Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 11:36 PM BST

PDB ID	:	2KQN
Title	:	Solution structure of the AL-09 H87Y immunoglobulin light chain variable domain
Authors	:	Volkman, B.F.; Peterson, F.C.; Ramirez-Alvarado, M.; Baden, E.M.
Deposited on	:	2009-11-11

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:

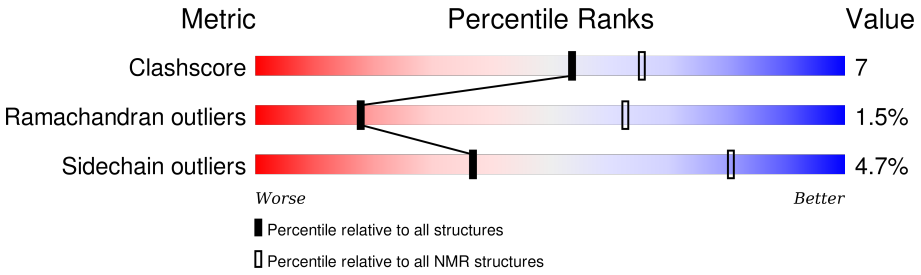
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 91%.

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	110	85% 14% .
1	B	110	77% 16% . . .

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:1-A:108, B:201-B:239, B:243-B:308 (213)	0.40	12

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3297 atoms, of which 1614 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ig kappa chain V-I region AU.

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1648	529	807	136	173	3	
1	B	108	Total	C	H	N	O	S	0
			1649	529	807	136	174	3	

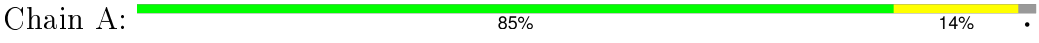
4 Residue-property plots (i)

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.

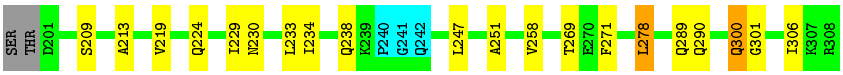
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

Chain B:



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

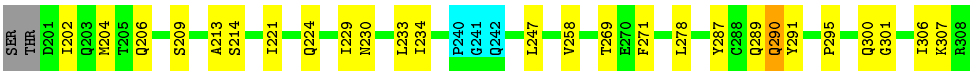
4.2.1 Score per residue for model 1

• Molecule 1: Ig kappa chain V-I region AU

Chain A:

• Molecule 1: Ig kappa chain V-I region AU

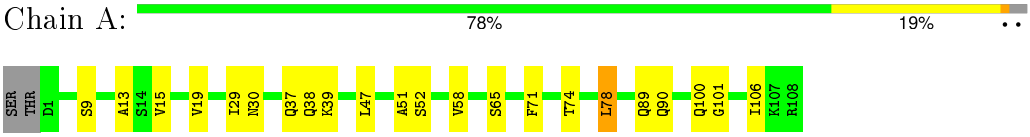
Chain B:



4.2.2 Score per residue for model 2

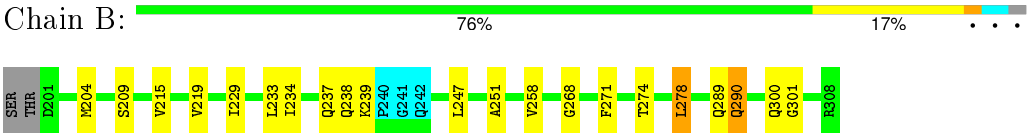
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

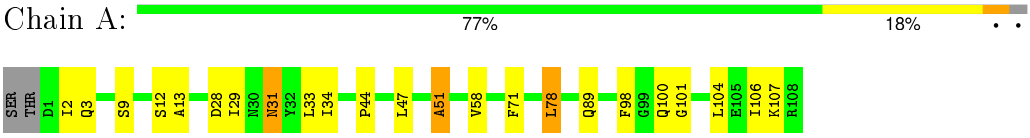
Chain B:



4.2.3 Score per residue for model 3

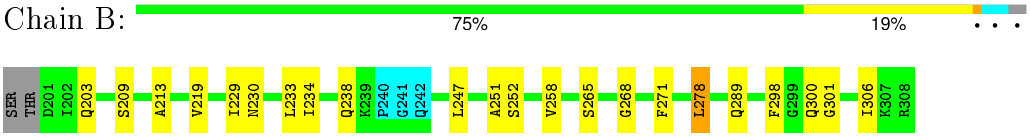
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

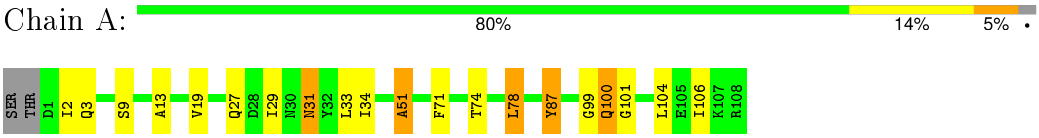
Chain B:



4.2.4 Score per residue for model 4

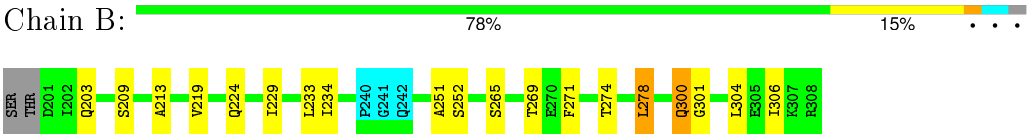
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

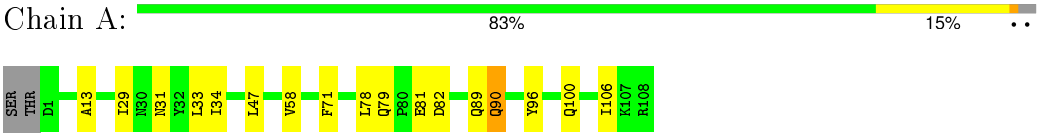
Chain B:



4.2.5 Score per residue for model 5

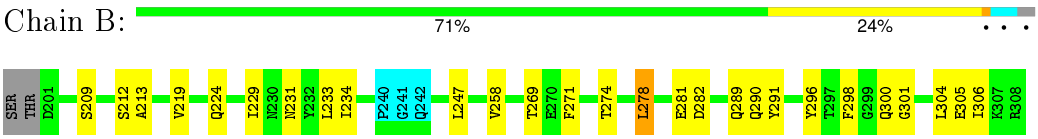
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

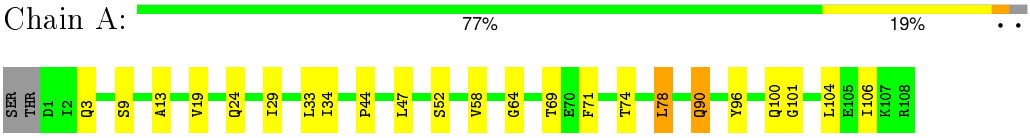
Chain B:



4.2.6 Score per residue for model 6

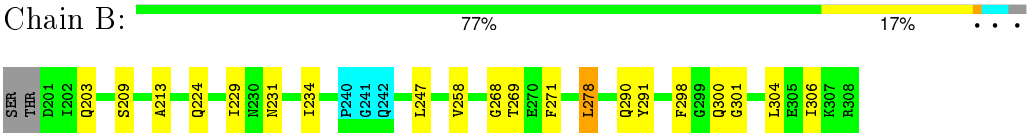
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

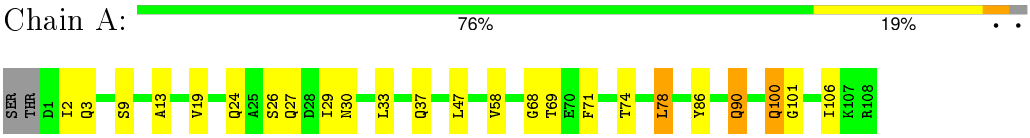
Chain B:



4.2.7 Score per residue for model 7

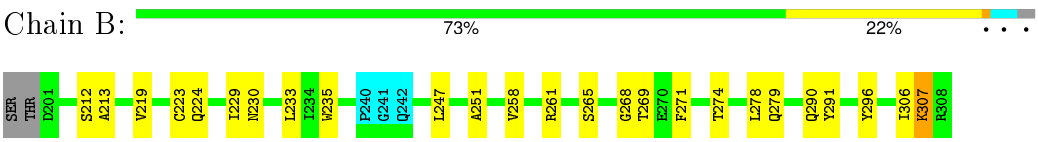
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

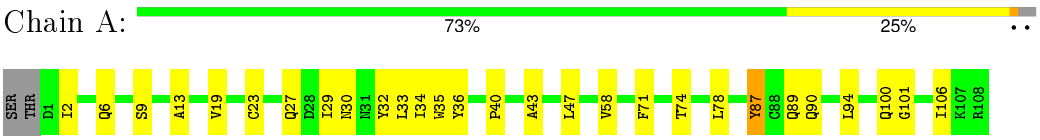
Chain B:



4.2.8 Score per residue for model 8

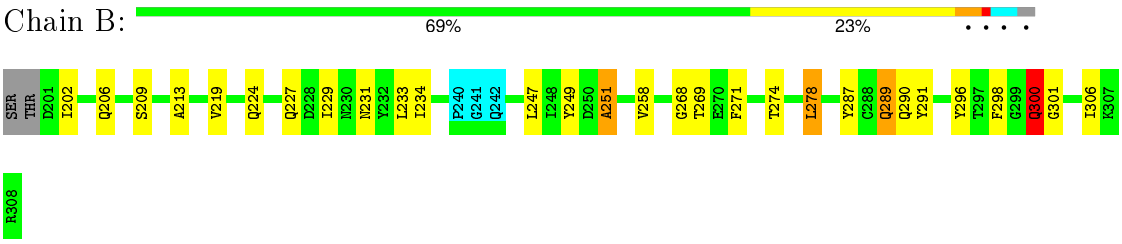
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

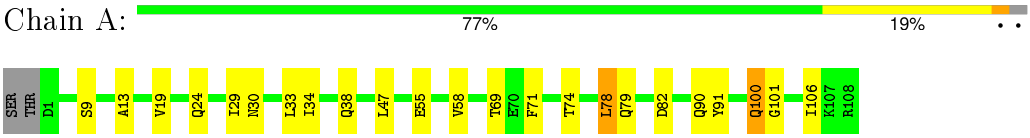
Chain B:



4.2.9 Score per residue for model 9

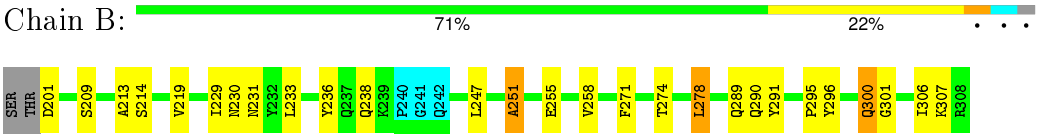
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

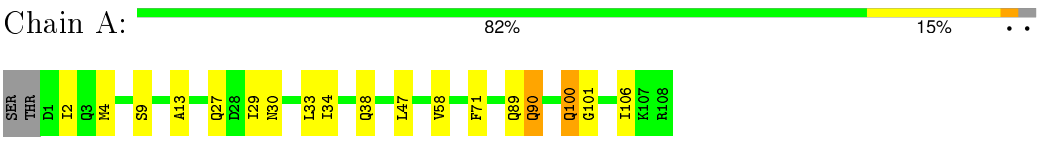
Chain B:



4.2.10 Score per residue for model 10

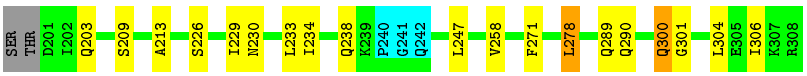
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

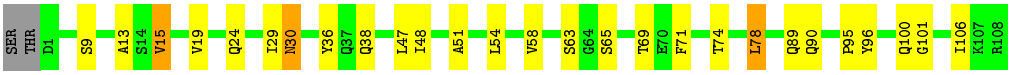
Chain B:



4.2.11 Score per residue for model 11

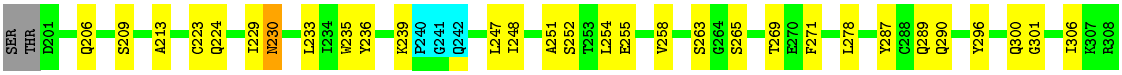
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

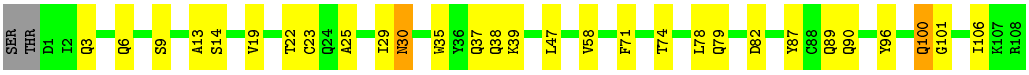
Chain B:



4.2.12 Score per residue for model 12 (medoid)

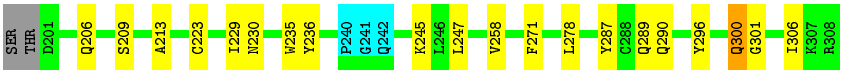
• Molecule 1: Ig kappa chain V-I region AU

Chain A:



• Molecule 1: Ig kappa chain V-I region AU

Chain B:



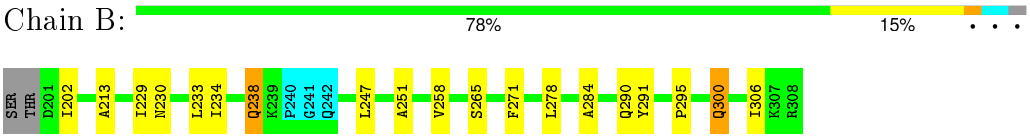
4.2.13 Score per residue for model 13

• Molecule 1: Ig kappa chain V-I region AU

Chain A:

• Molecule 1: Ig kappa chain V-I region AU

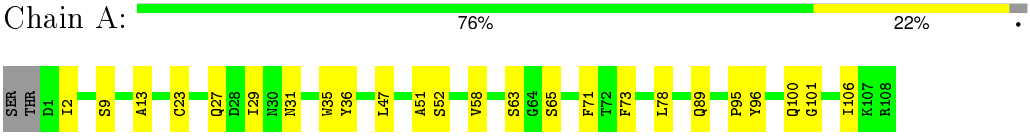
Chain B:



4.2.14 Score per residue for model 14

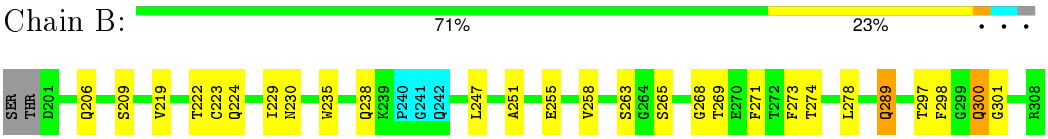
- Molecule 1: Ig kappa chain V-I region AU

Chain A:



- Molecule 1: Ig kappa chain V-I region AU

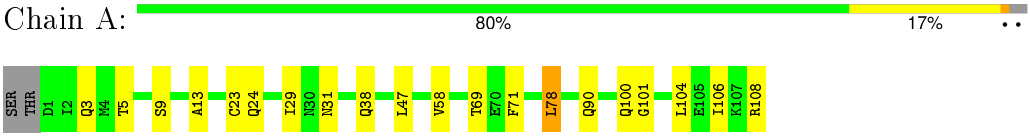
Chain B:



4.2.15 Score per residue for model 15

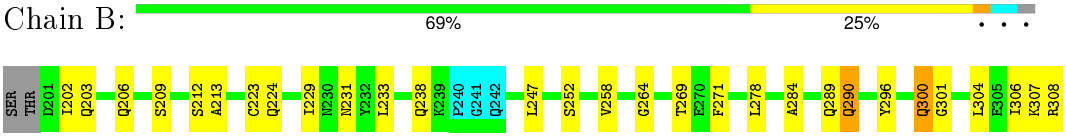
- Molecule 1: Ig kappa chain V-I region AU

Chain A:



- Molecule 1: Ig kappa chain V-I region AU

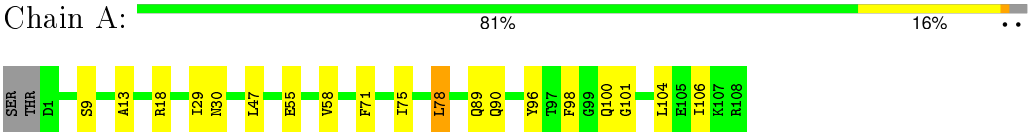
Chain B:



4.2.16 Score per residue for model 16

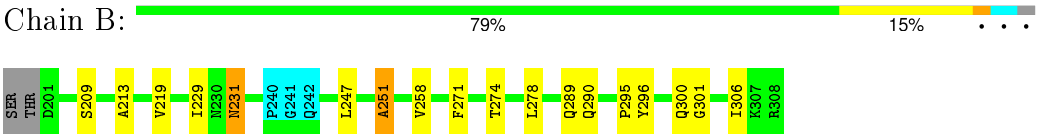
- Molecule 1: Ig kappa chain V-I region AU

Chain A:



- Molecule 1: Ig kappa chain V-I region AU

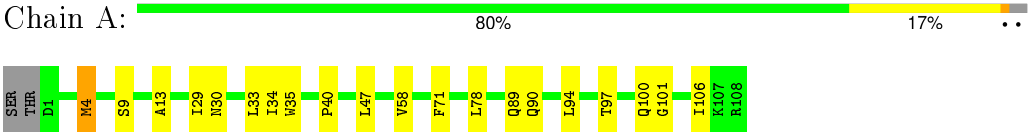
Chain B:



4.2.17 Score per residue for model 17

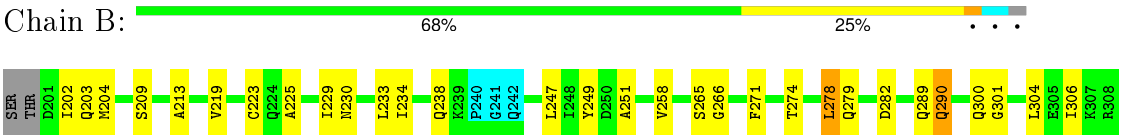
- Molecule 1: Ig kappa chain V-I region AU

Chain A:



- Molecule 1: Ig kappa chain V-I region AU

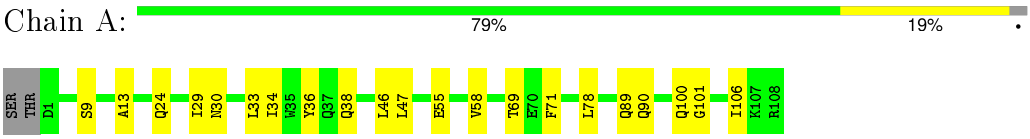
Chain B:



4.2.18 Score per residue for model 18

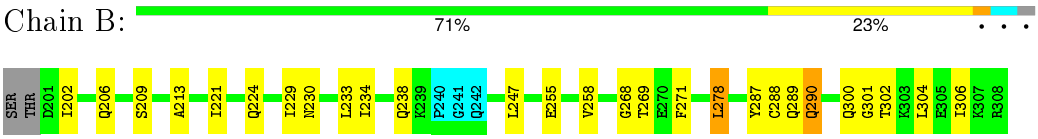
- Molecule 1: Ig kappa chain V-I region AU

Chain A:



- Molecule 1: Ig kappa chain V-I region AU

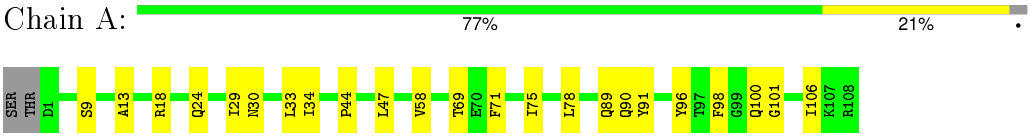
Chain B:



4.2.19 Score per residue for model 19

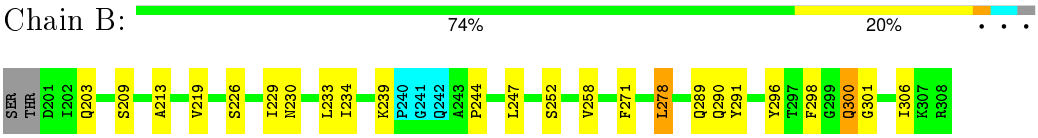
- Molecule 1: Ig kappa chain V-I region AU

Chain A:



- Molecule 1: Ig kappa chain V-I region AU

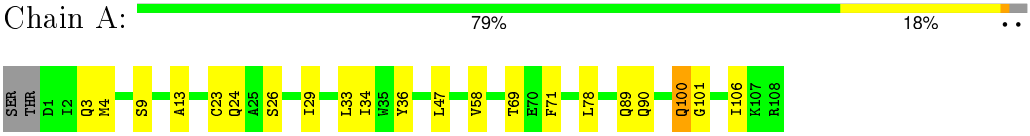
Chain B:



4.2.20 Score per residue for model 20

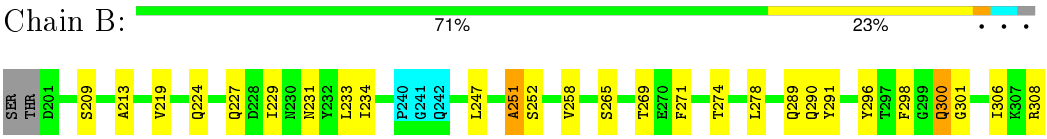
- Molecule 1: Ig kappa chain V-I region AU

Chain A:



- Molecule 1: Ig kappa chain V-I region AU

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

Of the 100 calculated structures, 20 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
Xplor-NIH	refinement	2.9.3

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 16607
Number of chemical shift lists	1
Total number of shifts	5248
Number of shifts mapped to atoms	2628
Number of unparsed shifts	2620
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	841	807	809	11±3
1	B	822	789	788	12±3
All	All	33260	31920	31940	440

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:GLN:NE2	1:A:100:GLN:H	0.69	1.85	4	2
1:A:9:SER:HA	1:A:101:GLY:O	0.67	1.90	17	19
1:B:213:ALA:O	1:B:306:ILE:HA	0.65	1.92	10	18
1:B:209:SER:HA	1:B:301:GLY:O	0.65	1.92	8	18
1:A:13:ALA:O	1:A:106:ILE:HA	0.65	1.91	10	20
1:B:251:ALA:O	1:B:265:SER:HA	0.64	1.92	7	7
1:B:300:GLN:H	1:B:300:GLN:NE2	0.61	1.93	15	5
1:B:206:GLN:NE2	1:B:287:TYR:HA	0.61	2.10	1	2
1:B:289:GLN:NE2	1:B:296:TYR:HB3	0.61	2.11	9	4
1:B:204:MET:SD	1:B:290:GLN:HG3	0.61	2.36	17	2
1:A:6:GLN:NE2	1:A:87:TYR:HA	0.60	2.12	13	2
1:A:51:ALA:O	1:A:65:SER:HA	0.59	1.97	14	3
1:B:219:VAL:O	1:B:274:THR:HA	0.58	1.98	14	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:278:LEU:HD21	1:B:304:LEU:HD21	0.57	1.76	5	6
1:B:231:ASN:O	1:B:251:ALA:HB2	0.57	2.00	9	4
1:A:29:ILE:HD11	1:A:71:PHE:CZ	0.56	2.35	2	19
1:B:229:ILE:HD11	1:B:271:PHE:CZ	0.56	2.36	18	20
1:A:89:GLN:NE2	1:A:96:TYR:HB3	0.55	2.16	13	3
1:B:247:LEU:O	1:B:258:VAL:HG21	0.55	2.02	14	19
1:B:223:CYS:SG	1:B:235:TRP:CH2	0.55	3.00	14	3
1:A:47:LEU:O	1:A:58:VAL:HG21	0.54	2.02	13	19
1:A:78:LEU:HD21	1:A:104:LEU:HD21	0.54	1.80	15	5
1:A:29:ILE:HD11	1:A:71:PHE:CE2	0.53	2.39	19	5
1:A:23:CYS:SG	1:A:35:TRP:CH2	0.52	3.02	12	3
1:B:233:LEU:HD13	1:B:234:ILE:N	0.52	2.19	20	11
1:A:3:GLN:HB2	1:A:26:SER:OG	0.52	2.05	20	1
1:A:100:GLN:H	1:A:100:GLN:NE2	0.52	2.03	7	2
1:A:24:GLN:HA	1:A:69:THR:O	0.51	2.05	1	9
1:B:224:GLN:HA	1:B:269:THR:O	0.51	2.06	7	11
1:B:234:ILE:HD11	1:B:291:TYR:CD1	0.51	2.40	1	3
1:B:289:GLN:HB2	1:B:298:PHE:CD2	0.51	2.40	3	1
1:B:203:GLN:HB2	1:B:226:SER:HB2	0.51	1.83	19	1
1:B:204:MET:HE2	1:B:223:CYS:SG	0.50	2.47	17	1
1:A:63:SER:O	1:A:73:PHE:HA	0.50	2.06	14	2
1:A:79:GLN:HB2	1:A:82:ASP:OD2	0.50	2.07	13	4
1:A:52:SER:HA	1:A:64:GLY:O	0.50	2.07	1	2
1:B:203:GLN:O	1:B:225:ALA:HA	0.50	2.06	17	1
1:A:33:LEU:HD22	1:A:71:PHE:CG	0.50	2.41	9	2
1:A:3:GLN:O	1:A:25:ALA:HA	0.50	2.06	12	1
1:A:2:ILE:HB	1:A:90:GLN:NE2	0.49	2.22	7	1
1:B:223:CYS:HB2	1:B:235:TRP:CH2	0.49	2.43	7	1
1:A:43:ALA:HB2	1:B:300:GLN:HB3	0.49	1.85	8	1
1:B:279:GLN:HB2	1:B:282:ASP:OD2	0.49	2.07	17	1
1:B:229:ILE:HD11	1:B:271:PHE:CE2	0.49	2.42	8	7
1:A:34:ILE:HD11	1:A:91:TYR:CD1	0.49	2.43	9	1
1:B:289:GLN:HE22	1:B:296:TYR:HB3	0.48	1.68	19	4
1:A:19:VAL:O	1:A:74:THR:HA	0.48	2.08	8	8
1:A:31:ASN:O	1:A:51:ALA:HB2	0.48	2.09	4	2
1:A:37:GLN:CD	1:A:39:LYS:HE3	0.48	2.29	12	2
1:B:229:ILE:HD11	1:B:271:PHE:CE1	0.48	2.43	9	2
1:B:212:SER:O	1:B:307:LYS:HE3	0.47	2.08	7	1
1:A:87:TYR:HA	1:A:99:GLY:O	0.47	2.09	4	1
1:A:95:PRO:HB3	1:B:255:GLU:OE2	0.47	2.09	11	1
1:B:219:VAL:CG2	1:B:278:LEU:HD23	0.47	2.40	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:291:TYR:HA	1:B:296:TYR:CE1	0.47	2.45	9	6
1:A:33:LEU:HD13	1:A:34:ILE:N	0.47	2.24	17	11
1:A:15:VAL:HA	1:A:78:LEU:O	0.47	2.10	11	1
1:A:90:GLN:OE1	1:A:96:TYR:HA	0.47	2.10	5	2
1:B:206:GLN:OE1	1:B:287:TYR:HA	0.47	2.10	11	3
1:A:89:GLN:HB2	1:A:98:PHE:CD1	0.47	2.44	3	1
1:B:206:GLN:HE22	1:B:287:TYR:HA	0.46	1.69	1	2
1:A:94:LEU:HD13	1:B:249:TYR:CD1	0.46	2.44	17	2
1:B:202:ILE:HB	1:B:290:GLN:NE2	0.46	2.26	1	2
1:A:95:PRO:HB3	1:B:255:GLU:OE1	0.46	2.11	14	1
1:B:206:GLN:OE1	1:B:302:THR:HB	0.46	2.10	18	1
1:A:4:MET:HG3	1:A:97:THR:O	0.46	2.11	17	1
1:A:6:GLN:OE1	1:A:87:TYR:HA	0.46	2.11	12	2
1:A:89:GLN:HE22	1:A:96:TYR:HB3	0.46	1.69	13	4
1:A:89:GLN:HB2	1:A:98:PHE:CD2	0.46	2.46	16	1
1:B:202:ILE:HD12	1:B:290:GLN:HE21	0.46	1.71	17	2
1:B:219:VAL:HG21	1:B:278:LEU:HD23	0.46	1.87	2	4
1:A:2:ILE:HD13	1:A:29:ILE:HG22	0.45	1.87	7	3
1:A:44:PRO:HB2	1:B:298:PHE:CE1	0.45	2.46	3	1
1:B:212:SER:O	1:B:307:LYS:HE2	0.45	2.12	15	1
1:B:233:LEU:HD22	1:B:271:PHE:CG	0.45	2.46	9	5
1:A:55:GLU:OE1	1:B:295:PRO:HB3	0.45	2.12	13	3
1:A:19:VAL:HG21	1:A:78:LEU:HD23	0.45	1.89	9	3
1:B:261:ARG:NH1	1:B:279:GLN:HG3	0.45	2.27	7	1
1:B:201:ASP:N	1:B:295:PRO:HD2	0.45	2.27	9	1
1:B:234:ILE:O	1:B:288:CYS:HA	0.44	2.11	18	1
1:B:300:GLN:NE2	1:B:300:GLN:H	0.44	2.10	10	2
1:A:3:GLN:HB2	1:A:26:SER:HB2	0.44	1.89	7	2
1:B:202:ILE:HD13	1:B:229:ILE:CG2	0.44	2.42	13	1
1:A:14:SER:HA	1:A:106:ILE:HG23	0.44	1.90	12	1
1:B:238:GLN:O	1:B:284:ALA:HB1	0.44	2.13	13	1
1:B:206:GLN:OE1	1:B:221:ILE:HG21	0.44	2.13	18	2
1:B:206:GLN:HG3	1:B:223:CYS:SG	0.44	2.52	15	1
1:B:237:GLN:CD	1:B:239:LYS:HE3	0.44	2.33	2	1
1:B:229:ILE:HG12	1:B:268:GLY:O	0.44	2.12	7	3
1:A:48:ILE:HG12	1:A:54:LEU:HD23	0.44	1.89	11	1
1:B:203:GLN:HB3	1:B:226:SER:HB2	0.44	1.90	10	1
1:A:91:TYR:HA	1:A:96:TYR:CE1	0.44	2.48	13	3
1:A:36:TYR:CE1	1:B:298:PHE:HE1	0.44	2.31	14	1
1:A:36:TYR:CE2	1:B:298:PHE:HE1	0.44	2.31	8	1
1:A:44:PRO:HG2	1:B:298:PHE:CE2	0.43	2.48	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:252:SER:OG	1:B:265:SER:HA	0.43	2.13	20	1
1:A:5:THR:O	1:A:23:CYS:HA	0.43	2.12	15	1
1:B:236:TYR:HE2	1:B:289:GLN:CB	0.43	2.26	11	1
1:A:12:SER:O	1:A:107:LYS:HE2	0.43	2.14	3	1
1:A:29:ILE:HD11	1:A:71:PHE:CE1	0.43	2.49	7	1
1:A:33:LEU:HD22	1:A:71:PHE:CD1	0.43	2.48	7	1
1:A:18:ARG:HA	1:A:75:ILE:O	0.43	2.14	16	2
1:A:6:GLN:OE1	1:A:102:THR:HB	0.43	2.13	13	1
1:B:236:TYR:HE1	1:B:289:GLN:HB3	0.43	1.73	9	1
1:B:248:ILE:HG12	1:B:254:LEU:HD23	0.43	1.91	11	1
1:A:4:MET:SD	1:A:90:GLN:HG3	0.42	2.54	10	1
1:B:202:ILE:HG12	1:B:227:GLN:HB2	0.42	1.90	8	1
1:B:206:GLN:HA	1:B:222:THR:O	0.42	2.14	14	1
1:B:214:SER:HB2	1:B:307:LYS:HB2	0.42	1.92	1	1
1:B:202:ILE:HD13	1:B:229:ILE:HG22	0.42	1.92	1	1
1:B:214:SER:OG	1:B:307:LYS:HB2	0.42	2.15	9	1
1:A:33:LEU:HD22	1:A:71:PHE:CD2	0.42	2.50	13	1
1:A:2:ILE:HG12	1:A:27:GLN:HB2	0.42	1.91	8	1
1:A:38:GLN:O	1:A:84:ALA:HB1	0.41	2.14	13	1
1:B:239:LYS:HA	1:B:239:LYS:HE2	0.41	1.91	19	1
1:A:33:LEU:HD12	1:A:35:TRP:NE1	0.41	2.30	17	1
1:A:36:TYR:CE1	1:B:298:PHE:HE2	0.41	2.33	20	1
1:B:212:SER:HA	1:B:305:GLU:O	0.41	2.14	5	1
1:A:6:GLN:HA	1:A:22:THR:O	0.41	2.15	12	1
1:B:289:GLN:HA	1:B:297:THR:O	0.41	2.15	14	1
1:B:289:GLN:HB3	1:B:298:PHE:CD1	0.41	2.49	5	1
1:B:236:TYR:HA	1:B:245:LYS:O	0.41	2.15	12	1
1:B:236:TYR:HE2	1:B:289:GLN:HB3	0.41	1.75	11	1
1:A:98:PHE:CE2	1:B:244:PRO:HG2	0.41	2.51	19	1
1:B:263:SER:O	1:B:273:PHE:HA	0.41	2.16	14	1
1:A:2:ILE:HG12	1:A:27:GLN:HB3	0.41	1.92	7	4
1:A:36:TYR:HE2	1:A:89:GLN:HB3	0.41	1.75	11	2
1:B:266:GLY:HA3	1:B:271:PHE:HA	0.41	1.92	17	1
1:A:34:ILE:CG2	1:A:46:LEU:HG	0.40	2.46	18	1
1:A:4:MET:CE	1:A:23:CYS:SG	0.40	3.09	20	1
1:B:252:SER:HA	1:B:264:GLY:O	0.40	2.16	15	1
1:A:29:ILE:HD12	1:A:32:TYR:O	0.40	2.16	8	1
1:A:29:ILE:HG12	1:A:68:GLY:O	0.40	2.16	1	1
1:A:37:GLN:HB3	1:A:86:TYR:CE1	0.40	2.51	7	1
1:A:6:GLN:HE22	1:A:87:TYR:HA	0.40	1.73	13	1
1:B:284:ALA:O	1:B:304:LEU:HB3	0.40	2.17	15	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	106/110 (96%)	98±2 (92±2%)	7±2 (6±2%)	1±1 (1±1%)	19 64
1	B	103/110 (94%)	95±2 (92±2%)	6±2 (6±2%)	2±1 (2±1%)	17 61
All	All	4180/4400 (95%)	3859 (92%)	259 (6%)	62 (1%)	18 63

All 15 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	30	ASN	13
1	B	230	ASN	12
1	A	31	ASN	5
1	B	251	ALA	5
1	B	252	SER	4
1	B	268	GLY	4
1	B	231	ASN	4
1	A	100	GLN	3
1	B	300	GLN	3
1	A	40	PRO	2
1	A	51	ALA	2
1	A	52	SER	2
1	B	263	SER	1
1	A	63	SER	1
1	A	68	GLY	1

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	95/97 (98%)	91±1 (95±1%)	4±1 (5±1%)	38 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	93/97 (96%)	89±1 (95±1%)	4±1 (5±1%)	37 80
All	All	3760/3880 (97%)	3584 (95%)	176 (5%)	37 80

All 29 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	100	GLN	20
1	B	278	LEU	20
1	B	300	GLN	19
1	A	78	LEU	19
1	A	90	GLN	17
1	B	290	GLN	17
1	B	238	GLN	9
1	B	289	GLN	8
1	A	38	GLN	8
1	A	89	GLN	7
1	B	203	GLN	4
1	A	3	GLN	4
1	A	15	VAL	2
1	B	255	GLU	2
1	A	55	GLU	2
1	A	4	MET	2
1	A	30	ASN	2
1	A	87	TYR	2
1	B	308	ARG	2
1	B	227	GLN	1
1	B	215	VAL	1
1	B	230	ASN	1
1	B	307	LYS	1
1	A	28	ASP	1
1	A	108	ARG	1
1	A	81	GLU	1
1	B	204	MET	1
1	B	282	ASP	1
1	B	281	GLU	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16607

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	5248
Number of shifts mapped to atoms	2628
Number of unparsed shifts	2620
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

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

- Chemical shift has been reported more than once. All 2620 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2627	A	1	ASP	H	8.433	0.02	1
2628	B	201	ASP	H	8.433	0.02	1
2629	A	1	ASP	HA	4.671	0.02	1
2630	B	201	ASP	HA	4.671	0.02	1
2631	A	1	ASP	HB2	2.671	0.02	2
2632	B	201	ASP	HB2	2.671	0.02	2
2633	A	1	ASP	HB3	2.591	0.02	2
2634	B	201	ASP	HB3	2.591	0.02	2
2635	A	1	ASP	C	175.700	0.1	1
2636	B	201	ASP	C	175.700	0.1	1
2637	A	1	ASP	CA	54.100	0.1	1
2638	B	201	ASP	CA	54.100	0.1	1
2639	A	1	ASP	CB	41.300	0.1	1
2640	B	201	ASP	CB	41.300	0.1	1
2641	A	1	ASP	N	124.000	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2642	B	201	ASP	N	124.000	0.1	1
2643	A	2	ILE	H	8.594	0.02	1
2644	B	202	ILE	H	8.594	0.02	1
2645	A	2	ILE	HA	3.803	0.02	1
2646	B	202	ILE	HA	3.803	0.02	1
2647	A	2	ILE	HB	1.769	0.02	1
2648	B	202	ILE	HB	1.769	0.02	1
2649	A	2	ILE	HD11	0.804	0.02	1
2650	B	202	ILE	HD11	0.804	0.02	1
2651	A	2	ILE	HD12	0.804	0.02	1
2652	B	202	ILE	HD12	0.804	0.02	1
2653	A	2	ILE	HD13	0.804	0.02	1
2654	B	202	ILE	HD13	0.804	0.02	1
2655	A	2	ILE	HG12	1.578	0.02	2
2656	B	202	ILE	HG12	1.578	0.02	2
2657	A	2	ILE	HG13	0.740	0.02	2
2658	B	202	ILE	HG13	0.740	0.02	2
2659	A	2	ILE	HG21	0.860	0.02	1
2660	B	202	ILE	HG21	0.860	0.02	1
2661	A	2	ILE	HG22	0.860	0.02	1
2662	B	202	ILE	HG22	0.860	0.02	1
2663	A	2	ILE	HG23	0.860	0.02	1
2664	B	202	ILE	HG23	0.860	0.02	1
2665	A	2	ILE	C	175.707	0.1	1
2666	B	202	ILE	C	175.707	0.1	1
2667	A	2	ILE	CA	62.340	0.1	1
2668	B	202	ILE	CA	62.340	0.1	1
2669	A	2	ILE	CB	38.387	0.1	1
2670	B	202	ILE	CB	38.387	0.1	1
2671	A	2	ILE	CD1	13.794	0.1	1
2672	B	202	ILE	CD1	13.794	0.1	1
2673	A	2	ILE	CG1	28.118	0.1	1
2674	B	202	ILE	CG1	28.118	0.1	1
2675	A	2	ILE	CG2	18.486	0.1	1
2676	B	202	ILE	CG2	18.486	0.1	1
2677	A	2	ILE	N	124.009	0.1	1
2678	B	202	ILE	N	124.009	0.1	1
2679	A	3	GLN	H	8.717	0.02	1
2680	B	203	GLN	H	8.717	0.02	1
2681	A	3	GLN	HA	4.562	0.02	1
2682	B	203	GLN	HA	4.562	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2683	A	3	GLN	HB2	2.030	0.02	2
2684	B	203	GLN	HB2	2.030	0.02	2
2685	A	3	GLN	HB3	2.135	0.02	2
2686	B	203	GLN	HB3	2.135	0.02	2
2687	A	3	GLN	HE21	7.691	0.02	2
2688	B	203	GLN	HE21	7.691	0.02	2
2689	A	3	GLN	HE22	6.869	0.02	2
2690	B	203	GLN	HE22	6.869	0.02	2
2691	A	3	GLN	HG2	2.449	0.02	2
2692	B	203	GLN	HG2	2.449	0.02	2
2693	A	3	GLN	HG3	2.407	0.02	2
2694	B	203	GLN	HG3	2.407	0.02	2
2695	A	3	GLN	C	175.652	0.1	1
2696	B	203	GLN	C	175.652	0.1	1
2697	A	3	GLN	CA	55.188	0.1	1
2698	B	203	GLN	CA	55.188	0.1	1
2699	A	3	GLN	CB	30.685	0.1	1
2700	B	203	GLN	CB	30.685	0.1	1
2701	A	3	GLN	CG	34.246	0.1	1
2702	B	203	GLN	CG	34.246	0.1	1
2703	A	3	GLN	N	128.596	0.1	1
2704	B	203	GLN	N	128.596	0.1	1
2705	A	3	GLN	NE2	113.109	0.1	1
2706	B	203	GLN	NE2	113.109	0.1	1
2707	A	4	MET	H	9.088	0.02	1
2708	B	204	MET	H	9.088	0.02	1
2709	A	4	MET	HA	5.670	0.02	1
2710	B	204	MET	HA	5.670	0.02	1
2711	A	4	MET	HB2	2.398	0.02	2
2712	B	204	MET	HB2	2.398	0.02	2
2713	A	4	MET	HB3	2.398	0.02	2
2714	B	204	MET	HB3	2.398	0.02	2
2715	A	4	MET	HE1	1.650	0.02	1
2716	B	204	MET	HE1	1.650	0.02	1
2717	A	4	MET	HE2	1.650	0.02	1
2718	B	204	MET	HE2	1.650	0.02	1
2719	A	4	MET	HE3	1.650	0.02	1
2720	B	204	MET	HE3	1.650	0.02	1
2721	A	4	MET	HG2	1.899	0.02	2
2722	B	204	MET	HG2	1.899	0.02	2
2723	A	4	MET	HG3	1.654	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2724	B	204	MET	HG3	1.654	0.02	2
2725	A	4	MET	C	176.659	0.1	1
2726	B	204	MET	C	176.659	0.1	1
2727	A	4	MET	CA	51.877	0.1	1
2728	B	204	MET	CA	51.877	0.1	1
2729	A	4	MET	CB	30.900	0.1	1
2730	B	204	MET	CB	30.900	0.1	1
2731	A	4	MET	CE	16.631	0.1	1
2732	B	204	MET	CE	16.631	0.1	1
2733	A	4	MET	CG	30.800	0.1	1
2734	B	204	MET	CG	30.800	0.1	1
2735	A	4	MET	N	124.118	0.1	1
2736	B	204	MET	N	124.118	0.1	1
2737	A	5	THR	H	9.614	0.02	1
2738	B	205	THR	H	9.614	0.02	1
2739	A	5	THR	HA	4.829	0.02	1
2740	B	205	THR	HA	4.829	0.02	1
2741	A	5	THR	HB	4.212	0.02	1
2742	B	205	THR	HB	4.212	0.02	1
2743	A	5	THR	HG21	1.314	0.02	1
2744	B	205	THR	HG21	1.314	0.02	1
2745	A	5	THR	HG22	1.314	0.02	1
2746	B	205	THR	HG22	1.314	0.02	1
2747	A	5	THR	HG23	1.314	0.02	1
2748	B	205	THR	HG23	1.314	0.02	1
2749	A	5	THR	C	173.970	0.1	1
2750	B	205	THR	C	173.970	0.1	1
2751	A	5	THR	CA	62.399	0.1	1
2752	B	205	THR	CA	62.399	0.1	1
2753	A	5	THR	CB	70.314	0.1	1
2754	B	205	THR	CB	70.314	0.1	1
2755	A	5	THR	CG2	21.352	0.1	1
2756	B	205	THR	CG2	21.352	0.1	1
2757	A	5	THR	N	120.262	0.1	1
2758	B	205	THR	N	120.262	0.1	1
2759	A	6	GLN	H	9.780	0.02	1
2760	B	206	GLN	H	9.780	0.02	1
2761	A	6	GLN	HA	5.667	0.02	1
2762	B	206	GLN	HA	5.667	0.02	1
2763	A	6	GLN	HB2	2.356	0.02	2
2764	B	206	GLN	HB2	2.356	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2765	A	6	GLN	HB3	2.143	0.02	2
2766	B	206	GLN	HB3	2.143	0.02	2
2767	A	6	GLN	HE21	7.699	0.02	2
2768	B	206	GLN	HE21	7.699	0.02	2
2769	A	6	GLN	HE22	7.169	0.02	2
2770	B	206	GLN	HE22	7.169	0.02	2
2771	A	6	GLN	HG2	2.318	0.02	2
2772	B	206	GLN	HG2	2.318	0.02	2
2773	A	6	GLN	HG3	2.830	0.02	2
2774	B	206	GLN	HG3	2.830	0.02	2
2775	A	6	GLN	C	175.268	0.1	1
2776	B	206	GLN	C	175.268	0.1	1
2777	A	6	GLN	CA	54.600	0.1	1
2778	B	206	GLN	CA	54.600	0.1	1
2779	A	6	GLN	CB	31.200	0.1	1
2780	B	206	GLN	CB	31.200	0.1	1
2781	A	6	GLN	CG	34.500	0.1	1
2782	B	206	GLN	CG	34.500	0.1	1
2783	A	6	GLN	N	132.000	0.1	1
2784	B	206	GLN	N	132.000	0.1	1
2785	A	6	GLN	NE2	110.407	0.1	1
2786	B	206	GLN	NE2	110.407	0.1	1
2787	A	7	SER	H	9.073	0.02	1
2788	B	207	SER	H	9.073	0.02	1
2789	A	7	SER	HA	4.856	0.02	1
2790	B	207	SER	HA	4.856	0.02	1
2791	A	7	SER	HB2	3.815	0.02	2
2792	B	207	SER	HB2	3.815	0.02	2
2793	A	7	SER	HB3	3.815	0.02	2
2794	B	207	SER	HB3	3.815	0.02	2
2795	A	7	SER	C	171.266	0.1	1
2796	B	207	SER	C	171.266	0.1	1
2797	A	7	SER	CA	55.457	0.1	1
2798	B	207	SER	CA	55.457	0.1	1
2799	A	7	SER	CB	65.810	0.1	1
2800	B	207	SER	CB	65.810	0.1	1
2801	A	7	SER	N	120.581	0.1	1
2802	B	207	SER	N	120.581	0.1	1
2803	A	8	PRO	HA	5.231	0.02	1
2804	B	208	PRO	HA	5.231	0.02	1
2805	A	8	PRO	HB2	2.690	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2806	B	208	PRO	HB2	2.690	0.02	2
2807	A	8	PRO	HB3	2.565	0.02	2
2808	B	208	PRO	HB3	2.565	0.02	2
2809	A	8	PRO	HD2	3.789	0.02	2
2810	B	208	PRO	HD2	3.789	0.02	2
2811	A	8	PRO	HD3	3.845	0.02	2
2812	B	208	PRO	HD3	3.845	0.02	2
2813	A	8	PRO	HG2	2.266	0.02	2
2814	B	208	PRO	HG2	2.266	0.02	2
2815	A	8	PRO	HG3	1.698	0.02	2
2816	B	208	PRO	HG3	1.698	0.02	2
2817	A	8	PRO	CA	63.222	0.1	1
2818	B	208	PRO	CA	63.222	0.1	1
2819	A	8	PRO	CB	35.073	0.1	1
2820	B	208	PRO	CB	35.073	0.1	1
2821	A	8	PRO	CD	49.309	0.1	1
2822	B	208	PRO	CD	49.309	0.1	1
2823	A	8	PRO	CG	25.690	0.1	1
2824	B	208	PRO	CG	25.690	0.1	1
2825	A	9	SER	HA	5.005	0.02	1
2826	B	209	SER	HA	5.005	0.02	1
2827	A	9	SER	HB2	4.150	0.02	2
2828	B	209	SER	HB2	4.150	0.02	2
2829	A	9	SER	HB3	4.150	0.02	2
2830	B	209	SER	HB3	4.150	0.02	2
2831	A	9	SER	C	175.843	0.1	1
2832	B	209	SER	C	175.843	0.1	1
2833	A	9	SER	CA	60.911	0.1	1
2834	B	209	SER	CA	60.911	0.1	1
2835	A	9	SER	CB	63.300	0.1	1
2836	B	209	SER	CB	63.300	0.1	1
2837	A	10	SER	H	7.840	0.02	1
2838	B	210	SER	H	7.840	0.02	1
2839	A	10	SER	HA	5.313	0.02	1
2840	B	210	SER	HA	5.313	0.02	1
2841	A	10	SER	HB2	3.972	0.02	2
2842	B	210	SER	HB2	3.972	0.02	2
2843	A	10	SER	HB3	3.972	0.02	2
2844	B	210	SER	HB3	3.972	0.02	2
2845	A	10	SER	C	172.071	0.1	1
2846	B	210	SER	C	172.071	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2847	A	10	SER	CA	57.474	0.1	1
2848	B	210	SER	CA	57.474	0.1	1
2849	A	10	SER	CB	65.214	0.1	1
2850	B	210	SER	CB	65.214	0.1	1
2851	A	10	SER	N	115.700	0.1	1
2852	B	210	SER	N	115.700	0.1	1
2853	A	11	LEU	H	8.689	0.02	1
2854	B	211	LEU	H	8.689	0.02	1
2855	A	11	LEU	HA	4.709	0.02	1
2856	B	211	LEU	HA	4.709	0.02	1
2857	A	11	LEU	HB2	1.662	0.02	2
2858	B	211	LEU	HB2	1.662	0.02	2
2859	A	11	LEU	HB3	1.559	0.02	2
2860	B	211	LEU	HB3	1.559	0.02	2
2861	A	11	LEU	HD11	0.991	0.02	2
2862	B	211	LEU	HD11	0.991	0.02	2
2863	A	11	LEU	HD12	0.991	0.02	2
2864	B	211	LEU	HD12	0.991	0.02	2
2865	A	11	LEU	HD13	0.991	0.02	2
2866	B	211	LEU	HD13	0.991	0.02	2
2867	A	11	LEU	HD21	0.980	0.02	2
2868	B	211	LEU	HD21	0.980	0.02	2
2869	A	11	LEU	HD22	0.980	0.02	2
2870	B	211	LEU	HD22	0.980	0.02	2
2871	A	11	LEU	HD23	0.980	0.02	2
2872	B	211	LEU	HD23	0.980	0.02	2
2873	A	11	LEU	HG	1.606	0.02	1
2874	B	211	LEU	HG	1.606	0.02	1
2875	A	11	LEU	C	174.260	0.1	1
2876	B	211	LEU	C	174.260	0.1	1
2877	A	11	LEU	CA	55.423	0.1	1
2878	B	211	LEU	CA	55.423	0.1	1
2879	A	11	LEU	CB	46.800	0.1	1
2880	B	211	LEU	CB	46.800	0.1	1
2883	A	11	LEU	CG	27.259	0.1	1
2884	B	211	LEU	CG	27.259	0.1	1
2885	A	11	LEU	N	124.247	0.1	1
2886	B	211	LEU	N	124.247	0.1	1
2887	A	12	SER	H	8.541	0.02	1
2888	B	212	SER	H	8.541	0.02	1
2889	A	12	SER	HA	5.459	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2890	B	212	SER	HA	5.459	0.02	1
2891	A	12	SER	HB2	3.720	0.02	2
2892	B	212	SER	HB2	3.720	0.02	2
2893	A	12	SER	HB3	3.720	0.02	2
2894	B	212	SER	HB3	3.720	0.02	2
2895	A	12	SER	C	173.588	0.1	1
2896	B	212	SER	C	173.588	0.1	1
2897	A	12	SER	CA	56.478	0.1	1
2898	B	212	SER	CA	56.478	0.1	1
2899	A	12	SER	CB	64.214	0.1	1
2900	B	212	SER	CB	64.214	0.1	1
2901	A	12	SER	N	119.600	0.1	1
2902	B	212	SER	N	119.600	0.1	1
2903	A	13	ALA	H	8.620	0.02	1
2904	B	213	ALA	H	8.620	0.02	1
2905	A	13	ALA	HA	4.780	0.02	1
2906	B	213	ALA	HA	4.780	0.02	1
2907	A	13	ALA	HB1	1.403	0.02	1
2908	B	213	ALA	HB1	1.403	0.02	1
2909	A	13	ALA	HB2	1.403	0.02	1
2910	B	213	ALA	HB2	1.403	0.02	1
2911	A	13	ALA	HB3	1.403	0.02	1
2912	B	213	ALA	HB3	1.403	0.02	1
2913	A	13	ALA	C	175.124	0.1	1
2914	B	213	ALA	C	175.124	0.1	1
2915	A	13	ALA	CA	51.085	0.1	1
2916	B	213	ALA	CA	51.085	0.1	1
2917	A	13	ALA	CB	23.200	0.1	1
2918	B	213	ALA	CB	23.200	0.1	1
2919	A	13	ALA	N	128.300	0.1	1
2920	B	213	ALA	N	128.300	0.1	1
2921	A	14	SER	H	8.696	0.02	1
2922	B	214	SER	H	8.696	0.02	1
2923	A	14	SER	HA	4.968	0.02	1
2924	B	214	SER	HA	4.968	0.02	1
2925	A	14	SER	HB2	3.936	0.02	2
2926	B	214	SER	HB2	3.936	0.02	2
2927	A	14	SER	HB3	3.689	0.02	2
2928	B	214	SER	HB3	3.689	0.02	2
2929	A	14	SER	C	173.972	0.1	1
2930	B	214	SER	C	173.972	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2931	A	14	SER	CA	57.855	0.1	1
2932	B	214	SER	CA	57.855	0.1	1
2933	A	14	SER	CB	64.956	0.1	1
2934	B	214	SER	CB	64.956	0.1	1
2935	A	14	SER	N	116.525	0.1	1
2936	B	214	SER	N	116.525	0.1	1
2937	A	15	VAL	H	8.590	0.02	1
2938	B	215	VAL	H	8.590	0.02	1
2939	A	15	VAL	HA	3.518	0.02	1
2940	B	215	VAL	HA	3.518	0.02	1
2941	A	15	VAL	HB	1.981	0.02	1
2942	B	215	VAL	HB	1.981	0.02	1
2943	A	15	VAL	HG11	1.081	0.02	2
2944	B	215	VAL	HG11	1.081	0.02	2
2945	A	15	VAL	HG12	1.081	0.02	2
2946	B	215	VAL	HG12	1.081	0.02	2
2947	A	15	VAL	HG13	1.081	0.02	2
2948	B	215	VAL	HG13	1.081	0.02	2
2949	A	15	VAL	HG21	1.025	0.02	2
2950	B	215	VAL	HG21	1.025	0.02	2
2951	A	15	VAL	HG22	1.025	0.02	2
2952	B	215	VAL	HG22	1.025	0.02	2
2953	A	15	VAL	HG23	1.025	0.02	2
2954	B	215	VAL	HG23	1.025	0.02	2
2955	A	15	VAL	C	178.003	0.1	1
2956	B	215	VAL	C	178.003	0.1	1
2957	A	15	VAL	CA	65.426	0.1	1
2958	B	215	VAL	CA	65.426	0.1	1
2959	A	15	VAL	CB	31.405	0.1	1
2960	B	215	VAL	CB	31.405	0.1	1
2961	A	15	VAL	CG1	21.035	0.1	1
2962	B	215	VAL	CG1	21.035	0.1	1
2963	A	15	VAL	CG2	23.200	0.1	1
2964	B	215	VAL	CG2	23.200	0.1	1
2965	A	15	VAL	N	122.738	0.1	1
2966	B	215	VAL	N	122.738	0.1	1
2967	A	16	GLY	H	10.039	0.02	1
2968	B	216	GLY	H	10.039	0.02	1
2969	A	16	GLY	HA2	4.406	0.02	2
2970	B	216	GLY	HA2	4.406	0.02	2
2971	A	16	GLY	HA3	3.780	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2972	B	216	GLY	HA3	3.780	0.02	2
2973	A	16	GLY	C	174.980	0.1	1
2974	B	216	GLY	C	174.980	0.1	1
2975	A	16	GLY	CA	44.624	0.1	1
2976	B	216	GLY	CA	44.624	0.1	1
2977	A	16	GLY	N	117.732	0.1	1
2978	B	216	GLY	N	117.732	0.1	1
2979	A	17	ASP	H	8.131	0.02	1
2980	B	217	ASP	H	8.131	0.02	1
2981	A	17	ASP	HA	4.638	0.02	1
2982	B	217	ASP	HA	4.638	0.02	1
2983	A	17	ASP	HB2	2.957	0.02	2
2984	B	217	ASP	HB2	2.957	0.02	2
2985	A	17	ASP	HB3	2.613	0.02	2
2986	B	217	ASP	HB3	2.613	0.02	2
2987	A	17	ASP	C	175.220	0.1	1
2988	B	217	ASP	C	175.220	0.1	1
2989	A	17	ASP	CA	55.012	0.1	1
2990	B	217	ASP	CA	55.012	0.1	1
2991	A	17	ASP	CB	41.796	0.1	1
2992	B	217	ASP	CB	41.796	0.1	1
2993	A	17	ASP	N	122.036	0.1	1
2994	B	217	ASP	N	122.036	0.1	1
2995	A	18	ARG	H	8.256	0.02	1
2996	B	218	ARG	H	8.256	0.02	1
2997	A	18	ARG	HA	4.965	0.02	1
2998	B	218	ARG	HA	4.965	0.02	1
2999	A	18	ARG	HB2	1.795	0.02	2
3000	B	218	ARG	HB2	1.795	0.02	2
3001	A	18	ARG	HB3	1.714	0.02	2
3002	B	218	ARG	HB3	1.714	0.02	2
3003	A	18	ARG	HD2	3.147	0.02	2
3004	B	218	ARG	HD2	3.147	0.02	2
3005	A	18	ARG	HD3	3.147	0.02	2
3006	B	218	ARG	HD3	3.147	0.02	2
3007	A	18	ARG	HG2	1.521	0.02	2
3008	B	218	ARG	HG2	1.521	0.02	2
3009	A	18	ARG	HG3	1.299	0.02	2
3010	B	218	ARG	HG3	1.299	0.02	2
3011	A	18	ARG	C	176.879	0.1	1
3012	B	218	ARG	C	176.879	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3013	A	18	ARG	CA	54.954	0.1	1
3014	B	218	ARG	CA	54.954	0.1	1
3015	A	18	ARG	CB	31.600	0.1	1
3016	B	218	ARG	CB	31.600	0.1	1
3017	A	18	ARG	CD	43.500	0.1	1
3018	B	218	ARG	CD	43.500	0.1	1
3019	A	18	ARG	CG	28.149	0.1	1
3020	B	218	ARG	CG	28.149	0.1	1
3021	A	18	ARG	N	120.476	0.1	1
3022	B	218	ARG	N	120.476	0.1	1
3023	A	19	VAL	H	8.630	0.02	1
3024	B	219	VAL	H	8.630	0.02	1
3025	A	19	VAL	HA	4.515	0.02	1
3026	B	219	VAL	HA	4.515	0.02	1
3027	A	19	VAL	HB	1.841	0.02	1
3028	B	219	VAL	HB	1.841	0.02	1
3029	A	19	VAL	HG11	0.807	0.02	2
3030	B	219	VAL	HG11	0.807	0.02	2
3031	A	19	VAL	HG12	0.807	0.02	2
3032	B	219	VAL	HG12	0.807	0.02	2
3033	A	19	VAL	HG13	0.807	0.02	2
3034	B	219	VAL	HG13	0.807	0.02	2
3035	A	19	VAL	HG21	0.801	0.02	2
3036	B	219	VAL	HG21	0.801	0.02	2
3037	A	19	VAL	HG22	0.801	0.02	2
3038	B	219	VAL	HG22	0.801	0.02	2
3039	A	19	VAL	HG23	0.801	0.02	2
3040	B	219	VAL	HG23	0.801	0.02	2
3041	A	19	VAL	C	173.972	0.1	1
3042	B	219	VAL	C	173.972	0.1	1
3043	A	19	VAL	CA	60.581	0.1	1
3044	B	219	VAL	CA	60.581	0.1	1
3045	A	19	VAL	CB	35.800	0.1	1
3046	B	219	VAL	CB	35.800	0.1	1
3047	A	19	VAL	CG1	21.416	0.1	1
3048	B	219	VAL	CG1	21.416	0.1	1
3049	A	19	VAL	CG2	21.924	0.1	1
3050	B	219	VAL	CG2	21.924	0.1	1
3051	A	19	VAL	N	124.630	0.1	1
3052	B	219	VAL	N	124.630	0.1	1
3053	A	20	THR	H	8.155	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3054	B	220	THR	H	8.155	0.02	1
3055	A	20	THR	HA	5.237	0.02	1
3056	B	220	THR	HA	5.237	0.02	1
3057	A	20	THR	HB	3.782	0.02	1
3058	B	220	THR	HB	3.782	0.02	1
3059	A	20	THR	HG21	1.093	0.02	1
3060	B	220	THR	HG21	1.093	0.02	1
3061	A	20	THR	HG22	1.093	0.02	1
3062	B	220	THR	HG22	1.093	0.02	1
3063	A	20	THR	HG23	1.093	0.02	1
3064	B	220	THR	HG23	1.093	0.02	1
3065	A	20	THR	C	173.205	0.1	1
3066	B	220	THR	C	173.205	0.1	1
3067	A	20	THR	CA	61.578	0.1	1
3068	B	220	THR	CA	61.578	0.1	1
3069	A	20	THR	CB	71.714	0.1	1
3070	B	220	THR	CB	71.714	0.1	1
3071	A	20	THR	CG2	21.797	0.1	1
3072	B	220	THR	CG2	21.797	0.1	1
3073	A	20	THR	N	119.277	0.1	1
3074	B	220	THR	N	119.277	0.1	1
3075	A	21	ILE	H	9.477	0.02	1
3076	B	221	ILE	H	9.477	0.02	1
3077	A	21	ILE	HA	4.626	0.02	1
3078	B	221	ILE	HA	4.626	0.02	1
3079	A	21	ILE	HB	1.718	0.02	1
3080	B	221	ILE	HB	1.718	0.02	1
3081	A	21	ILE	HD11	0.662	0.02	1
3082	B	221	ILE	HD11	0.662	0.02	1
3083	A	21	ILE	HD12	0.662	0.02	1
3084	B	221	ILE	HD12	0.662	0.02	1
3085	A	21	ILE	HD13	0.662	0.02	1
3086	B	221	ILE	HD13	0.662	0.02	1
3087	A	21	ILE	HG12	1.062	0.02	2
3088	B	221	ILE	HG12	1.062	0.02	2
3089	A	21	ILE	HG13	1.549	0.02	2
3090	B	221	ILE	HG13	1.549	0.02	2
3091	A	21	ILE	HG21	1.269	0.02	1
3092	B	221	ILE	HG21	1.269	0.02	1
3093	A	21	ILE	HG22	1.269	0.02	1
3094	B	221	ILE	HG22	1.269	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3095	A	21	ILE	HG23	1.269	0.02	1
3096	B	221	ILE	HG23	1.269	0.02	1
3097	A	21	ILE	C	174.500	0.1	1
3098	B	221	ILE	C	174.500	0.1	1
3099	A	21	ILE	CA	60.845	0.1	1
3100	B	221	ILE	CA	60.845	0.1	1
3101	A	21	ILE	CB	42.090	0.1	1
3102	B	221	ILE	CB	42.090	0.1	1
3103	A	21	ILE	CD1	13.686	0.1	1
3104	B	221	ILE	CD1	13.686	0.1	1
3105	A	21	ILE	CG1	28.022	0.1	1
3106	B	221	ILE	CG1	28.022	0.1	1
3107	A	21	ILE	CG2	18.748	0.1	1
3108	B	221	ILE	CG2	18.748	0.1	1
3109	A	21	ILE	N	127.300	0.1	1
3110	B	221	ILE	N	127.300	0.1	1
3111	A	22	THR	H	9.162	0.02	1
3112	B	222	THR	H	9.162	0.02	1
3113	A	22	THR	HA	5.719	0.02	1
3114	B	222	THR	HA	5.719	0.02	1
3115	A	22	THR	HB	4.332	0.02	1
3116	B	222	THR	HB	4.332	0.02	1
3117	A	22	THR	HG21	1.320	0.02	1
3118	B	222	THR	HG21	1.320	0.02	1
3119	A	22	THR	HG22	1.320	0.02	1
3120	B	222	THR	HG22	1.320	0.02	1
3121	A	22	THR	HG23	1.320	0.02	1
3122	B	222	THR	HG23	1.320	0.02	1
3123	A	22	THR	C	175.028	0.1	1
3124	B	222	THR	C	175.028	0.1	1
3125	A	22	THR	CA	61.255	0.1	1
3126	B	222	THR	CA	61.255	0.1	1
3127	A	22	THR	CB	72.414	0.1	1
3128	B	222	THR	CB	72.414	0.1	1
3129	A	22	THR	CG2	21.416	0.1	1
3130	B	222	THR	CG2	21.416	0.1	1
3131	A	22	THR	N	117.440	0.1	1
3132	B	222	THR	N	117.440	0.1	1
3133	A	23	CYS	H	9.519	0.02	1
3134	B	223	CYS	H	9.519	0.02	1
3135	A	23	CYS	HA	5.549	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3136	B	223	CYS	HA	5.549	0.02	1
3137	A	23	CYS	HB2	2.843	0.02	2
3138	B	223	CYS	HB2	2.843	0.02	2
3139	A	23	CYS	HB3	3.125	0.02	2
3140	B	223	CYS	HB3	3.125	0.02	2
3141	A	23	CYS	C	172.437	0.1	1
3142	B	223	CYS	C	172.437	0.1	1
3143	A	23	CYS	CA	56.155	0.1	1
3144	B	223	CYS	CA	56.155	0.1	1
3145	A	23	CYS	CB	49.400	0.1	1
3146	B	223	CYS	CB	49.400	0.1	1
3147	A	23	CYS	N	121.413	0.1	1
3148	B	223	CYS	N	121.413	0.1	1
3149	A	24	GLN	H	9.163	0.02	1
3150	B	224	GLN	H	9.163	0.02	1
3151	A	24	GLN	HA	5.809	0.02	1
3152	B	224	GLN	HA	5.809	0.02	1
3153	A	24	GLN	HB2	2.237	0.02	2
3154	B	224	GLN	HB2	2.237	0.02	2
3155	A	24	GLN	HB3	2.115	0.02	2
3156	B	224	GLN	HB3	2.115	0.02	2
3157	A	24	GLN	HE21	7.963	0.02	2
3158	B	224	GLN	HE21	7.963	0.02	2
3159	A	24	GLN	HE22	6.792	0.02	2
3160	B	224	GLN	HE22	6.792	0.02	2
3161	A	24	GLN	HG2	2.472	0.02	2
3162	B	224	GLN	HG2	2.472	0.02	2
3163	A	24	GLN	HG3	2.512	0.02	2
3164	B	224	GLN	HG3	2.512	0.02	2
3165	A	24	GLN	C	175.028	0.1	1
3166	B	224	GLN	C	175.028	0.1	1
3167	A	24	GLN	CA	53.811	0.1	1
3168	B	224	GLN	CA	53.811	0.1	1
3169	A	24	GLN	CB	32.742	0.1	1
3170	B	224	GLN	CB	32.742	0.1	1
3171	A	24	GLN	CG	34.627	0.1	1
3172	B	224	GLN	CG	34.627	0.1	1
3173	A	24	GLN	N	123.700	0.1	1
3174	B	224	GLN	N	123.700	0.1	1
3175	A	24	GLN	NE2	112.271	0.1	1
3176	B	224	GLN	NE2	112.271	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3177	A	25	ALA	H	9.184	0.02	1
3178	B	225	ALA	H	9.184	0.02	1
3179	A	25	ALA	HA	5.609	0.02	1
3180	B	225	ALA	HA	5.609	0.02	1
3181	A	25	ALA	HB1	1.629	0.02	1
3182	B	225	ALA	HB1	1.629	0.02	1
3183	A	25	ALA	HB2	1.629	0.02	1
3184	B	225	ALA	HB2	1.629	0.02	1
3185	A	25	ALA	HB3	1.629	0.02	1
3186	B	225	ALA	HB3	1.629	0.02	1
3187	A	25	ALA	C	178.626	0.1	1
3188	B	225	ALA	C	178.626	0.1	1
3189	A	25	ALA	CA	50.411	0.1	1
3190	B	225	ALA	CA	50.411	0.1	1
3191	A	25	ALA	CB	24.100	0.1	1
3192	B	225	ALA	CB	24.100	0.1	1
3193	A	25	ALA	N	128.300	0.1	1
3194	B	225	ALA	N	128.300	0.1	1
3195	A	26	SER	H	8.281	0.02	1
3196	B	226	SER	H	8.281	0.02	1
3197	A	26	SER	HA	4.387	0.02	1
3198	B	226	SER	HA	4.387	0.02	1
3199	A	26	SER	HB2	4.178	0.02	2
3200	B	226	SER	HB2	4.178	0.02	2
3201	A	26	SER	HB3	4.078	0.02	2
3202	B	226	SER	HB3	4.078	0.02	2
3203	A	26	SER	C	173.492	0.1	1
3204	B	226	SER	C	173.492	0.1	1
3205	A	26	SER	CA	60.639	0.1	1
3206	B	226	SER	CA	60.639	0.1	1
3207	A	26	SER	CB	63.369	0.1	1
3208	B	226	SER	CB	63.369	0.1	1
3209	A	26	SER	N	113.935	0.1	1
3210	B	226	SER	N	113.935	0.1	1
3211	A	27	GLN	H	7.470	0.02	1
3212	B	227	GLN	H	7.470	0.02	1
3213	A	27	GLN	HA	4.556	0.02	1
3214	B	227	GLN	HA	4.556	0.02	1
3215	A	27	GLN	HB2	1.928	0.02	2
3216	B	227	GLN	HB2	1.928	0.02	2
3217	A	27	GLN	HB3	2.127	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3218	B	227	GLN	HB3	2.127	0.02	2
3219	A	27	GLN	HE21	7.976	0.02	2
3220	B	227	GLN	HE21	7.976	0.02	2
3221	A	27	GLN	HE22	6.852	0.02	2
3222	B	227	GLN	HE22	6.852	0.02	2
3223	A	27	GLN	HG2	2.127	0.02	2
3224	B	227	GLN	HG2	2.127	0.02	2
3225	A	27	GLN	HG3	2.218	0.02	2
3226	B	227	GLN	HG3	2.218	0.02	2
3227	A	27	GLN	C	172.341	0.1	1
3228	B	227	GLN	C	172.341	0.1	1
3229	A	27	GLN	CA	53.600	0.1	1
3230	B	227	GLN	CA	53.600	0.1	1
3231	A	27	GLN	CB	32.801	0.1	1
3232	B	227	GLN	CB	32.801	0.1	1
3233	A	27	GLN	CG	33.132	0.1	1
3234	B	227	GLN	CG	33.132	0.1	1
3235	A	27	GLN	N	116.158	0.1	1
3236	B	227	GLN	N	116.158	0.1	1
3237	A	27	GLN	NE2	114.125	0.1	1
3238	B	227	GLN	NE2	114.125	0.1	1
3239	A	28	ASP	H	8.143	0.02	1
3240	B	228	ASP	H	8.143	0.02	1
3241	A	28	ASP	HA	4.099	0.02	1
3242	B	228	ASP	HA	4.099	0.02	1
3243	A	28	ASP	HB2	2.544	0.02	2
3244	B	228	ASP	HB2	2.544	0.02	2
3245	A	28	ASP	HB3	2.851	0.02	2
3246	B	228	ASP	HB3	2.851	0.02	2
3247	A	28	ASP	C	177.427	0.1	1
3248	B	228	ASP	C	177.427	0.1	1
3249	A	28	ASP	CA	55.800	0.1	1
3250	B	228	ASP	CA	55.800	0.1	1
3251	A	28	ASP	CB	41.600	0.1	1
3252	B	228	ASP	CB	41.600	0.1	1
3253	A	28	ASP	N	118.000	0.1	1
3254	B	228	ASP	N	118.000	0.1	1
3255	A	29	ILE	H	8.588	0.02	1
3256	B	229	ILE	H	8.588	0.02	1
3257	A	29	ILE	HA	4.652	0.02	1
3258	B	229	ILE	HA	4.652	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3259	A	29	ILE	HB	2.377	0.02	1
3260	B	229	ILE	HB	2.377	0.02	1
3261	A	29	ILE	HD11	0.502	0.02	1
3262	B	229	ILE	HD11	0.502	0.02	1
3263	A	29	ILE	HD12	0.502	0.02	1
3264	B	229	ILE	HD12	0.502	0.02	1
3265	A	29	ILE	HD13	0.502	0.02	1
3266	B	229	ILE	HD13	0.502	0.02	1
3267	A	29	ILE	HG12	1.284	0.02	2
3268	B	229	ILE	HG12	1.284	0.02	2
3269	A	29	ILE	HG13	1.284	0.02	2
3270	B	229	ILE	HG13	1.284	0.02	2
3271	A	29	ILE	HG21	0.978	0.02	1
3272	B	229	ILE	HG21	0.978	0.02	1
3273	A	29	ILE	HG22	0.978	0.02	1
3274	B	229	ILE	HG22	0.978	0.02	1
3275	A	29	ILE	HG23	0.978	0.02	1
3276	B	229	ILE	HG23	0.978	0.02	1
3277	A	29	ILE	C	175.364	0.1	1
3278	B	229	ILE	C	175.364	0.1	1
3279	A	29	ILE	CA	60.816	0.1	1
3280	B	229	ILE	CA	60.816	0.1	1
3281	A	29	ILE	CB	39.000	0.1	1
3282	B	229	ILE	CB	39.000	0.1	1
3283	A	29	ILE	CD1	16.207	0.1	1
3284	B	229	ILE	CD1	16.207	0.1	1
3285	A	29	ILE	CG1	26.661	0.1	1
3286	B	229	ILE	CG1	26.661	0.1	1
3287	A	29	ILE	CG2	17.859	0.1	1
3288	B	229	ILE	CG2	17.859	0.1	1
3289	A	29	ILE	N	122.302	0.1	1
3290	B	229	ILE	N	122.302	0.1	1
3291	A	30	ASN	H	9.224	0.02	1
3292	B	230	ASN	H	9.224	0.02	1
3293	A	30	ASN	HA	4.214	0.02	1
3294	B	230	ASN	HA	4.214	0.02	1
3295	A	30	ASN	HB2	2.777	0.02	2
3296	B	230	ASN	HB2	2.777	0.02	2
3297	A	30	ASN	HB3	2.684	0.02	2
3298	B	230	ASN	HB3	2.684	0.02	2
3299	A	30	ASN	HD21	7.338	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3300	B	230	ASN	HD21	7.338	0.02	2
3301	A	30	ASN	HD22	6.837	0.02	2
3302	B	230	ASN	HD22	6.837	0.02	2
3303	A	30	ASN	C	173.396	0.1	1
3304	B	230	ASN	C	173.396	0.1	1
3305	A	30	ASN	CA	55.502	0.1	1
3306	B	230	ASN	CA	55.502	0.1	1
3307	A	30	ASN	CB	37.700	0.1	1
3308	B	230	ASN	CB	37.700	0.1	1
3309	A	30	ASN	N	120.008	0.1	1
3310	B	230	ASN	N	120.008	0.1	1
3311	A	30	ASN	ND2	114.174	0.1	1
3312	B	230	ASN	ND2	114.174	0.1	1
3313	A	31	ASN	H	7.503	0.02	1
3314	B	231	ASN	H	7.503	0.02	1
3315	A	31	ASN	HA	4.903	0.02	1
3316	B	231	ASN	HA	4.903	0.02	1
3317	A	31	ASN	HB2	2.852	0.02	2
3318	B	231	ASN	HB2	2.852	0.02	2
3319	A	31	ASN	HB3	2.852	0.02	2
3320	B	231	ASN	HB3	2.852	0.02	2
3321	A	31	ASN	HD21	7.217	0.02	2
3322	B	231	ASN	HD21	7.217	0.02	2
3323	A	31	ASN	HD22	6.601	0.02	2
3324	B	231	ASN	HD22	6.601	0.02	2
3325	A	31	ASN	C	175.268	0.1	1
3326	B	231	ASN	C	175.268	0.1	1
3327	A	31	ASN	CA	52.359	0.1	1
3328	B	231	ASN	CA	52.359	0.1	1
3329	A	31	ASN	CB	37.958	0.1	1
3330	B	231	ASN	CB	37.958	0.1	1
3331	A	31	ASN	N	117.745	0.1	1
3332	B	231	ASN	N	117.745	0.1	1
3333	A	31	ASN	ND2	110.107	0.1	1
3334	B	231	ASN	ND2	110.107	0.1	1
3335	A	32	TYR	H	7.942	0.02	1
3336	B	232	TYR	H	7.942	0.02	1
3337	A	32	TYR	HA	4.103	0.02	1
3338	B	232	TYR	HA	4.103	0.02	1
3339	A	32	TYR	HB2	2.641	0.02	2
3340	B	232	TYR	HB2	2.641	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3341	A	32	TYR	HB3	1.169	0.02	2
3342	B	232	TYR	HB3	1.169	0.02	2
3343	A	32	TYR	HD1	7.104	0.02	1
3344	B	232	TYR	HD1	7.104	0.02	1
3345	A	32	TYR	HD2	7.104	0.02	1
3346	B	232	TYR	HD2	7.104	0.02	1
3347	A	32	TYR	HE1	6.949	0.02	1
3348	B	232	TYR	HE1	6.949	0.02	1
3349	A	32	TYR	HE2	6.949	0.02	1
3350	B	232	TYR	HE2	6.949	0.02	1
3351	A	32	TYR	C	173.588	0.1	1
3352	B	232	TYR	C	173.588	0.1	1
3353	A	32	TYR	CA	56.361	0.1	1
3354	B	232	TYR	CA	56.361	0.1	1
3355	A	32	TYR	CB	34.636	0.1	1
3356	B	232	TYR	CB	34.636	0.1	1
3357	A	32	TYR	CD1	133.341	0.1	1
3358	B	232	TYR	CD1	133.341	0.1	1
3359	A	32	TYR	CE1	118.329	0.1	1
3360	B	232	TYR	CE1	118.329	0.1	1
3361	A	32	TYR	N	120.590	0.1	1
3362	B	232	TYR	N	120.590	0.1	1
3363	A	33	LEU	H	7.893	0.02	1
3364	B	233	LEU	H	7.893	0.02	1
3365	A	33	LEU	HA	4.748	0.02	1
3366	B	233	LEU	HA	4.748	0.02	1
3367	A	33	LEU	HB2	0.145	0.02	2
3368	B	233	LEU	HB2	0.145	0.02	2
3369	A	33	LEU	HB3	0.779	0.02	2
3370	B	233	LEU	HB3	0.779	0.02	2
3371	A	33	LEU	HD11	-0.029	0.02	2
3372	B	233	LEU	HD11	-0.029	0.02	2
3373	A	33	LEU	HD12	-0.029	0.02	2
3374	B	233	LEU	HD12	-0.029	0.02	2
3375	A	33	LEU	HD13	-0.029	0.02	2
3376	B	233	LEU	HD13	-0.029	0.02	2
3377	A	33	LEU	HD21	-0.072	0.02	2
3378	B	233	LEU	HD21	-0.072	0.02	2
3379	A	33	LEU	HD22	-0.072	0.02	2
3380	B	233	LEU	HD22	-0.072	0.02	2
3381	A	33	LEU	HD23	-0.072	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3382	B	233	LEU	HD23	-0.072	0.02	2
3383	A	33	LEU	HG	0.622	0.02	1
3384	B	233	LEU	HG	0.622	0.02	1
3385	A	33	LEU	C	175.700	0.1	1
3386	B	233	LEU	C	175.700	0.1	1
3387	A	33	LEU	CA	52.961	0.1	1
3388	B	233	LEU	CA	52.961	0.1	1
3389	A	33	LEU	CB	46.400	0.1	1
3390	B	233	LEU	CB	46.400	0.1	1
3391	A	33	LEU	CD1	25.000	0.1	1
3392	B	233	LEU	CD1	25.000	0.1	1
3393	A	33	LEU	CD2	24.720	0.1	1
3394	B	233	LEU	CD2	24.720	0.1	1
3395	A	33	LEU	CG	26.014	0.1	1
3396	B	233	LEU	CG	26.014	0.1	1
3397	A	33	LEU	N	125.500	0.1	1
3398	B	233	LEU	N	125.500	0.1	1
3399	A	34	ILE	H	8.752	0.02	1
3400	B	234	ILE	H	8.752	0.02	1
3401	A	34	ILE	HA	4.892	0.02	1
3402	B	234	ILE	HA	4.892	0.02	1
3403	A	34	ILE	HB	1.140	0.02	1
3404	B	234	ILE	HB	1.140	0.02	1
3405	A	34	ILE	HD11	0.107	0.02	1
3406	B	234	ILE	HD11	0.107	0.02	1
3407	A	34	ILE	HD12	0.107	0.02	1
3408	B	234	ILE	HD12	0.107	0.02	1
3409	A	34	ILE	HD13	0.107	0.02	1
3410	B	234	ILE	HD13	0.107	0.02	1
3411	A	34	ILE	HG12	1.781	0.02	2
3412	B	234	ILE	HG12	1.781	0.02	2
3413	A	34	ILE	HG13	0.768	0.02	2
3414	B	234	ILE	HG13	0.768	0.02	2
3415	A	34	ILE	HG21	0.096	0.02	1
3416	B	234	ILE	HG21	0.096	0.02	1
3417	A	34	ILE	HG22	0.096	0.02	1
3418	B	234	ILE	HG22	0.096	0.02	1
3419	A	34	ILE	HG23	0.096	0.02	1
3420	B	234	ILE	HG23	0.096	0.02	1
3421	A	34	ILE	C	175.843	0.1	1
3422	B	234	ILE	C	175.843	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3423	A	34	ILE	CA	59.057	0.1	1
3424	B	234	ILE	CA	59.057	0.1	1
3425	A	34	ILE	CB	43.618	0.1	1
3426	B	234	ILE	CB	43.618	0.1	1
3427	A	34	ILE	CD1	14.810	0.1	1
3428	B	234	ILE	CD1	14.810	0.1	1
3429	A	34	ILE	CG1	29.896	0.1	1
3430	B	234	ILE	CG1	29.896	0.1	1
3431	A	34	ILE	CG2	18.240	0.1	1
3432	B	234	ILE	CG2	18.240	0.1	1
3433	A	34	ILE	N	127.763	0.1	1
3434	B	234	ILE	N	127.763	0.1	1
3435	A	35	TRP	H	8.114	0.02	1
3436	B	235	TRP	H	8.114	0.02	1
3437	A	35	TRP	HA	5.316	0.02	1
3438	B	235	TRP	HA	5.316	0.02	1
3439	A	35	TRP	HB2	2.683	0.02	2
3440	B	235	TRP	HB2	2.683	0.02	2
3441	A	35	TRP	HB3	2.547	0.02	2
3442	B	235	TRP	HB3	2.547	0.02	2
3443	A	35	TRP	HD1	6.667	0.02	1
3444	B	235	TRP	HD1	6.667	0.02	1
3445	A	35	TRP	HE1	11.544	0.02	1
3446	B	235	TRP	HE1	11.544	0.02	1
3447	A	35	TRP	HE3	6.863	0.02	1
3448	B	235	TRP	HE3	6.863	0.02	1
3449	A	35	TRP	HH2	6.817	0.02	1
3450	B	235	TRP	HH2	6.817	0.02	1
3451	A	35	TRP	HZ2	7.035	0.02	1
3452	B	235	TRP	HZ2	7.035	0.02	1
3453	A	35	TRP	HZ3	6.708	0.02	1
3454	B	235	TRP	HZ3	6.708	0.02	1
3455	A	35	TRP	C	176.000	0.1	1
3456	B	235	TRP	C	176.000	0.1	1
3457	A	35	TRP	CA	56.000	0.1	1
3458	B	235	TRP	CA	56.000	0.1	1
3459	A	35	TRP	CB	32.272	0.1	1
3460	B	235	TRP	CB	32.272	0.1	1
3461	A	35	TRP	CD1	125.576	0.1	1
3462	B	235	TRP	CD1	125.576	0.1	1
3463	A	35	TRP	CE3	120.141	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3464	B	235	TRP	CE3	120.141	0.1	1
3465	A	35	TRP	CH2	126.094	0.1	1
3466	B	235	TRP	CH2	126.094	0.1	1
3467	A	35	TRP	CZ2	114.188	0.1	1
3468	B	235	TRP	CZ2	114.188	0.1	1
3469	A	35	TRP	CZ3	121.694	0.1	1
3470	B	235	TRP	CZ3	121.694	0.1	1
3471	A	35	TRP	N	121.554	0.1	1
3472	B	235	TRP	N	121.554	0.1	1
3473	A	35	TRP	NE1	134.000	0.1	1
3474	B	235	TRP	NE1	134.000	0.1	1
3475	A	36	TYR	H	9.616	0.02	1
3476	B	236	TYR	H	9.616	0.02	1
3477	A	36	TYR	HA	5.463	0.02	1
3478	B	236	TYR	HA	5.463	0.02	1
3479	A	36	TYR	HB2	2.797	0.02	2
3480	B	236	TYR	HB2	2.797	0.02	2
3481	A	36	TYR	HB3	2.672	0.02	2
3482	B	236	TYR	HB3	2.672	0.02	2
3483	A	36	TYR	HD1	6.568	0.02	1
3484	B	236	TYR	HD1	6.568	0.02	1
3485	A	36	TYR	HD2	6.568	0.02	1
3486	B	236	TYR	HD2	6.568	0.02	1
3487	A	36	TYR	HE1	6.726	0.02	1
3488	B	236	TYR	HE1	6.726	0.02	1
3489	A	36	TYR	HE2	6.726	0.02	1
3490	B	236	TYR	HE2	6.726	0.02	1
3491	A	36	TYR	C	175.172	0.1	1
3492	B	236	TYR	C	175.172	0.1	1
3493	A	36	TYR	CA	57.152	0.1	1
3494	B	236	TYR	CA	57.152	0.1	1
3495	A	36	TYR	CB	44.559	0.1	1
3496	B	236	TYR	CB	44.559	0.1	1
3497	A	36	TYR	CD1	132.306	0.1	1
3498	B	236	TYR	CD1	132.306	0.1	1
3499	A	36	TYR	CE1	118.847	0.1	1
3500	B	236	TYR	CE1	118.847	0.1	1
3501	A	36	TYR	N	119.300	0.1	1
3502	B	236	TYR	N	119.300	0.1	1
3503	A	37	GLN	H	9.194	0.02	1
3504	B	237	GLN	H	9.194	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3505	A	37	GLN	HA	4.172	0.02	1
3506	B	237	GLN	HA	4.172	0.02	1
3507	A	37	GLN	HB2	1.882	0.02	2
3508	B	237	GLN	HB2	1.882	0.02	2
3509	A	37	GLN	HB3	2.196	0.02	2
3510	B	237	GLN	HB3	2.196	0.02	2
3511	A	37	GLN	HE21	7.822	0.02	2
3512	B	237	GLN	HE21	7.822	0.02	2
3513	A	37	GLN	HE22	8.073	0.02	2
3514	B	237	GLN	HE22	8.073	0.02	2
3515	A	37	GLN	HG2	1.517	0.02	2
3516	B	237	GLN	HG2	1.517	0.02	2
3517	A	37	GLN	HG3	1.517	0.02	2
3518	B	237	GLN	HG3	1.517	0.02	2
3519	A	37	GLN	C	174.010	0.1	1
3520	B	237	GLN	C	174.010	0.1	1
3521	A	37	GLN	CA	54.309	0.1	1
3522	B	237	GLN	CA	54.309	0.1	1
3523	A	37	GLN	CB	35.073	0.1	1
3524	B	237	GLN	CB	35.073	0.1	1
3525	A	37	GLN	CG	35.800	0.1	1
3526	B	237	GLN	CG	35.800	0.1	1
3527	A	37	GLN	N	120.527	0.1	1
3528	B	237	GLN	N	120.527	0.1	1
3529	A	37	GLN	NE2	112.426	0.1	1
3530	B	237	GLN	NE2	112.426	0.1	1
3531	A	38	GLN	H	9.525	0.02	1
3532	B	238	GLN	H	9.525	0.02	1
3533	A	38	GLN	HA	4.826	0.02	1
3534	B	238	GLN	HA	4.826	0.02	1
3535	A	38	GLN	HB2	2.342	0.02	2
3536	B	238	GLN	HB2	2.342	0.02	2
3537	A	38	GLN	HB3	2.342	0.02	2
3538	B	238	GLN	HB3	2.342	0.02	2
3539	A	38	GLN	HE21	7.980	0.02	2
3540	B	238	GLN	HE21	7.980	0.02	2
3541	A	38	GLN	HE22	7.429	0.02	2
3542	B	238	GLN	HE22	7.429	0.02	2
3543	A	38	GLN	HG2	2.145	0.02	2
3544	B	238	GLN	HG2	2.145	0.02	2
3545	A	38	GLN	HG3	1.945	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3546	B	238	GLN	HG3	1.945	0.02	2
3547	A	38	GLN	C	175.384	0.1	1
3548	B	238	GLN	C	175.384	0.1	1
3549	A	38	GLN	CA	55.071	0.1	1
3550	B	238	GLN	CA	55.071	0.1	1
3551	A	38	GLN	CB	31.500	0.1	1
3552	B	238	GLN	CB	31.500	0.1	1
3553	A	38	GLN	CG	34.103	0.1	1
3554	B	238	GLN	CG	34.103	0.1	1
3555	A	38	GLN	N	128.647	0.1	1
3556	B	238	GLN	N	128.647	0.1	1
3557	A	38	GLN	NE2	110.064	0.1	1
3558	B	238	GLN	NE2	110.064	0.1	1
3559	A	39	LYS	H	9.194	0.02	1
3560	B	239	LYS	H	9.194	0.02	1
3561	A	39	LYS	HA	4.539	0.02	1
3562	B	239	LYS	HA	4.539	0.02	1
3563	A	39	LYS	HB2	1.992	0.02	2
3564	B	239	LYS	HB2	1.992	0.02	2
3565	A	39	LYS	HB3	1.520	0.02	2
3566	B	239	LYS	HB3	1.520	0.02	2
3567	A	39	LYS	HD2	1.816	0.02	2
3568	B	239	LYS	HD2	1.816	0.02	2
3569	A	39	LYS	HD3	1.816	0.02	2
3570	B	239	LYS	HD3	1.816	0.02	2
3571	A	39	LYS	HE2	3.129	0.02	2
3572	B	239	LYS	HE2	3.129	0.02	2
3573	A	39	LYS	HE3	3.016	0.02	2
3574	B	239	LYS	HE3	3.016	0.02	2
3575	A	39	LYS	HG2	1.517	0.02	2
3576	B	239	LYS	HG2	1.517	0.02	2
3577	A	39	LYS	HG3	1.517	0.02	2
3578	B	239	LYS	HG3	1.517	0.02	2
3579	A	39	LYS	C	173.182	0.1	1
3580	B	239	LYS	C	173.182	0.1	1
3581	A	39	LYS	CA	55.500	0.1	1
3582	B	239	LYS	CA	55.500	0.1	1
3583	A	39	LYS	CB	31.191	0.1	1
3584	B	239	LYS	CB	31.191	0.1	1
3585	A	39	LYS	CD	29.573	0.1	1
3586	B	239	LYS	CD	29.573	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3587	A	39	LYS	CE	42.191	0.1	1
3588	B	239	LYS	CE	42.191	0.1	1
3589	A	39	LYS	CG	26.984	0.1	1
3590	B	239	LYS	CG	26.984	0.1	1
3591	A	39	LYS	N	132.971	0.1	1
3592	B	239	LYS	N	132.971	0.1	1
3593	A	40	PRO	HA	4.314	0.02	1
3594	B	240	PRO	HA	4.314	0.02	1
3595	A	40	PRO	HB2	2.323	0.02	2
3596	B	240	PRO	HB2	2.323	0.02	2
3597	A	40	PRO	HB3	1.981	0.02	2
3598	B	240	PRO	HB3	1.981	0.02	2
3599	A	40	PRO	HD2	3.684	0.02	2
3600	B	240	PRO	HD2	3.684	0.02	2
3601	A	40	PRO	HD3	3.838	0.02	2
3602	B	240	PRO	HD3	3.838	0.02	2
3603	A	40	PRO	HG2	2.206	0.02	2
3604	B	240	PRO	HG2	2.206	0.02	2
3605	A	40	PRO	HG3	2.034	0.02	2
3606	B	240	PRO	HG3	2.034	0.02	2
3607	A	40	PRO	CA	64.512	0.1	1
3608	B	240	PRO	CA	64.512	0.1	1
3609	A	40	PRO	CB	31.838	0.1	1
3610	B	240	PRO	CB	31.838	0.1	1
3611	A	40	PRO	CD	50.280	0.1	1
3612	B	240	PRO	CD	50.280	0.1	1
3613	A	40	PRO	CG	28.279	0.1	1
3614	B	240	PRO	CG	28.279	0.1	1
3615	A	41	GLY	HA2	4.232	0.02	2
3616	B	241	GLY	HA2	4.232	0.02	2
3617	A	41	GLY	HA3	3.785	0.02	2
3618	B	241	GLY	HA3	3.785	0.02	2
3619	A	41	GLY	C	174.260	0.1	1
3620	B	241	GLY	C	174.260	0.1	1
3621	A	41	GLY	CA	46.023	0.1	1
3622	B	241	GLY	CA	46.023	0.1	1
3623	A	42	GLN	H	8.083	0.02	1
3624	B	242	GLN	H	8.083	0.02	1
3625	A	42	GLN	HA	4.947	0.02	1
3626	B	242	GLN	HA	4.947	0.02	1
3627	A	42	GLN	HB2	2.386	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3628	B	242	GLN	HB2	2.386	0.02	2
3629	A	42	GLN	HB3	2.076	0.02	2
3630	B	242	GLN	HB3	2.076	0.02	2
3631	A	42	GLN	HE21	7.621	0.02	2
3632	B	242	GLN	HE21	7.621	0.02	2
3633	A	42	GLN	HE22	6.953	0.02	2
3634	B	242	GLN	HE22	6.953	0.02	2
3635	A	42	GLN	HG2	2.345	0.02	2
3636	B	242	GLN	HG2	2.345	0.02	2
3637	A	42	GLN	HG3	2.345	0.02	2
3638	B	242	GLN	HG3	2.345	0.02	2
3639	A	42	GLN	C	175.020	0.1	1
3640	B	242	GLN	C	175.020	0.1	1
3641	A	42	GLN	CA	54.221	0.1	1
3642	B	242	GLN	CA	54.221	0.1	1
3643	A	42	GLN	CB	32.507	0.1	1
3644	B	242	GLN	CB	32.507	0.1	1
3645	A	42	GLN	CG	34.119	0.1	1
3646	B	242	GLN	CG	34.119	0.1	1
3647	A	42	GLN	N	119.261	0.1	1
3648	B	242	GLN	N	119.261	0.1	1
3649	A	42	GLN	NE2	112.260	0.1	1
3650	B	242	GLN	NE2	112.260	0.1	1
3651	A	43	ALA	H	8.386	0.02	1
3652	B	243	ALA	H	8.386	0.02	1
3653	A	43	ALA	HA	4.160	0.02	1
3654	B	243	ALA	HA	4.160	0.02	1
3655	A	43	ALA	HB1	1.354	0.02	1
3656	B	243	ALA	HB1	1.354	0.02	1
3657	A	43	ALA	HB2	1.354	0.02	1
3658	B	243	ALA	HB2	1.354	0.02	1
3659	A	43	ALA	HB3	1.354	0.02	1
3660	B	243	ALA	HB3	1.354	0.02	1
3661	A	43	ALA	C	175.505	0.1	1
3662	B	243	ALA	C	175.505	0.1	1
3663	A	43	ALA	CA	50.280	0.1	1
3664	B	243	ALA	CA	50.280	0.1	1
3665	A	43	ALA	CB	18.286	0.1	1
3666	B	243	ALA	CB	18.286	0.1	1
3667	A	43	ALA	N	120.919	0.1	1
3668	B	243	ALA	N	120.919	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3669	A	44	PRO	HA	4.055	0.02	1
3670	B	244	PRO	HA	4.055	0.02	1
3671	A	44	PRO	HB2	0.588	0.02	2
3672	B	244	PRO	HB2	0.588	0.02	2
3673	A	44	PRO	HB3	1.069	0.02	2
3674	B	244	PRO	HB3	1.069	0.02	2
3675	A	44	PRO	HD2	2.443	0.02	2
3676	B	244	PRO	HD2	2.443	0.02	2
3677	A	44	PRO	HD3	1.427	0.02	2
3678	B	244	PRO	HD3	1.427	0.02	2
3679	A	44	PRO	HG2	0.584	0.02	2
3680	B	244	PRO	HG2	0.584	0.02	2
3681	A	44	PRO	HG3	-0.016	0.02	2
3682	B	244	PRO	HG3	-0.016	0.02	2
3683	A	44	PRO	C	174.212	0.1	1
3684	B	244	PRO	C	174.212	0.1	1
3685	A	44	PRO	CA	62.978	0.1	1
3686	B	244	PRO	CA	62.978	0.1	1
3687	A	44	PRO	CB	30.904	0.1	1
3688	B	244	PRO	CB	30.904	0.1	1
3689	A	44	PRO	CD	48.986	0.1	1
3690	B	244	PRO	CD	48.986	0.1	1
3691	A	44	PRO	CG	26.337	0.1	1
3692	B	244	PRO	CG	26.337	0.1	1
3693	A	45	LYS	H	9.085	0.02	1
3694	B	245	LYS	H	9.085	0.02	1
3695	A	45	LYS	HA	4.697	0.02	1
3696	B	245	LYS	HA	4.697	0.02	1
3697	A	45	LYS	HB2	1.939	0.02	2
3698	B	245	LYS	HB2	1.939	0.02	2
3699	A	45	LYS	HB3	2.117	0.02	2
3700	B	245	LYS	HB3	2.117	0.02	2
3701	A	45	LYS	HD2	1.887	0.02	2
3702	B	245	LYS	HD2	1.887	0.02	2
3703	A	45	LYS	HD3	1.808	0.02	2
3704	B	245	LYS	HD3	1.808	0.02	2
3705	A	45	LYS	HE2	3.160	0.02	2
3706	B	245	LYS	HE2	3.160	0.02	2
3707	A	45	LYS	HE3	3.091	0.02	2
3708	B	245	LYS	HE3	3.091	0.02	2
3709	A	45	LYS	HG2	1.625	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3710	B	245	LYS	HG2	1.625	0.02	2
3711	A	45	LYS	HG3	1.433	0.02	2
3712	B	245	LYS	HG3	1.433	0.02	2
3713	A	45	LYS	C	175.707	0.1	1
3714	B	245	LYS	C	175.707	0.1	1
3715	A	45	LYS	CA	55.159	0.1	1
3716	B	245	LYS	CA	55.159	0.1	1
3717	A	45	LYS	CB	35.799	0.1	1
3718	B	245	LYS	CB	35.799	0.1	1
3719	A	45	LYS	CD	29.600	0.1	1
3720	B	245	LYS	CD	29.600	0.1	1
3721	A	45	LYS	CE	42.800	0.1	1
3722	B	245	LYS	CE	42.800	0.1	1
3723	A	45	LYS	CG	25.400	0.1	1
3724	B	245	LYS	CG	25.400	0.1	1
3725	A	45	LYS	N	123.672	0.1	1
3726	B	245	LYS	N	123.672	0.1	1
3727	A	46	LEU	H	9.103	0.02	1
3728	B	246	LEU	H	9.103	0.02	1
3729	A	46	LEU	HA	3.882	0.02	1
3730	B	246	LEU	HA	3.882	0.02	1
3731	A	46	LEU	HB2	1.862	0.02	2
3732	B	246	LEU	HB2	1.862	0.02	2
3733	A	46	LEU	HB3	1.862	0.02	2
3734	B	246	LEU	HB3	1.862	0.02	2
3735	A	46	LEU	HD11	0.807	0.02	2
3736	B	246	LEU	HD11	0.807	0.02	2
3737	A	46	LEU	HD12	0.807	0.02	2
3738	B	246	LEU	HD12	0.807	0.02	2
3739	A	46	LEU	HD13	0.807	0.02	2
3740	B	246	LEU	HD13	0.807	0.02	2
3741	A	46	LEU	HD21	0.844	0.02	2
3742	B	246	LEU	HD21	0.844	0.02	2
3743	A	46	LEU	HD22	0.844	0.02	2
3744	B	246	LEU	HD22	0.844	0.02	2
3745	A	46	LEU	HD23	0.844	0.02	2
3746	B	246	LEU	HD23	0.844	0.02	2
3747	A	46	LEU	HG	1.467	0.02	1
3748	B	246	LEU	HG	1.467	0.02	1
3749	A	46	LEU	C	175.173	0.1	1
3750	B	246	LEU	C	175.173	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3751	A	46	LEU	CA	59.100	0.1	1
3752	B	246	LEU	CA	59.100	0.1	1
3753	A	46	LEU	CB	42.200	0.1	1
3754	B	246	LEU	CB	42.200	0.1	1
3755	A	46	LEU	CD1	26.014	0.1	1
3756	B	246	LEU	CD1	26.014	0.1	1
3757	A	46	LEU	CD2	28.926	0.1	1
3758	B	246	LEU	CD2	28.926	0.1	1
3759	A	46	LEU	CG	27.955	0.1	1
3760	B	246	LEU	CG	27.955	0.1	1
3761	A	46	LEU	N	131.133	0.1	1
3762	B	246	LEU	N	131.133	0.1	1
3763	A	47	LEU	HA	4.960	0.02	1
3764	B	247	LEU	HA	4.960	0.02	1
3765	A	47	LEU	HB2	1.847	0.02	2
3766	B	247	LEU	HB2	1.847	0.02	2
3767	A	47	LEU	HB3	1.444	0.02	2
3768	B	247	LEU	HB3	1.444	0.02	2
3769	A	47	LEU	HD11	0.714	0.02	2
3770	B	247	LEU	HD11	0.714	0.02	2
3771	A	47	LEU	HD12	0.714	0.02	2
3772	B	247	LEU	HD12	0.714	0.02	2
3773	A	47	LEU	HD13	0.714	0.02	2
3774	B	247	LEU	HD13	0.714	0.02	2
3775	A	47	LEU	HD21	0.759	0.02	2
3776	B	247	LEU	HD21	0.759	0.02	2
3777	A	47	LEU	HD22	0.759	0.02	2
3778	B	247	LEU	HD22	0.759	0.02	2
3779	A	47	LEU	HD23	0.759	0.02	2
3780	B	247	LEU	HD23	0.759	0.02	2
3781	A	47	LEU	HG	1.522	0.02	1
3782	B	247	LEU	HG	1.522	0.02	1
3783	A	47	LEU	C	175.508	0.1	1
3784	B	247	LEU	C	175.508	0.1	1
3785	A	47	LEU	CA	55.476	0.1	1
3786	B	247	LEU	CA	55.476	0.1	1
3787	A	47	LEU	CB	45.200	0.1	1
3788	B	247	LEU	CB	45.200	0.1	1
3789	A	47	LEU	CD1	27.300	0.1	1
3790	B	247	LEU	CD1	27.300	0.1	1
3791	A	47	LEU	CD2	22.178	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3792	B	247	LEU	CD2	22.178	0.1	1
3793	A	47	LEU	CG	27.900	0.1	1
3794	B	247	LEU	CG	27.900	0.1	1
3795	A	48	ILE	H	7.334	0.02	1
3796	B	248	ILE	H	7.334	0.02	1
3797	A	48	ILE	HA	5.273	0.02	1
3798	B	248	ILE	HA	5.273	0.02	1
3799	A	48	ILE	HB	1.712	0.02	1
3800	B	248	ILE	HB	1.712	0.02	1
3801	A	48	ILE	HD11	0.786	0.02	1
3802	B	248	ILE	HD11	0.786	0.02	1
3803	A	48	ILE	HD12	0.786	0.02	1
3804	B	248	ILE	HD12	0.786	0.02	1
3805	A	48	ILE	HD13	0.786	0.02	1
3806	B	248	ILE	HD13	0.786	0.02	1
3807	A	48	ILE	HG12	1.149	0.02	2
3808	B	248	ILE	HG12	1.149	0.02	2
3809	A	48	ILE	HG13	1.654	0.02	2
3810	B	248	ILE	HG13	1.654	0.02	2
3811	A	48	ILE	HG21	0.822	0.02	1
3812	B	248	ILE	HG21	0.822	0.02	1
3813	A	48	ILE	HG22	0.822	0.02	1
3814	B	248	ILE	HG22	0.822	0.02	1
3815	A	48	ILE	HG23	0.822	0.02	1
3816	B	248	ILE	HG23	0.822	0.02	1
3817	A	48	ILE	C	174.644	0.1	1
3818	B	248	ILE	C	174.644	0.1	1
3819	A	48	ILE	CA	58.530	0.1	1
3820	B	248	ILE	CA	58.530	0.1	1
3821	A	48	ILE	CB	44.734	0.1	1
3822	B	248	ILE	CB	44.734	0.1	1
3823	A	48	ILE	CD1	14.175	0.1	1
3824	B	248	ILE	CD1	14.175	0.1	1
3825	A	48	ILE	CG1	28.800	0.1	1
3826	B	248	ILE	CG1	28.800	0.1	1
3827	A	48	ILE	CG2	17.605	0.1	1
3828	B	248	ILE	CG2	17.605	0.1	1
3829	A	48	ILE	N	117.200	0.1	1
3830	B	248	ILE	N	117.200	0.1	1
3831	A	49	TYR	H	9.079	0.02	1
3832	B	249	TYR	H	9.079	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3833	A	49	TYR	HA	5.402	0.02	1
3834	B	249	TYR	HA	5.402	0.02	1
3835	A	49	TYR	HB2	2.866	0.02	2
3836	B	249	TYR	HB2	2.866	0.02	2
3837	A	49	TYR	HB3	2.684	0.02	2
3838	B	249	TYR	HB3	2.684	0.02	2
3839	A	49	TYR	HD1	6.897	0.02	1
3840	B	249	TYR	HD1	6.897	0.02	1
3841	A	49	TYR	HD2	6.897	0.02	1
3842	B	249	TYR	HD2	6.897	0.02	1
3843	A	49	TYR	HE1	6.722	0.02	1
3844	B	249	TYR	HE1	6.722	0.02	1
3845	A	49	TYR	HE2	6.722	0.02	1
3846	B	249	TYR	HE2	6.722	0.02	1
3847	A	49	TYR	C	172.485	0.1	1
3848	B	249	TYR	C	172.485	0.1	1
3849	A	49	TYR	CA	55.364	0.1	1
3850	B	249	TYR	CA	55.364	0.1	1
3851	A	49	TYR	CB	40.678	0.1	1
3852	B	249	TYR	CB	40.678	0.1	1
3853	A	49	TYR	CD1	133.859	0.1	1
3854	B	249	TYR	CD1	133.859	0.1	1
3855	A	49	TYR	CE1	118.000	0.1	1
3856	B	249	TYR	CE1	118.000	0.1	1
3857	A	49	TYR	N	121.662	0.1	1
3858	B	249	TYR	N	121.662	0.1	1
3859	A	50	ASP	H	8.674	0.02	1
3860	B	250	ASP	H	8.674	0.02	1
3861	A	50	ASP	HA	5.132	0.02	1
3862	B	250	ASP	HA	5.132	0.02	1
3863	A	50	ASP	HB2	2.700	0.02	2
3864	B	250	ASP	HB2	2.700	0.02	2
3865	A	50	ASP	HB3	3.170	0.02	2
3866	B	250	ASP	HB3	3.170	0.02	2
3867	A	50	ASP	C	179.058	0.1	1
3868	B	250	ASP	C	179.058	0.1	1
3869	A	50	ASP	CA	56.302	0.1	1
3870	B	250	ASP	CA	56.302	0.1	1
3871	A	50	ASP	CB	40.343	0.1	1
3872	B	250	ASP	CB	40.343	0.1	1
3873	A	50	ASP	N	119.859	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3874	B	250	ASP	N	119.859	0.1	1
3875	A	51	ALA	H	9.025	0.02	1
3876	B	251	ALA	H	9.025	0.02	1
3877	A	51	ALA	HA	3.757	0.02	1
3878	B	251	ALA	HA	3.757	0.02	1
3879	A	51	ALA	HB1	1.930	0.02	1
3880	B	251	ALA	HB1	1.930	0.02	1
3881	A	51	ALA	HB2	1.930	0.02	1
3882	B	251	ALA	HB2	1.930	0.02	1
3883	A	51	ALA	HB3	1.930	0.02	1
3884	B	251	ALA	HB3	1.930	0.02	1
3885	A	51	ALA	C	179.490	0.1	1
3886	B	251	ALA	C	179.490	0.1	1
3887	A	51	ALA	CA	57.800	0.1	1
3888	B	251	ALA	CA	57.800	0.1	1
3889	A	51	ALA	CB	19.386	0.1	1
3890	B	251	ALA	CB	19.386	0.1	1
3891	A	51	ALA	N	114.075	0.1	1
3892	B	251	ALA	N	114.075	0.1	1
3893	A	52	SER	H	8.675	0.02	1
3894	B	252	SER	H	8.675	0.02	1
3895	A	52	SER	HA	4.869	0.02	1
3896	B	252	SER	HA	4.869	0.02	1
3897	A	52	SER	HB2	4.230	0.02	2
3898	B	252	SER	HB2	4.230	0.02	2
3899	A	52	SER	HB3	3.863	0.02	2
3900	B	252	SER	HB3	3.863	0.02	2
3901	A	52	SER	C	175.268	0.1	1
3902	B	252	SER	C	175.268	0.1	1
3903	A	52	SER	CA	57.898	0.1	1
3904	B	252	SER	CA	57.898	0.1	1
3905	A	52	SER	CB	66.814	0.1	1
3906	B	252	SER	CB	66.814	0.1	1
3907	A	52	SER	N	111.188	0.1	1
3908	B	252	SER	N	111.188	0.1	1
3909	A	53	THR	H	9.045	0.02	1
3910	B	253	THR	H	9.045	0.02	1
3911	A	53	THR	HA	4.255	0.02	1
3912	B	253	THR	HA	4.255	0.02	1
3913	A	53	THR	HB	3.214	0.02	1
3914	B	253	THR	HB	3.214	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3915	A	53	THR	HG21	0.888	0.02	1
3916	B	253	THR	HG21	0.888	0.02	1
3917	A	53	THR	HG22	0.888	0.02	1
3918	B	253	THR	HG22	0.888	0.02	1
3919	A	53	THR	HG23	0.888	0.02	1
3920	B	253	THR	HG23	0.888	0.02	1
3921	A	53	THR	C	172.149	0.1	1
3922	B	253	THR	C	172.149	0.1	1
3923	A	53	THR	CA	63.500	0.1	1
3924	B	253	THR	CA	63.500	0.1	1
3925	A	53	THR	CB	68.600	0.1	1
3926	B	253	THR	CB	68.600	0.1	1
3927	A	53	THR	CG2	23.100	0.1	1
3928	B	253	THR	CG2	23.100	0.1	1
3929	A	53	THR	N	123.672	0.1	1
3930	B	253	THR	N	123.672	0.1	1
3931	A	54	LEU	H	8.484	0.02	1
3932	B	254	LEU	H	8.484	0.02	1
3933	A	54	LEU	HA	4.571	0.02	1
3934	B	254	LEU	HA	4.571	0.02	1
3935	A	54	LEU	HB2	1.605	0.02	2
3936	B	254	LEU	HB2	1.605	0.02	2
3937	A	54	LEU	HB3	1.828	0.02	2
3938	B	254	LEU	HB3	1.828	0.02	2
3939	A	54	LEU	HD11	0.998	0.02	2
3940	B	254	LEU	HD11	0.998	0.02	2
3941	A	54	LEU	HD12	0.998	0.02	2
3942	B	254	LEU	HD12	0.998	0.02	2
3943	A	54	LEU	HD13	0.998	0.02	2
3944	B	254	LEU	HD13	0.998	0.02	2
3945	A	54	LEU	HD21	1.050	0.02	2
3946	B	254	LEU	HD21	1.050	0.02	2
3947	A	54	LEU	HD22	1.050	0.02	2
3948	B	254	LEU	HD22	1.050	0.02	2
3949	A	54	LEU	HD23	1.050	0.02	2
3950	B	254	LEU	HD23	1.050	0.02	2
3951	A	54	LEU	HG	1.782	0.02	1
3952	B	254	LEU	HG	1.782	0.02	1
3953	A	54	LEU	C	177.955	0.1	1
3954	B	254	LEU	C	177.955	0.1	1
3955	A	54	LEU	CA	55.774	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3956	B	254	LEU	CA	55.774	0.1	1
3957	A	54	LEU	CB	43.500	0.1	1
3958	B	254	LEU	CB	43.500	0.1	1
3959	A	54	LEU	CD1	24.973	0.1	1
3960	B	254	LEU	CD1	24.973	0.1	1
3961	A	54	LEU	CD2	24.800	0.1	1
3962	B	254	LEU	CD2	24.800	0.1	1
3963	A	54	LEU	CG	29.249	0.1	1
3964	B	254	LEU	CG	29.249	0.1	1
3965	A	54	LEU	N	129.316	0.1	1
3966	B	254	LEU	N	129.316	0.1	1
3967	A	55	GLU	H	8.082	0.02	1
3968	B	255	GLU	H	8.082	0.02	1
3969	A	55	GLU	HA	4.734	0.02	1
3970	B	255	GLU	HA	4.734	0.02	1
3971	A	55	GLU	HB2	1.830	0.02	2
3972	B	255	GLU	HB2	1.830	0.02	2
3973	A	55	GLU	HB3	2.027	0.02	2
3974	B	255	GLU	HB3	2.027	0.02	2
3975	A	55	GLU	HG2	2.697	0.02	2
3976	B	255	GLU	HG2	2.697	0.02	2
3977	A	55	GLU	HG3	2.396	0.02	2
3978	B	255	GLU	HG3	2.396	0.02	2
3979	A	55	GLU	C	176.179	0.1	1
3980	B	255	GLU	C	176.179	0.1	1
3981	A	55	GLU	CA	55.979	0.1	1
3982	B	255	GLU	CA	55.979	0.1	1
3983	A	55	GLU	CB	30.626	0.1	1
3984	B	255	GLU	CB	30.626	0.1	1
3985	A	55	GLU	CG	36.400	0.1	1
3986	B	255	GLU	CG	36.400	0.1	1
3987	A	55	GLU	N	126.000	0.1	1
3988	B	255	GLU	N	126.000	0.1	1
3989	A	56	THR	H	8.454	0.02	1
3990	B	256	THR	H	8.454	0.02	1
3991	A	56	THR	HA	4.051	0.02	1
3992	B	256	THR	HA	4.051	0.02	1
3993	A	56	THR	HB	4.129	0.02	1
3994	B	256	THR	HB	4.129	0.02	1
3995	A	56	THR	HG21	1.348	0.02	1
3996	B	256	THR	HG21	1.348	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3997	A	56	THR	HG22	1.348	0.02	1
3998	B	256	THR	HG22	1.348	0.02	1
3999	A	56	THR	HG23	1.348	0.02	1
4000	B	256	THR	HG23	1.348	0.02	1
4001	A	56	THR	C	175.652	0.1	1
4002	B	256	THR	C	175.652	0.1	1
4003	A	56	THR	CA	64.978	0.1	1
4004	B	256	THR	CA	64.978	0.1	1
4005	A	56	THR	CB	69.369	0.1	1
4006	B	256	THR	CB	69.369	0.1	1
4007	A	56	THR	CG2	21.670	0.1	1
4008	B	256	THR	CG2	21.670	0.1	1
4009	A	56	THR	N	120.402	0.1	1
4010	B	256	THR	N	120.402	0.1	1
4011	A	57	GLY	H	8.983	0.02	1
4012	B	257	GLY	H	8.983	0.02	1
4013	A	57	GLY	HA2	4.288	0.02	2
4014	B	257	GLY	HA2	4.288	0.02	2
4015	A	57	GLY	HA3	3.813	0.02	2
4016	B	257	GLY	HA3	3.813	0.02	2
4017	A	57	GLY	C	174.548	0.1	1
4018	B	257	GLY	C	174.548	0.1	1
4019	A	57	GLY	CA	45.500	0.1	1
4020	B	257	GLY	CA	45.500	0.1	1
4021	A	57	GLY	N	114.813	0.1	1
4022	B	257	GLY	N	114.813	0.1	1
4023	A	58	VAL	H	7.738	0.02	1
4024	B	258	VAL	H	7.738	0.02	1
4025	A	58	VAL	HA	4.398	0.02	1
4026	B	258	VAL	HA	4.398	0.02	1
4027	A	58	VAL	HB	2.408	0.02	1
4028	B	258	VAL	HB	2.408	0.02	1
4029	A	58	VAL	HG11	1.323	0.02	2
4030	B	258	VAL	HG11	1.323	0.02	2
4031	A	58	VAL	HG12	1.323	0.02	2
4032	B	258	VAL	HG12	1.323	0.02	2
4033	A	58	VAL	HG13	1.323	0.02	2
4034	B	258	VAL	HG13	1.323	0.02	2
4035	A	58	VAL	HG21	1.266	0.02	2
4036	B	258	VAL	HG21	1.266	0.02	2
4037	A	58	VAL	HG22	1.266	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4038	B	258	VAL	HG22	1.266	0.02	2
4039	A	58	VAL	HG23	1.266	0.02	2
4040	B	258	VAL	HG23	1.266	0.02	2
4041	A	58	VAL	C	174.417	0.1	1
4042	B	258	VAL	C	174.417	0.1	1
4043	A	58	VAL	CA	60.957	0.1	1
4044	B	258	VAL	CA	60.957	0.1	1
4045	A	58	VAL	CB	33.132	0.1	1
4046	B	258	VAL	CB	33.132	0.1	1
4047	A	58	VAL	CG1	22.778	0.1	1
4048	B	258	VAL	CG1	22.778	0.1	1
4049	A	58	VAL	CG2	23.749	0.1	1
4050	B	258	VAL	CG2	23.749	0.1	1
4051	A	58	VAL	N	125.000	0.1	1
4052	B	258	VAL	N	125.000	0.1	1
4053	A	59	PRO	HA	4.532	0.02	1
4054	B	259	PRO	HA	4.532	0.02	1
4055	A	59	PRO	HB2	1.768	0.02	2
4056	B	259	PRO	HB2	1.768	0.02	2
4057	A	59	PRO	HB3	2.491	0.02	2
4058	B	259	PRO	HB3	2.491	0.02	2
4059	A	59	PRO	HD2	3.792	0.02	2
4060	B	259	PRO	HD2	3.792	0.02	2
4061	A	59	PRO	HD3	4.151	0.02	2
4062	B	259	PRO	HD3	4.151	0.02	2
4063	A	59	PRO	HG2	2.147	0.02	2
4064	B	259	PRO	HG2	2.147	0.02	2
4065	A	59	PRO	HG3	2.044	0.02	2
4066	B	259	PRO	HG3	2.044	0.02	2
4067	A	59	PRO	C	176.707	0.1	1
4068	B	259	PRO	C	176.707	0.1	1
4069	A	59	PRO	CA	63.628	0.1	1
4070	B	259	PRO	CA	63.628	0.1	1
4071	A	59	PRO	CB	33.854	0.1	1
4072	B	259	PRO	CB	33.854	0.1	1
4073	A	59	PRO	CD	51.600	0.1	1
4074	B	259	PRO	CD	51.600	0.1	1
4075	A	59	PRO	CG	27.700	0.1	1
4076	B	259	PRO	CG	27.700	0.1	1
4077	A	60	SER	H	8.419	0.02	1
4078	B	260	SER	H	8.419	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4079	A	60	SER	HA	4.324	0.02	1
4080	B	260	SER	HA	4.324	0.02	1
4081	A	60	SER	HB2	4.158	0.02	2
4082	B	260	SER	HB2	4.158	0.02	2
4083	A	60	SER	HB3	4.017	0.02	2
4084	B	260	SER	HB3	4.017	0.02	2
4085	A	60	SER	C	174.692	0.1	1
4086	B	260	SER	C	174.692	0.1	1
4087	A	60	SER	CA	60.000	0.1	1
4088	B	260	SER	CA	60.000	0.1	1
4089	A	60	SER	CB	63.300	0.1	1
4090	B	260	SER	CB	63.300	0.1	1
4091	A	60	SER	N	114.139	0.1	1
4092	B	260	SER	N	114.139	0.1	1
4093	A	61	ARG	H	6.918	0.02	1
4094	B	261	ARG	H	6.918	0.02	1
4095	A	61	ARG	HA	4.318	0.02	1
4096	B	261	ARG	HA	4.318	0.02	1
4097	A	61	ARG	HB2	1.720	0.02	2
4098	B	261	ARG	HB2	1.720	0.02	2
4099	A	61	ARG	HB3	1.790	0.02	2
4100	B	261	ARG	HB3	1.790	0.02	2
4101	A	61	ARG	HD2	3.182	0.02	2
4102	B	261	ARG	HD2	3.182	0.02	2
4103	A	61	ARG	HD3	3.119	0.02	2
4104	B	261	ARG	HD3	3.119	0.02	2
4105	A	61	ARG	HG2	1.523	0.02	2
4106	B	261	ARG	HG2	1.523	0.02	2
4107	A	61	ARG	HG3	1.307	0.02	2
4108	B	261	ARG	HG3	1.307	0.02	2
4109	A	61	ARG	C	175.364	0.1	1
4110	B	261	ARG	C	175.364	0.1	1
4111	A	61	ARG	CA	56.771	0.1	1
4112	B	261	ARG	CA	56.771	0.1	1
4113	A	61	ARG	CB	29.896	0.1	1
4114	B	261	ARG	CB	29.896	0.1	1
4115	A	61	ARG	CD	42.515	0.1	1
4116	B	261	ARG	CD	42.515	0.1	1
4117	A	61	ARG	CG	27.632	0.1	1
4118	B	261	ARG	CG	27.632	0.1	1
4119	A	61	ARG	N	116.026	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4120	B	261	ARG	N	116.026	0.1	1
4121	A	62	PHE	H	7.725	0.02	1
4122	B	262	PHE	H	7.725	0.02	1
4123	A	62	PHE	HA	5.101	0.02	1
4124	B	262	PHE	HA	5.101	0.02	1
4125	A	62	PHE	HB2	3.216	0.02	2
4126	B	262	PHE	HB2	3.216	0.02	2
4127	A	62	PHE	HB3	2.761	0.02	2
4128	B	262	PHE	HB3	2.761	0.02	2
4129	A	62	PHE	HD1	7.254	0.02	1
4130	B	262	PHE	HD1	7.254	0.02	1
4131	A	62	PHE	HD2	7.254	0.02	1
4132	B	262	PHE	HD2	7.254	0.02	1
4133	A	62	PHE	HE1	7.322	0.02	1
4134	B	262	PHE	HE1	7.322	0.02	1
4135	A	62	PHE	HE2	7.322	0.02	1
4136	B	262	PHE	HE2	7.322	0.02	1
4137	A	62	PHE	HZ	7.505	0.02	1
4138	B	262	PHE	HZ	7.505	0.02	1
4139	A	62	PHE	C	174.212	0.1	1
4140	B	262	PHE	C	174.212	0.1	1
4141	A	62	PHE	CA	56.126	0.1	1
4142	B	262	PHE	CA	56.126	0.1	1
4143	A	62	PHE	CB	39.914	0.1	1
4144	B	262	PHE	CB	39.914	0.1	1
4145	A	62	PHE	CD1	131.788	0.1	1
4146	B	262	PHE	CD1	131.788	0.1	1
4147	A	62	PHE	CE1	131.012	0.1	1
4148	B	262	PHE	CE1	131.012	0.1	1
4149	A	62	PHE	CZ	130.700	0.1	1
4150	B	262	PHE	CZ	130.700	0.1	1
4151	A	62	PHE	N	121.900	0.1	1
4152	B	262	PHE	N	121.900	0.1	1
4153	A	63	SER	H	8.362	0.02	1
4154	B	263	SER	H	8.362	0.02	1
4155	A	63	SER	HA	4.598	0.02	1
4156	B	263	SER	HA	4.598	0.02	1
4157	A	63	SER	HB2	3.800	0.02	2
4158	B	263	SER	HB2	3.800	0.02	2
4159	A	63	SER	HB3	3.800	0.02	2
4160	B	263	SER	HB3	3.800	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4161	A	63	SER	C	171.861	0.1	1
4162	B	263	SER	C	171.861	0.1	1
4163	A	63	SER	CA	58.000	0.1	1
4164	B	263	SER	CA	58.000	0.1	1
4165	A	63	SER	CB	66.309	0.1	1
4166	B	263	SER	CB	66.309	0.1	1
4167	A	63	SER	N	111.581	0.1	1
4168	B	263	SER	N	111.581	0.1	1
4169	A	64	GLY	H	8.759	0.02	1
4170	B	264	GLY	H	8.759	0.02	1
4171	A	64	GLY	HA2	5.379	0.02	2
4172	B	264	GLY	HA2	5.379	0.02	2
4173	A	64	GLY	HA3	3.964	0.02	2
4174	B	264	GLY	HA3	3.964	0.02	2
4175	A	64	GLY	C	172.965	0.1	1
4176	B	264	GLY	C	172.965	0.1	1
4177	A	64	GLY	CA	44.607	0.1	1
4178	B	264	GLY	CA	44.607	0.1	1
4179	A	64	GLY	N	107.681	0.1	1
4180	B	264	GLY	N	107.681	0.1	1
4181	A	65	SER	H	9.112	0.02	1
4182	B	265	SER	H	9.112	0.02	1
4183	A	65	SER	HA	4.893	0.02	1
4184	B	265	SER	HA	4.893	0.02	1
4185	A	65	SER	HB2	3.800	0.02	2
4186	B	265	SER	HB2	3.800	0.02	2
4187	A	65	SER	HB3	3.901	0.02	2
4188	B	265	SER	HB3	3.901	0.02	2
4189	A	65	SER	C	174.356	0.1	1
4190	B	265	SER	C	174.356	0.1	1
4191	A	65	SER	CA	57.327	0.1	1
4192	B	265	SER	CA	57.327	0.1	1
4193	A	65	SER	CB	66.214	0.1	1
4194	B	265	SER	CB	66.214	0.1	1
4195	A	65	SER	N	114.425	0.1	1
4196	B	265	SER	N	114.425	0.1	1
4197	A	66	GLY	H	8.468	0.02	1
4198	B	266	GLY	H	8.468	0.02	1
4199	A	66	GLY	HA2	4.956	0.02	2
4200	B	266	GLY	HA2	4.956	0.02	2
4201	A	66	GLY	HA3	3.832	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4202	B	266	GLY	HA3	3.832	0.02	2
4203	A	66	GLY	C	171.861	0.1	1
4204	B	266	GLY	C	171.861	0.1	1
4205	A	66	GLY	CA	45.200	0.1	1
4206	B	266	GLY	CA	45.200	0.1	1
4207	A	66	GLY	N	111.600	0.1	1
4208	B	266	GLY	N	111.600	0.1	1
4209	A	67	SER	H	7.030	0.02	1
4210	B	267	SER	H	7.030	0.02	1
4211	A	67	SER	HA	4.446	0.02	1
4212	B	267	SER	HA	4.446	0.02	1
4213	A	67	SER	HB2	3.778	0.02	2
4214	B	267	SER	HB2	3.778	0.02	2
4215	A	67	SER	HB3	3.778	0.02	2
4216	B	267	SER	HB3	3.778	0.02	2
4217	A	67	SER	C	174.452	0.1	1
4218	B	267	SER	C	174.452	0.1	1
4219	A	67	SER	CA	58.441	0.1	1
4220	B	267	SER	CA	58.441	0.1	1
4221	A	67	SER	CB	64.914	0.1	1
4222	B	267	SER	CB	64.914	0.1	1
4223	A	67	SER	N	109.300	0.1	1
4224	B	267	SER	N	109.300	0.1	1
4225	A	68	GLY	H	9.097	0.02	1
4226	B	268	GLY	H	9.097	0.02	1
4227	A	68	GLY	HA2	4.258	0.02	2
4228	B	268	GLY	HA2	4.258	0.02	2
4229	A	68	GLY	HA3	4.035	0.02	2
4230	B	268	GLY	HA3	4.035	0.02	2
4231	A	68	GLY	C	172.917	0.1	1
4232	B	268	GLY	C	172.917	0.1	1
4233	A	68	GLY	CA	47.393	0.1	1
4234	B	268	GLY	CA	47.393	0.1	1
4235	A	68	GLY	N	112.566	0.1	1
4236	B	268	GLY	N	112.566	0.1	1
4237	A	69	THR	H	8.228	0.02	1
4238	B	269	THR	H	8.228	0.02	1
4239	A	69	THR	HA	4.824	0.02	1
4240	B	269	THR	HA	4.824	0.02	1
4241	A	69	THR	HB	4.874	0.02	1
4242	B	269	THR	HB	4.874	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4243	A	69	THR	HG21	1.018	0.02	1
4244	B	269	THR	HG21	1.018	0.02	1
4245	A	69	THR	HG22	1.018	0.02	1
4246	B	269	THR	HG22	1.018	0.02	1
4247	A	69	THR	HG23	1.018	0.02	1
4248	B	269	THR	HG23	1.018	0.02	1
4249	A	69	THR	C	174.356	0.1	1
4250	B	269	THR	C	174.356	0.1	1
4251	A	69	THR	CA	61.519	0.1	1
4252	B	269	THR	CA	61.519	0.1	1
4253	A	69	THR	CB	71.129	0.1	1
4254	B	269	THR	CB	71.129	0.1	1
4255	A	69	THR	CG2	21.162	0.1	1
4256	B	269	THR	CG2	21.162	0.1	1
4257	A	69	THR	N	112.926	0.1	1
4258	B	269	THR	N	112.926	0.1	1
4259	A	70	GLU	H	7.062	0.02	1
4260	B	270	GLU	H	7.062	0.02	1
4261	A	70	GLU	HA	5.024	0.02	1
4262	B	270	GLU	HA	5.024	0.02	1
4263	A	70	GLU	HB2	2.005	0.02	2
4264	B	270	GLU	HB2	2.005	0.02	2
4265	A	70	GLU	HB3	1.918	0.02	2
4266	B	270	GLU	HB3	1.918	0.02	2
4267	A	70	GLU	HG2	2.270	0.02	2
4268	B	270	GLU	HG2	2.270	0.02	2
4269	A	70	GLU	HG3	2.184	0.02	2
4270	B	270	GLU	HG3	2.184	0.02	2
4271	A	70	GLU	C	174.068	0.1	1
4272	B	270	GLU	C	174.068	0.1	1
4273	A	70	GLU	CA	56.683	0.1	1
4274	B	270	GLU	CA	56.683	0.1	1
4275	A	70	GLU	CB	32.919	0.1	1
4276	B	270	GLU	CB	32.919	0.1	1
4277	A	70	GLU	CG	36.787	0.1	1
4278	B	270	GLU	CG	36.787	0.1	1
4279	A	70	GLU	N	121.600	0.1	1
4280	B	270	GLU	N	121.600	0.1	1
4281	A	71	PHE	H	8.897	0.02	1
4282	B	271	PHE	H	8.897	0.02	1
4283	A	71	PHE	HA	5.326	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4284	B	271	PHE	HA	5.326	0.02	1
4285	A	71	PHE	HB2	2.883	0.02	2
4286	B	271	PHE	HB2	2.883	0.02	2
4287	A	71	PHE	HB3	3.689	0.02	2
4288	B	271	PHE	HB3	3.689	0.02	2
4289	A	71	PHE	HD1	6.893	0.02	1
4290	B	271	PHE	HD1	6.893	0.02	1
4291	A	71	PHE	HD2	6.893	0.02	1
4292	B	271	PHE	HD2	6.893	0.02	1
4293	A	71	PHE	HE1	7.279	0.02	1
4294	B	271	PHE	HE1	7.279	0.02	1
4295	A	71	PHE	HE2	7.279	0.02	1
4296	B	271	PHE	HE2	7.279	0.02	1
4297	A	71	PHE	C	175.939	0.1	1
4298	B	271	PHE	C	175.939	0.1	1
4299	A	71	PHE	CA	57.357	0.1	1
4300	B	271	PHE	CA	57.357	0.1	1
4301	A	71	PHE	CB	43.500	0.1	1
4302	B	271	PHE	CB	43.500	0.1	1
4303	A	71	PHE	CD1	130.753	0.1	1
4304	B	271	PHE	CD1	130.753	0.1	1
4305	A	71	PHE	CE1	129.977	0.1	1
4306	B	271	PHE	CE1	129.977	0.1	1
4307	A	71	PHE	N	123.395	0.1	1
4308	B	271	PHE	N	123.395	0.1	1
4309	A	72	THR	H	9.046	0.02	1
4310	B	272	THR	H	9.046	0.02	1
4311	A	72	THR	HA	5.462	0.02	1
4312	B	272	THR	HA	5.462	0.02	1
4313	A	72	THR	HB	3.926	0.02	1
4314	B	272	THR	HB	3.926	0.02	1
4315	A	72	THR	HG21	1.128	0.02	1
4316	B	272	THR	HG21	1.128	0.02	1
4317	A	72	THR	HG22	1.128	0.02	1
4318	B	272	THR	HG22	1.128	0.02	1
4319	A	72	THR	HG23	1.128	0.02	1
4320	B	272	THR	HG23	1.128	0.02	1
4321	A	72	THR	C	172.053	0.1	1
4322	B	272	THR	C	172.053	0.1	1
4323	A	72	THR	CA	61.313	0.1	1
4324	B	272	THR	CA	61.313	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4325	A	72	THR	CB	72.614	0.1	1
4326	B	272	THR	CB	72.614	0.1	1
4327	A	72	THR	CG2	21.797	0.1	1
4328	B	272	THR	CG2	21.797	0.1	1
4329	A	72	THR	N	115.454	0.1	1
4330	B	272	THR	N	115.454	0.1	1
4331	A	73	PHE	H	9.050	0.02	1
4332	B	273	PHE	H	9.050	0.02	1
4333	A	73	PHE	HA	4.798	0.02	1
4334	B	273	PHE	HA	4.798	0.02	1
4335	A	73	PHE	HB2	1.240	0.02	2
4336	B	273	PHE	HB2	1.240	0.02	2
4337	A	73	PHE	HB3	0.160	0.02	2
4338	B	273	PHE	HB3	0.160	0.02	2
4339	A	73	PHE	HE1	6.143	0.02	1
4340	B	273	PHE	HE1	6.143	0.02	1
4341	A	73	PHE	HE2	6.143	0.02	1
4342	B	273	PHE	HE2	6.143	0.02	1
4343	A	73	PHE	HZ	6.331	0.02	1
4344	B	273	PHE	HZ	6.331	0.02	1
4345	A	73	PHE	C	173.444	0.1	1
4346	B	273	PHE	C	173.444	0.1	1
4347	A	73	PHE	CA	55.540	0.1	1
4348	B	273	PHE	CA	55.540	0.1	1
4349	A	73	PHE	CB	39.300	0.1	1
4350	B	273	PHE	CB	39.300	0.1	1
4351	A	73	PHE	CE1	131.012	0.1	1
4352	B	273	PHE	CE1	131.012	0.1	1
4353	A	73	PHE	CZ	128.941	0.1	1
4354	B	273	PHE	CZ	128.941	0.1	1
4355	A	73	PHE	N	128.473	0.1	1
4356	B	273	PHE	N	128.473	0.1	1
4357	A	74	THR	H	8.349	0.02	1
4358	B	274	THR	H	8.349	0.02	1
4359	A	74	THR	HA	5.105	0.02	1
4360	B	274	THR	HA	5.105	0.02	1
4361	A	74	THR	HB	3.478	0.02	1
4362	B	274	THR	HB	3.478	0.02	1
4363	A	74	THR	HG21	0.827	0.02	1
4364	B	274	THR	HG21	0.827	0.02	1
4365	A	74	THR	HG22	0.827	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4366	B	274	THR	HG22	0.827	0.02	1
4367	A	74	THR	HG23	0.827	0.02	1
4368	B	274	THR	HG23	0.827	0.02	1
4369	A	74	THR	C	172.923	0.1	1
4370	B	274	THR	C	172.923	0.1	1
4371	A	74	THR	CA	60.400	0.1	1
4372	B	274	THR	CA	60.400	0.1	1
4373	A	74	THR	CB	72.014	0.1	1
4374	B	274	THR	CB	72.014	0.1	1
4375	A	74	THR	CG2	20.837	0.1	1
4376	B	274	THR	CG2	20.837	0.1	1
4377	A	74	THR	N	122.400	0.1	1
4378	B	274	THR	N	122.400	0.1	1
4379	A	75	ILE	H	8.412	0.02	1
4380	B	275	ILE	H	8.412	0.02	1
4381	A	75	ILE	HA	4.286	0.02	1
4382	B	275	ILE	HA	4.286	0.02	1
4383	A	75	ILE	HB	1.446	0.02	1
4384	B	275	ILE	HB	1.446	0.02	1
4385	A	75	ILE	HD11	0.500	0.02	1
4386	B	275	ILE	HD11	0.500	0.02	1
4387	A	75	ILE	HD12	0.500	0.02	1
4388	B	275	ILE	HD12	0.500	0.02	1
4389	A	75	ILE	HD13	0.500	0.02	1
4390	B	275	ILE	HD13	0.500	0.02	1
4391	A	75	ILE	HG12	0.517	0.02	2
4392	B	275	ILE	HG12	0.517	0.02	2
4393	A	75	ILE	HG13	0.975	0.02	2
4394	B	275	ILE	HG13	0.975	0.02	2
4395	A	75	ILE	HG21	0.494	0.02	1
4396	B	275	ILE	HG21	0.494	0.02	1
4397	A	75	ILE	HG22	0.494	0.02	1
4398	B	275	ILE	HG22	0.494	0.02	1
4399	A	75	ILE	HG23	0.494	0.02	1
4400	B	275	ILE	HG23	0.494	0.02	1
4401	A	75	ILE	C	176.707	0.1	1
4402	B	275	ILE	C	176.707	0.1	1
4403	A	75	ILE	CA	60.229	0.1	1
4404	B	275	ILE	CA	60.229	0.1	1
4405	A	75	ILE	CB	39.300	0.1	1
4406	B	275	ILE	CB	39.300	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4407	A	75	ILE	CD1	13.386	0.1	1
4408	B	275	ILE	CD1	13.386	0.1	1
4409	A	75	ILE	CG1	26.337	0.1	1
4410	B	275	ILE	CG1	26.337	0.1	1
4411	A	75	ILE	CG2	17.224	0.1	1
4412	B	275	ILE	CG2	17.224	0.1	1
4413	A	75	ILE	N	123.807	0.1	1
4414	B	275	ILE	N	123.807	0.1	1
4415	A	76	SER	H	9.193	0.02	1
4416	B	276	SER	H	9.193	0.02	1
4417	A	76	SER	HA	3.902	0.02	1
4418	B	276	SER	HA	3.902	0.02	1
4419	A	76	SER	HB2	3.818	0.02	2
4420	B	276	SER	HB2	3.818	0.02	2
4421	A	76	SER	HB3	3.818	0.02	2
4422	B	276	SER	HB3	3.818	0.02	2
4423	A	76	SER	C	174.260	0.1	1
4424	B	276	SER	C	174.260	0.1	1
4425	A	76	SER	CA	60.992	0.1	1
4426	B	276	SER	CA	60.992	0.1	1
4427	A	76	SER	CB	62.919	0.1	1
4428	B	276	SER	CB	62.919	0.1	1
4429	A	76	SER	N	121.707	0.1	1
4430	B	276	SER	N	121.707	0.1	1
4431	A	77	SER	H	6.223	0.02	1
4432	B	277	SER	H	6.223	0.02	1
4433	A	77	SER	HA	3.990	0.02	1
4434	B	277	SER	HA	3.990	0.02	1
4435	A	77	SER	HB2	3.641	0.02	2
4436	B	277	SER	HB2	3.641	0.02	2
4437	A	77	SER	HB3	3.641	0.02	2
4438	B	277	SER	HB3	3.641	0.02	2
4439	A	77	SER	C	174.068	0.1	1
4440	B	277	SER	C	174.068	0.1	1
4441	A	77	SER	CA	56.684	0.1	1
4442	B	277	SER	CA	56.684	0.1	1
4443	A	77	SER	CB	62.600	0.1	1
4444	B	277	SER	CB	62.600	0.1	1
4445	A	77	SER	N	113.400	0.1	1
4446	B	277	SER	N	113.400	0.1	1
4447	A	78	LEU	H	9.001	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4448	B	278	LEU	H	9.001	0.02	1
4449	A	78	LEU	HA	4.000	0.02	1
4450	B	278	LEU	HA	4.000	0.02	1
4451	A	78	LEU	HB2	1.476	0.02	2
4452	B	278	LEU	HB2	1.476	0.02	2
4453	A	78	LEU	HB3	1.882	0.02	2
4454	B	278	LEU	HB3	1.882	0.02	2
4455	A	78	LEU	HD11	0.977	0.02	2
4456	B	278	LEU	HD11	0.977	0.02	2
4457	A	78	LEU	HD12	0.977	0.02	2
4458	B	278	LEU	HD12	0.977	0.02	2
4459	A	78	LEU	HD13	0.977	0.02	2
4460	B	278	LEU	HD13	0.977	0.02	2
4461	A	78	LEU	HD21	0.709	0.02	2
4462	B	278	LEU	HD21	0.709	0.02	2
4463	A	78	LEU	HD22	0.709	0.02	2
4464	B	278	LEU	HD22	0.709	0.02	2
4465	A	78	LEU	HD23	0.709	0.02	2
4466	B	278	LEU	HD23	0.709	0.02	2
4467	A	78	LEU	HG	1.553	0.02	1
4468	B	278	LEU	HG	1.553	0.02	1
4469	A	78	LEU	C	176.515	0.1	1
4470	B	278	LEU	C	176.515	0.1	1
4471	A	78	LEU	CA	57.152	0.1	1
4472	B	278	LEU	CA	57.152	0.1	1
4473	A	78	LEU	CB	42.900	0.1	1
4474	B	278	LEU	CB	42.900	0.1	1
4475	A	78	LEU	CD1	26.900	0.1	1
4476	B	278	LEU	CD1	26.900	0.1	1
4477	A	78	LEU	CD2	26.900	0.1	1
4478	B	278	LEU	CD2	26.900	0.1	1
4479	A	78	LEU	CG	26.700	0.1	1
4480	B	278	LEU	CG	26.700	0.1	1
4481	A	78	LEU	N	127.974	0.1	1
4482	B	278	LEU	N	127.974	0.1	1
4483	A	79	GLN	H	9.099	0.02	1
4484	B	279	GLN	H	9.099	0.02	1
4485	A	79	GLN	HA	4.955	0.02	1
4486	B	279	GLN	HA	4.955	0.02	1
4487	A	79	GLN	HB2	2.522	0.02	2
4488	B	279	GLN	HB2	2.522	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4489	A	79	GLN	HB3	1.599	0.02	2
4490	B	279	GLN	HB3	1.599	0.02	2
4491	A	79	GLN	HE21	6.960	0.02	2
4492	B	279	GLN	HE21	6.960	0.02	2
4493	A	79	GLN	HE22	6.839	0.02	2
4494	B	279	GLN	HE22	6.839	0.02	2
4495	A	79	GLN	HG2	2.545	0.02	2
4496	B	279	GLN	HG2	2.545	0.02	2
4497	A	79	GLN	HG3	2.273	0.02	2
4498	B	279	GLN	HG3	2.273	0.02	2
4499	A	79	GLN	C	174.786	0.1	1
4500	B	279	GLN	C	174.786	0.1	1
4501	A	79	GLN	CA	52.868	0.1	1
4502	B	279	GLN	CA	52.868	0.1	1
4503	A	79	GLN	CB	29.573	0.1	1
4504	B	279	GLN	CB	29.573	0.1	1
4505	A	79	GLN	CG	33.132	0.1	1
4506	B	279	GLN	CG	33.132	0.1	1
4507	A	79	GLN	N	125.700	0.1	1
4508	B	279	GLN	N	125.700	0.1	1
4509	A	79	GLN	NE2	114.104	0.1	1
4510	B	279	GLN	NE2	114.104	0.1	1
4511	A	80	PRO	HA	4.101	0.02	1
4512	B	280	PRO	HA	4.101	0.02	1
4513	A	80	PRO	HB2	2.460	0.02	2
4514	B	280	PRO	HB2	2.460	0.02	2
4515	A	80	PRO	HB3	2.069	0.02	2
4516	B	280	PRO	HB3	2.069	0.02	2
4517	A	80	PRO	HD2	3.968	0.02	2
4518	B	280	PRO	HD2	3.968	0.02	2
4519	A	80	PRO	HD3	3.723	0.02	2
4520	B	280	PRO	HD3	3.723	0.02	2
4521	A	80	PRO	HG2	2.028	0.02	2
4522	B	280	PRO	HG2	2.028	0.02	2
4523	A	80	PRO	HG3	2.357	0.02	2
4524	B	280	PRO	HG3	2.357	0.02	2
4525	A	80	PRO	C	178.722	0.1	1
4526	B	280	PRO	C	178.722	0.1	1
4527	A	80	PRO	CA	66.582	0.1	1
4528	B	280	PRO	CA	66.582	0.1	1
4529	A	80	PRO	CB	32.101	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4530	B	280	PRO	CB	32.101	0.1	1
4531	A	80	PRO	CD	50.280	0.1	1
4532	B	280	PRO	CD	50.280	0.1	1
4533	A	80	PRO	CG	28.279	0.1	1
4534	B	280	PRO	CG	28.279	0.1	1
4535	A	81	GLU	H	9.548	0.02	1
4536	B	281	GLU	H	9.548	0.02	1
4537	A	81	GLU	HA	4.412	0.02	1
4538	B	281	GLU	HA	4.412	0.02	1
4539	A	81	GLU	HB2	2.262	0.02	2
4540	B	281	GLU	HB2	2.262	0.02	2
4541	A	81	GLU	HB3	2.170	0.02	2
4542	B	281	GLU	HB3	2.170	0.02	2
4543	A	81	GLU	HG2	2.353	0.02	2
4544	B	281	GLU	HG2	2.353	0.02	2
4545	A	81	GLU	HG3	2.232	0.02	2
4546	B	281	GLU	HG3	2.232	0.02	2
4547	A	81	GLU	C	176.313	0.1	1
4548	B	281	GLU	C	176.313	0.1	1
4549	A	81	GLU	CA	57.915	0.1	1
4550	B	281	GLU	CA	57.915	0.1	1
4551	A	81	GLU	CB	28.451	0.1	1
4552	B	281	GLU	CB	28.451	0.1	1
4553	A	81	GLU	CG	35.771	0.1	1
4554	B	281	GLU	CG	35.771	0.1	1
4555	A	81	GLU	N	114.700	0.1	1
4556	B	281	GLU	N	114.700	0.1	1
4557	A	82	ASP	H	8.352	0.02	1
4558	B	282	ASP	H	8.352	0.02	1
4559	A	82	ASP	HA	4.697	0.02	1
4560	B	282	ASP	HA	4.697	0.02	1
4561	A	82	ASP	HB2	3.148	0.02	2
4562	B	282	ASP	HB2	3.148	0.02	2
4563	A	82	ASP	HB3	3.035	0.02	2
4564	B	282	ASP	HB3	3.035	0.02	2
4565	A	82	ASP	C	177.475	0.1	1
4566	B	282	ASP	C	177.475	0.1	1
4567	A	82	ASP	CA	54.660	0.1	1
4568	B	282	ASP	CA	54.660	0.1	1
4569	A	82	ASP	CB	40.900	0.1	1
4570	B	282	ASP	CB	40.900	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4571	A	82	ASP	N	120.836	0.1	1
4572	B	282	ASP	N	120.836	0.1	1
4573	A	83	LEU	H	7.191	0.02	1
4574	B	283	LEU	H	7.191	0.02	1
4575	A	83	LEU	HA	4.115	0.02	1
4576	B	283	LEU	HA	4.115	0.02	1
4577	A	83	LEU	HB2	1.958	0.02	2
4578	B	283	LEU	HB2	1.958	0.02	2
4579	A	83	LEU	HB3	1.860	0.02	2
4580	B	283	LEU	HB3	1.860	0.02	2
4581	A	83	LEU	HD11	1.186	0.02	2
4582	B	283	LEU	HD11	1.186	0.02	2
4583	A	83	LEU	HD12	1.186	0.02	2
4584	B	283	LEU	HD12	1.186	0.02	2
4585	A	83	LEU	HD13	1.186	0.02	2
4586	B	283	LEU	HD13	1.186	0.02	2
4587	A	83	LEU	HD21	0.974	0.02	2
4588	B	283	LEU	HD21	0.974	0.02	2
4589	A	83	LEU	HD22	0.974	0.02	2
4590	B	283	LEU	HD22	0.974	0.02	2
4591	A	83	LEU	HD23	0.974	0.02	2
4592	B	283	LEU	HD23	0.974	0.02	2
4593	A	83	LEU	HG	1.952	0.02	1
4594	B	283	LEU	HG	1.952	0.02	1
4595	A	83	LEU	C	175.172	0.1	1
4596	B	283	LEU	C	175.172	0.1	1
4597	A	83	LEU	CA	58.032	0.1	1
4598	B	283	LEU	CA	58.032	0.1	1
4599	A	83	LEU	CB	41.600	0.1	1
4600	B	283	LEU	CB	41.600	0.1	1
4601	A	83	LEU	CD1	26.014	0.1	1
4602	B	283	LEU	CD1	26.014	0.1	1
4603	A	83	LEU	CD2	24.592	0.1	1
4604	B	283	LEU	CD2	24.592	0.1	1
4605	A	83	LEU	CG	27.300	0.1	1
4606	B	283	LEU	CG	27.300	0.1	1
4607	A	83	LEU	N	122.669	0.1	1
4608	B	283	LEU	N	122.669	0.1	1
4609	A	84	ALA	H	7.822	0.02	1
4610	B	284	ALA	H	7.822	0.02	1
4611	A	84	ALA	HA	4.420	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4612	B	284	ALA	HA	4.420	0.02	1
4613	A	84	ALA	HB1	1.043	0.02	1
4614	B	284	ALA	HB1	1.043	0.02	1
4615	A	84	ALA	HB2	1.043	0.02	1
4616	B	284	ALA	HB2	1.043	0.02	1
4617	A	84	ALA	HB3	1.043	0.02	1
4618	B	284	ALA	HB3	1.043	0.02	1
4619	A	84	ALA	C	175.364	0.1	1
4620	B	284	ALA	C	175.364	0.1	1
4621	A	84	ALA	CA	52.300	0.1	1
4622	B	284	ALA	CA	52.300	0.1	1
4623	A	84	ALA	CB	20.886	0.1	1
4624	B	284	ALA	CB	20.886	0.1	1
4625	A	84	ALA	N	126.545	0.1	1
4626	B	284	ALA	N	126.545	0.1	1
4627	A	85	THR	H	7.832	0.02	1
4628	B	285	THR	H	7.832	0.02	1
4629	A	85	THR	HA	5.294	0.02	1
4630	B	285	THR	HA	5.294	0.02	1
4631	A	85	THR	HB	3.835	0.02	1
4632	B	285	THR	HB	3.835	0.02	1
4633	A	85	THR	HG21	0.621	0.02	1
4634	B	285	THR	HG21	0.621	0.02	1
4635	A	85	THR	HG22	0.621	0.02	1
4636	B	285	THR	HG22	0.621	0.02	1
4637	A	85	THR	HG23	0.621	0.02	1
4638	B	285	THR	HG23	0.621	0.02	1
4639	A	85	THR	C	172.960	0.1	1
4640	B	285	THR	C	172.960	0.1	1
4641	A	85	THR	CA	62.163	0.1	1
4642	B	285	THR	CA	62.163	0.1	1
4643	A	85	THR	CB	69.414	0.1	1
4644	B	285	THR	CB	69.414	0.1	1
4645	A	85	THR	CG2	20.781	0.1	1
4646	B	285	THR	CG2	20.781	0.1	1
4647	A	85	THR	N	114.400	0.1	1
4648	B	285	THR	N	114.400	0.1	1
4649	A	86	TYR	H	8.623	0.02	1
4650	B	286	TYR	H	8.623	0.02	1
4651	A	86	TYR	HA	5.313	0.02	1
4652	B	286	TYR	HA	5.313	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4653	A	86	TYR	HB2	2.554	0.02	2
4654	B	286	TYR	HB2	2.554	0.02	2
4655	A	86	TYR	HB3	2.611	0.02	2
4656	B	286	TYR	HB3	2.611	0.02	2
4657	A	86	TYR	HD1	6.824	0.02	1
4658	B	286	TYR	HD1	6.824	0.02	1
4659	A	86	TYR	HD2	6.824	0.02	1
4660	B	286	TYR	HD2	6.824	0.02	1
4661	A	86	TYR	HE1	6.774	0.02	1
4662	B	286	TYR	HE1	6.774	0.02	1
4663	A	86	TYR	HE2	6.774	0.02	1
4664	B	286	TYR	HE2	6.774	0.02	1
4665	A	86	TYR	HH	10.619	0.02	1
4666	B	286	TYR	HH	10.619	0.02	1
4667	A	86	TYR	C	176.707	0.1	1
4668	B	286	TYR	C	176.707	0.1	1
4669	A	86	TYR	CA	56.500	0.1	1
4670	B	286	TYR	CA	56.500	0.1	1
4671	A	86	TYR	CB	41.600	0.1	1
4672	B	286	TYR	CB	41.600	0.1	1
4673	A	86	TYR	CD1	133.600	0.1	1
4674	B	286	TYR	CD1	133.600	0.1	1
4675	A	86	TYR	CE1	117.553	0.1	1
4676	B	286	TYR	CE1	117.553	0.1	1
4677	A	86	TYR	N	124.630	0.1	1
4678	B	286	TYR	N	124.630	0.1	1
4679	A	87	TYR	H	9.036	0.02	1
4680	B	287	TYR	H	9.036	0.02	1
4681	A	87	TYR	HA	5.532	0.02	1
4682	B	287	TYR	HA	5.532	0.02	1
4683	A	87	TYR	HB2	3.435	0.02	2
4684	B	287	TYR	HB2	3.435	0.02	2
4685	A	87	TYR	HB3	2.625	0.02	2
4686	B	287	TYR	HB3	2.625	0.02	2
4687	A	87	TYR	HD1	7.110	0.02	1
4688	B	287	TYR	HD1	7.110	0.02	1
4689	A	87	TYR	HD2	7.110	0.02	1
4690	B	287	TYR	HD2	7.110	0.02	1
4691	A	87	TYR	HE1	6.740	0.02	1
4692	B	287	TYR	HE1	6.740	0.02	1
4693	A	87	TYR	HE2	6.740	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4694	B	287	TYR	HE2	6.740	0.02	1
4695	A	87	TYR	C	174.836	0.1	1
4696	B	287	TYR	C	174.836	0.1	1
4697	A	87	TYR	CA	58.100	0.1	1
4698	B	287	TYR	CA	58.100	0.1	1
4699	A	87	TYR	CB	45.800	0.1	1
4700	B	287	TYR	CB	45.800	0.1	1
4701	A	87	TYR	CD1	132.047	0.1	1
4702	B	287	TYR	CD1	132.047	0.1	1
4703	A	87	TYR	CE1	118.847	0.1	1
4704	B	287	TYR	CE1	118.847	0.1	1
4705	A	87	TYR	N	119.084	0.1	1
4706	B	287	TYR	N	119.084	0.1	1
4707	A	88	CYS	H	7.482	0.02	1
4708	B	288	CYS	H	7.482	0.02	1
4709	A	88	CYS	HA	5.458	0.02	1
4710	B	288	CYS	HA	5.458	0.02	1
4711	A	88	CYS	HB2	2.353	0.02	2
4712	B	288	CYS	HB2	2.353	0.02	2
4713	A	88	CYS	HB3	1.169	0.02	2
4714	B	288	CYS	HB3	1.169	0.02	2
4715	A	88	CYS	C	172.773	0.1	1
4716	B	288	CYS	C	172.773	0.1	1
4717	A	88	CYS	CA	52.375	0.1	1
4718	B	288	CYS	CA	52.375	0.1	1
4719	A	88	CYS	CB	45.750	0.1	1
4720	B	288	CYS	CB	45.750	0.1	1
4721	A	88	CYS	N	114.893	0.1	1
4722	B	288	CYS	N	114.893	0.1	1
4723	A	89	GLN	H	8.761	0.02	1
4724	B	289	GLN	H	8.761	0.02	1
4725	A	89	GLN	HA	4.909	0.02	1
4726	B	289	GLN	HA	4.909	0.02	1
4727	A	89	GLN	HB2	1.186	0.02	2
4728	B	289	GLN	HB2	1.186	0.02	2
4729	A	89	GLN	HB3	1.768	0.02	2
4730	B	289	GLN	HB3	1.768	0.02	2
4731	A	89	GLN	HE21	6.025	0.02	2
4732	B	289	GLN	HE21	6.025	0.02	2
4733	A	89	GLN	HE22	6.025	0.02	2
4734	B	289	GLN	HE22	6.025	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4735	A	89	GLN	HG2	0.882	0.02	2
4736	B	289	GLN	HG2	0.882	0.02	2
4737	A	89	GLN	HG3	1.663	0.02	2
4738	B	289	GLN	HG3	1.663	0.02	2
4739	A	89	GLN	C	174.548	0.1	1
4740	B	289	GLN	C	174.548	0.1	1
4741	A	89	GLN	CA	54.514	0.1	1
4742	B	289	GLN	CA	54.514	0.1	1
4743	A	89	GLN	CB	32.808	0.1	1
4744	B	289	GLN	CB	32.808	0.1	1
4745	A	89	GLN	CG	33.779	0.1	1
4746	B	289	GLN	CG	33.779	0.1	1
4747	A	89	GLN	N	121.900	0.1	1
4748	B	289	GLN	N	121.900	0.1	1
4749	A	89	GLN	NE2	111.908	0.1	1
4750	B	289	GLN	NE2	111.908	0.1	1
4751	A	90	GLN	H	8.190	0.02	1
4752	B	290	GLN	H	8.190	0.02	1
4753	A	90	GLN	HA	5.325	0.02	1
4754	B	290	GLN	HA	5.325	0.02	1
4755	A	90	GLN	HB2	2.580	0.02	2
4756	B	290	GLN	HB2	2.580	0.02	2
4757	A	90	GLN	HB3	1.960	0.02	2
4758	B	290	GLN	HB3	1.960	0.02	2
4759	A	90	GLN	HE21	7.355	0.02	2
4760	B	290	GLN	HE21	7.355	0.02	2
4761	A	90	GLN	HE22	7.528	0.02	2
4762	B	290	GLN	HE22	7.528	0.02	2
4763	A	90	GLN	HG2	2.251	0.02	2
4764	B	290	GLN	HG2	2.251	0.02	2
4765	A	90	GLN	HG3	2.914	0.02	2
4766	B	290	GLN	HG3	2.914	0.02	2
4767	A	90	GLN	C	175.172	0.1	1
4768	B	290	GLN	C	175.172	0.1	1
4769	A	90	GLN	CA	53.137	0.1	1
4770	B	290	GLN	CA	53.137	0.1	1
4771	A	90	GLN	CB	28.900	0.1	1
4772	B	290	GLN	CB	28.900	0.1	1
4773	A	90	GLN	CG	31.514	0.1	1
4774	B	290	GLN	CG	31.514	0.1	1
4775	A	90	GLN	N	125.000	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4776	B	290	GLN	N	125.000	0.1	1
4777	A	90	GLN	NE2	110.444	0.1	1
4778	B	290	GLN	NE2	110.444	0.1	1
4779	A	91	TYR	H	7.860	0.02	1
4780	B	291	TYR	H	7.860	0.02	1
4781	A	91	TYR	HA	4.243	0.02	1
4782	B	291	TYR	HA	4.243	0.02	1
4783	A	91	TYR	HB2	2.520	0.02	2
4784	B	291	TYR	HB2	2.520	0.02	2
4785	A	91	TYR	HB3	1.426	0.02	2
4786	B	291	TYR	HB3	1.426	0.02	2
4787	A	91	TYR	HD1	6.748	0.02	1
4788	B	291	TYR	HD1	6.748	0.02	1
4789	A	91	TYR	HD2	6.748	0.02	1
4790	B	291	TYR	HD2	6.748	0.02	1
4791	A	91	TYR	HE1	6.657	0.02	1
4792	B	291	TYR	HE1	6.657	0.02	1
4793	A	91	TYR	HE2	6.657	0.02	1
4794	B	291	TYR	HE2	6.657	0.02	1
4795	A	91	TYR	C	174.212	0.1	1
4796	B	291	TYR	C	174.212	0.1	1
4797	A	91	TYR	CA	55.200	0.1	1
4798	B	291	TYR	CA	55.200	0.1	1
4799	A	91	TYR	CB	36.035	0.1	1
4800	B	291	TYR	CB	36.035	0.1	1
4801	A	91	TYR	CD1	134.894	0.1	1
4802	B	291	TYR	CD1	134.894	0.1	1
4803	A	91	TYR	CE1	118.070	0.1	1
4804	B	291	TYR	CE1	118.070	0.1	1
4805	A	91	TYR	N	118.082	0.1	1
4806	B	291	TYR	N	118.082	0.1	1
4807	A	92	ASP	H	8.683	0.02	1
4808	B	292	ASP	H	8.683	0.02	1
4809	A	92	ASP	HA	4.196	0.02	1
4810	B	292	ASP	HA	4.196	0.02	1
4811	A	92	ASP	HB2	2.662	0.02	2
4812	B	292	ASP	HB2	2.662	0.02	2
4813	A	92	ASP	HB3	2.954	0.02	2
4814	B	292	ASP	HB3	2.954	0.02	2
4815	A	92	ASP	C	176.803	0.1	1
4816	B	292	ASP	C	176.803	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4817	A	92	ASP	CA	56.800	0.1	1
4818	B	292	ASP	CA	56.800	0.1	1
4819	A	92	ASP	CB	43.500	0.1	1
4820	B	292	ASP	CB	43.500	0.1	1
4821	A	92	ASP	N	122.100	0.1	1
4822	B	292	ASP	N	122.100	0.1	1
4823	A	93	ASN	H	8.226	0.02	1
4824	B	293	ASN	H	8.226	0.02	1
4825	A	93	ASN	HA	4.910	0.02	1
4826	B	293	ASN	HA	4.910	0.02	1
4827	A	93	ASN	HB2	2.563	0.02	2
4828	B	293	ASN	HB2	2.563	0.02	2
4829	A	93	ASN	HB3	2.657	0.02	2
4830	B	293	ASN	HB3	2.657	0.02	2
4831	A	93	ASN	HD21	7.649	0.02	2
4832	B	293	ASN	HD21	7.649	0.02	2
4833	A	93	ASN	HD22	6.656	0.02	2
4834	B	293	ASN	HD22	6.656	0.02	2
4835	A	93	ASN	C	173.540	0.1	1
4836	B	293	ASN	C	173.540	0.1	1
4837	A	93	ASN	CA	52.405	0.1	1
4838	B	293	ASN	CA	52.405	0.1	1
4839	A	93	ASN	CB	43.500	0.1	1
4840	B	293	ASN	CB	43.500	0.1	1
4841	A	93	ASN	N	113.400	0.1	1
4842	B	293	ASN	N	113.400	0.1	1
4843	A	93	ASN	ND2	113.657	0.1	1
4844	B	293	ASN	ND2	113.657	0.1	1
4845	A	94	LEU	H	8.269	0.02	1
4846	B	294	LEU	H	8.269	0.02	1
4847	A	94	LEU	HA	3.678	0.02	1
4848	B	294	LEU	HA	3.678	0.02	1
4849	A	94	LEU	HB2	1.280	0.02	2
4850	B	294	LEU	HB2	1.280	0.02	2
4851	A	94	LEU	HB3	0.340	0.02	2
4852	B	294	LEU	HB3	0.340	0.02	2
4853	A	94	LEU	HD11	0.576	0.02	2
4854	B	294	LEU	HD11	0.576	0.02	2
4855	A	94	LEU	HD12	0.576	0.02	2
4856	B	294	LEU	HD12	0.576	0.02	2
4857	A	94	LEU	HD13	0.576	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4858	B	294	LEU	HD13	0.576	0.02	2
4859	A	94	LEU	HD21	-0.459	0.02	2
4860	B	294	LEU	HD21	-0.459	0.02	2
4861	A	94	LEU	HD22	-0.459	0.02	2
4862	B	294	LEU	HD22	-0.459	0.02	2
4863	A	94	LEU	HD23	-0.459	0.02	2
4864	B	294	LEU	HD23	-0.459	0.02	2
4865	A	94	LEU	HG	1.045	0.02	1
4866	B	294	LEU	HG	1.045	0.02	1
4867	A	94	LEU	C	175.320	0.1	1
4868	B	294	LEU	C	175.320	0.1	1
4869	A	94	LEU	CA	53.192	0.1	1
4870	B	294	LEU	CA	53.192	0.1	1
4871	A	94	LEU	CB	42.191	0.1	1
4872	B	294	LEU	CB	42.191	0.1	1
4873	A	94	LEU	CD1	25.600	0.1	1
4874	B	294	LEU	CD1	25.600	0.1	1
4875	A	94	LEU	CD2	22.778	0.1	1
4876	B	294	LEU	CD2	22.778	0.1	1
4877	A	94	LEU	CG	27.308	0.1	1
4878	B	294	LEU	CG	27.308	0.1	1
4879	A	94	LEU	N	123.400	0.1	1
4880	B	294	LEU	N	123.400	0.1	1
4881	A	95	PRO	HA	3.449	0.02	1
4882	B	295	PRO	HA	3.449	0.02	1
4883	A	95	PRO	HB2	2.029	0.02	2
4884	B	295	PRO	HB2	2.029	0.02	2
4885	A	95	PRO	HB3	2.029	0.02	2
4886	B	295	PRO	HB3	2.029	0.02	2
4887	A	95	PRO	HD2	3.215	0.02	2
4888	B	295	PRO	HD2	3.215	0.02	2
4889	A	95	PRO	HD3	3.773	0.02	2
4890	B	295	PRO	HD3	3.773	0.02	2
4891	A	95	PRO	HG2	2.032	0.02	2
4892	B	295	PRO	HG2	2.032	0.02	2
4893	A	95	PRO	HG3	2.032	0.02	2
4894	B	295	PRO	HG3	2.032	0.02	2
4895	A	95	PRO	CA	61.927	0.1	1
4896	B	295	PRO	CA	61.927	0.1	1
4897	A	95	PRO	CB	34.750	0.1	1
4898	B	295	PRO	CB	34.750	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4899	A	95	PRO	CD	50.603	0.1	1
4900	B	295	PRO	CD	50.603	0.1	1
4901	A	95	PRO	CG	24.720	0.1	1
4902	B	295	PRO	CG	24.720	0.1	1
4903	A	96	TYR	H	5.290	0.02	1
4904	B	296	TYR	H	5.290	0.02	1
4905	A	96	TYR	HA	5.074	0.02	1
4906	B	296	TYR	HA	5.074	0.02	1
4907	A	96	TYR	HB2	2.754	0.02	2
4908	B	296	TYR	HB2	2.754	0.02	2
4909	A	96	TYR	HB3	3.288	0.02	2
4910	B	296	TYR	HB3	3.288	0.02	2
4911	A	96	TYR	HD1	6.648	0.02	1
4912	B	296	TYR	HD1	6.648	0.02	1
4913	A	96	TYR	HD2	6.648	0.02	1
4914	B	296	TYR	HD2	6.648	0.02	1
4915	A	96	TYR	HE1	6.020	0.02	1
4916	B	296	TYR	HE1	6.020	0.02	1
4917	A	96	TYR	HE2	6.020	0.02	1
4918	B	296	TYR	HE2	6.020	0.02	1
4919	A	96	TYR	C	175.795	0.1	1
4920	B	296	TYR	C	175.795	0.1	1
4921	A	96	TYR	CA	55.457	0.1	1
4922	B	296	TYR	CA	55.457	0.1	1
4923	A	96	TYR	CB	36.700	0.1	1
4924	B	296	TYR	CB	36.700	0.1	1
4925	A	96	TYR	CD1	131.271	0.1	1
4926	B	296	TYR	CD1	131.271	0.1	1
4927	A	96	TYR	CE1	118.847	0.1	1
4928	B	296	TYR	CE1	118.847	0.1	1
4929	A	96	TYR	N	122.184	0.1	1
4930	B	296	TYR	N	122.184	0.1	1
4931	A	97	THR	H	7.254	0.02	1
4932	B	297	THR	H	7.254	0.02	1
4933	A	97	THR	HA	4.898	0.02	1
4934	B	297	THR	HA	4.898	0.02	1
4935	A	97	THR	HB	4.626	0.02	1
4936	B	297	THR	HB	4.626	0.02	1
4937	A	97	THR	HG21	1.497	0.02	1
4938	B	297	THR	HG21	1.497	0.02	1
4939	A	97	THR	HG22	1.497	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4940	B	297	THR	HG22	1.497	0.02	1
4941	A	97	THR	HG23	1.497	0.02	1
4942	B	297	THR	HG23	1.497	0.02	1
4943	A	97	THR	C	173.205	0.1	1
4944	B	297	THR	C	173.205	0.1	1
4945	A	97	THR	CA	60.113	0.1	1
4946	B	297	THR	CA	60.113	0.1	1
4947	A	97	THR	CB	72.314	0.1	1
4948	B	297	THR	CB	72.314	0.1	1
4949	A	97	THR	CG2	24.211	0.1	1
4950	B	297	THR	CG2	24.211	0.1	1
4951	A	97	THR	N	111.900	0.1	1
4952	B	297	THR	N	111.900	0.1	1
4953	A	98	PHE	H	8.779	0.02	1
4954	B	298	PHE	H	8.779	0.02	1
4955	A	98	PHE	HA	5.384	0.02	1
4956	B	298	PHE	HA	5.384	0.02	1
4957	A	98	PHE	HB2	2.943	0.02	2
4958	B	298	PHE	HB2	2.943	0.02	2
4959	A	98	PHE	HB3	3.709	0.02	2
4960	B	298	PHE	HB3	3.709	0.02	2
4961	A	98	PHE	HD1	7.109	0.02	1
4962	B	298	PHE	HD1	7.109	0.02	1
4963	A	98	PHE	HD2	7.109	0.02	1
4964	B	298	PHE	HD2	7.109	0.02	1
4965	A	98	PHE	HE1	6.628	0.02	1
4966	B	298	PHE	HE1	6.628	0.02	1
4967	A	98	PHE	HE2	6.628	0.02	1
4968	B	298	PHE	HE2	6.628	0.02	1
4969	A	98	PHE	HZ	6.235	0.02	1
4970	B	298	PHE	HZ	6.235	0.02	1
4971	A	98	PHE	C	179.682	0.1	1
4972	B	298	PHE	C	179.682	0.1	1
4973	A	98	PHE	CA	57.240	0.1	1
4974	B	298	PHE	CA	57.240	0.1	1
4975	A	98	PHE	CB	43.559	0.1	1
4976	B	298	PHE	CB	43.559	0.1	1
4977	A	98	PHE	CD1	132.047	0.1	1
4978	B	298	PHE	CD1	132.047	0.1	1
4979	A	98	PHE	CE1	131.012	0.1	1
4980	B	298	PHE	CE1	131.012	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4981	A	98	PHE	CZ	128.682	0.1	1
4982	B	298	PHE	CZ	128.682	0.1	1
4983	A	98	PHE	N	120.867	0.1	1
4984	B	298	PHE	N	120.867	0.1	1
4985	A	99	GLY	H	8.922	0.02	1
4986	B	299	GLY	H	8.922	0.02	1
4987	A	99	GLY	HA2	4.395	0.02	2
4988	B	299	GLY	HA2	4.395	0.02	2
4989	A	99	GLY	HA3	4.395	0.02	2
4990	B	299	GLY	HA3	4.395	0.02	2
4991	A	99	GLY	C	173.396	0.1	1
4992	B	299	GLY	C	173.396	0.1	1
4993	A	99	GLY	CA	45.135	0.1	1
4994	B	299	GLY	CA	45.135	0.1	1
4995	A	99	GLY	N	107.500	0.1	1
4996	B	299	GLY	N	107.500	0.1	1
4997	A	100	GLN	H	8.474	0.02	1
4998	B	300	GLN	H	8.474	0.02	1
4999	A	100	GLN	HA	4.454	0.02	1
5000	B	300	GLN	HA	4.454	0.02	1
5001	A	100	GLN	HB2	2.495	0.02	2
5002	B	300	GLN	HB2	2.495	0.02	2
5003	A	100	GLN	HB3	2.606	0.02	2
5004	B	300	GLN	HB3	2.606	0.02	2
5005	A	100	GLN	HE21	7.825	0.02	2
5006	B	300	GLN	HE21	7.825	0.02	2
5007	A	100	GLN	HE22	7.381	0.02	2
5008	B	300	GLN	HE22	7.381	0.02	2
5009	A	100	GLN	HG2	2.869	0.02	2
5010	B	300	GLN	HG2	2.869	0.02	2
5011	A	100	GLN	HG3	2.869	0.02	2
5012	B	300	GLN	HG3	2.869	0.02	2
5013	A	100	GLN	C	177.283	0.1	1
5014	B	300	GLN	C	177.283	0.1	1
5015	A	100	GLN	CA	58.852	0.1	1
5016	B	300	GLN	CA	58.852	0.1	1
5017	A	100	GLN	CB	28.300	0.1	1
5018	B	300	GLN	CB	28.300	0.1	1
5019	A	100	GLN	CG	34.119	0.1	1
5020	B	300	GLN	CG	34.119	0.1	1
5021	A	100	GLN	N	113.400	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
5022	B	300	GLN	N	113.400	0.1	1
5023	A	100	GLN	NE2	112.973	0.1	1
5024	B	300	GLN	NE2	112.973	0.1	1
5025	A	101	GLY	H	7.088	0.02	1
5026	B	301	GLY	H	7.088	0.02	1
5027	A	101	GLY	HA2	3.697	0.02	2
5028	B	301	GLY	HA2	3.697	0.02	2
5029	A	101	GLY	HA3	4.004	0.02	2
5030	B	301	GLY	HA3	4.004	0.02	2
5031	A	101	GLY	C	172.677	0.1	1
5032	B	301	GLY	C	172.677	0.1	1
5033	A	101	GLY	CA	45.832	0.1	1
5034	B	301	GLY	CA	45.832	0.1	1
5035	A	101	GLY	N	106.701	0.1	1
5036	B	301	GLY	N	106.701	0.1	1
5037	A	102	THR	H	7.986	0.02	1
5038	B	302	THR	H	7.986	0.02	1
5039	A	102	THR	HA	4.780	0.02	1
5040	B	302	THR	HA	4.780	0.02	1
5041	A	102	THR	HB	3.735	0.02	1
5042	B	302	THR	HB	3.735	0.02	1
5043	A	102	THR	HG21	1.032	0.02	1
5044	B	302	THR	HG21	1.032	0.02	1
5045	A	102	THR	HG22	1.032	0.02	1
5046	B	302	THR	HG22	1.032	0.02	1
5047	A	102	THR	HG23	1.032	0.02	1
5048	B	302	THR	HG23	1.032	0.02	1
5049	A	102	THR	C	174.051	0.1	1
5050	B	302	THR	C	174.051	0.1	1
5051	A	102	THR	CA	61.636	0.1	1
5052	B	302	THR	CA	61.636	0.1	1
5053	A	102	THR	CB	72.658	0.1	1
5054	B	302	THR	CB	72.658	0.1	1
5055	A	102	THR	CG2	21.543	0.1	1
5056	B	302	THR	CG2	21.543	0.1	1
5057	A	102	THR	N	116.700	0.1	1
5058	B	302	THR	N	116.700	0.1	1
5059	A	103	LYS	H	8.310	0.02	1
5060	B	303	LYS	H	8.310	0.02	1
5061	A	103	LYS	HA	4.642	0.02	1
5062	B	303	LYS	HA	4.642	0.02	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
5063	A	103	LYS	HB2	1.813	0.02	2
5064	B	303	LYS	HB2	1.813	0.02	2
5065	A	103	LYS	HB3	1.985	0.02	2
5066	B	303	LYS	HB3	1.985	0.02	2
5067	A	103	LYS	HD2	1.741	0.02	2
5068	B	303	LYS	HD2	1.741	0.02	2
5069	A	103	LYS	HD3	1.649	0.02	2
5070	B	303	LYS	HD3	1.649	0.02	2
5071	A	103	LYS	HE2	3.044	0.02	2
5072	B	303	LYS	HE2	3.044	0.02	2
5073	A	103	LYS	HE3	2.974	0.02	2
5074	B	303	LYS	HE3	2.974	0.02	2
5075	A	103	LYS	HG2	1.472	0.02	2
5076	B	303	LYS	HG2	1.472	0.02	2
5077	A	103	LYS	HG3	1.375	0.02	2
5078	B	303	LYS	HG3	1.375	0.02	2
5079	A	103	LYS	C	174.172	0.1	1
5080	B	303	LYS	C	174.172	0.1	1
5081	A	103	LYS	CA	56.800	0.1	1
5082	B	303	LYS	CA	56.800	0.1	1
5083	A	103	LYS	CB	33.500	0.1	1
5084	B	303	LYS	CB	33.500	0.1	1
5085	A	103	LYS	CD	29.800	0.1	1
5086	B	303	LYS	CD	29.800	0.1	1
5087	A	103	LYS	CE	42.200	0.1	1
5088	B	303	LYS	CE	42.200	0.1	1
5089	A	103	LYS	CG	25.227	0.1	1
5090	B	303	LYS	CG	25.227	0.1	1
5091	A	103	LYS	N	129.800	0.1	1
5092	B	303	LYS	N	129.800	0.1	1
5093	A	104	LEU	H	8.497	0.02	1
5094	B	304	LEU	H	8.497	0.02	1
5095	A	104	LEU	HA	5.276	0.02	1
5096	B	304	LEU	HA	5.276	0.02	1
5097	A	104	LEU	HB2	1.704	0.02	2
5098	B	304	LEU	HB2	1.704	0.02	2
5099	A	104	LEU	HB3	2.230	0.02	2
5100	B	304	LEU	HB3	2.230	0.02	2
5101	A	104	LEU	HD11	0.933	0.02	2
5102	B	304	LEU	HD11	0.933	0.02	2
5103	A	104	LEU	HD12	0.933	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
5104	B	304	LEU	HD12	0.933	0.02	2
5105	A	104	LEU	HD13	0.933	0.02	2
5106	B	304	LEU	HD13	0.933	0.02	2
5107	A	104	LEU	HD21	0.949	0.02	2
5108	B	304	LEU	HD21	0.949	0.02	2
5109	A	104	LEU	HD22	0.949	0.02	2
5110	B	304	LEU	HD22	0.949	0.02	2
5111	A	104	LEU	HD23	0.949	0.02	2
5112	B	304	LEU	HD23	0.949	0.02	2
5113	A	104	LEU	HG	1.801	0.02	1
5114	B	304	LEU	HG	1.801	0.02	1
5115	A	104	LEU	C	175.316	0.1	1
5116	B	304	LEU	C	175.316	0.1	1
5117	A	104	LEU	CA	54.500	0.1	1
5118	B	304	LEU	CA	54.500	0.1	1
5119	A	104	LEU	CB	44.800	0.1	1
5120	B	304	LEU	CB	44.800	0.1	1
5121	A	104	LEU	CD1	26.400	0.1	1
5122	B	304	LEU	CD1	26.400	0.1	1
5123	A	104	LEU	CD2	26.400	0.1	1
5124	B	304	LEU	CD2	26.400	0.1	1
5125	A	104	LEU	CG	28.279	0.1	1
5126	B	304	LEU	CG	28.279	0.1	1
5127	A	104	LEU	N	129.808	0.1	1
5128	B	304	LEU	N	129.808	0.1	1
5129	A	105	GLU	H	8.805	0.02	1
5130	B	305	GLU	H	8.805	0.02	1
5131	A	105	GLU	HA	4.710	0.02	1
5132	B	305	GLU	HA	4.710	0.02	1
5133	A	105	GLU	HB2	2.089	0.02	2
5134	B	305	GLU	HB2	2.089	0.02	2
5135	A	105	GLU	HB3	1.976	0.02	2
5136	B	305	GLU	HB3	1.976	0.02	2
5137	A	105	GLU	HG2	2.219	0.02	2
5138	B	305	GLU	HG2	2.219	0.02	2
5139	A	105	GLU	HG3	2.219	0.02	2
5140	B	305	GLU	HG3	2.219	0.02	2
5141	A	105	GLU	C	174.452	0.1	1
5142	B	305	GLU	C	174.452	0.1	1
5143	A	105	GLU	CA	54.700	0.1	1
5144	B	305	GLU	CA	54.700	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
5145	A	105	GLU	CB	33.200	0.1	1
5146	B	305	GLU	CB	33.200	0.1	1
5147	A	105	GLU	CG	37.041	0.1	1
5148	B	305	GLU	CG	37.041	0.1	1
5149	A	105	GLU	N	124.200	0.1	1
5150	B	305	GLU	N	124.200	0.1	1
5151	A	106	ILE	H	7.852	0.02	1
5152	B	306	ILE	H	7.852	0.02	1
5153	A	106	ILE	HA	4.969	0.02	1
5154	B	306	ILE	HA	4.969	0.02	1
5155	A	106	ILE	HB	1.829	0.02	1
5156	B	306	ILE	HB	1.829	0.02	1
5157	A	106	ILE	HD11	0.849	0.02	1
5158	B	306	ILE	HD11	0.849	0.02	1
5159	A	106	ILE	HD12	0.849	0.02	1
5160	B	306	ILE	HD12	0.849	0.02	1
5161	A	106	ILE	HD13	0.849	0.02	1
5162	B	306	ILE	HD13	0.849	0.02	1
5163	A	106	ILE	HG12	1.209	0.02	2
5164	B	306	ILE	HG12	1.209	0.02	2
5165	A	106	ILE	HG13	1.582	0.02	2
5166	B	306	ILE	HG13	1.582	0.02	2
5167	A	106	ILE	HG21	0.917	0.02	1
5168	B	306	ILE	HG21	0.917	0.02	1
5169	A	106	ILE	HG22	0.917	0.02	1
5170	B	306	ILE	HG22	0.917	0.02	1
5171	A	106	ILE	HG23	0.917	0.02	1
5172	B	306	ILE	HG23	0.917	0.02	1
5173	A	106	ILE	C	176.475	0.1	1
5174	B	306	ILE	C	176.475	0.1	1
5175	A	106	ILE	CA	59.100	0.1	1
5176	B	306	ILE	CA	59.100	0.1	1
5177	A	106	ILE	CB	39.300	0.1	1
5178	B	306	ILE	CB	39.300	0.1	1
5179	A	106	ILE	CD1	13.286	0.1	1
5180	B	306	ILE	CD1	13.286	0.1	1
5181	A	106	ILE	CG1	28.657	0.1	1
5182	B	306	ILE	CG1	28.657	0.1	1
5183	A	106	ILE	CG2	18.186	0.1	1
5184	B	306	ILE	CG2	18.186	0.1	1
5185	A	106	ILE	N	120.775	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
5186	B	306	ILE	N	120.775	0.1	1
5187	A	107	LYS	H	8.531	0.02	1
5188	B	307	LYS	H	8.531	0.02	1
5189	A	107	LYS	HA	4.303	0.02	1
5190	B	307	LYS	HA	4.303	0.02	1
5191	A	107	LYS	HB2	1.600	0.02	2
5192	B	307	LYS	HB2	1.600	0.02	2
5193	A	107	LYS	HB3	1.763	0.02	2
5194	B	307	LYS	HB3	1.763	0.02	2
5195	A	107	LYS	HD2	1.652	0.02	2
5196	B	307	LYS	HD2	1.652	0.02	2
5197	A	107	LYS	HD3	1.652	0.02	2
5198	B	307	LYS	HD3	1.652	0.02	2
5199	A	107	LYS	HE2	2.960	0.02	2
5200	B	307	LYS	HE2	2.960	0.02	2
5201	A	107	LYS	HE3	2.960	0.02	2
5202	B	307	LYS	HE3	2.960	0.02	2
5203	A	107	LYS	HG2	1.375	0.02	2
5204	B	307	LYS	HG2	1.375	0.02	2
5205	A	107	LYS	HG3	1.375	0.02	2
5206	B	307	LYS	HG3	1.375	0.02	2
5207	A	107	LYS	C	175.263	0.1	1
5208	B	307	LYS	C	175.263	0.1	1
5209	A	107	LYS	CA	56.654	0.1	1
5210	B	307	LYS	CA	56.654	0.1	1
5211	A	107	LYS	CB	33.565	0.1	1
5212	B	307	LYS	CB	33.565	0.1	1
5213	A	107	LYS	CD	29.673	0.1	1
5214	B	307	LYS	CD	29.673	0.1	1
5215	A	107	LYS	CE	42.191	0.1	1
5216	B	307	LYS	CE	42.191	0.1	1
5217	A	107	LYS	CG	25.100	0.1	1
5218	B	307	LYS	CG	25.100	0.1	1
5219	A	107	LYS	N	129.321	0.1	1
5220	B	307	LYS	N	129.321	0.1	1
5221	A	108	ARG	H	8.153	0.02	1
5222	B	308	ARG	H	8.153	0.02	1
5223	A	108	ARG	HA	4.263	0.02	1
5224	B	308	ARG	HA	4.263	0.02	1
5225	A	108	ARG	HB2	1.918	0.02	2
5226	B	308	ARG	HB2	1.918	0.02	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
5227	A	108	ARG	HB3	1.788	0.02	2
5228	B	308	ARG	HB3	1.788	0.02	2
5229	A	108	ARG	HD2	3.261	0.02	2
5230	B	308	ARG	HD2	3.261	0.02	2
5231	A	108	ARG	HD3	3.261	0.02	2
5232	B	308	ARG	HD3	3.261	0.02	2
5233	A	108	ARG	HG2	1.697	0.02	2
5234	B	308	ARG	HG2	1.697	0.02	2
5235	A	108	ARG	HG3	1.697	0.02	2
5236	B	308	ARG	HG3	1.697	0.02	2
5237	A	108	ARG	C	180.978	0.1	1
5238	B	308	ARG	C	180.978	0.1	1
5239	A	108	ARG	CA	57.721	0.1	1
5240	B	308	ARG	CA	57.721	0.1	1
5241	A	108	ARG	CB	31.870	0.1	1
5242	B	308	ARG	CB	31.870	0.1	1
5243	A	108	ARG	CD	43.809	0.1	1
5244	B	308	ARG	CD	43.809	0.1	1
5245	A	108	ARG	CG	27.308	0.1	1
5246	B	308	ARG	CG	27.308	0.1	1
5247	A	108	ARG	N	129.640	0.1	1
5248	B	308	ARG	N	129.640	0.1	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	216	-0.25 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	200	-0.24 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	210	0.20 ± 0.08	None needed (< 0.5 ppm)
^{15}N	200	-0.67 ± 0.26	Should be applied

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 91%, i.e. 2312 atoms were assigned a chemical shift out of a possible 2528. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1032/1043 (99%)	412/415 (99%)	421/426 (99%)	199/202 (99%)
Sidechain	1124/1277 (88%)	700/752 (93%)	397/472 (84%)	27/53 (51%)
Aromatic	156/208 (75%)	102/108 (94%)	52/98 (53%)	2/2 (100%)
Overall	2312/2528 (91%)	1214/1275 (95%)	870/996 (87%)	228/257 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 2340 atoms were assigned a chemical shift out of a possible 2560. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1042/1056 (99%)	416/420 (99%)	426/432 (99%)	200/204 (98%)
Sidechain	1142/1296 (88%)	712/764 (93%)	402/478 (84%)	28/54 (52%)
Aromatic	156/208 (75%)	102/108 (94%)	52/98 (53%)	2/2 (100%)
Overall	2340/2560 (91%)	1230/1292 (95%)	880/1008 (87%)	230/260 (88%)

7.1.4 Statistically unusual chemical shifts (i)

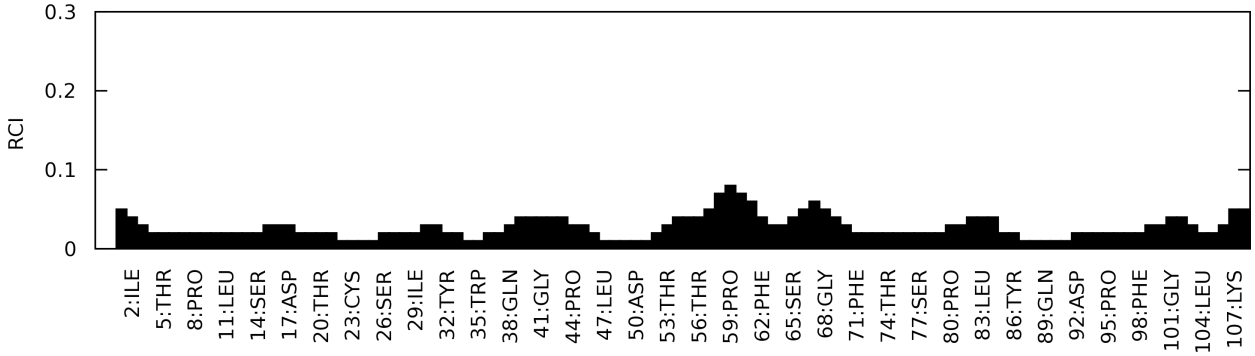
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	73	PHE	HB3	0.16	4.85 – 1.05	-7.3
1	B	273	PHE	HB3	0.16	4.85 – 1.05	-7.3
1	A	44	PRO	HG3	-0.02	3.56 – 0.26	-5.8
1	B	244	PRO	HG3	-0.02	3.56 – 0.26	-5.8
1	B	244	PRO	HD3	1.43	5.52 – 1.72	-5.8
1	A	44	PRO	HD3	1.43	5.52 – 1.72	-5.8
1	A	89	GLN	HG2	0.88	3.67 – 0.97	-5.3
1	B	289	GLN	HG2	0.88	3.67 – 0.97	-5.3

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: