118	LYS	HG2	1.21	0.02	1
3107	A	18	LYS	HG3	1.21	0.02	1
3108	B	118	LYS	HG3	1.21	0.02	1
3109	A	18	LYS	HD2	1.53	0.02	1
3110	B	118	LYS	HD2	1.53	0.02	1
3111	A	18	LYS	HD3	1.53	0.02	1
3112	B	118	LYS	HD3	1.53	0.02	1
3113	A	18	LYS	HE2	2.88	0.02	2
3114	B	118	LYS	HE2	2.88	0.02	2
3115	A	18	LYS	HE3	3.01	0.02	2
3116	B	118	LYS	HE3	3.01	0.02	2
3117	A	18	LYS	C	178.43	0.2	1
3118	B	118	LYS	C	178.43	0.2	1
3119	A	18	LYS	CA	59.54	0.2	1
3120	B	118	LYS	CA	59.54	0.2	1
3121	A	18	LYS	CB	30.54	0.2	1
3122	B	118	LYS	CB	30.54	0.2	1
3123	A	18	LYS	CG	24.44	0.2	1
3124	B	118	LYS	CG	24.44	0.2	1
3125	A	18	LYS	CD	28.79	0.2	1
3126	B	118	LYS	CD	28.79	0.2	1
3127	A	18	LYS	CE	41.54	0.2	1
3128	B	118	LYS	CE	41.54	0.2	1
3129	A	18	LYS	N	118.96	0.1	1
3130	B	118	LYS	N	118.96	0.1	1
3131	A	19	ALA	H	7.76	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3132	B	119	ALA	H	7.76	0.02	1
3133	A	19	ALA	HA	4.30	0.02	1
3134	B	119	ALA	HA	4.30	0.02	1
3135	A	19	ALA	HB1	1.61	0.02	1
3136	B	119	ALA	HB1	1.61	0.02	1
3137	A	19	ALA	HB2	1.61	0.02	1
3138	B	119	ALA	HB2	1.61	0.02	1
3139	A	19	ALA	HB3	1.61	0.02	1
3140	B	119	ALA	HB3	1.61	0.02	1
3141	A	19	ALA	C	179.83	0.2	1
3142	B	119	ALA	C	179.83	0.2	1
3143	A	19	ALA	CA	54.79	0.2	1
3144	B	119	ALA	CA	54.79	0.2	1
3145	A	19	ALA	CB	18.22	0.2	1
3146	B	119	ALA	CB	18.22	0.2	1
3147	A	19	ALA	N	120.81	0.1	1
3148	B	119	ALA	N	120.81	0.1	1
3149	A	20	TYR	H	8.07	0.02	1
3150	B	120	TYR	H	8.07	0.02	1
3151	A	20	TYR	HA	4.20	0.02	1
3152	B	120	TYR	HA	4.20	0.02	1
3153	A	20	TYR	HD1	7.23	0.02	1
3154	B	120	TYR	HD1	7.23	0.02	1
3155	A	20	TYR	HD2	7.23	0.02	1
3156	B	120	TYR	HD2	7.23	0.02	1
3157	A	20	TYR	HE1	6.77	0.02	1
3158	B	120	TYR	HE1	6.77	0.02	1
3159	A	20	TYR	HE2	6.77	0.02	1
3160	B	120	TYR	HE2	6.77	0.02	1
3161	A	20	TYR	CA	58.22	0.2	1
3162	B	120	TYR	CA	58.22	0.2	1
3163	A	20	TYR	CB	39.16	0.2	1
3164	B	120	TYR	CB	39.16	0.2	1
3165	A	20	TYR	CD1	132.59	0.2	1
3166	B	120	TYR	CD1	132.59	0.2	1
3167	A	20	TYR	CD2	132.59	0.2	1
3168	B	120	TYR	CD2	132.59	0.2	1
3169	A	20	TYR	CE1	117.86	0.2	1
3170	B	120	TYR	CE1	117.86	0.2	1
3171	A	20	TYR	CE2	117.86	0.2	1
3172	B	120	TYR	CE2	117.86	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3173	A	20	TYR	N	117.73	0.1	1
3174	B	120	TYR	N	117.73	0.1	1
3175	A	21	ASP	H	8.16	0.02	1
3176	B	121	ASP	H	8.16	0.02	1
3177	A	21	ASP	HA	4.48	0.02	1
3178	B	121	ASP	HA	4.48	0.02	1
3179	A	21	ASP	HB2	2.63	0.02	2
3180	B	121	ASP	HB2	2.63	0.02	2
3181	A	21	ASP	HB3	3.18	0.02	2
3182	B	121	ASP	HB3	3.18	0.02	2
3183	A	21	ASP	C	175.27	0.2	1
3184	B	121	ASP	C	175.27	0.2	1
3185	A	21	ASP	CA	55.38	0.2	1
3186	B	121	ASP	CA	55.38	0.2	1
3187	A	21	ASP	CB	39.43	0.2	1
3188	B	121	ASP	CB	39.43	0.2	1
3189	A	21	ASP	N	118.03	0.1	1
3190	B	121	ASP	N	118.03	0.1	1
3191	A	22	VAL	H	7.85	0.02	1
3192	B	122	VAL	H	7.85	0.02	1
3193	A	22	VAL	HA	3.86	0.02	1
3194	B	122	VAL	HA	3.86	0.02	1
3195	A	22	VAL	HB	1.84	0.02	1
3196	B	122	VAL	HB	1.84	0.02	1
3197	A	22	VAL	HG11	0.90	0.02	2
3198	B	122	VAL	HG11	0.90	0.02	2
3199	A	22	VAL	HG12	0.90	0.02	2
3200	B	122	VAL	HG12	0.90	0.02	2
3201	A	22	VAL	HG13	0.90	0.02	2
3202	B	122	VAL	HG13	0.90	0.02	2
3203	A	22	VAL	HG21	1.13	0.02	2
3204	B	122	VAL	HG21	1.13	0.02	2
3205	A	22	VAL	HG22	1.13	0.02	2
3206	B	122	VAL	HG22	1.13	0.02	2
3207	A	22	VAL	HG23	1.13	0.02	2
3208	B	122	VAL	HG23	1.13	0.02	2
3209	A	22	VAL	C	176.16	0.2	1
3210	B	122	VAL	C	176.16	0.2	1
3211	A	22	VAL	CA	63.03	0.2	1
3212	B	122	VAL	CA	63.03	0.2	1
3213	A	22	VAL	CB	32.80	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3214	B	122	VAL	CB	32.80	0.2	1
3215	A	22	VAL	CG1	21.14	0.2	2
3216	B	122	VAL	CG1	21.14	0.2	2
3217	A	22	VAL	CG2	23.33	0.2	2
3218	B	122	VAL	CG2	23.33	0.2	2
3219	A	22	VAL	N	118.96	0.1	1
3220	B	122	VAL	N	118.96	0.1	1
3221	A	23	ASN	H	8.77	0.02	1
3222	B	123	ASN	H	8.77	0.02	1
3223	A	23	ASN	HA	4.83	0.02	1
3224	B	123	ASN	HA	4.83	0.02	1
3225	A	23	ASN	HB2	2.98	0.02	2
3226	B	123	ASN	HB2	2.98	0.02	2
3227	A	23	ASN	HB3	3.25	0.02	2
3228	B	123	ASN	HB3	3.25	0.02	2
3229	A	23	ASN	HD21	7.19	0.02	2
3230	B	123	ASN	HD21	7.19	0.02	2
3231	A	23	ASN	HD22	7.89	0.02	2
3232	B	123	ASN	HD22	7.89	0.02	2
3233	A	23	ASN	C	175.60	0.2	1
3234	B	123	ASN	C	175.60	0.2	1
3235	A	23	ASN	CA	52.41	0.2	1
3236	B	123	ASN	CA	52.41	0.2	1
3237	A	23	ASN	CB	37.05	0.2	1
3238	B	123	ASN	CB	37.05	0.2	1
3239	A	23	ASN	N	124.51	0.1	1
3240	B	123	ASN	N	124.51	0.1	1
3241	A	23	ASN	ND2	112.29	0.1	1
3242	B	123	ASN	ND2	112.29	0.1	1
3243	A	24	ILE	H	8.38	0.02	1
3244	B	124	ILE	H	8.38	0.02	1
3245	A	24	ILE	HA	3.63	0.02	1
3246	B	124	ILE	HA	3.63	0.02	1
3247	A	24	ILE	HB	2.22	0.02	1
3248	B	124	ILE	HB	2.22	0.02	1
3249	A	24	ILE	HG12	1.38	0.02	2
3250	B	124	ILE	HG12	1.38	0.02	2
3251	A	24	ILE	HG13	1.84	0.02	2
3252	B	124	ILE	HG13	1.84	0.02	2
3253	A	24	ILE	HG21	1.02	0.02	1
3254	B	124	ILE	HG21	1.02	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3255	A	24	ILE	HG22	1.02	0.02	1
3256	B	124	ILE	HG22	1.02	0.02	1
3257	A	24	ILE	HG23	1.02	0.02	1
3258	B	124	ILE	HG23	1.02	0.02	1
3259	A	24	ILE	HD11	0.90	0.02	1
3260	B	124	ILE	HD11	0.90	0.02	1
3261	A	24	ILE	HD12	0.90	0.02	1
3262	B	124	ILE	HD12	0.90	0.02	1
3263	A	24	ILE	HD13	0.90	0.02	1
3264	B	124	ILE	HD13	0.90	0.02	1
3265	A	24	ILE	C	177.57	0.2	1
3266	B	124	ILE	C	177.57	0.2	1
3267	A	24	ILE	CA	64.85	0.2	1
3268	B	124	ILE	CA	64.85	0.2	1
3269	A	24	ILE	CB	37.17	0.2	1
3270	B	124	ILE	CB	37.17	0.2	1
3271	A	24	ILE	CG1	28.79	0.2	1
3272	B	124	ILE	CG1	28.79	0.2	1
3273	A	24	ILE	CG2	17.87	0.2	1
3274	B	124	ILE	CG2	17.87	0.2	1
3275	A	24	ILE	CD1	12.00	0.2	1
3276	B	124	ILE	CD1	12.00	0.2	1
3277	A	24	ILE	N	130.68	0.1	1
3278	B	124	ILE	N	130.68	0.1	1
3279	A	25	SER	H	8.72	0.02	1
3280	B	125	SER	H	8.72	0.02	1
3281	A	25	SER	HA	4.37	0.02	1
3282	B	125	SER	HA	4.37	0.02	1
3283	A	25	SER	HB2	4.15	0.02	2
3284	B	125	SER	HB2	4.15	0.02	2
3285	A	25	SER	HB3	4.22	0.02	2
3286	B	125	SER	HB3	4.22	0.02	2
3287	A	25	SER	C	176.50	0.2	1
3288	B	125	SER	C	176.50	0.2	1
3289	A	25	SER	CA	63.64	0.2	1
3290	B	125	SER	CA	63.64	0.2	1
3291	A	25	SER	CB	68.58	0.2	1
3292	B	125	SER	CB	68.58	0.2	1
3293	A	25	SER	N	116.80	0.1	1
3294	B	125	SER	N	116.80	0.1	1
3295	A	26	GLY	H	8.06	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3296	B	126	GLY	H	8.06	0.02	1
3297	A	26	GLY	HA2	3.82	0.02	2
3298	B	126	GLY	HA2	3.82	0.02	2
3299	A	26	GLY	HA3	3.96	0.02	2
3300	B	126	GLY	HA3	3.96	0.02	2
3301	A	26	GLY	C	175.95	0.2	1
3302	B	126	GLY	C	175.95	0.2	1
3303	A	26	GLY	CA	47.53	0.2	1
3304	B	126	GLY	CA	47.53	0.2	1
3305	A	26	GLY	N	109.71	0.1	1
3306	B	126	GLY	N	109.71	0.1	1
3307	A	27	LEU	H	8.01	0.02	1
3308	B	127	LEU	H	8.01	0.02	1
3309	A	27	LEU	HA	4.29	0.02	1
3310	B	127	LEU	HA	4.29	0.02	1
3311	A	27	LEU	HB2	1.75	0.02	2
3312	B	127	LEU	HB2	1.75	0.02	2
3313	A	27	LEU	HB3	2.06	0.02	2
3314	B	127	LEU	HB3	2.06	0.02	2
3315	A	27	LEU	HD11	0.90	0.02	2
3316	B	127	LEU	HD11	0.90	0.02	2
3317	A	27	LEU	HD12	0.90	0.02	2
3318	B	127	LEU	HD12	0.90	0.02	2
3319	A	27	LEU	HD13	0.90	0.02	2
3320	B	127	LEU	HD13	0.90	0.02	2
3321	A	27	LEU	HD21	0.95	0.02	2
3322	B	127	LEU	HD21	0.95	0.02	2
3323	A	27	LEU	HD22	0.95	0.02	2
3324	B	127	LEU	HD22	0.95	0.02	2
3325	A	27	LEU	HD23	0.95	0.02	2
3326	B	127	LEU	HD23	0.95	0.02	2
3327	A	27	LEU	C	180.07	0.2	1
3328	B	127	LEU	C	180.07	0.2	1
3329	A	27	LEU	CA	58.29	0.2	1
3330	B	127	LEU	CA	58.29	0.2	1
3331	A	27	LEU	CB	42.28	0.2	1
3332	B	127	LEU	CB	42.28	0.2	1
3333	A	27	LEU	CD1	26.60	0.2	2
3334	B	127	LEU	CD1	26.60	0.2	2
3335	A	27	LEU	CD2	23.69	0.2	2
3336	B	127	LEU	CD2	23.69	0.2	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3337	A	27	LEU	N	124.51	0.1	1
3338	B	127	LEU	N	124.51	0.1	1
3339	A	28	VAL	H	8.77	0.02	1
3340	B	128	VAL	H	8.77	0.02	1
3341	A	28	VAL	HA	3.57	0.02	1
3342	B	128	VAL	HA	3.57	0.02	1
3343	A	28	VAL	HB	2.23	0.02	1
3344	B	128	VAL	HB	2.23	0.02	1
3345	A	28	VAL	HG11	1.05	0.02	2
3346	B	128	VAL	HG11	1.05	0.02	2
3347	A	28	VAL	HG12	1.05	0.02	2
3348	B	128	VAL	HG12	1.05	0.02	2
3349	A	28	VAL	HG13	1.05	0.02	2
3350	B	128	VAL	HG13	1.05	0.02	2
3351	A	28	VAL	HG21	1.14	0.02	2
3352	B	128	VAL	HG21	1.14	0.02	2
3353	A	28	VAL	HG22	1.14	0.02	2
3354	B	128	VAL	HG22	1.14	0.02	2
3355	A	28	VAL	HG23	1.14	0.02	2
3356	B	128	VAL	HG23	1.14	0.02	2
3357	A	28	VAL	C	177.48	0.2	1
3358	B	128	VAL	C	177.48	0.2	1
3359	A	28	VAL	CA	67.40	0.2	1
3360	B	128	VAL	CA	67.40	0.2	1
3361	A	28	VAL	CB	31.70	0.2	1
3362	B	128	VAL	CB	31.70	0.2	1
3363	A	28	VAL	CG1	23.20	0.2	2
3364	B	128	VAL	CG1	23.20	0.2	2
3365	A	28	VAL	CG2	23.69	0.2	2
3366	B	128	VAL	CG2	23.69	0.2	2
3367	A	28	VAL	N	119.88	0.1	1
3368	B	128	VAL	N	119.88	0.1	1
3369	A	29	SER	H	9.03	0.02	1
3370	B	129	SER	H	9.03	0.02	1
3371	A	29	SER	HA	4.34	0.02	1
3372	B	129	SER	HA	4.34	0.02	1
3373	A	29	SER	HB2	4.27	0.02	1
3374	B	129	SER	HB2	4.27	0.02	1
3375	A	29	SER	HB3	4.27	0.02	1
3376	B	129	SER	HB3	4.27	0.02	1
3377	A	29	SER	C	177.86	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3378	B	129	SER	C	177.86	0.2	1
3379	A	29	SER	CA	63.32	0.2	1
3380	B	129	SER	CA	63.32	0.2	1
3381	A	29	SER	CB	65.99	0.2	1
3382	B	129	SER	CB	65.99	0.2	1
3383	A	29	SER	N	115.57	0.1	1
3384	B	129	SER	N	115.57	0.1	1
3385	A	30	THR	H	8.52	0.02	1
3386	B	130	THR	H	8.52	0.02	1
3387	A	30	THR	HA	4.09	0.02	1
3388	B	130	THR	HA	4.09	0.02	1
3389	A	30	THR	HB	4.38	0.02	1
3390	B	130	THR	HB	4.38	0.02	1
3391	A	30	THR	HG21	1.38	0.02	1
3392	B	130	THR	HG21	1.38	0.02	1
3393	A	30	THR	HG22	1.38	0.02	1
3394	B	130	THR	HG22	1.38	0.02	1
3395	A	30	THR	HG23	1.38	0.02	1
3396	B	130	THR	HG23	1.38	0.02	1
3397	A	30	THR	C	176.26	0.2	1
3398	B	130	THR	C	176.26	0.2	1
3399	A	30	THR	CA	67.00	0.2	1
3400	B	130	THR	CA	67.00	0.2	1
3401	A	30	THR	CB	68.86	0.2	1
3402	B	130	THR	CB	68.86	0.2	1
3403	A	30	THR	CG2	21.56	0.2	1
3404	B	130	THR	CG2	21.56	0.2	1
3405	A	30	THR	N	117.11	0.1	1
3406	B	130	THR	N	117.11	0.1	1
3407	A	31	THR	H	7.89	0.02	1
3408	B	131	THR	H	7.89	0.02	1
3409	A	31	THR	HA	4.16	0.02	1
3410	B	131	THR	HA	4.16	0.02	1
3411	A	31	THR	HB	4.49	0.02	1
3412	B	131	THR	HB	4.49	0.02	1
3413	A	31	THR	HG21	1.39	0.02	1
3414	B	131	THR	HG21	1.39	0.02	1
3415	A	31	THR	HG22	1.39	0.02	1
3416	B	131	THR	HG22	1.39	0.02	1
3417	A	31	THR	HG23	1.39	0.02	1
3418	B	131	THR	HG23	1.39	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3419	A	31	THR	C	176.96	0.2	1
3420	B	131	THR	C	176.96	0.2	1
3421	A	31	THR	CA	66.00	0.2	1
3422	B	131	THR	CA	66.00	0.2	1
3423	A	31	THR	CB	67.77	0.2	1
3424	B	131	THR	CB	67.77	0.2	1
3425	A	31	THR	CG2	21.14	0.2	1
3426	B	131	THR	CG2	21.14	0.2	1
3427	A	31	THR	N	118.65	0.1	1
3428	B	131	THR	N	118.65	0.1	1
3429	A	32	MET	H	8.53	0.02	1
3430	B	132	MET	H	8.53	0.02	1
3431	A	32	MET	HA	3.98	0.02	1
3432	B	132	MET	HA	3.98	0.02	1
3433	A	32	MET	HB2	2.40	0.02	2
3434	B	132	MET	HB2	2.40	0.02	2
3435	A	32	MET	HB3	2.48	0.02	2
3436	B	132	MET	HB3	2.48	0.02	2
3437	A	32	MET	HG2	2.99	0.02	2
3438	B	132	MET	HG2	2.99	0.02	2
3439	A	32	MET	HG3	3.16	0.02	2
3440	B	132	MET	HG3	3.16	0.02	2
3441	A	32	MET	HE1	2.10	0.02	1
3442	B	132	MET	HE1	2.10	0.02	1
3443	A	32	MET	HE2	2.10	0.02	1
3444	B	132	MET	HE2	2.10	0.02	1
3445	A	32	MET	HE3	2.10	0.02	1
3446	B	132	MET	HE3	2.10	0.02	1
3447	A	32	MET	C	177.57	0.2	1
3448	B	132	MET	C	177.57	0.2	1
3449	A	32	MET	CA	60.72	0.2	1
3450	B	132	MET	CA	60.72	0.2	1
3451	A	32	MET	CB	33.53	0.2	1
3452	B	132	MET	CB	33.53	0.2	1
3453	A	32	MET	CG	31.34	0.2	1
3454	B	132	MET	CG	31.34	0.2	1
3455	A	32	MET	CE	17.86	0.2	1
3456	B	132	MET	CE	17.86	0.2	1
3457	A	32	MET	N	120.19	0.1	1
3458	B	132	MET	N	120.19	0.1	1
3459	A	33	GLN	H	8.64	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3460	B	133	GLN	H	8.64	0.02	1
3461	A	33	GLN	HA	4.30	0.02	1
3462	B	133	GLN	HA	4.30	0.02	1
3463	A	33	GLN	HB2	2.04	0.02	2
3464	B	133	GLN	HB2	2.04	0.02	2
3465	A	33	GLN	HB3	2.26	0.02	2
3466	B	133	GLN	HB3	2.26	0.02	2
3467	A	33	GLN	HG2	2.48	0.02	2
3468	B	133	GLN	HG2	2.48	0.02	2
3469	A	33	GLN	HG3	2.66	0.02	2
3470	B	133	GLN	HG3	2.66	0.02	2
3471	A	33	GLN	HE21	7.01	0.02	2
3472	B	133	GLN	HE21	7.01	0.02	2
3473	A	33	GLN	HE22	7.40	0.02	2
3474	B	133	GLN	HE22	7.40	0.02	2
3475	A	33	GLN	C	179.07	0.2	1
3476	B	133	GLN	C	179.07	0.2	1
3477	A	33	GLN	CA	59.16	0.2	1
3478	B	133	GLN	CA	59.16	0.2	1
3479	A	33	GLN	CB	29.23	0.2	1
3480	B	133	GLN	CB	29.23	0.2	1
3481	A	33	GLN	N	119.58	0.1	1
3482	B	133	GLN	N	119.58	0.1	1
3483	A	33	GLN	NE2	111.69	0.1	1
3484	B	133	GLN	NE2	111.69	0.1	1
3485	A	34	ASN	H	8.55	0.02	1
3486	B	134	ASN	H	8.55	0.02	1
3487	A	34	ASN	HA	4.59	0.02	1
3488	B	134	ASN	HA	4.59	0.02	1
3489	A	34	ASN	HB2	2.99	0.02	2
3490	B	134	ASN	HB2	2.99	0.02	2
3491	A	34	ASN	HB3	3.16	0.02	2
3492	B	134	ASN	HB3	3.16	0.02	2
3493	A	34	ASN	HD21	7.06	0.02	2
3494	B	134	ASN	HD21	7.06	0.02	2
3495	A	34	ASN	HD22	7.85	0.02	2
3496	B	134	ASN	HD22	7.85	0.02	2
3497	A	34	ASN	C	178.31	0.2	1
3498	B	134	ASN	C	178.31	0.2	1
3499	A	34	ASN	CA	56.97	0.2	1
3500	B	134	ASN	CA	56.97	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3501	A	34	ASN	CB	37.90	0.2	1
3502	B	134	ASN	CB	37.90	0.2	1
3503	A	34	ASN	N	118.96	0.1	1
3504	B	134	ASN	N	118.96	0.1	1
3505	A	34	ASN	ND2	112.22	0.1	1
3506	B	134	ASN	ND2	112.22	0.1	1
3507	A	35	GLU	H	8.34	0.02	1
3508	B	135	GLU	H	8.34	0.02	1
3509	A	35	GLU	HA	4.60	0.02	1
3510	B	135	GLU	HA	4.60	0.02	1
3511	A	35	GLU	C	177.99	0.2	1
3512	B	135	GLU	C	177.99	0.2	1
3513	A	35	GLU	CA	58.31	0.2	1
3514	B	135	GLU	CA	58.31	0.2	1
3515	A	35	GLU	CB	30.21	0.2	1
3516	B	135	GLU	CB	30.21	0.2	1
3517	A	35	GLU	N	122.66	0.1	1
3518	B	135	GLU	N	122.66	0.1	1
3519	A	36	ALA	H	8.63	0.02	1
3520	B	136	ALA	H	8.63	0.02	1
3521	A	36	ALA	HA	4.03	0.02	1
3522	B	136	ALA	HA	4.03	0.02	1
3523	A	36	ALA	HB1	1.62	0.02	1
3524	B	136	ALA	HB1	1.62	0.02	1
3525	A	36	ALA	HB2	1.62	0.02	1
3526	B	136	ALA	HB2	1.62	0.02	1
3527	A	36	ALA	HB3	1.62	0.02	1
3528	B	136	ALA	HB3	1.62	0.02	1
3529	A	36	ALA	C	179.00	0.2	1
3530	B	136	ALA	C	179.00	0.2	1
3531	A	36	ALA	CA	55.38	0.2	1
3532	B	136	ALA	CA	55.38	0.2	1
3533	A	36	ALA	CB	17.87	0.2	1
3534	B	136	ALA	CB	17.87	0.2	1
3535	A	36	ALA	N	121.73	0.1	1
3536	B	136	ALA	N	121.73	0.1	1
3537	A	37	ARG	H	7.92	0.02	1
3538	B	137	ARG	H	7.92	0.02	1
3539	A	37	ARG	HA	4.01	0.02	1
3540	B	137	ARG	HA	4.01	0.02	1
3541	A	37	ARG	HB2	2.05	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3542	B	137	ARG	HB2	2.05	0.02	1
3543	A	37	ARG	HB3	2.05	0.02	1
3544	B	137	ARG	HB3	2.05	0.02	1
3545	A	37	ARG	HG2	1.70	0.02	2
3546	B	137	ARG	HG2	1.70	0.02	2
3547	A	37	ARG	HG3	1.93	0.02	2
3548	B	137	ARG	HG3	1.93	0.02	2
3549	A	37	ARG	HD2	2.98	0.02	2
3550	B	137	ARG	HD2	2.98	0.02	2
3551	A	37	ARG	HD3	3.31	0.02	2
3552	B	137	ARG	HD3	3.31	0.02	2
3553	A	37	ARG	C	179.02	0.2	1
3554	B	137	ARG	C	179.02	0.2	1
3555	A	37	ARG	CA	59.39	0.2	1
3556	B	137	ARG	CA	59.39	0.2	1
3557	A	37	ARG	CB	30.25	0.2	1
3558	B	137	ARG	CB	30.25	0.2	1
3559	A	37	ARG	CG	27.85	0.2	1
3560	B	137	ARG	CG	27.85	0.2	1
3561	A	37	ARG	CD	43.00	0.2	1
3562	B	137	ARG	CD	43.00	0.2	1
3563	A	37	ARG	N	116.80	0.1	1
3564	B	137	ARG	N	116.80	0.1	1
3565	A	38	ARG	H	7.83	0.02	1
3566	B	138	ARG	H	7.83	0.02	1
3567	A	38	ARG	HA	4.10	0.02	1
3568	B	138	ARG	HA	4.10	0.02	1
3569	A	38	ARG	HB2	2.14	0.02	1
3570	B	138	ARG	HB2	2.14	0.02	1
3571	A	38	ARG	HB3	2.14	0.02	1
3572	B	138	ARG	HB3	2.14	0.02	1
3573	A	38	ARG	HD2	3.31	0.02	1
3574	B	138	ARG	HD2	3.31	0.02	1
3575	A	38	ARG	HD3	3.31	0.02	1
3576	B	138	ARG	HD3	3.31	0.02	1
3577	A	38	ARG	C	178.90	0.2	1
3578	B	138	ARG	C	178.90	0.2	1
3579	A	38	ARG	CA	59.79	0.2	1
3580	B	138	ARG	CA	59.79	0.2	1
3581	A	38	ARG	CB	30.32	0.2	1
3582	B	138	ARG	CB	30.32	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3583	A	38	ARG	CD	43.85	0.2	1
3584	B	138	ARG	CD	43.85	0.2	1
3585	A	38	ARG	N	121.12	0.1	1
3586	B	138	ARG	N	121.12	0.1	1
3587	A	39	LEU	H	8.41	0.02	1
3588	B	139	LEU	H	8.41	0.02	1
3589	A	39	LEU	HA	3.96	0.02	1
3590	B	139	LEU	HA	3.96	0.02	1
3591	A	39	LEU	HB2	1.11	0.02	2
3592	B	139	LEU	HB2	1.11	0.02	2
3593	A	39	LEU	HB3	1.76	0.02	2
3594	B	139	LEU	HB3	1.76	0.02	2
3595	A	39	LEU	HG	1.69	0.02	1
3596	B	139	LEU	HG	1.69	0.02	1
3597	A	39	LEU	HD11	0.68	0.02	2
3598	B	139	LEU	HD11	0.68	0.02	2
3599	A	39	LEU	HD12	0.68	0.02	2
3600	B	139	LEU	HD12	0.68	0.02	2
3601	A	39	LEU	HD13	0.68	0.02	2
3602	B	139	LEU	HD13	0.68	0.02	2
3603	A	39	LEU	HD21	0.76	0.02	2
3604	B	139	LEU	HD21	0.76	0.02	2
3605	A	39	LEU	HD22	0.76	0.02	2
3606	B	139	LEU	HD22	0.76	0.02	2
3607	A	39	LEU	HD23	0.76	0.02	2
3608	B	139	LEU	HD23	0.76	0.02	2
3609	A	39	LEU	C	176.81	0.2	1
3610	B	139	LEU	C	176.81	0.2	1
3611	A	39	LEU	CA	57.57	0.2	1
3612	B	139	LEU	CA	57.57	0.2	1
3613	A	39	LEU	CB	41.90	0.2	1
3614	B	139	LEU	CB	41.90	0.2	1
3615	A	39	LEU	CG	27.28	0.2	1
3616	B	139	LEU	CG	27.28	0.2	1
3617	A	39	LEU	CD1	22.60	0.2	2
3618	B	139	LEU	CD1	22.60	0.2	2
3619	A	39	LEU	CD2	25.88	0.2	2
3620	B	139	LEU	CD2	25.88	0.2	2
3621	A	39	LEU	N	119.27	0.1	1
3622	B	139	LEU	N	119.27	0.1	1
3623	A	40	ARG	H	8.29	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3624	B	140	ARG	H	8.29	0.02	1
3625	A	40	ARG	HA	4.51	0.02	1
3626	B	140	ARG	HA	4.51	0.02	1
3627	A	40	ARG	HB2	1.88	0.02	1
3628	B	140	ARG	HB2	1.88	0.02	1
3629	A	40	ARG	HB3	1.88	0.02	1
3630	B	140	ARG	HB3	1.88	0.02	1
3631	A	40	ARG	HG2	1.58	0.02	1
3632	B	140	ARG	HG2	1.58	0.02	1
3633	A	40	ARG	HG3	1.58	0.02	1
3634	B	140	ARG	HG3	1.58	0.02	1
3635	A	40	ARG	C	176.46	0.2	1
3636	B	140	ARG	C	176.46	0.2	1
3637	A	40	ARG	CA	55.75	0.2	1
3638	B	140	ARG	CA	55.75	0.2	1
3639	A	40	ARG	CB	33.07	0.2	1
3640	B	140	ARG	CB	33.07	0.2	1
3641	A	40	ARG	N	120.50	0.1	1
3642	B	140	ARG	N	120.50	0.1	1
3643	A	41	ALA	H	8.30	0.02	1
3644	B	141	ALA	H	8.30	0.02	1
3645	A	41	ALA	HA	4.34	0.02	1
3646	B	141	ALA	HA	4.34	0.02	1
3647	A	41	ALA	HB1	1.48	0.02	1
3648	B	141	ALA	HB1	1.48	0.02	1
3649	A	41	ALA	HB2	1.48	0.02	1
3650	B	141	ALA	HB2	1.48	0.02	1
3651	A	41	ALA	HB3	1.48	0.02	1
3652	B	141	ALA	HB3	1.48	0.02	1
3653	A	41	ALA	C	178.11	0.2	1
3654	B	141	ALA	C	178.11	0.2	1
3655	A	41	ALA	CA	53.56	0.2	1
3656	B	141	ALA	CA	53.56	0.2	1
3657	A	41	ALA	CB	19.78	0.2	1
3658	B	141	ALA	CB	19.78	0.2	1
3659	A	41	ALA	N	124.82	0.1	1
3660	B	141	ALA	N	124.82	0.1	1
3661	A	42	GLU	H	8.34	0.02	1
3662	B	142	GLU	H	8.34	0.02	1
3663	A	42	GLU	HA	4.33	0.02	1
3664	B	142	GLU	HA	4.33	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3665	A	42	GLU	HB2	2.05	0.02	2
3666	B	142	GLU	HB2	2.05	0.02	2
3667	A	42	GLU	HB3	2.13	0.02	2
3668	B	142	GLU	HB3	2.13	0.02	2
3669	A	42	GLU	HG2	2.34	0.02	1
3670	B	142	GLU	HG2	2.34	0.02	1
3671	A	42	GLU	HG3	2.34	0.02	1
3672	B	142	GLU	HG3	2.34	0.02	1
3673	A	42	GLU	CA	57.20	0.2	1
3674	B	142	GLU	CA	57.20	0.2	1
3675	A	42	GLU	CB	30.17	0.2	1
3676	B	142	GLU	CB	30.17	0.2	1
3677	A	42	GLU	CG	36.44	0.2	1
3678	B	142	GLU	CG	36.44	0.2	1
3679	A	42	GLU	N	119.64	0.1	1
3680	B	142	GLU	N	119.64	0.1	1
3681	A	44	TRP	HD1	7.34	0.02	1
3682	B	144	TRP	HD1	7.34	0.02	1
3683	A	44	TRP	HE1	10.19	0.02	1
3684	B	144	TRP	HE1	10.19	0.02	1
3685	A	44	TRP	HE3	7.65	0.02	1
3686	B	144	TRP	HE3	7.65	0.02	1
3687	A	44	TRP	HZ2	7.51	0.02	1
3688	B	144	TRP	HZ2	7.51	0.02	1
3689	A	44	TRP	HZ3	7.18	0.02	1
3690	B	144	TRP	HZ3	7.18	0.02	1
3691	A	44	TRP	HH2	7.26	0.02	1
3692	B	144	TRP	HH2	7.26	0.02	1
3693	A	44	TRP	CD1	127.10	0.2	1
3694	B	144	TRP	CD1	127.10	0.2	1
3695	A	44	TRP	CE3	121.00	0.2	1
3696	B	144	TRP	CE3	121.00	0.2	1
3697	A	44	TRP	CZ2	114.58	0.2	1
3698	B	144	TRP	CZ2	114.58	0.2	1
3699	A	44	TRP	CZ3	121.93	0.2	1
3700	B	144	TRP	CZ3	121.93	0.2	1
3701	A	44	TRP	CH2	124.59	0.2	1
3702	B	144	TRP	CH2	124.59	0.2	1
3703	A	44	TRP	NE1	129.20	0.2	1
3704	B	144	TRP	NE1	129.20	0.2	1
3705	A	55	VAL	C	175.98	0.2	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3706	B	155	VAL	C	175.98	0.2	1
3707	A	56	ALA	H	8.24	0.02	1
3708	B	156	ALA	H	8.24	0.02	1
3709	A	56	ALA	CA	52.73	0.2	1
3710	B	156	ALA	CA	52.73	0.2	1
3711	A	56	ALA	N	126.68	0.1	1
3712	B	156	ALA	N	126.68	0.1	1
3713	A	58	PHE	C	175.49	0.2	1
3714	B	158	PHE	C	175.49	0.2	1
3715	A	59	ILE	H	7.95	0.02	1
3716	B	159	ILE	H	7.95	0.02	1
3717	A	59	ILE	HA	4.03	0.02	1
3718	B	159	ILE	HA	4.03	0.02	1
3719	A	59	ILE	C	175.58	0.2	1
3720	B	159	ILE	C	175.58	0.2	1
3721	A	59	ILE	CA	61.53	0.2	1
3722	B	159	ILE	CA	61.53	0.2	1
3723	A	59	ILE	CB	39.16	0.2	1
3724	B	159	ILE	CB	39.16	0.2	1
3725	A	59	ILE	N	122.40	0.1	1
3726	B	159	ILE	N	122.40	0.1	1
3727	A	60	GLU	H	8.34	0.02	1
3728	B	160	GLU	H	8.34	0.02	1
3729	A	60	GLU	N	124.50	0.1	1
3730	B	160	GLU	N	124.50	0.1	1
3731	A	62	ASN	C	176.48	0.2	1
3732	B	162	ASN	C	176.48	0.2	1
3733	A	63	GLY	H	8.40	0.02	1
3734	B	163	GLY	H	8.40	0.02	1
3735	A	63	GLY	HA2	3.95	0.02	1
3736	B	163	GLY	HA2	3.95	0.02	1
3737	A	63	GLY	HA3	3.95	0.02	1
3738	B	163	GLY	HA3	3.95	0.02	1
3739	A	63	GLY	C	174.52	0.2	1
3740	B	163	GLY	C	174.52	0.2	1
3741	A	63	GLY	CA	45.74	0.2	1
3742	B	163	GLY	CA	45.74	0.2	1
3743	A	63	GLY	N	114.65	0.1	1
3744	B	163	GLY	N	114.65	0.1	1
3745	A	64	SER	H	8.35	0.02	1
3746	B	164	SER	H	8.35	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3747	A	64	SER	C	176.13	0.2	1
3748	B	164	SER	C	176.13	0.2	1
3749	A	64	SER	CA	58.62	0.2	1
3750	B	164	SER	CA	58.62	0.2	1
3751	A	64	SER	CB	63.76	0.2	1
3752	B	164	SER	CB	63.76	0.2	1
3753	A	64	SER	N	113.88	0.1	1
3754	B	164	SER	N	113.88	0.1	1
3755	A	65	PHE	H	8.33	0.02	1
3756	B	165	PHE	H	8.33	0.02	1
3757	A	65	PHE	N	122.00	0.1	1
3758	B	165	PHE	N	122.00	0.1	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	134	-0.60 ± 0.06	Should be applied
$^{13}\text{C}_\beta$	122	-0.01 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	126	-0.40 ± 0.08	None needed (< 0.5 ppm)
^{15}N	130	-0.03 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 1388 atoms were assigned a chemical shift out of a possible 1836. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	650/720 (90%)	260/288 (90%)	260/288 (90%)	130/144 (90%)
Sidechain	642/1000 (64%)	400/582 (69%)	228/356 (64%)	14/62 (23%)
Aromatic	96/116 (83%)	56/60 (93%)	36/52 (69%)	4/4 (100%)
Overall	1388/1836 (76%)	716/930 (77%)	524/696 (75%)	148/210 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1388 atoms were assigned a chemical shift out of a possible 1836. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	650/720 (90%)	260/288 (90%)	260/288 (90%)	130/144 (90%)
Sidechain	642/1000 (64%)	400/582 (69%)	228/356 (64%)	14/62 (23%)
Aromatic	96/116 (83%)	56/60 (93%)	36/52 (69%)	4/4 (100%)
Overall	1388/1836 (76%)	716/930 (77%)	524/696 (75%)	148/210 (70%)

7.1.4 Statistically unusual chemical shifts [i](#)

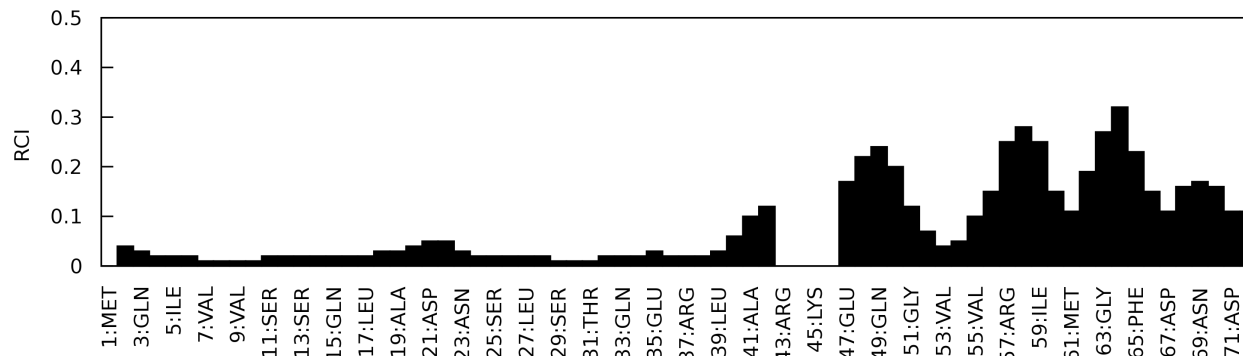
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	54	GLU	HB2	3.44	3.08 – 0.98	6.7
1	B	154	GLU	HB2	3.44	3.08 – 0.98	6.7
1	B	154	GLU	HB3	3.44	3.10 – 0.90	6.5
1	A	54	GLU	HB3	3.44	3.10 – 0.90	6.5

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:

