



Full wwPDB NMR Structure Validation Report ⓘ

Oct 10, 2016 – 12:36 PM EDT

PDB ID : 5JPW
Title : Molecular basis for protein recognition specificity of the DYNLT1/Tctex1 canonical binding groove. Characterization of the interaction with activin receptor IIB
Authors : Rodriguez-Crespo, I.; Merino-Gracia, J.; Bruix, M.; Zamora-Carreras, H.
Deposited on : 2016-05-04

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027939
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

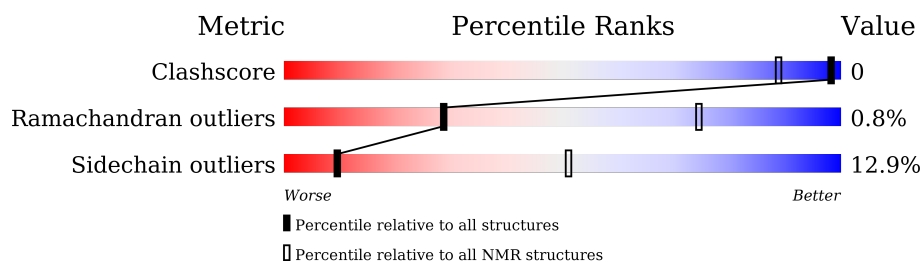
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	143	 72% 5% 23%
1	B	143	 73% . 23%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:13-A:114, A:130-A:137, B:156-B:257, B:273-B:280 (220)	0.92	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4284 atoms, of which 2124 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms						Trace
1	A	143	Total	C	H	N	O	S	0
			2142	678	1062	179	215	8	
1	B	143	Total	C	H	N	O	S	0
			2142	678	1062	179	215	8	

There are 18 discrepancies between the modelled and reference sequences:

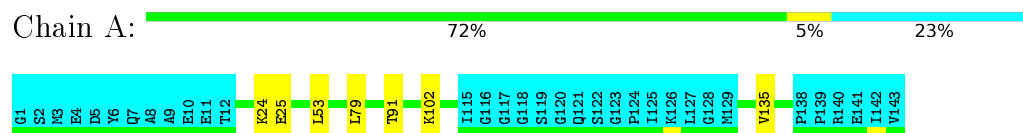
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P63172
A	2	SER	-	expression tag	UNP P63172
A	116	GLY	-	linker	UNP P63172
A	117	GLY	-	linker	UNP P63172
A	118	GLY	-	linker	UNP P63172
A	119	SER	-	linker	UNP P63172
A	120	GLY	-	linker	UNP P63172
A	121	GLN	-	linker	UNP P63172
A	122	SER	-	linker	UNP P63172
B	144	GLY	-	expression tag	UNP P63172
B	145	SER	-	expression tag	UNP P63172
B	259	GLY	-	linker	UNP P63172
B	260	GLY	-	linker	UNP P63172
B	261	GLY	-	linker	UNP P63172
B	262	SER	-	linker	UNP P63172
B	263	GLY	-	linker	UNP P63172
B	264	GLN	-	linker	UNP P63172
B	265	SER	-	linker	UNP P63172

4 Residue-property plots

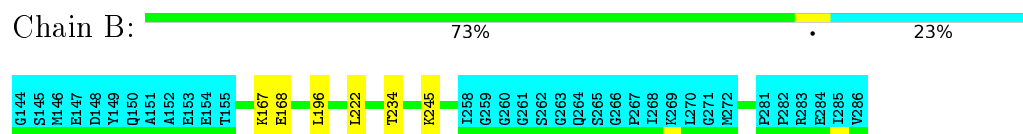
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2



- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

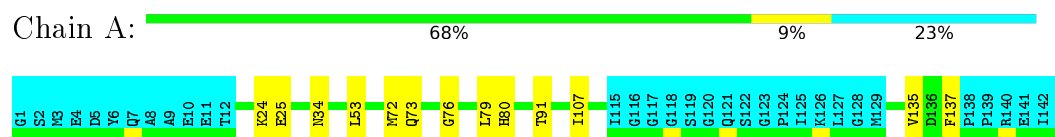


4.2 Scores per residue for each member of the ensemble

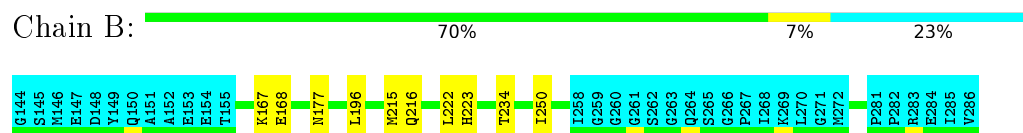
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

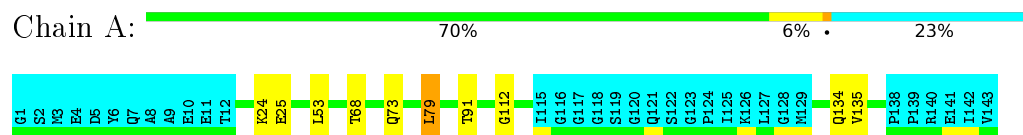


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

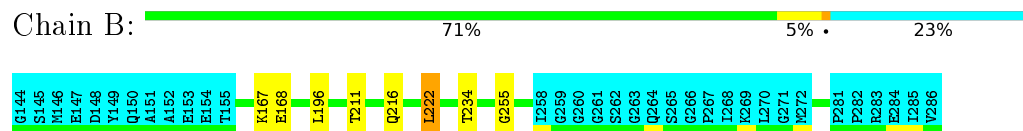


4.2.2 Score per residue for model 2

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

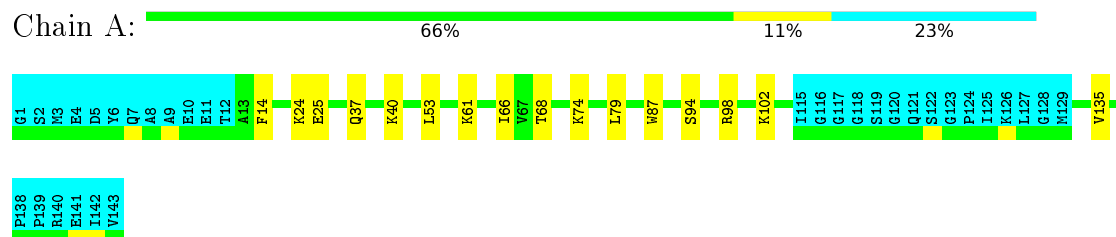


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

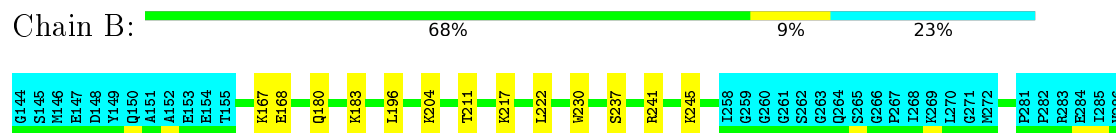


4.2.3 Score per residue for model 3

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

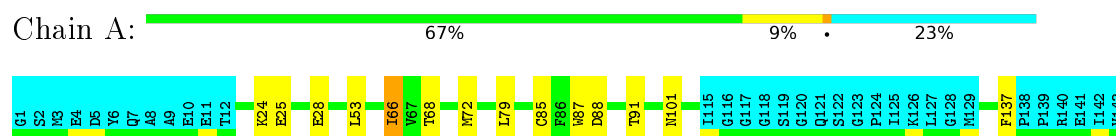


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2



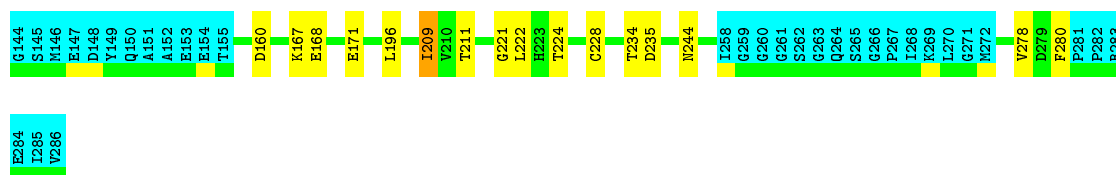
4.2.4 Score per residue for model 4

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2



- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2





4.2.5 Score per residue for model 5

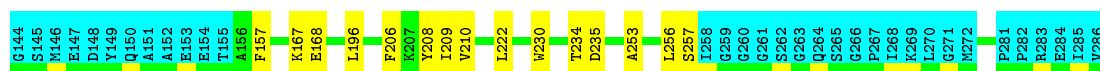
- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain A: 71% 6% 23%



- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain B: 66% 10% 23%



4.2.6 Score per residue for model 6

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain A: 69% 8% 23%



- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain B: 69% 8% 23%

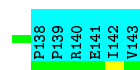


4.2.7 Score per residue for model 7

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain A: 65% 12% 23%





- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

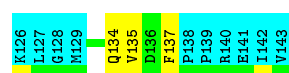
Chain B: 69% 8% 23%



4.2.8 Score per residue for model 8

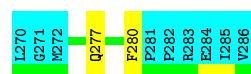
- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain A: 61% 15% 23%



- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

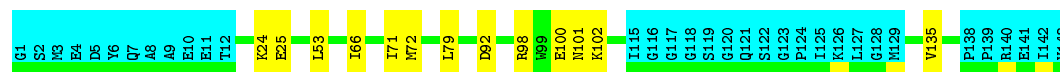
Chain B: 62% 15% 23%



4.2.9 Score per residue for model 9

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain A: 68% 9% 23%



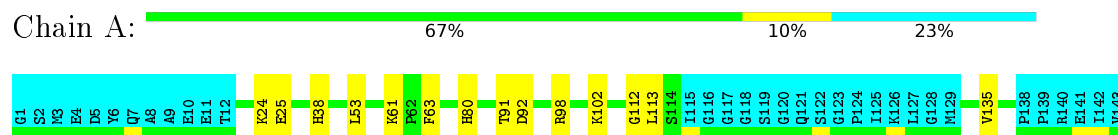
- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain B: 67% 10% 23%

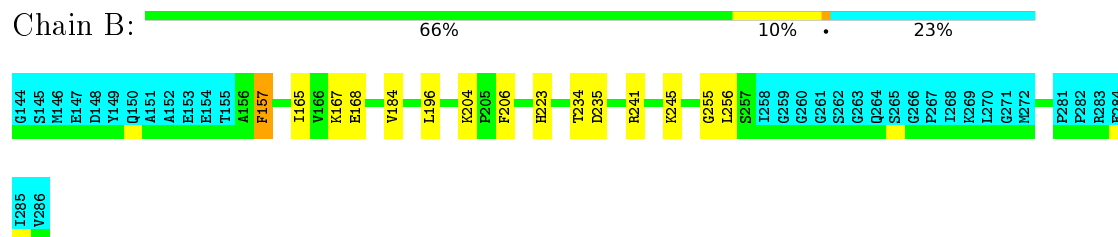


4.2.10 Score per residue for model 10

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

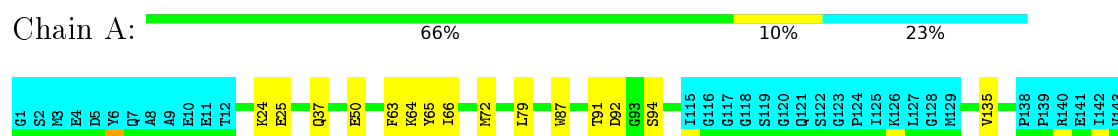


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

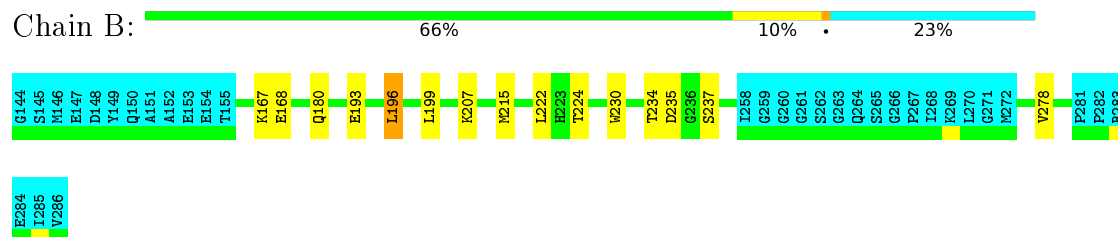


4.2.11 Score per residue for model 11

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

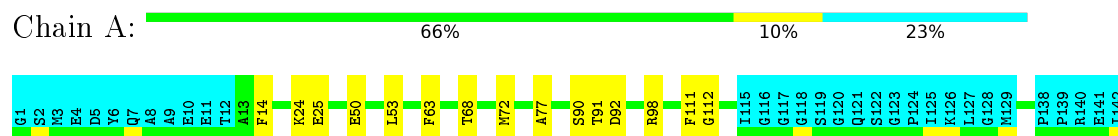


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2



4.2.12 Score per residue for model 12

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2



V143

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

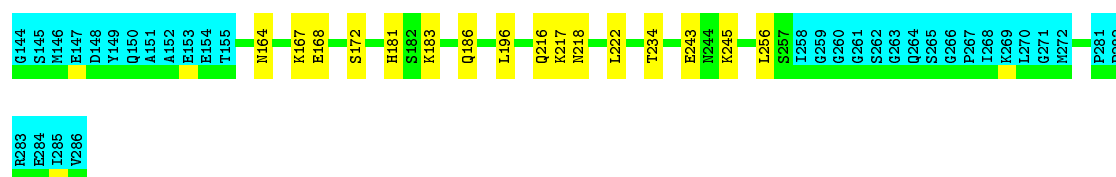
Chain B: 

4.2.13 Score per residue for model 13

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

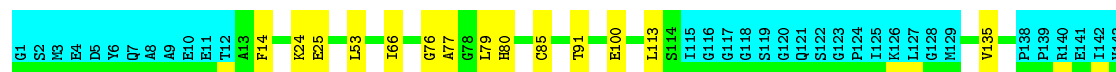
Chain A: 

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain B: 

4.2.14 Score per residue for model 14

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain A: 

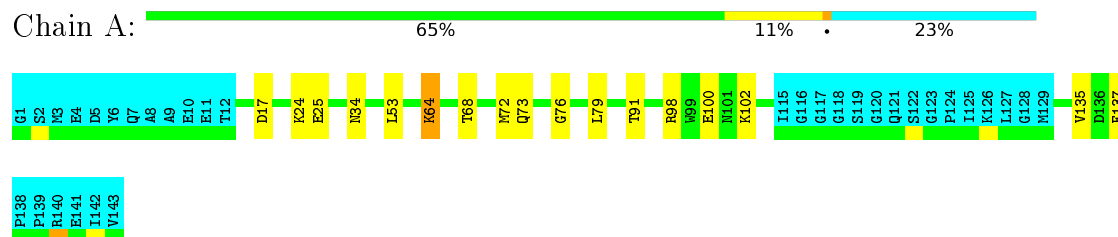
- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

Chain B: 

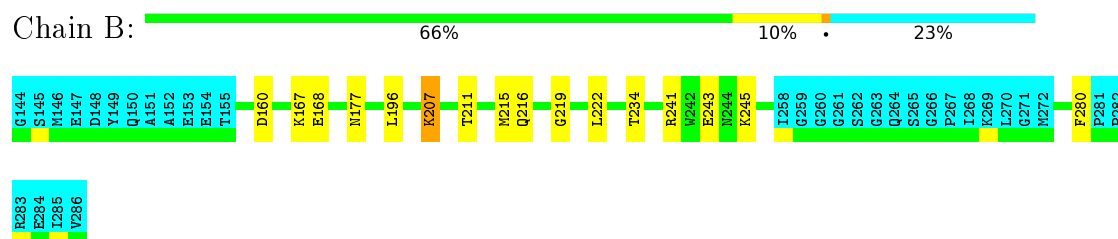
T285
Y286

4.2.15 Score per residue for model 15

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

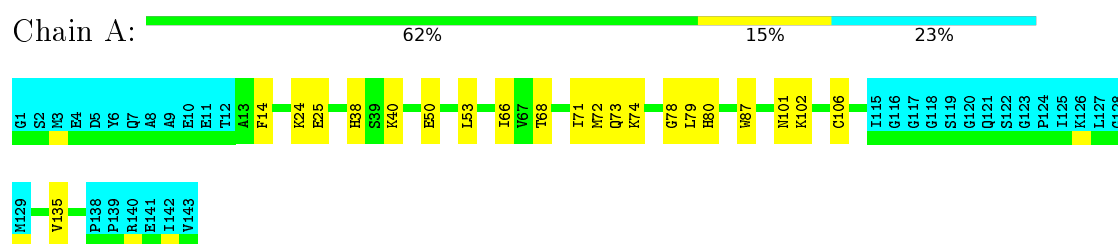


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

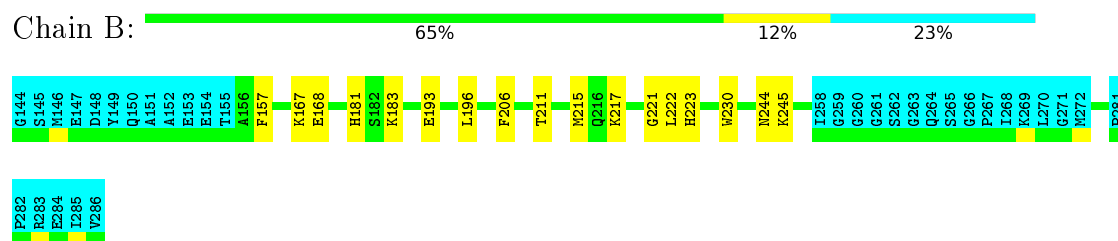


4.2.16 Score per residue for model 16

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

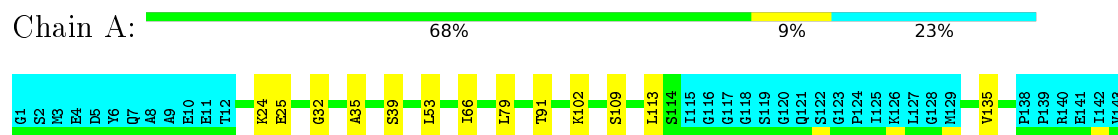


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

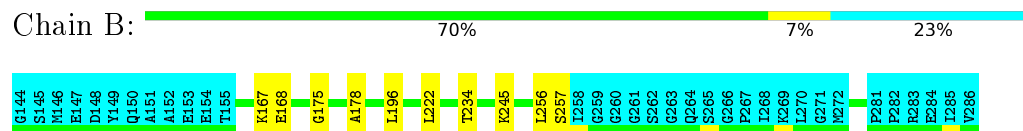


4.2.17 Score per residue for model 17

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

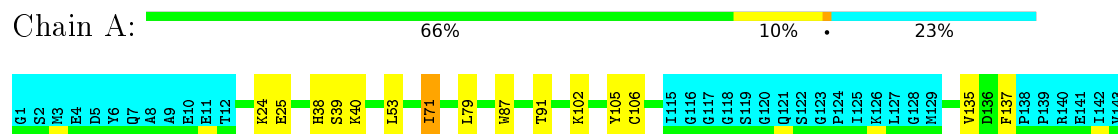


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

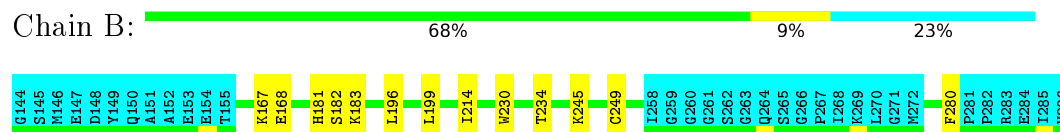


4.2.18 Score per residue for model 18

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

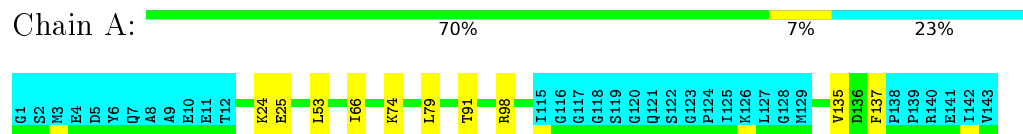


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

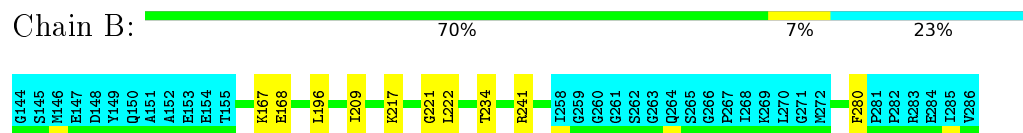


4.2.19 Score per residue for model 19

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

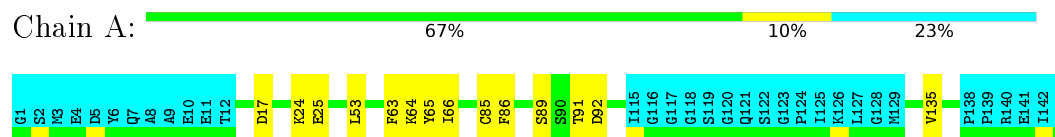


- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2

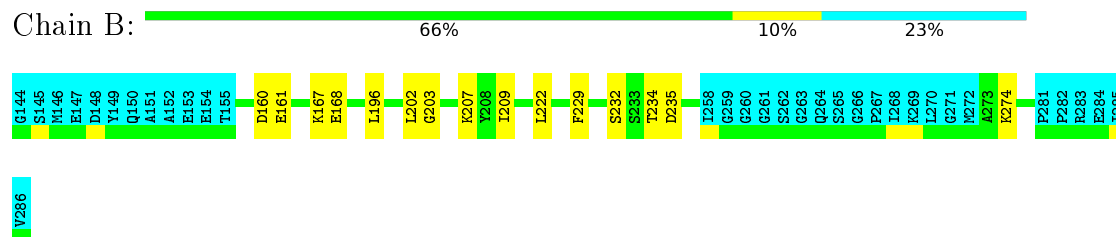


4.2.20 Score per residue for model 20

- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2



- Molecule 1: Dynein light chain Tctex-type 1,Cytoplasmic dynein 1 intermediate chain 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

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

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

Software name	Classification	Version
AMBER	refinement	

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)	5jpw_cs.cif
Number of chemical shift lists	1
Total number of shifts	2748
Number of shifts mapped to atoms	0
Number of unparsed shifts	2748
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.69±0.02	0±0/863 (0.0±0.0%)	0.95±0.02	0±0/1173 (0.0±0.0%)
1	B	0.69±0.02	0±0/863 (0.0±0.0%)	0.95±0.02	0±0/1173 (0.0±0.0%)
All	All	0.69	1/34520 (0.0%)	0.95	0/46920 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.2
All	All	0	1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	39	SER	CA-CB	5.34	1.60	1.52	17	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	208	TYR	Sidechain	1

6.2 Too-close contacts [i](#)

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

averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	846	836	834	1±2
1	A	846	836	834	1±2
All	All	33840	33440	33360	31

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:CYS:SG	1:B:209:ILE:HD11	0.56	2.41	14	4
1:A:66:ILE:HD11	1:B:228:CYS:SG	0.55	2.42	4	2
1:A:79:LEU:HD13	1:B:222:LEU:HD13	0.55	1.77	14	1
1:A:79:LEU:HD11	1:B:220:ALA:HB1	0.52	1.82	14	1
1:B:224:THR:HB	1:B:278:VAL:HG13	0.51	1.83	12	3
1:A:79:LEU:HD13	1:B:222:LEU:HD11	0.51	1.80	6	1
1:B:159:VAL:HA	1:B:162:VAL:HG22	0.51	1.82	12	1
1:A:19:VAL:HG13	1:A:56:LEU:HD22	0.51	1.82	7	1
1:A:77:ALA:HB1	1:B:222:LEU:HD11	0.50	1.82	14	1
1:A:71:ILE:HD12	1:A:106:CYS:CB	0.47	2.39	18	3
1:B:214:ILE:HD12	1:B:249:CYS:HB2	0.46	1.87	8	1
1:A:64:LYS:HE3	1:B:254:PHE:CE2	0.46	2.46	8	1
1:B:162:VAL:HG13	1:B:199:LEU:HD22	0.46	1.87	7	2
1:A:71:ILE:HD12	1:A:106:CYS:HB2	0.45	1.87	8	1
1:A:77:ALA:HB1	1:B:222:LEU:CD1	0.43	2.43	14	1
1:A:79:LEU:CD1	1:B:220:ALA:HB1	0.43	2.42	14	1
1:B:214:ILE:HD12	1:B:249:CYS:CB	0.43	2.44	8	2
1:B:210:VAL:HG12	1:B:253:ALA:HB2	0.42	1.90	5	1
1:A:79:LEU:HD22	1:B:222:LEU:HD22	0.41	1.91	2	1
1:B:157:PHE:CZ	1:B:165:ILE:HD11	0.40	2.51	10	1
1:B:196:LEU:HD13	1:B:199:LEU:HD11	0.40	1.93	11	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	110/143 (77%)	98±3 (89±2%)	11±3 (10±2%)	1±1 (1±1%)	31	76
1	B	110/143 (77%)	97±3 (89±3%)	12±3 (10±3%)	1±1 (1±1%)	26	73
All	All	4400/5720 (77%)	3910 (89%)	454 (10%)	36 (1%)	29	74

All 19 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	112	GLY	4
1	B	255	GLY	4
1	A	76	GLY	3
1	B	221	GLY	3
1	B	219	GLY	3
1	B	207	LYS	3
1	A	38	HIS	2
1	B	203	GLY	2
1	B	181	HIS	2
1	B	182	SER	1
1	A	35	ALA	1
1	A	77	ALA	1
1	A	39	SER	1
1	B	178	ALA	1
1	B	175	GLY	1
1	A	63	PHE	1
1	A	32	GLY	1
1	A	78	GLY	1
1	A	64	LYS	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	95/119 (80%)	82±3 (87±3%)	13±3 (13±3%)	9	50
1	B	95/119 (80%)	83±3 (88±3%)	12±3 (12±3%)	10	52
All	All	3800/4760 (80%)	3310 (87%)	490 (13%)	9	51

All 98 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	168	GLU	20
1	A	25	GLU	20
1	B	167	LYS	20
1	A	24	LYS	20
1	A	53	LEU	18
1	A	135	VAL	18
1	B	196	LEU	18
1	B	222	LEU	16
1	A	91	THR	16
1	B	234	THR	16
1	A	79	LEU	12
1	B	245	LYS	11
1	A	102	LYS	11
1	A	72	MET	10
1	B	235	ASP	9
1	A	66	ILE	8
1	B	241	ARG	8
1	A	87	TRP	8
1	A	98	ARG	8
1	A	68	THR	8
1	A	92	ASP	7
1	B	206	PHE	7
1	B	211	THR	7
1	B	256	LEU	7
1	A	137	PHE	6
1	A	80	HIS	6
1	B	157	PHE	6
1	B	215	MET	6
1	B	230	TRP	6
1	B	223	HIS	6
1	A	14	PHE	5
1	B	280	PHE	5
1	A	74	LYS	5
1	B	217	LYS	5
1	A	63	PHE	5
1	B	243	GLU	5
1	A	73	GLN	5
1	B	183	LYS	5
1	A	113	LEU	5
1	B	216	GLN	4
1	A	100	GLU	4
1	A	64	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	40	LYS	4
1	B	218	ASN	3
1	A	71	ILE	3
1	A	75	ASN	3
1	B	193	GLU	3
1	A	101	ASN	3
1	B	244	ASN	3
1	A	50	GLU	3
1	A	94	SER	3
1	B	160	ASP	3
1	B	207	LYS	2
1	A	65	TYR	2
1	A	21	ASN	2
1	B	257	SER	2
1	B	209	ILE	2
1	A	34	ASN	2
1	B	177	ASN	2
1	A	37	GLN	2
1	B	237	SER	2
1	A	111	PHE	2
1	B	180	GLN	2
1	B	229	PHE	2
1	A	61	LYS	2
1	B	164	ASN	2
1	A	17	ASP	2
1	A	134	GLN	2
1	B	204	LYS	2
1	A	29	SER	1
1	B	274	LYS	1
1	B	161	GLU	1
1	A	107	ILE	1
1	A	88	ASP	1
1	A	89	SER	1
1	A	90	SER	1
1	B	277	GLN	1
1	A	38	HIS	1
1	B	250	ILE	1
1	B	186	GLN	1
1	B	199	LEU	1
1	B	184	VAL	1
1	B	202	LEU	1
1	B	172	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	B	247	MET	1
1	A	109	SER	1
1	B	248	TYR	1
1	A	86	PHE	1
1	A	106	CYS	1
1	A	105	TYR	1
1	A	28	GLU	1
1	B	171	GLU	1
1	B	232	SER	1
1	A	43	GLN	1
1	B	181	HIS	1
1	B	238	CYS	1
1	B	233	SER	1
1	B	224	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: 5jpw_cs.cif

Chemical shift list name: *Tctex-IC_dimer.bmrB*

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	2748
Number of shifts mapped to atoms	0
Number of unparsed shifts	2748
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Entity instance (chain) must be specified. All 2748 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	1	GLY	CA	45.216	0.002	1
2	?	2	SER	N	115.595	0.028	1
3	?	2	SER	H	8.229	0.002	1
4	?	2	SER	CA	58.516	0.046	1
5	?	2	SER	CB	63.991	0.026	1
6	?	3	MET	N	121.950	0.001	1
7	?	3	MET	H	8.563	0.003	1
8	?	3	MET	CA	56.091	0.024	1
9	?	3	MET	HA	4.401	0.012	1
10	?	3	MET	CB	32.280	0.004	1
11	?	3	MET	HB2	1.951	0.004	2
12	?	3	MET	HB3	2.038	0.001	2
13	?	3	MET	CG	31.978	0.000	1
14	?	3	MET	HG2	2.469	0.005	2
15	?	3	MET	HG3	2.545	0.005	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	4	GLU	N	120.702	0.010	1
17	?	4	GLU	H	8.323	0.006	1
18	?	4	GLU	CA	57.223	0.006	1
19	?	4	GLU	HA	4.132	0.011	1
20	?	4	GLU	CB	29.703	0.006	1
21	?	4	GLU	HB2	1.893	0.004	2
22	?	4	GLU	HB3	1.975	0.006	2
23	?	4	GLU	CG	36.514	0.000	1
24	?	4	GLU	HG2	2.192	0.008	2
25	?	4	GLU	HG3	2.192	0.008	2
26	?	5	ASP	N	120.565	0.087	1
27	?	5	ASP	H	8.081	0.008	1
28	?	5	ASP	CA	54.544	0.005	1
29	?	5	ASP	HA	4.455	0.009	1
30	?	5	ASP	CB	40.913	0.003	1
31	?	5	ASP	HB2	2.471	0.006	2
32	?	5	ASP	HB3	2.556	0.008	2
33	?	6	TYR	N	120.512	0.011	1
34	?	6	TYR	H	7.914	0.006	1
35	?	6	TYR	CA	58.290	0.039	1
36	?	6	TYR	HA	4.427	0.014	1
37	?	6	TYR	CB	38.581	0.016	1
38	?	6	TYR	HB2	2.910	0.008	2
39	?	6	TYR	HB3	2.952	0.012	2
40	?	6	TYR	CD1	133.082	0.025	1
41	?	6	TYR	HD1	7.088	0.011	1
42	?	6	TYR	CE1	118.139	0.095	1
43	?	6	TYR	HE1	6.849	0.034	1
44	?	6	TYR	HE2	6.849	0.034	1
45	?	6	TYR	HD2	7.088	0.011	1
46	?	7	GLN	N	122.489	0.010	1
47	?	7	GLN	H	8.021	0.017	1
48	?	7	GLN	CA	55.568	0.013	1
49	?	7	GLN	HA	4.153	0.010	1
50	?	7	GLN	CB	29.380	0.011	1
51	?	7	GLN	HB2	1.836	0.003	2
52	?	7	GLN	HB3	1.934	0.003	2
53	?	7	GLN	CG	33.655	0.018	1
54	?	7	GLN	HG2	2.195	0.003	2
55	?	7	GLN	HG3	2.195	0.003	2
56	?	8	ALA	N	125.378	0.013	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	8	ALA	H	8.105	0.009	1
58	?	8	ALA	CA	52.531	0.021	1
59	?	8	ALA	HA	4.150	0.008	1
60	?	8	ALA	HB1	1.328	0.009	1
61	?	8	ALA	HB2	1.328	0.009	1
62	?	8	ALA	HB3	1.328	0.009	1
63	?	8	ALA	CB	19.172	0.033	1
64	?	9	ALA	N	123.529	0.033	1
65	?	9	ALA	H	8.151	0.005	1
66	?	9	ALA	CA	52.690	0.057	1
67	?	9	ALA	HA	4.206	0.013	1
68	?	9	ALA	HB1	1.349	0.016	1
69	?	9	ALA	HB2	1.349	0.016	1
70	?	9	ALA	HB3	1.349	0.016	1
71	?	9	ALA	CB	19.133	0.043	1
72	?	10	GLU	N	119.820	0.092	1
73	?	10	GLU	H	8.371	0.007	1
74	?	10	GLU	CA	57.420	0.003	1
75	?	10	GLU	HA	4.712	0.013	1
76	?	10	GLU	CB	29.895	0.003	1
77	?	10	GLU	HB2	1.886	0.004	2
78	?	10	GLU	HB3	1.962	0.012	2
79	?	10	GLU	HG2	2.211	0.003	2
80	?	10	GLU	HG3	2.211	0.003	2
81	?	11	GLU	N	119.997	0.006	1
82	?	11	GLU	H	8.371	0.006	1
83	?	11	GLU	CA	57.481	0.006	1
84	?	11	GLU	HA	4.689	0.015	1
85	?	11	GLU	CB	29.961	0.035	1
86	?	11	GLU	HB2	1.975	0.002	2
87	?	11	GLU	HB3	2.032	0.013	2
88	?	11	GLU	CG	36.518	0.004	1
89	?	11	GLU	HG2	2.212	0.004	2
90	?	11	GLU	HG3	2.212	0.004	2
91	?	12	THR	N	110.500	0.002	1
92	?	12	THR	H	7.866	0.017	1
93	?	12	THR	CA	60.996	0.040	1
94	?	12	THR	HA	4.304	0.007	1
95	?	12	THR	CB	69.488	0.030	1
96	?	12	THR	HB	4.276	0.010	1
97	?	12	THR	HG21	1.076	0.005	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	12	THR	HG22	1.076	0.005	1
99	?	12	THR	HG23	1.076	0.005	1
100	?	12	THR	CG2	21.662	0.000	1
101	?	13	ALA	N	124.206	0.015	1
102	?	13	ALA	H	7.713	0.006	1
103	?	13	ALA	CA	51.835	0.061	1
104	?	13	ALA	HA	4.561	0.009	1
105	?	13	ALA	HB1	1.311	0.003	1
106	?	13	ALA	HB2	1.311	0.003	1
107	?	13	ALA	HB3	1.311	0.003	1
108	?	13	ALA	CB	20.491	0.046	1
109	?	14	PHE	N	122.698	0.005	1
110	?	14	PHE	H	8.738	0.007	1
111	?	14	PHE	CA	57.978	0.024	1
112	?	14	PHE	HA	3.885	0.013	1
113	?	14	PHE	CB	38.187	0.008	1
114	?	14	PHE	HB2	2.345	0.009	2
115	?	14	PHE	HB3	2.832	0.004	2
116	?	14	PHE	HD1	6.654	0.011	1
117	?	14	PHE	HD2	6.654	0.011	1
118	?	15	VAL	N	131.417	0.231	1
119	?	15	VAL	H	8.427	0.009	1
120	?	15	VAL	CA	61.627	0.007	1
121	?	15	VAL	HA	4.061	0.013	1
122	?	15	VAL	CB	31.345	0.003	1
123	?	15	VAL	HB	1.764	0.027	1
124	?	15	VAL	HG11	0.731	0.009	2
125	?	15	VAL	HG12	0.731	0.009	2
126	?	15	VAL	HG13	0.731	0.009	2
127	?	15	VAL	HG21	0.746	0.006	2
128	?	15	VAL	HG22	0.746	0.006	2
129	?	15	VAL	HG23	0.746	0.006	2
130	?	15	VAL	CG1	20.304	0.000	1
131	?	15	VAL	CG2	21.137	0.028	1
132	?	16	VAL	N	129.080	0.019	1
133	?	16	VAL	H	8.648	0.013	1
134	?	16	VAL	CA	67.617	0.038	1
135	?	16	VAL	HA	3.184	0.010	1
136	?	16	VAL	CB	31.763	0.081	1
137	?	16	VAL	HB	2.062	0.010	1
138	?	16	VAL	HG11	1.009	0.003	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	16	VAL	HG12	1.009	0.003	2
140	?	16	VAL	HG13	1.009	0.003	2
141	?	16	VAL	HG21	1.241	0.007	2
142	?	16	VAL	HG22	1.241	0.007	2
143	?	16	VAL	HG23	1.241	0.007	2
144	?	16	VAL	CG1	21.134	0.005	1
145	?	16	VAL	CG2	22.605	0.009	1
146	?	17	ASP	N	118.704	0.013	1
147	?	17	ASP	H	8.787	0.012	1
148	?	17	ASP	CA	57.623	0.021	1
149	?	17	ASP	HA	4.250	0.010	1
150	?	17	ASP	CB	40.218	0.034	1
151	?	17	ASP	HB2	2.411	0.010	2
152	?	17	ASP	HB3	2.493	0.014	2
153	?	18	GLU	N	118.212	0.031	1
154	?	18	GLU	H	6.604	0.010	1
155	?	18	GLU	CA	58.106	0.017	1
156	?	18	GLU	HA	3.979	0.010	1
157	?	18	GLU	CB	30.248	0.044	1
158	?	18	GLU	HB2	1.887	0.003	2
159	?	18	GLU	HB3	1.971	0.017	2
160	?	18	GLU	CG	36.410	0.005	1
161	?	18	GLU	HG2	1.951	0.018	2
162	?	18	GLU	HG3	1.951	0.018	2
163	?	19	VAL	N	120.306	0.019	1
164	?	19	VAL	H	7.375	0.012	1
165	?	19	VAL	CA	66.491	0.034	1
166	?	19	VAL	HA	3.178	0.018	1
167	?	19	VAL	CB	31.181	0.059	1
168	?	19	VAL	HB	1.626	0.004	1
169	?	19	VAL	HG11	0.101	0.007	2
170	?	19	VAL	HG12	0.101	0.007	2
171	?	19	VAL	HG13	0.101	0.007	2
172	?	19	VAL	HG21	0.617	0.011	2
173	?	19	VAL	HG22	0.617	0.011	2
174	?	19	VAL	HG23	0.617	0.011	2
175	?	19	VAL	CG1	21.089	0.023	1
176	?	19	VAL	CG2	21.751	0.001	1
177	?	20	SER	N	115.603	0.010	1
178	?	20	SER	H	8.881	0.007	1
179	?	20	SER	CA	62.098	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	20	SER	HA	3.857	0.012	1
181	?	20	SER	CB	62.750	0.004	1
182	?	20	SER	HB2	3.783	0.009	2
183	?	20	SER	HB3	3.783	0.009	2
184	?	21	ASN	N	118.310	0.009	1
185	?	21	ASN	H	7.465	0.011	1
186	?	21	ASN	CA	56.603	0.004	1
187	?	21	ASN	HA	4.361	0.009	1
188	?	21	ASN	CB	38.135	0.002	1
189	?	21	ASN	HB2	2.746	0.011	2
190	?	21	ASN	HB3	2.746	0.011	2
191	?	22	ILE	N	121.294	0.017	1
192	?	22	ILE	H	7.170	0.009	1
193	?	22	ILE	CA	65.363	0.052	1
194	?	22	ILE	HA	3.534	0.012	1
195	?	22	ILE	CB	38.649	0.035	1
196	?	22	ILE	HB	1.859	0.009	1
197	?	22	ILE	HG21	0.773	0.006	1
198	?	22	ILE	HG22	0.773	0.006	1
199	?	22	ILE	HG23	0.773	0.006	1
200	?	22	ILE	CG2	17.784	0.056	1
201	?	22	ILE	CG1	29.826	0.035	1
202	?	22	ILE	HG12	0.889	0.009	2
203	?	22	ILE	HG13	1.698	0.006	2
204	?	22	ILE	HD11	0.566	0.005	1
205	?	22	ILE	HD12	0.566	0.005	1
206	?	22	ILE	HD13	0.566	0.005	1
207	?	22	ILE	CD1	14.302	0.027	1
208	?	23	VAL	N	120.404	0.009	1
209	?	23	VAL	H	8.223	0.010	1
210	?	23	VAL	CA	66.371	0.158	1
211	?	23	VAL	HA	3.396	0.008	1
212	?	23	VAL	CB	31.457	0.007	1
213	?	23	VAL	HB	2.017	0.004	1
214	?	23	VAL	HG11	0.649	0.002	2
215	?	23	VAL	HG12	0.649	0.002	2
216	?	23	VAL	HG13	0.649	0.002	2
217	?	23	VAL	HG21	0.732	0.021	2
218	?	23	VAL	HG22	0.732	0.021	2
219	?	23	VAL	HG23	0.732	0.021	2
220	?	23	VAL	CG1	22.349	0.004	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	23	VAL	CG2	22.972	0.006	1
222	?	24	LYS	N	118.400	0.000	1
223	?	24	LYS	H	8.447	0.013	1
224	?	24	LYS	CA	60.848	0.011	1
225	?	24	LYS	HA	3.585	0.006	1
226	?	24	LYS	CB	32.480	0.028	1
227	?	24	LYS	HB2	1.833	0.005	2
228	?	24	LYS	HB3	1.884	0.003	2
229	?	24	LYS	CG	26.503	0.007	1
230	?	24	LYS	HG2	1.368	0.005	2
231	?	24	LYS	HG3	1.582	0.002	2
232	?	24	LYS	CD	29.702	0.023	1
233	?	24	LYS	HD2	1.671	0.005	2
234	?	24	LYS	HD3	1.671	0.005	2
235	?	24	LYS	CE	42.212	0.008	1
236	?	24	LYS	HE2	2.916	0.002	2
237	?	24	LYS	HE3	2.916	0.002	2
238	?	25	GLU	N	117.300	0.001	1
239	?	25	GLU	H	7.734	0.006	1
240	?	25	GLU	CA	59.153	0.025	1
241	?	25	GLU	HA	3.874	0.008	1
242	?	25	GLU	CB	28.760	0.064	1
243	?	25	GLU	HB2	1.894	0.007	2
244	?	25	GLU	HB3	1.960	0.002	2
245	?	25	GLU	CG	36.534	0.002	1
246	?	25	GLU	HG2	2.068	0.007	2
247	?	25	GLU	HG3	2.264	0.002	2
248	?	26	ALA	N	123.785	0.065	1
249	?	26	ALA	H	7.900	0.008	1
250	?	26	ALA	CA	55.149	0.064	1
251	?	26	ALA	HA	3.877	0.012	1
252	?	26	ALA	HB1	1.325	0.007	1
253	?	26	ALA	HB2	1.325	0.007	1
254	?	26	ALA	HB3	1.325	0.007	1
255	?	26	ALA	CB	18.581	0.041	1
256	?	27	ILE	N	118.299	0.080	1
257	?	27	ILE	H	8.093	0.013	1
258	?	27	ILE	CA	65.948	0.036	1
259	?	27	ILE	HA	2.981	0.010	1
260	?	27	ILE	CB	39.039	0.024	1
261	?	27	ILE	HB	1.126	0.009	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	27	ILE	HG21	-0.801	0.007	1
263	?	27	ILE	HG22	-0.801	0.007	1
264	?	27	ILE	HG23	-0.801	0.007	1
265	?	27	ILE	CG2	15.045	0.017	1
266	?	27	ILE	CG1	28.509	0.010	1
267	?	27	ILE	HG12	0.333	0.002	2
268	?	27	ILE	HG13	1.619	0.004	2
269	?	27	ILE	HD11	0.385	0.008	1
270	?	27	ILE	HD12	0.385	0.008	1
271	?	27	ILE	HD13	0.385	0.008	1
272	?	27	ILE	CD1	14.758	0.181	1
273	?	28	GLU	N	117.899	0.004	1
274	?	28	GLU	H	7.839	0.008	1
275	?	28	GLU	CA	59.407	0.015	1
276	?	28	GLU	HA	3.452	0.011	1
277	?	28	GLU	CB	28.717	0.051	1
278	?	28	GLU	HB2	1.881	0.002	2
279	?	28	GLU	HB3	1.922	0.002	2
280	?	28	GLU	CG	36.084	0.025	1
281	?	28	GLU	HG2	2.060	0.020	2
282	?	28	GLU	HG3	2.267	0.002	2
283	?	29	SER	N	112.399	0.003	1
284	?	29	SER	H	8.034	0.010	1
285	?	29	SER	CA	60.842	0.014	1
286	?	29	SER	HA	3.950	0.007	1
287	?	29	SER	CB	63.090	0.008	1
288	?	29	SER	HB2	3.795	0.002	2
289	?	29	SER	HB3	3.795	0.002	2
290	?	30	ALA	N	121.292	0.018	1
291	?	30	ALA	H	7.457	0.010	1
292	?	30	ALA	CA	54.053	0.036	1
293	?	30	ALA	HA	4.083	0.008	1
294	?	30	ALA	HB1	1.190	0.010	1
295	?	30	ALA	HB2	1.190	0.010	1
296	?	30	ALA	HB3	1.190	0.010	1
297	?	30	ALA	CB	20.687	0.019	1
298	?	31	ILE	N	110.000	0.001	1
299	?	31	ILE	H	7.657	0.010	1
300	?	31	ILE	CA	61.792	0.039	1
301	?	31	ILE	HA	3.020	0.008	1
302	?	31	ILE	CB	39.252	0.071	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	31	ILE	HB	1.228	0.011	1
304	?	31	ILE	HG21	0.159	0.002	1
305	?	31	ILE	HG22	0.159	0.002	1
306	?	31	ILE	HG23	0.159	0.002	1
307	?	31	ILE	CG2	18.792	0.011	1
308	?	31	ILE	CG1	26.322	0.012	1
309	?	31	ILE	HG12	0.187	0.007	2
310	?	31	ILE	HG13	0.561	0.007	2
311	?	31	ILE	HD11	0.224	0.006	1
312	?	31	ILE	HD12	0.224	0.006	1
313	?	31	ILE	HD13	0.224	0.006	1
314	?	31	ILE	CD1	13.974	0.021	1
315	?	32	GLY	N	108.601	0.002	1
316	?	32	GLY	H	7.334	0.008	1
317	?	32	GLY	CA	47.499	0.016	1
318	?	32	GLY	HA2	3.805	0.006	2
319	?	32	GLY	HA3	3.805	0.006	2
320	?	33	GLY	N	112.801	0.004	1
321	?	33	GLY	H	8.865	0.052	1
322	?	33	GLY	CA	45.058	0.022	1
323	?	33	GLY	HA2	3.975	0.012	2
324	?	33	GLY	HA3	3.975	0.012	2
325	?	34	ASN	N	118.507	0.025	1
326	?	34	ASN	H	7.597	0.010	1
327	?	34	ASN	CA	53.272	0.046	1
328	?	34	ASN	HA	4.545	0.012	1
329	?	34	ASN	CB	40.703	0.008	1
330	?	34	ASN	HB2	2.009	0.006	2
331	?	34	ASN	HB3	2.303	0.008	2
332	?	35	ALA	N	121.309	0.015	1
333	?	35	ALA	H	8.240	0.005	1
334	?	35	ALA	CA	49.906	0.067	1
335	?	35	ALA	HA	4.577	0.009	1
336	?	35	ALA	HB1	1.403	0.009	1
337	?	35	ALA	HB2	1.403	0.009	1
338	?	35	ALA	HB3	1.403	0.009	1
339	?	35	ALA	CB	20.169	0.008	1
340	?	36	TYR	N	121.045	0.035	1
341	?	36	TYR	H	8.687	0.014	1
342	?	36	TYR	CA	62.433	0.044	1
343	?	36	TYR	HA	4.050	0.009	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	36	TYR	CB	38.698	0.018	1
345	?	36	TYR	HB2	2.887	0.015	2
346	?	36	TYR	HB3	3.022	0.014	2
347	?	37	GLN	N	125.686	0.031	1
348	?	37	GLN	H	5.502	0.013	1
349	?	37	GLN	CA	54.825	0.005	1
350	?	37	GLN	HA	4.232	0.007	1
351	?	37	GLN	CB	31.901	0.002	1
352	?	37	GLN	HB2	1.546	0.002	2
353	?	37	GLN	HB3	1.773	0.002	2
354	?	37	GLN	CG	33.820	0.003	1
355	?	37	GLN	HG2	2.256	0.002	2
356	?	37	GLN	HG3	2.348	0.001	2
357	?	38	HIS	N	122.101	0.000	1
358	?	38	HIS	H	8.371	0.000	1
359	?	39	SER	CA	59.797	0.011	1
360	?	39	SER	HA	3.806	0.006	1
361	?	39	SER	CB	62.507	0.085	1
362	?	39	SER	HB2	3.558	0.005	2
363	?	39	SER	HB3	3.691	0.007	2
364	?	40	LYS	N	117.996	0.012	1
365	?	40	LYS	H	6.530	0.021	1
366	?	40	LYS	CA	55.415	0.005	1
367	?	40	LYS	HA	3.949	0.012	1
368	?	40	LYS	CB	34.043	0.005	1
369	?	40	LYS	HB2	1.734	0.003	2
370	?	40	LYS	HB3	1.734	0.003	2
371	?	40	LYS	CG	24.750	0.005	1
372	?	40	LYS	HG2	0.878	0.004	2
373	?	40	LYS	HG3	0.878	0.004	2
374	?	40	LYS	CD	28.781	0.002	1
375	?	40	LYS	HD2	1.347	0.004	2
376	?	40	LYS	HD3	1.487	0.003	2
377	?	40	LYS	CE	42.271	0.003	1
378	?	40	LYS	HE2	2.791	0.004	2
379	?	40	LYS	HE3	2.791	0.004	2
380	?	41	VAL	N	117.680	0.038	1
381	?	41	VAL	H	6.430	0.010	1
382	?	41	VAL	CA	64.678	0.033	1
383	?	41	VAL	HA	3.117	0.012	1
384	?	41	VAL	CB	30.501	0.008	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	41	VAL	HB	1.105	0.009	1
386	?	41	VAL	HG11	0.811	0.010	2
387	?	41	VAL	HG12	0.811	0.010	2
388	?	41	VAL	HG13	0.811	0.010	2
389	?	41	VAL	HG21	0.037	0.011	2
390	?	41	VAL	HG22	0.037	0.011	2
391	?	41	VAL	HG23	0.037	0.011	2
392	?	41	VAL	CG1	22.211	0.015	1
393	?	41	VAL	CG2	18.322	0.040	1
394	?	42	ASN	N	118.200	0.088	1
395	?	42	ASN	H	7.835	0.008	1
396	?	42	ASN	CA	55.696	0.008	1
397	?	42	ASN	HA	4.430	0.009	1
398	?	42	ASN	CB	37.472	0.009	1
399	?	42	ASN	HB2	2.455	0.005	2
400	?	42	ASN	HB3	2.515	0.012	2
401	?	43	GLN	N	120.008	0.018	1
402	?	43	GLN	H	7.423	0.009	1
403	?	43	GLN	CA	57.807	0.005	1
404	?	43	GLN	HA	4.000	0.006	1
405	?	43	GLN	CB	27.460	0.001	1
406	?	43	GLN	HB2	1.948	0.004	2
407	?	43	GLN	HB3	1.948	0.004	2
408	?	44	TRP	H	7.398	0.006	1
409	?	44	TRP	CA	58.520	0.006	1
410	?	44	TRP	HA	4.458	0.006	1
411	?	44	TRP	CB	28.481	0.035	1
412	?	44	TRP	HB2	2.691	0.012	2
413	?	44	TRP	HB3	3.359	0.013	2
414	?	44	TRP	NE1	128.759	0.043	1
415	?	44	TRP	HD1	7.117	0.001	1
416	?	44	TRP	HE3	6.844	0.000	1
417	?	44	TRP	CZ3	124.809	0.015	1
418	?	44	TRP	CZ2	114.607	0.012	1
419	?	44	TRP	HE1	9.989	0.008	1
420	?	44	TRP	HZ3	6.923	0.002	1
421	?	44	TRP	CH2	123.796	0.007	1
422	?	44	TRP	HZ2	7.169	0.002	1
423	?	44	TRP	HH2	7.433	0.009	1
424	?	45	THR	N	109.998	0.008	1
425	?	45	THR	H	8.485	0.011	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	45	THR	CA	65.389	0.078	1
427	?	45	THR	HA	3.835	0.010	1
428	?	45	THR	CB	67.304	0.012	1
429	?	45	THR	HB	3.961	0.011	1
430	?	45	THR	HG21	1.223	0.006	1
431	?	45	THR	HG22	1.223	0.006	1
432	?	45	THR	HG23	1.223	0.006	1
433	?	45	THR	CG2	23.069	0.017	1
434	?	46	THR	N	117.101	0.002	1
435	?	46	THR	H	7.076	0.015	1
436	?	46	THR	CA	67.060	0.025	1
437	?	46	THR	HA	3.486	0.011	1
438	?	46	THR	CB	68.649	0.025	1
439	?	46	THR	HB	4.135	0.011	1
440	?	46	THR	HG21	1.096	0.009	1
441	?	46	THR	HG22	1.096	0.009	1
442	?	46	THR	HG23	1.096	0.009	1
443	?	46	THR	CG2	21.604	0.008	1
444	?	47	ASN	N	120.378	0.022	1
445	?	47	ASN	H	8.316	0.005	1
446	?	47	ASN	CA	56.117	0.013	1
447	?	47	ASN	HA	4.426	0.009	1
448	?	47	ASN	CB	38.293	0.006	1
449	?	47	ASN	HB2	2.778	0.017	2
450	?	47	ASN	HB3	2.937	0.010	2
451	?	48	VAL	N	119.914	0.023	1
452	?	48	VAL	H	8.334	0.010	1
453	?	48	VAL	CA	67.338	0.022	1
454	?	48	VAL	HA	3.209	0.011	1
455	?	48	VAL	CB	31.695	0.006	1
456	?	48	VAL	HB	2.046	0.020	1
457	?	48	VAL	HG11	0.554	0.004	2
458	?	48	VAL	HG12	0.554	0.004	2
459	?	48	VAL	HG13	0.554	0.004	2
460	?	48	VAL	HG21	0.767	0.020	2
461	?	48	VAL	HG22	0.767	0.020	2
462	?	48	VAL	HG23	0.767	0.020	2
463	?	48	VAL	CG1	21.999	0.004	1
464	?	48	VAL	CG2	23.251	0.023	1
465	?	49	VAL	N	120.000	0.097	1
466	?	49	VAL	H	7.586	0.012	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	49	VAL	CA	67.255	0.014	1
468	?	49	VAL	HA	3.203	0.014	1
469	?	49	VAL	CB	31.679	0.000	1
470	?	49	VAL	HB	2.009	0.003	1
471	?	49	VAL	HG11	0.638	0.011	2
472	?	49	VAL	HG12	0.638	0.011	2
473	?	49	VAL	HG13	0.638	0.011	2
474	?	49	VAL	HG21	0.738	0.001	2
475	?	49	VAL	HG22	0.738	0.001	2
476	?	49	VAL	HG23	0.738	0.001	2
477	?	49	VAL	CG1	21.150	0.002	1
478	?	49	VAL	CG2	23.283	0.007	1
479	?	50	GLU	N	118.710	0.030	1
480	?	50	GLU	H	8.891	0.005	1
481	?	50	GLU	CA	60.365	0.007	1
482	?	50	GLU	HA	4.436	0.004	1
483	?	50	GLU	CB	29.819	0.008	1
484	?	51	GLN	N	119.000	0.000	1
485	?	51	GLN	H	8.559	0.010	1
486	?	51	GLN	CA	59.086	0.006	1
487	?	51	GLN	HA	3.967	0.006	1
488	?	51	GLN	CB	28.152	0.002	1
489	?	51	GLN	HB2	1.848	0.006	2
490	?	51	GLN	HB3	2.102	0.002	2
491	?	51	GLN	CG	34.011	0.001	1
492	?	51	GLN	HG2	2.281	0.002	2
493	?	51	GLN	HG3	2.315	0.004	2
494	?	52	THR	N	115.406	0.012	1
495	?	52	THR	H	7.711	0.012	1
496	?	52	THR	CA	68.064	0.032	1
497	?	52	THR	HA	3.337	0.008	1
498	?	52	THR	CB	68.078	0.038	1
499	?	52	THR	HB	3.851	0.162	1
500	?	52	THR	HG21	0.783	0.007	1
501	?	52	THR	HG22	0.783	0.007	1
502	?	52	THR	HG23	0.783	0.007	1
503	?	52	THR	CG2	22.950	0.022	1
504	?	53	LEU	N	119.013	0.016	1
505	?	53	LEU	H	8.088	0.009	1
506	?	53	LEU	CA	58.518	0.022	1
507	?	53	LEU	HA	3.567	0.007	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	?	53	LEU	CB	42.223	0.059	1
509	?	53	LEU	HB2	1.119	0.004	2
510	?	53	LEU	HB3	1.799	0.012	2
511	?	53	LEU	CG	26.644	0.008	1
512	?	53	LEU	HG	0.655	0.003	1
513	?	53	LEU	HD11	0.644	0.003	2
514	?	53	LEU	HD12	0.644	0.003	2
515	?	53	LEU	HD13	0.644	0.003	2
516	?	53	LEU	HD21	0.644	0.003	2
517	?	53	LEU	HD22	0.644	0.003	2
518	?	53	LEU	HD23	0.644	0.003	2
519	?	53	LEU	CD1	25.128	0.031	1
520	?	54	SER	N	114.299	0.003	1
521	?	54	SER	H	8.250	0.006	1
522	?	54	SER	CA	61.723	0.011	1
523	?	54	SER	HA	4.018	0.009	1
524	?	54	SER	CB	62.447	0.010	1
525	?	55	GLN	N	118.442	0.145	1
526	?	55	GLN	H	7.875	0.013	1
527	?	55	GLN	CA	58.328	0.005	1
528	?	55	GLN	HA	3.875	0.010	1
529	?	55	GLN	CB	29.193	0.003	1
530	?	55	GLN	HB2	1.808	0.002	2
531	?	55	GLN	HB3	1.992	0.001	2
532	?	55	GLN	CG	33.851	0.002	1
533	?	55	GLN	HG2	2.323	0.003	2
534	?	55	GLN	HG3	2.505	0.003	2
535	?	56	LEU	N	119.587	0.020	1
536	?	56	LEU	H	8.259	0.007	1
537	?	56	LEU	CA	57.531	0.038	1
538	?	56	LEU	HA	3.667	0.016	1
539	?	56	LEU	CB	39.881	0.015	1
540	?	56	LEU	HB2	-0.229	0.004	2
541	?	56	LEU	HB3	1.128	0.006	2
542	?	56	LEU	CG	25.632	0.018	1
543	?	56	LEU	HG	0.109	0.005	1
544	?	56	LEU	HD11	0.101	0.004	2
545	?	56	LEU	HD12	0.101	0.004	2
546	?	56	LEU	HD13	0.101	0.004	2
547	?	56	LEU	HD21	0.338	0.006	2
548	?	56	LEU	HD22	0.338	0.006	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	?	56	LEU	HD23	0.338	0.006	2
550	?	56	LEU	CD1	25.469	0.000	1
551	?	56	LEU	CD2	23.216	0.022	1
552	?	57	THR	N	110.745	0.047	1
553	?	57	THR	H	7.962	0.010	1
554	?	57	THR	CA	65.352	0.019	1
555	?	57	THR	HA	3.885	0.007	1
556	?	57	THR	CB	68.888	0.023	1
557	?	57	THR	HB	3.748	0.010	1
558	?	57	THR	HG21	0.366	0.006	1
559	?	57	THR	HG22	0.366	0.006	1
560	?	57	THR	HG23	0.366	0.006	1
561	?	57	THR	CG2	20.546	0.004	1
562	?	58	LYS	N	121.897	0.012	1
563	?	58	LYS	H	7.177	0.010	1
564	?	58	LYS	CA	58.001	0.006	1
565	?	58	LYS	HA	3.999	0.010	1
566	?	58	LYS	CB	32.323	0.031	1
567	?	58	LYS	HB2	1.725	0.002	2
568	?	58	LYS	HB3	1.854	0.002	2
569	?	58	LYS	CG	25.500	0.002	1
570	?	58	LYS	HG2	1.343	0.002	2
571	?	58	LYS	HG3	1.509	0.002	2
572	?	58	LYS	CD	29.160	0.002	1
573	?	58	LYS	HD2	1.453	0.002	2
574	?	58	LYS	HD3	1.525	0.002	2
575	?	58	LYS	CE	42.159	0.002	1
576	?	58	LYS	HE2	2.802	0.005	2
577	?	58	LYS	HE3	2.922	0.004	2
578	?	59	LEU	N	116.504	0.014	1
579	?	59	LEU	H	7.276	0.018	1
580	?	59	LEU	CA	56.516	0.021	1
581	?	59	LEU	HA	4.047	0.011	1
582	?	59	LEU	CB	41.814	0.014	1
583	?	59	LEU	HB2	1.267	0.005	2
584	?	59	LEU	HB3	2.003	0.006	2
585	?	59	LEU	CG	26.045	0.003	1
586	?	59	LEU	HG	1.841	0.006	1
587	?	59	LEU	HD11	0.666	0.010	2
588	?	59	LEU	HD12	0.666	0.010	2
589	?	59	LEU	HD13	0.666	0.010	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	?	59	LEU	HD21	0.669	0.009	2
591	?	59	LEU	HD22	0.669	0.009	2
592	?	59	LEU	HD23	0.669	0.009	2
593	?	59	LEU	CD1	21.800	0.008	1
594	?	59	LEU	CD2	25.501	0.018	1
595	?	60	GLY	N	103.900	0.001	1
596	?	60	GLY	H	7.587	0.010	1
597	?	60	GLY	CA	46.663	0.042	1
598	?	60	GLY	HA2	3.875	0.014	2
599	?	60	GLY	HA3	3.875	0.014	2
600	?	61	LYS	N	119.837	0.044	1
601	?	61	LYS	H	8.256	0.008	1
602	?	61	LYS	CA	54.203	0.000	1
603	?	61	LYS	CB	32.633	0.000	1
604	?	62	PRO	CD	49.780	0.004	1
605	?	62	PRO	CA	62.639	0.008	1
606	?	62	PRO	HA	4.336	0.006	1
607	?	62	PRO	CB	32.148	0.001	1
608	?	62	PRO	HB2	1.747	0.001	2
609	?	62	PRO	HB3	2.161	0.001	2
610	?	62	PRO	CG	27.169	0.003	1
611	?	62	PRO	HG2	1.905	0.001	2
612	?	62	PRO	HG3	1.905	0.001	2
613	?	62	PRO	HD2	3.502	0.005	2
614	?	62	PRO	HD3	3.502	0.005	2
615	?	63	PHE	N	124.100	0.001	1
616	?	63	PHE	H	8.086	0.007	1
617	?	63	PHE	CA	57.697	0.020	1
618	?	63	PHE	HA	4.711	0.032	1
619	?	63	PHE	CB	42.821	0.002	1
620	?	63	PHE	HB2	1.931	0.002	2
621	?	63	PHE	HB3	2.177	0.001	2
622	?	63	PHE	CD1	132.023	0.000	1
623	?	63	PHE	HD1	6.676	0.004	1
624	?	63	PHE	HD2	6.676	0.004	1
625	?	64	LYS	N	116.605	0.024	1
626	?	64	LYS	H	8.642	0.010	1
627	?	64	LYS	CA	55.933	0.001	1
628	?	64	LYS	HA	4.631	0.000	1
629	?	65	TYR	N	115.600	0.001	1
630	?	65	TYR	H	8.896	0.010	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	?	65	TYR	CA	56.638	0.073	1
632	?	65	TYR	HA	6.286	0.016	1
633	?	65	TYR	CB	44.652	0.008	1
634	?	65	TYR	HB2	2.448	0.009	2
635	?	65	TYR	HB3	2.795	0.007	2
636	?	66	ILE	N	121.323	0.027	1
637	?	66	ILE	H	8.749	0.012	1
638	?	66	ILE	CA	60.749	0.032	1
639	?	66	ILE	HA	4.401	0.008	1
640	?	66	ILE	CB	41.979	0.014	1
641	?	66	ILE	HB	1.387	0.005	1
642	?	66	ILE	HG21	-0.278	0.004	1
643	?	66	ILE	HG22	-0.278	0.004	1
644	?	66	ILE	HG23	-0.278	0.004	1
645	?	66	ILE	CG2	16.581	0.028	1
646	?	66	ILE	CG1	28.031	0.009	1
647	?	66	ILE	HG12	0.892	0.004	2
648	?	66	ILE	HG13	1.207	0.002	2
649	?	66	ILE	HD11	0.560	0.006	1
650	?	66	ILE	HD12	0.560	0.006	1
651	?	66	ILE	HD13	0.560	0.006	1
652	?	66	ILE	CD1	15.545	0.491	1
653	?	67	VAL	N	125.399	0.016	1
654	?	67	VAL	H	8.397	0.007	1
655	?	67	VAL	CA	60.526	0.021	1
656	?	67	VAL	HA	5.258	0.010	1
657	?	67	VAL	CB	35.976	0.035	1
658	?	67	VAL	HB	1.597	0.009	1
659	?	67	VAL	HG11	0.710	0.005	2
660	?	67	VAL	HG12	0.710	0.005	2
661	?	67	VAL	HG13	0.710	0.005	2
662	?	67	VAL	HG21	0.780	0.001	2
663	?	67	VAL	HG22	0.780	0.001	2
664	?	67	VAL	HG23	0.780	0.001	2
665	?	67	VAL	CG1	21.543	0.007	1
666	?	67	VAL	CG2	22.515	0.002	1
667	?	68	THR	N	116.302	0.008	1
668	?	68	THR	H	9.103	0.012	1
669	?	68	THR	CA	59.125	0.066	1
670	?	68	THR	HA	5.175	0.011	1
671	?	68	THR	CB	71.016	0.071	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	?	68	THR	HB	4.281	0.011	1
673	?	68	THR	HG21	1.144	0.004	1
674	?	68	THR	HG22	1.144	0.004	1
675	?	68	THR	HG23	1.144	0.004	1
676	?	68	THR	CG2	20.989	0.012	1
677	?	69	CYS	N	122.348	0.059	1
678	?	69	CYS	H	9.162	0.084	1
679	?	69	CYS	CA	57.261	0.055	1
680	?	69	CYS	HA	5.173	0.010	1
681	?	69	CYS	CB	30.475	0.149	1
682	?	69	CYS	HB2	2.580	0.104	2
683	?	69	CYS	HB3	2.797	0.051	2
684	?	70	VAL	N	130.904	0.011	1
685	?	70	VAL	H	8.965	0.008	1
686	?	70	VAL	CA	60.733	0.053	1
687	?	70	VAL	HA	4.882	0.015	1
688	?	70	VAL	CB	35.229	0.022	1
689	?	70	VAL	HB	2.125	0.024	1
690	?	70	VAL	HG11	0.898	0.002	2
691	?	70	VAL	HG12	0.898	0.002	2
692	?	70	VAL	HG13	0.898	0.002	2
693	?	70	VAL	HG21	1.004	0.012	2
694	?	70	VAL	HG22	1.004	0.012	2
695	?	70	VAL	HG23	1.004	0.012	2
696	?	70	VAL	CG1	21.439	0.009	1
697	?	70	VAL	CG2	21.439	0.009	1
698	?	71	ILE	N	125.698	0.004	1
699	?	71	ILE	H	9.613	0.008	1
700	?	71	ILE	CA	61.064	0.033	1
701	?	71	ILE	HA	5.185	0.009	1
702	?	71	ILE	CB	41.823	0.032	1
703	?	71	ILE	HB	1.559	0.010	1
704	?	71	ILE	HG21	1.020	0.003	1
705	?	71	ILE	HG22	1.020	0.003	1
706	?	71	ILE	HG23	1.020	0.003	1
707	?	71	ILE	CG2	17.817	0.026	1
708	?	71	ILE	CG1	29.204	0.011	1
709	?	71	ILE	HG12	0.987	0.004	2
710	?	71	ILE	HG13	1.692	0.002	2
711	?	71	ILE	HD11	0.855	0.010	1
712	?	71	ILE	HD12	0.855	0.010	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	?	71	ILE	HD13	0.855	0.010	1
714	?	71	ILE	CD1	14.021	0.028	1
715	?	72	MET	N	126.397	0.007	1
716	?	72	MET	H	8.807	0.003	1
717	?	72	MET	CA	53.131	0.013	1
718	?	72	MET	HA	5.327	0.005	1
719	?	72	MET	CB	31.704	0.005	1
720	?	72	MET	CG	31.543	0.000	1
721	?	72	MET	CE	18.280	0.000	1
722	?	73	GLN	N	127.607	0.025	1
723	?	73	GLN	H	8.272	0.003	1
724	?	73	GLN	CA	55.677	0.054	1
725	?	73	GLN	HA	3.941	0.006	1
726	?	73	GLN	CB	28.737	0.019	1
727	?	73	GLN	HB2	1.847	0.001	2
728	?	73	GLN	HB3	1.923	0.001	2
729	?	73	GLN	CG	34.039	0.002	1
730	?	73	GLN	HG2	2.209	0.003	2
731	?	73	GLN	HG3	2.209	0.003	2
732	?	74	LYS	N	127.268	0.044	1
733	?	74	LYS	H	8.067	0.006	1
734	?	74	LYS	CA	57.002	0.002	1
735	?	74	LYS	HA	4.250	0.000	1
736	?	74	LYS	CB	33.821	0.000	1
737	?	75	ASN	H	8.053	0.000	1
738	?	75	ASN	CA	53.989	0.010	1
739	?	75	ASN	HA	4.473	0.008	1
740	?	75	ASN	CB	41.190	0.001	1
741	?	75	ASN	HB2	2.462	0.017	2
742	?	75	ASN	HB3	2.548	0.015	2
743	?	76	GLY	N	105.197	0.006	1
744	?	76	GLY	H	7.979	0.006	1
745	?	76	GLY	CA	45.310	0.010	1
746	?	76	GLY	HA2	3.582	0.004	2
747	?	76	GLY	HA3	3.582	0.004	2
748	?	77	ALA	N	123.500	0.001	1
749	?	77	ALA	H	7.669	0.008	1
750	?	77	ALA	CA	52.040	0.043	1
751	?	77	ALA	HA	4.290	0.009	1
752	?	77	ALA	HB1	1.459	0.006	1
753	?	77	ALA	HB2	1.459	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	?	77	ALA	HB3	1.459	0.006	1
755	?	77	ALA	CB	19.532	0.007	1
756	?	78	GLY	N	109.300	0.000	1
757	?	78	GLY	H	8.425	0.005	1
758	?	78	GLY	CA	45.041	0.017	1
759	?	78	GLY	HA2	3.827	0.005	2
760	?	78	GLY	HA3	3.827	0.005	2
761	?	79	LEU	CA	54.264	0.060	1
762	?	79	LEU	HA	4.924	0.014	1
763	?	79	LEU	CB	44.995	0.008	1
764	?	79	LEU	HB2	1.453	0.010	2
765	?	79	LEU	HB3	1.917	0.002	2
766	?	79	LEU	CG	27.924	0.041	1
767	?	79	LEU	HD11	0.752	0.003	2
768	?	79	LEU	HD12	0.752	0.003	2
769	?	79	LEU	HD13	0.752	0.003	2
770	?	79	LEU	HD21	0.899	0.004	2
771	?	79	LEU	HD22	0.899	0.004	2
772	?	79	LEU	HD23	0.899	0.004	2
773	?	79	LEU	CD1	26.023	0.038	1
774	?	79	LEU	CD2	23.244	0.032	1
775	?	80	HIS	N	124.868	0.043	1
776	?	80	HIS	H	8.764	0.002	1
777	?	80	HIS	CA	59.357	0.000	1
778	?	81	THR	N	113.256	0.867	1
779	?	81	THR	H	8.847	0.542	1
780	?	81	THR	CA	59.448	0.033	1
781	?	81	THR	HA	5.935	0.011	1
782	?	81	THR	CB	71.886	0.083	1
783	?	81	THR	HB	4.276	0.005	1
784	?	81	THR	HG21	1.104	0.014	1
785	?	81	THR	HG22	1.104	0.014	1
786	?	81	THR	HG23	1.104	0.014	1
787	?	81	THR	CG2	22.348	0.009	1
788	?	82	ALA	N	122.627	0.163	1
789	?	82	ALA	H	9.006	0.015	1
790	?	82	ALA	CA	51.249	0.054	1
791	?	82	ALA	HA	5.563	0.009	1
792	?	82	ALA	HB1	1.248	0.006	1
793	?	82	ALA	HB2	1.248	0.006	1
794	?	82	ALA	HB3	1.248	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	?	82	ALA	CB	22.716	0.014	1
796	?	83	SER	N	112.176	0.142	1
797	?	83	SER	H	8.630	0.024	1
798	?	83	SER	CA	57.062	0.023	1
799	?	83	SER	HA	5.458	0.011	1
800	?	83	SER	CB	67.000	0.001	1
801	?	83	SER	HB2	3.863	0.007	2
802	?	83	SER	HB3	3.980	0.013	2
803	?	84	SER	N	111.500	0.000	1
804	?	84	SER	H	8.523	0.011	1
805	?	84	SER	CA	56.853	0.019	1
806	?	84	SER	HA	4.332	0.012	1
807	?	84	SER	CB	63.176	0.004	1
808	?	84	SER	HB2	3.044	0.003	2
809	?	84	SER	HB3	4.023	0.005	2
810	?	85	CYS	N	115.201	0.003	1
811	?	85	CYS	H	7.801	0.006	1
812	?	85	CYS	CA	54.392	0.116	1
813	?	85	CYS	HA	5.271	0.010	1
814	?	85	CYS	CB	33.183	0.025	1
815	?	85	CYS	HB2	2.123	0.008	2
816	?	85	CYS	HB3	2.830	0.005	2
817	?	86	PHE	N	124.294	0.020	1
818	?	86	PHE	H	9.337	0.008	1
819	?	86	PHE	CA	57.497	0.027	1
820	?	86	PHE	HA	5.209	0.009	1
821	?	86	PHE	CB	41.402	0.005	1
822	?	86	PHE	HB2	2.939	0.004	2
823	?	86	PHE	HB3	3.146	0.021	2
824	?	87	TRP	N	122.505	0.012	1
825	?	87	TRP	H	8.987	0.013	1
826	?	87	TRP	CA	54.516	0.007	1
827	?	87	TRP	HA	5.348	0.011	1
828	?	87	TRP	CB	31.542	0.002	1
829	?	87	TRP	HB2	2.844	0.002	2
830	?	87	TRP	HB3	3.221	0.001	2
831	?	87	TRP	NE1	127.605	0.034	1
832	?	87	TRP	HD1	7.393	0.000	1
833	?	87	TRP	CZ3	124.085	0.021	1
834	?	87	TRP	CZ2	114.590	0.017	1
835	?	87	TRP	HE1	10.017	0.014	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	?	87	TRP	HZ3	7.016	0.003	1
837	?	87	TRP	CH2	122.397	0.006	1
838	?	87	TRP	HZ2	7.437	0.005	1
839	?	87	TRP	HH2	7.014	0.008	1
840	?	88	ASP	N	119.500	0.001	1
841	?	88	ASP	H	8.577	0.005	1
842	?	88	ASP	CA	52.307	0.094	1
843	?	88	ASP	HA	4.998	0.005	1
844	?	88	ASP	CB	41.355	0.047	1
845	?	88	ASP	HB2	1.923	0.006	2
846	?	88	ASP	HB3	2.930	0.010	2
847	?	89	SER	N	121.024	0.041	1
848	?	89	SER	H	8.700	0.008	1
849	?	89	SER	CA	60.399	0.034	1
850	?	89	SER	HA	4.693	0.010	1
851	?	89	SER	CB	63.253	0.006	1
852	?	89	SER	HB2	3.591	0.009	2
853	?	89	SER	HB3	3.970	0.000	2
854	?	90	SER	N	117.053	0.058	1
855	?	90	SER	H	8.644	0.007	1
856	?	90	SER	CA	60.749	0.040	1
857	?	90	SER	HA	4.315	0.008	1
858	?	90	SER	CB	63.593	0.100	1
859	?	90	SER	HB2	3.899	0.005	2
860	?	90	SER	HB3	3.899	0.005	2
861	?	91	THR	N	109.501	0.002	1
862	?	91	THR	H	6.874	0.010	1
863	?	91	THR	CA	62.234	0.055	1
864	?	91	THR	HA	4.455	0.007	1
865	?	91	THR	CB	71.447	0.025	1
866	?	91	THR	HB	4.067	0.007	1
867	?	91	THR	HG21	0.930	0.013	1
868	?	91	THR	HG22	0.930	0.013	1
869	?	91	THR	HG23	0.930	0.013	1
870	?	91	THR	CG2	20.694	0.009	1
871	?	92	ASP	N	124.875	0.088	1
872	?	92	ASP	H	7.741	0.017	1
873	?	92	ASP	CA	54.146	0.010	1
874	?	92	ASP	HA	4.729	0.006	1
875	?	92	ASP	CB	41.261	0.006	1
876	?	92	ASP	HB2	2.333	0.011	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	?	92	ASP	HB3	2.807	0.010	2
878	?	93	GLY	N	105.149	0.048	1
879	?	93	GLY	H	7.956	0.008	1
880	?	93	GLY	CA	45.353	0.004	1
881	?	93	GLY	HA2	4.022	0.008	2
882	?	93	GLY	HA3	4.022	0.008	2
883	?	94	SER	N	111.497	0.008	1
884	?	94	SER	H	8.233	0.008	1
885	?	94	SER	CA	56.572	0.007	1
886	?	94	SER	HA	5.168	0.013	1
887	?	94	SER	CB	68.249	0.092	1
888	?	94	SER	HB2	3.365	0.007	2
889	?	94	SER	HB3	3.848	0.003	2
890	?	95	CYS	N	116.903	0.013	1
891	?	95	CYS	H	8.706	0.009	1
892	?	95	CYS	CA	57.240	0.040	1
893	?	95	CYS	HA	4.731	0.004	1
894	?	95	CYS	CB	30.801	0.040	1
895	?	95	CYS	HB2	2.668	0.004	2
896	?	95	CYS	HB3	2.825	0.006	2
897	?	96	THR	N	122.094	0.008	1
898	?	96	THR	H	8.561	0.013	1
899	?	96	THR	CA	62.371	0.091	1
900	?	96	THR	HA	5.108	0.011	1
901	?	96	THR	CB	71.331	0.028	1
902	?	96	THR	HB	3.674	0.007	1
903	?	96	THR	HG21	0.814	0.004	1
904	?	96	THR	HG22	0.814	0.004	1
905	?	96	THR	HG23	0.814	0.004	1
906	?	96	THR	CG2	20.452	0.048	1
907	?	97	VAL	N	129.451	0.031	1
908	?	97	VAL	H	9.449	0.006	1
909	?	97	VAL	CA	61.431	0.022	1
910	?	97	VAL	HA	4.218	0.009	1
911	?	97	VAL	CB	35.321	0.027	1
912	?	97	VAL	HB	1.739	0.010	1
913	?	97	VAL	HG11	0.802	0.007	2
914	?	97	VAL	HG12	0.802	0.007	2
915	?	97	VAL	HG13	0.802	0.007	2
916	?	97	VAL	HG21	0.846	0.004	2
917	?	97	VAL	HG22	0.846	0.004	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	?	97	VAL	HG23	0.846	0.004	2
919	?	97	VAL	CG1	21.497	0.002	1
920	?	97	VAL	CG2	21.497	0.002	1
921	?	98	ARG	N	125.494	0.013	1
922	?	98	ARG	H	8.455	0.009	1
923	?	98	ARG	CA	54.035	0.021	1
924	?	98	ARG	HA	5.079	0.008	1
925	?	98	ARG	CB	32.611	0.011	1
926	?	98	ARG	HB2	1.718	0.001	2
927	?	98	ARG	HB3	1.718	0.001	2
928	?	98	ARG	CG	26.701	0.003	1
929	?	98	ARG	HG2	1.479	0.003	2
930	?	98	ARG	HG3	1.591	0.001	2
931	?	98	ARG	CD	43.912	0.002	1
932	?	98	ARG	HD2	2.930	0.004	2
933	?	98	ARG	HD3	3.042	0.003	2
934	?	99	TRP	N	128.068	0.045	1
935	?	99	TRP	H	9.304	0.007	1
936	?	99	TRP	CA	57.786	0.010	1
937	?	99	TRP	HA	4.726	0.002	1
938	?	99	TRP	CB	34.452	0.007	1
939	?	99	TRP	HB2	2.865	0.006	2
940	?	99	TRP	HB3	2.951	0.014	2
941	?	99	TRP	CE3	124.209	0.009	1
942	?	99	TRP	NE1	130.099	0.011	1
943	?	99	TRP	HD1	7.204	0.000	1
944	?	99	TRP	HE3	7.431	0.007	1
945	?	99	TRP	CZ3	124.600	0.000	1
946	?	99	TRP	CZ2	113.896	0.006	1
947	?	99	TRP	HE1	10.368	0.014	1
948	?	99	TRP	HZ3	6.981	0.000	1
949	?	99	TRP	CH2	123.904	0.006	1
950	?	99	TRP	HZ2	7.317	0.004	1
951	?	99	TRP	HH2	7.086	0.005	1
952	?	100	GLU	N	123.736	0.044	1
953	?	100	GLU	H	7.468	0.008	1
954	?	100	GLU	CA	54.811	0.008	1
955	?	100	GLU	HA	5.045	0.008	1
956	?	100	GLU	CB	35.406	0.004	1
957	?	100	GLU	HB2	1.879	0.009	2
958	?	100	GLU	HB3	1.976	0.005	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	?	101	ASN	N	122.099	0.037	1
960	?	101	ASN	H	8.380	0.004	1
961	?	101	ASN	CA	50.652	0.010	1
962	?	101	ASN	HA	4.287	0.011	1
963	?	101	ASN	CB	38.872	0.003	1
964	?	101	ASN	HB2	2.490	0.005	2
965	?	101	ASN	HB3	3.302	0.000	2
966	?	102	LYS	H	8.342	0.002	1
967	?	102	LYS	CA	60.312	0.009	1
968	?	102	LYS	HA	3.881	0.006	1
969	?	102	LYS	CB	32.669	0.006	1
970	?	102	LYS	HB2	1.802	0.002	2
971	?	102	LYS	HB3	1.848	0.001	2
972	?	102	LYS	CG	25.483	0.006	1
973	?	102	LYS	HG2	1.357	0.005	2
974	?	102	LYS	HG3	1.468	0.003	2
975	?	102	LYS	CD	29.142	0.004	1
976	?	102	LYS	HD2	1.620	0.004	2
977	?	102	LYS	HD3	1.620	0.004	2
978	?	102	LYS	CE	42.261	0.004	1
979	?	102	LYS	HE2	2.909	0.001	2
980	?	102	LYS	HE3	2.909	0.001	2
981	?	103	THR	N	101.100	0.001	1
982	?	103	THR	H	7.679	0.011	1
983	?	103	THR	CA	61.688	0.007	1
984	?	103	THR	HA	4.778	0.005	1
985	?	103	THR	CB	72.207	0.006	1
986	?	103	THR	HB	4.664	0.001	1
987	?	103	THR	HG21	1.264	0.005	1
988	?	103	THR	HG22	1.264	0.005	1
989	?	103	THR	HG23	1.264	0.005	1
990	?	103	THR	CG2	21.567	0.004	1
991	?	104	MET	N	122.951	0.059	1
992	?	104	MET	H	8.292	0.007	1
993	?	104	MET	CA	56.176	0.028	1
994	?	104	MET	HA	5.267	0.012	1
995	?	104	MET	CB	39.103	0.014	1
996	?	104	MET	HB2	1.928	0.002	2
997	?	104	MET	HB3	2.178	0.006	2
998	?	104	MET	CG	34.124	0.010	1
999	?	104	MET	HG2	2.478	0.001	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1000	?	104	MET	HG3	2.560	0.000	2
1001	?	105	TYR	N	118.100	0.000	1
1002	?	105	TYR	H	8.489	0.013	1
1003	?	105	TYR	CA	55.711	0.010	1
1004	?	105	TYR	HA	5.098	0.010	1
1005	?	106	CYS	N	123.098	0.007	1
1006	?	106	CYS	H	9.406	0.009	1
1007	?	106	CYS	CA	56.629	0.039	1
1008	?	106	CYS	HA	5.783	0.015	1
1009	?	106	CYS	CB	30.569	0.009	1
1010	?	106	CYS	HB2	2.585	0.014	2
1011	?	106	CYS	HB3	2.727	0.001	2
1012	?	107	ILE	N	126.943	0.044	1
1013	?	107	ILE	H	9.102	0.010	1
1014	?	107	ILE	CA	60.058	0.095	1
1015	?	107	ILE	HA	5.180	0.007	1
1016	?	107	ILE	CB	42.360	0.007	1
1017	?	107	ILE	HB	1.545	0.002	1
1018	?	107	ILE	HG21	0.725	0.001	1
1019	?	107	ILE	HG22	0.725	0.001	1
1020	?	107	ILE	HG23	0.725	0.001	1
1021	?	107	ILE	CG2	18.096	0.003	1
1022	?	107	ILE	CG1	28.479	0.002	1
1023	?	107	ILE	HG12	0.944	0.000	2
1024	?	107	ILE	HG13	1.641	0.003	2
1025	?	107	ILE	HD11	0.833	0.002	1
1026	?	107	ILE	HD12	0.833	0.002	1
1027	?	107	ILE	HD13	0.833	0.002	1
1028	?	107	ILE	CD1	16.358	0.018	1
1029	?	108	VAL	N	129.881	0.012	1
1030	?	108	VAL	H	9.051	0.004	1
1031	?	108	VAL	CA	60.085	0.044	1
1032	?	108	VAL	HA	5.145	0.008	1
1033	?	108	VAL	CB	34.564	0.080	1
1034	?	108	VAL	HB	1.605	0.003	1
1035	?	108	VAL	HG11	0.754	0.012	2
1036	?	108	VAL	HG12	0.754	0.012	2
1037	?	108	VAL	HG13	0.754	0.012	2
1038	?	108	VAL	HG21	0.799	0.006	2
1039	?	108	VAL	HG22	0.799	0.006	2
1040	?	108	VAL	HG23	0.799	0.006	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1041	?	108	VAL	CG1	21.507	0.007	1
1042	?	108	VAL	CG2	24.024	0.027	1
1043	?	109	SER	N	121.903	0.025	1
1044	?	109	SER	H	8.572	0.009	1
1045	?	109	SER	CA	56.795	0.036	1
1046	?	109	SER	HA	5.308	0.009	1
1047	?	109	SER	CB	65.089	0.022	1
1048	?	109	SER	HB2	3.336	0.004	2
1049	?	109	SER	HB3	3.731	0.010	2
1050	?	110	ALA	N	124.803	0.018	1
1051	?	110	ALA	H	8.646	0.006	1
1052	?	110	ALA	CA	49.635	0.029	1
1053	?	110	ALA	HA	5.406	0.011	1
1054	?	110	ALA	HB1	0.976	0.009	1
1055	?	110	ALA	HB2	0.976	0.009	1
1056	?	110	ALA	HB3	0.976	0.009	1
1057	?	110	ALA	CB	21.718	0.008	1
1058	?	111	PHE	N	119.496	0.013	1
1059	?	111	PHE	H	9.329	0.005	1
1060	?	111	PHE	CA	56.064	0.034	1
1061	?	111	PHE	HA	4.952	0.011	1
1062	?	111	PHE	CB	42.618	0.007	1
1063	?	111	PHE	HB2	2.806	0.005	2
1064	?	111	PHE	HB3	2.861	0.022	2
1065	?	112	GLY	N	109.702	0.006	1
1066	?	112	GLY	H	8.954	0.009	1
1067	?	112	GLY	CA	45.208	0.006	1
1068	?	112	GLY	HA2	2.893	0.005	2
1069	?	112	GLY	HA3	2.893	0.005	2
1070	?	113	LEU	N	126.100	0.001	1
1071	?	113	LEU	H	8.927	0.007	1
1072	?	113	LEU	CA	52.470	0.010	1
1073	?	113	LEU	HA	4.768	0.010	1
1074	?	113	LEU	CB	42.493	0.044	1
1075	?	113	LEU	HB2	1.518	0.016	2
1076	?	113	LEU	HB3	1.706	0.073	2
1077	?	113	LEU	CG	28.922	0.030	1
1078	?	113	LEU	HG	1.842	0.004	1
1079	?	113	LEU	HD11	0.988	0.005	2
1080	?	113	LEU	HD12	0.988	0.005	2
1081	?	113	LEU	HD13	0.988	0.005	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1082	?	113	LEU	HD21	1.090	0.008	2
1083	?	113	LEU	HD22	1.090	0.008	2
1084	?	113	LEU	HD23	1.090	0.008	2
1085	?	113	LEU	CD1	26.614	0.022	1
1086	?	113	LEU	CD2	24.900	0.006	1
1087	?	114	SER	N	119.998	0.005	1
1088	?	114	SER	H	9.275	0.007	1
1089	?	114	SER	CA	58.523	0.044	1
1090	?	114	SER	HA	3.618	0.007	1
1091	?	114	SER	CB	63.185	0.031	1
1092	?	114	SER	HB2	3.503	0.012	2
1093	?	114	SER	HB3	3.606	0.003	2
1094	?	115	ILE	N	122.165	0.044	1
1095	?	115	ILE	H	7.680	0.010	1
1096	?	115	ILE	CA	62.011	0.010	1
1097	?	115	ILE	HA	4.072	0.018	1
1098	?	115	ILE	CB	38.580	0.008	1
1099	?	115	ILE	HB	1.748	0.022	1
1100	?	115	ILE	HG21	0.786	0.007	1
1101	?	115	ILE	HG22	0.786	0.007	1
1102	?	115	ILE	HG23	0.786	0.007	1
1103	?	115	ILE	CG2	18.215	0.022	1
1104	?	115	ILE	CG1	26.909	0.003	1
1105	?	115	ILE	HG12	1.071	0.004	2
1106	?	115	ILE	HG13	1.329	0.005	2
1107	?	115	ILE	HD11	0.768	0.005	1
1108	?	115	ILE	HD12	0.768	0.005	1
1109	?	115	ILE	HD13	0.768	0.005	1
1110	?	115	ILE	CD1	12.595	0.000	1
1111	?	116	GLY	N	110.200	0.002	1
1112	?	116	GLY	H	8.148	0.012	1
1113	?	116	GLY	CA	45.001	0.007	1
1114	?	116	GLY	HA2	3.863	0.014	2
1115	?	116	GLY	HA3	3.863	0.014	2
1116	?	117	GLY	N	108.682	0.035	1
1117	?	117	GLY	H	8.179	0.003	1
1118	?	117	GLY	CA	45.146	0.004	1
1119	?	117	GLY	HA2	3.849	0.005	2
1120	?	117	GLY	HA3	3.849	0.005	2
1121	?	118	GLY	N	108.703	0.006	1
1122	?	118	GLY	H	8.318	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1123	?	118	GLY	CA	45.220	0.010	1
1124	?	118	GLY	HA2	3.830	0.006	2
1125	?	118	GLY	HA3	3.830	0.006	2
1126	?	119	SER	N	115.703	0.006	1
1127	?	119	SER	H	8.290	0.006	1
1128	?	119	SER	CA	58.512	0.008	1
1129	?	119	SER	HA	4.698	0.001	1
1130	?	119	SER	CB	63.727	0.002	1
1131	?	119	SER	HB2	3.750	0.001	2
1132	?	119	SER	HB3	3.793	0.001	2
1133	?	120	GLY	N	110.798	0.007	1
1134	?	120	GLY	H	8.430	0.007	1
1135	?	120	GLY	CA	45.477	0.004	1
1136	?	121	GLN	N	119.803	0.007	1
1137	?	121	GLN	H	8.039	0.006	1
1138	?	121	GLN	CA	56.000	0.004	1
1139	?	121	GLN	HA	4.259	0.012	1
1140	?	121	GLN	CB	29.113	0.010	1
1141	?	121	GLN	HB2	1.849	0.003	2
1142	?	121	GLN	HB3	2.034	0.002	2
1143	?	121	GLN	CG	33.839	0.001	1
1144	?	121	GLN	HG2	2.210	0.001	2
1145	?	121	GLN	HG3	2.226	0.006	2
1146	?	122	SER	H	7.992	0.001	1
1147	?	122	SER	CA	58.271	0.008	1
1148	?	122	SER	HA	4.402	0.001	1
1149	?	122	SER	CB	63.843	0.044	1
1150	?	122	SER	HB2	3.742	0.001	2
1151	?	122	SER	HB3	3.789	0.001	2
1152	?	123	GLY	N	110.673	0.045	1
1153	?	123	GLY	H	7.948	0.008	1
1154	?	123	GLY	CA	44.376	0.004	1
1155	?	123	GLY	HA2	3.973	0.009	2
1156	?	123	GLY	HA3	4.031	0.007	2
1157	?	124	PRO	CD	49.771	0.004	1
1158	?	124	PRO	CA	62.777	0.024	1
1159	?	124	PRO	HA	4.344	0.007	1
1160	?	124	PRO	CB	31.960	0.004	1
1161	?	124	PRO	HB2	1.756	0.002	2
1162	?	124	PRO	HB3	2.161	0.004	2
1163	?	124	PRO	CG	27.162	0.005	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1164	?	124	PRO	HG2	1.907	0.005	2
1165	?	124	PRO	HG3	1.907	0.005	2
1166	?	124	PRO	HD2	3.505	0.005	2
1167	?	124	PRO	HD3	3.505	0.005	2
1168	?	125	ILE	N	122.096	0.098	1
1169	?	125	ILE	H	8.178	0.007	1
1170	?	125	ILE	CA	61.233	0.034	1
1171	?	125	ILE	HA	3.960	0.011	1
1172	?	125	ILE	CB	38.590	0.010	1
1173	?	125	ILE	HB	1.667	0.008	1
1174	?	125	ILE	HG21	0.723	0.001	1
1175	?	125	ILE	HG22	0.723	0.001	1
1176	?	125	ILE	HG23	0.723	0.001	1
1177	?	125	ILE	CG2	17.358	0.004	1
1178	?	125	ILE	CG1	27.406	0.002	1
1179	?	125	ILE	HG12	1.029	0.002	2
1180	?	125	ILE	HG13	1.388	0.003	2
1181	?	125	ILE	HD11	0.723	0.006	1
1182	?	125	ILE	HD12	0.723	0.006	1
1183	?	125	ILE	HD13	0.723	0.006	1
1184	?	125	ILE	CD1	13.496	0.006	1
1185	?	126	LYS	N	128.101	0.004	1
1186	?	126	LYS	H	8.351	0.007	1
1187	?	126	LYS	CA	55.220	0.004	1
1188	?	126	LYS	HA	4.352	0.009	1
1189	?	126	LYS	CB	32.660	0.003	1
1190	?	126	LYS	HB2	1.600	0.003	2
1191	?	126	LYS	HB3	1.733	0.006	2
1192	?	126	LYS	CG	24.511	0.002	1
1193	?	126	LYS	HG2	1.252	0.003	2
1194	?	126	LYS	HG3	1.328	0.002	2
1195	?	126	LYS	CD	29.087	0.005	1
1196	?	126	LYS	HD2	1.609	0.002	2
1197	?	126	LYS	HD3	1.609	0.002	2
1198	?	126	LYS	CE	42.157	0.004	1
1199	?	126	LYS	HE2	2.921	0.005	2
1200	?	126	LYS	HE3	2.921	0.005	2
1201	?	127	LEU	N	124.204	0.010	1
1202	?	127	LEU	H	8.003	0.009	1
1203	?	127	LEU	CA	53.071	0.047	1
1204	?	127	LEU	HA	4.531	0.008	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1205	?	127	LEU	CB	43.054	0.019	1
1206	?	127	LEU	HB2	0.245	0.005	2
1207	?	127	LEU	HB3	1.264	0.007	2
1208	?	127	LEU	CG	26.903	0.016	1
1209	?	127	LEU	HG	1.345	0.007	1
1210	?	127	LEU	HD11	0.427	0.074	2
1211	?	127	LEU	HD12	0.427	0.074	2
1212	?	127	LEU	HD13	0.427	0.074	2
1213	?	127	LEU	HD21	0.712	0.003	2
1214	?	127	LEU	HD22	0.712	0.003	2
1215	?	127	LEU	HD23	0.712	0.003	2
1216	?	127	LEU	CD1	24.088	0.012	1
1217	?	127	LEU	CD2	26.396	0.009	1
1218	?	128	GLY	N	107.602	0.006	1
1219	?	128	GLY	H	8.713	0.006	1
1220	?	128	GLY	CA	45.075	0.007	1
1221	?	128	GLY	HA2	3.962	0.008	2
1222	?	128	GLY	HA3	4.348	0.013	2
1223	?	129	MET	N	118.699	0.002	1
1224	?	129	MET	H	8.710	0.007	1
1225	?	129	MET	CA	54.607	0.005	1
1226	?	129	MET	HA	5.272	0.005	1
1227	?	129	MET	CB	33.189	0.003	1
1228	?	129	MET	HB2	2.096	0.003	2
1229	?	129	MET	HB3	2.096	0.003	2
1230	?	129	MET	CG	33.183	0.011	1
1231	?	129	MET	HG2	2.828	0.004	2
1232	?	129	MET	HG3	2.828	0.004	2
1233	?	130	ALA	N	127.483	0.045	1
1234	?	130	ALA	H	8.395	0.007	1
1235	?	130	ALA	CA	50.938	0.214	1
1236	?	130	ALA	HA	4.539	0.012	1
1237	?	130	ALA	HB1	0.986	0.006	1
1238	?	130	ALA	HB2	0.986	0.006	1
1239	?	130	ALA	HB3	0.986	0.006	1
1240	?	130	ALA	CB	20.278	0.007	1
1241	?	131	LYS	N	119.543	0.082	1
1242	?	131	LYS	H	8.242	0.005	1
1243	?	131	LYS	CA	56.390	0.021	1
1244	?	131	LYS	HA	4.258	0.006	1
1245	?	131	LYS	CB	32.611	0.004	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1246	?	131	LYS	HB2	1.776	0.002	2
1247	?	131	LYS	HB3	1.776	0.002	2
1248	?	131	LYS	CG	24.669	0.002	1
1249	?	131	LYS	HG2	1.430	0.001	2
1250	?	131	LYS	HG3	1.471	0.002	2
1251	?	131	LYS	CD	29.431	0.004	1
1252	?	131	LYS	HD2	1.684	0.001	2
1253	?	131	LYS	HD3	1.684	0.001	2
1254	?	131	LYS	CE	42.320	0.005	1
1255	?	131	LYS	HE2	3.003	0.004	2
1256	?	131	LYS	HE3	3.003	0.004	2
1257	?	132	ILE	N	125.690	0.031	1
1258	?	132	ILE	H	8.710	0.009	1
1259	?	132	ILE	CA	60.985	0.030	1
1260	?	132	ILE	HA	4.398	0.011	1
1261	?	132	ILE	CB	37.980	0.040	1
1262	?	132	ILE	HB	1.895	0.006	1
1263	?	132	ILE	HG21	0.789	0.006	1
1264	?	132	ILE	HG22	0.789	0.006	1
1265	?	132	ILE	HG23	0.789	0.006	1
1266	?	132	ILE	CG2	18.017	0.029	1
1267	?	132	ILE	CG1	27.996	0.008	1
1268	?	132	ILE	HG12	1.140	0.006	2
1269	?	132	ILE	HG13	1.608	0.009	2
1270	?	132	ILE	HD11	0.833	0.006	1
1271	?	132	ILE	HD12	0.833	0.006	1
1272	?	132	ILE	HD13	0.833	0.006	1
1273	?	132	ILE	CD1	13.419	0.023	1
1274	?	133	THR	N	121.801	0.002	1
1275	?	133	THR	H	8.120	0.008	1
1276	?	133	THR	CA	62.713	0.043	1
1277	?	133	THR	HA	4.431	0.008	1
1278	?	133	THR	CB	69.734	0.122	1
1279	?	133	THR	HB	4.002	0.013	1
1280	?	133	THR	HG21	1.053	0.004	1
1281	?	133	THR	HG22	1.053	0.004	1
1282	?	133	THR	HG23	1.053	0.004	1
1283	?	133	THR	CG2	20.751	0.007	1
1284	?	134	GLN	N	127.560	0.052	1
1285	?	134	GLN	H	8.992	0.009	1
1286	?	134	GLN	CA	54.773	0.009	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1287	?	134	GLN	HA	5.184	0.012	1
1288	?	134	GLN	CB	33.049	0.002	1
1289	?	134	GLN	HB2	1.915	0.005	2
1290	?	134	GLN	HB3	2.017	0.002	2
1291	?	134	GLN	CG	34.929	0.003	1
1292	?	134	GLN	HG2	2.108	0.001	2
1293	?	134	GLN	HG3	2.213	0.003	2
1294	?	135	VAL	N	123.297	0.031	1
1295	?	135	VAL	H	8.198	0.005	1
1296	?	135	VAL	CA	62.589	0.005	1
1297	?	135	VAL	HA	3.953	0.006	1
1298	?	135	VAL	CB	33.443	0.004	1
1299	?	135	VAL	HB	1.971	0.001	1
1300	?	135	VAL	HG11	0.524	0.008	2
1301	?	135	VAL	HG12	0.524	0.008	2
1302	?	135	VAL	HG13	0.524	0.008	2
1303	?	135	VAL	HG21	0.630	0.008	2
1304	?	135	VAL	HG22	0.630	0.008	2
1305	?	135	VAL	HG23	0.630	0.008	2
1306	?	135	VAL	CG1	22.002	0.003	1
1307	?	135	VAL	CG2	22.000	0.005	1
1308	?	136	ASP	N	126.000	0.001	1
1309	?	136	ASP	H	8.279	0.008	1
1310	?	136	ASP	CA	53.298	0.014	1
1311	?	136	ASP	HA	5.167	0.010	1
1312	?	136	ASP	CB	45.261	0.035	1
1313	?	136	ASP	HB2	2.482	0.007	2
1314	?	136	ASP	HB3	2.583	0.008	2
1315	?	137	PHE	N	125.108	0.016	1
1316	?	137	PHE	H	8.877	0.013	1
1317	?	137	PHE	CA	54.589	0.009	1
1318	?	137	PHE	HA	4.857	0.011	1
1319	?	137	PHE	CB	40.000	0.000	1
1320	?	137	PHE	HB2	2.465	0.000	2
1321	?	137	PHE	HB3	2.625	0.012	2
1322	?	140	ARG	H	8.334	0.001	1
1323	?	140	ARG	CA	55.768	0.003	1
1324	?	140	ARG	HA	4.282	0.001	1
1325	?	140	ARG	CB	32.003	0.003	1
1326	?	140	ARG	HB2	1.643	0.001	2
1327	?	140	ARG	HB3	1.740	0.001	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1328	?	140	ARG	CG	26.610	0.001	1
1329	?	140	ARG	HG2	1.517	0.004	2
1330	?	140	ARG	HG3	1.567	0.001	2
1331	?	140	ARG	CD	43.669	0.002	1
1332	?	140	ARG	HD2	3.090	0.003	2
1333	?	140	ARG	HD3	3.090	0.003	2
1334	?	141	GLU	N	121.715	0.037	1
1335	?	141	GLU	H	8.347	0.007	1
1336	?	141	GLU	CA	56.256	0.004	1
1337	?	141	GLU	HA	4.155	0.004	1
1338	?	141	GLU	CB	30.248	0.003	1
1339	?	141	GLU	HB2	1.832	0.003	2
1340	?	141	GLU	HB3	1.935	0.002	2
1341	?	141	GLU	CG	33.873	0.004	1
1342	?	141	GLU	HG2	2.238	0.004	2
1343	?	141	GLU	HG3	2.238	0.004	2
1344	?	142	ILE	N	123.235	0.037	1
1345	?	142	ILE	H	8.222	0.006	1
1346	?	142	ILE	CA	61.094	0.096	1
1347	?	142	ILE	HA	4.076	0.011	1
1348	?	142	ILE	CB	38.162	0.007	1
1349	?	142	ILE	HB	1.781	0.010	1
1350	?	142	ILE	HG21	0.782	0.005	1
1351	?	142	ILE	HG22	0.782	0.005	1
1352	?	142	ILE	HG23	0.782	0.005	1
1353	?	142	ILE	CG2	17.471	0.008	1
1354	?	142	ILE	CG1	27.166	0.011	1
1355	?	142	ILE	HG12	1.069	0.007	2
1356	?	142	ILE	HG13	1.335	0.006	2
1357	?	142	ILE	HD11	0.698	0.003	1
1358	?	142	ILE	HD12	0.698	0.003	1
1359	?	142	ILE	HD13	0.698	0.003	1
1360	?	142	ILE	CD1	12.383	0.006	1
1361	?	143	VAL	N	128.733	0.024	1
1362	?	143	VAL	H	7.591	0.006	1
1363	?	143	VAL	CA	63.391	0.021	1
1364	?	143	VAL	HA	3.968	0.008	1
1365	?	143	VAL	CB	33.328	0.015	1
1366	?	143	VAL	HB	1.977	0.003	1
1367	?	143	VAL	HG11	0.798	0.008	2
1368	?	143	VAL	HG12	0.798	0.008	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1369	?	143	VAL	HG13	0.798	0.008	2
1370	?	143	VAL	HG21	0.798	0.008	2
1371	?	143	VAL	HG22	0.798	0.008	2
1372	?	143	VAL	HG23	0.798	0.008	2
1373	?	143	VAL	CG1	20.160	0.003	1
1374	?	143	VAL	CG2	21.631	0.003	1
1375	?	144	GLY	CA	45.216	0.002	1
1376	?	145	SER	N	115.595	0.028	1
1377	?	145	SER	H	8.229	0.002	1
1378	?	145	SER	CA	58.516	0.046	1
1379	?	145	SER	CB	63.991	0.026	1
1380	?	146	MET	N	121.950	0.001	1
1381	?	146	MET	H	8.563	0.003	1
1382	?	146	MET	CA	56.091	0.024	1
1383	?	146	MET	HA	4.401	0.012	1
1384	?	146	MET	CB	32.280	0.004	1
1385	?	146	MET	HB2	1.951	0.004	2
1386	?	146	MET	HB3	2.038	0.001	2
1387	?	146	MET	CG	31.978	0.000	1
1388	?	146	MET	HG2	2.469	0.005	2
1389	?	146	MET	HG3	2.545	0.005	2
1390	?	147	GLU	N	120.702	0.010	1
1391	?	147	GLU	H	8.323	0.006	1
1392	?	147	GLU	CA	57.223	0.006	1
1393	?	147	GLU	HA	4.132	0.011	1
1394	?	147	GLU	CB	29.703	0.006	1
1395	?	147	GLU	HB2	1.893	0.004	2
1396	?	147	GLU	HB3	1.975	0.006	2
1397	?	147	GLU	CG	36.514	0.000	1
1398	?	147	GLU	HG2	2.192	0.008	2
1399	?	147	GLU	HG3	2.192	0.008	2
1400	?	148	ASP	N	120.565	0.087	1
1401	?	148	ASP	H	8.081	0.008	1
1402	?	148	ASP	CA	54.544	0.005	1
1403	?	148	ASP	HA	4.455	0.009	1
1404	?	148	ASP	CB	40.913	0.003	1
1405	?	148	ASP	HB2	2.471	0.006	2
1406	?	148	ASP	HB3	2.556	0.008	2
1407	?	149	TYR	N	120.512	0.011	1
1408	?	149	TYR	H	7.914	0.006	1
1409	?	149	TYR	CA	58.290	0.039	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1410	?	149	TYR	HA	4.427	0.014	1
1411	?	149	TYR	CB	38.581	0.016	1
1412	?	149	TYR	HB2	2.910	0.008	2
1413	?	149	TYR	HB3	2.952	0.012	2
1414	?	149	TYR	CD1	133.082	0.025	1
1415	?	149	TYR	HD1	7.088	0.011	1
1416	?	149	TYR	CE1	118.139	0.095	1
1417	?	149	TYR	HE1	6.849	0.034	1
1418	?	149	TYR	HE2	6.849	0.034	1
1419	?	149	TYR	HD2	7.088	0.011	1
1420	?	150	GLN	N	122.489	0.010	1
1421	?	150	GLN	H	8.021	0.017	1
1422	?	150	GLN	CA	55.568	0.013	1
1423	?	150	GLN	HA	4.153	0.010	1
1424	?	150	GLN	CB	29.380	0.011	1
1425	?	150	GLN	HB2	1.836	0.003	2
1426	?	150	GLN	HB3	1.934	0.003	2
1427	?	150	GLN	CG	33.655	0.018	1
1428	?	150	GLN	HG2	2.195	0.003	2
1429	?	150	GLN	HG3	2.195	0.003	2
1430	?	151	ALA	N	125.378	0.013	1
1431	?	151	ALA	H	8.105	0.009	1
1432	?	151	ALA	CA	52.531	0.021	1
1433	?	151	ALA	HA	4.150	0.008	1
1434	?	151	ALA	HB1	1.328	0.009	1
1435	?	151	ALA	HB2	1.328	0.009	1
1436	?	151	ALA	HB3	1.328	0.009	1
1437	?	151	ALA	CB	19.172	0.033	1
1438	?	152	ALA	N	123.529	0.033	1
1439	?	152	ALA	H	8.151	0.005	1
1440	?	152	ALA	CA	52.690	0.057	1
1441	?	152	ALA	HA	4.206	0.013	1
1442	?	152	ALA	HB1	1.349	0.016	1
1443	?	152	ALA	HB2	1.349	0.016	1
1444	?	152	ALA	HB3	1.349	0.016	1
1445	?	152	ALA	CB	19.133	0.043	1
1446	?	153	GLU	N	119.820	0.092	1
1447	?	153	GLU	H	8.371	0.007	1
1448	?	153	GLU	CA	57.420	0.003	1
1449	?	153	GLU	HA	4.712	0.013	1
1450	?	153	GLU	CB	29.895	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1451	?	153	GLU	HB2	1.886	0.004	2
1452	?	153	GLU	HB3	1.962	0.012	2
1453	?	153	GLU	HG2	2.211	0.003	2
1454	?	153	GLU	HG3	2.211	0.003	2
1455	?	154	GLU	N	119.997	0.006	1
1456	?	154	GLU	H	8.371	0.006	1
1457	?	154	GLU	CA	57.481	0.006	1
1458	?	154	GLU	HA	4.689	0.015	1
1459	?	154	GLU	CB	29.961	0.035	1
1460	?	154	GLU	HB2	1.975	0.002	2
1461	?	154	GLU	HB3	2.032	0.013	2
1462	?	154	GLU	CG	36.518	0.004	1
1463	?	154	GLU	HG2	2.212	0.004	2
1464	?	154	GLU	HG3	2.212	0.004	2
1465	?	155	THR	N	110.500	0.002	1
1466	?	155	THR	H	7.866	0.017	1
1467	?	155	THR	CA	60.996	0.040	1
1468	?	155	THR	HA	4.304	0.007	1
1469	?	155	THR	CB	69.488	0.030	1
1470	?	155	THR	HB	4.276	0.010	1
1471	?	155	THR	HG21	1.076	0.005	1
1472	?	155	THR	HG22	1.076	0.005	1
1473	?	155	THR	HG23	1.076	0.005	1
1474	?	155	THR	CG2	21.662	0.000	1
1475	?	156	ALA	N	124.206	0.015	1
1476	?	156	ALA	H	7.713	0.006	1
1477	?	156	ALA	CA	51.835	0.061	1
1478	?	156	ALA	HA	4.561	0.009	1
1479	?	156	ALA	HB1	1.311	0.003	1
1480	?	156	ALA	HB2	1.311	0.003	1
1481	?	156	ALA	HB3	1.311	0.003	1
1482	?	156	ALA	CB	20.491	0.046	1
1483	?	157	PHE	N	122.698	0.005	1
1484	?	157	PHE	H	8.738	0.007	1
1485	?	157	PHE	CA	57.978	0.024	1
1486	?	157	PHE	HA	3.885	0.013	1
1487	?	157	PHE	CB	38.187	0.008	1
1488	?	157	PHE	HB2	2.345	0.009	2
1489	?	157	PHE	HB3	2.832	0.004	2
1490	?	157	PHE	HD1	6.654	0.011	1
1491	?	157	PHE	HD2	6.654	0.011	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1492	?	158	VAL	N	131.417	0.231	1
1493	?	158	VAL	H	8.427	0.009	1
1494	?	158	VAL	CA	61.627	0.007	1
1495	?	158	VAL	HA	4.061	0.013	1
1496	?	158	VAL	CB	31.345	0.003	1
1497	?	158	VAL	HB	1.764	0.027	1
1498	?	158	VAL	HG11	0.731	0.009	2
1499	?	158	VAL	HG12	0.731	0.009	2
1500	?	158	VAL	HG13	0.731	0.009	2
1501	?	158	VAL	HG21	0.746	0.006	2
1502	?	158	VAL	HG22	0.746	0.006	2
1503	?	158	VAL	HG23	0.746	0.006	2
1504	?	158	VAL	CG1	20.304	0.000	1
1505	?	158	VAL	CG2	21.137	0.028	1
1506	?	159	VAL	N	129.080	0.019	1
1507	?	159	VAL	H	8.648	0.013	1
1508	?	159	VAL	CA	67.617	0.038	1
1509	?	159	VAL	HA	3.184	0.010	1
1510	?	159	VAL	CB	31.763	0.081	1
1511	?	159	VAL	HB	2.062	0.010	1
1512	?	159	VAL	HG11	1.009	0.003	2
1513	?	159	VAL	HG12	1.009	0.003	2
1514	?	159	VAL	HG13	1.009	0.003	2
1515	?	159	VAL	HG21	1.241	0.007	2
1516	?	159	VAL	HG22	1.241	0.007	2
1517	?	159	VAL	HG23	1.241	0.007	2
1518	?	159	VAL	CG1	21.134	0.005	1
1519	?	159	VAL	CG2	22.605	0.009	1
1520	?	160	ASP	N	118.704	0.013	1
1521	?	160	ASP	H	8.787	0.012	1
1522	?	160	ASP	CA	57.623	0.021	1
1523	?	160	ASP	HA	4.250	0.010	1
1524	?	160	ASP	CB	40.218	0.034	1
1525	?	160	ASP	HB2	2.411	0.010	2
1526	?	160	ASP	HB3	2.493	0.014	2
1527	?	161	GLU	N	118.212	0.031	1
1528	?	161	GLU	H	6.604	0.010	1
1529	?	161	GLU	CA	58.106	0.017	1
1530	?	161	GLU	HA	3.979	0.010	1
1531	?	161	GLU	CB	30.248	0.044	1
1532	?	161	GLU	HB2	1.887	0.003	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1533	?	161	GLU	HB3	1.971	0.017	2
1534	?	161	GLU	CG	36.410	0.005	1
1535	?	161	GLU	HG2	1.951	0.018	2
1536	?	161	GLU	HG3	1.951	0.018	2
1537	?	162	VAL	N	120.306	0.019	1
1538	?	162	VAL	H	7.375	0.012	1
1539	?	162	VAL	CA	66.491	0.034	1
1540	?	162	VAL	HA	3.178	0.018	1
1541	?	162	VAL	CB	31.181	0.059	1
1542	?	162	VAL	HB	1.626	0.004	1
1543	?	162	VAL	HG11	0.101	0.007	2
1544	?	162	VAL	HG12	0.101	0.007	2
1545	?	162	VAL	HG13	0.101	0.007	2
1546	?	162	VAL	HG21	0.617	0.011	2
1547	?	162	VAL	HG22	0.617	0.011	2
1548	?	162	VAL	HG23	0.617	0.011	2
1549	?	162	VAL	CG1	21.089	0.023	1
1550	?	162	VAL	CG2	21.751	0.001	1
1551	?	163	SER	N	115.603	0.010	1
1552	?	163	SER	H	8.881	0.007	1
1553	?	163	SER	CA	62.098	0.003	1
1554	?	163	SER	HA	3.857	0.012	1
1555	?	163	SER	CB	62.750	0.004	1
1556	?	163	SER	HB2	3.783	0.009	2
1557	?	163	SER	HB3	3.783	0.009	2
1558	?	164	ASN	N	118.310	0.009	1
1559	?	164	ASN	H	7.465	0.011	1
1560	?	164	ASN	CA	56.603	0.004	1
1561	?	164	ASN	HA	4.361	0.009	1
1562	?	164	ASN	CB	38.135	0.002	1
1563	?	164	ASN	HB2	2.746	0.011	2
1564	?	164	ASN	HB3	2.746	0.011	2
1565	?	165	ILE	N	121.294	0.017	1
1566	?	165	ILE	H	7.170	0.009	1
1567	?	165	ILE	CA	65.363	0.052	1
1568	?	165	ILE	HA	3.534	0.012	1
1569	?	165	ILE	CB	38.649	0.035	1
1570	?	165	ILE	HB	1.859	0.009	1
1571	?	165	ILE	HG21	0.773	0.006	1
1572	?	165	ILE	HG22	0.773	0.006	1
1573	?	165	ILE	HG23	0.773	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1574	?	165	ILE	CG2	17.784	0.056	1
1575	?	165	ILE	CG1	29.826	0.035	1
1576	?	165	ILE	HG12	0.889	0.009	2
1577	?	165	ILE	HG13	1.698	0.006	2
1578	?	165	ILE	HD11	0.566	0.005	1
1579	?	165	ILE	HD12	0.566	0.005	1
1580	?	165	ILE	HD13	0.566	0.005	1
1581	?	165	ILE	CD1	14.302	0.027	1
1582	?	166	VAL	N	120.404	0.009	1
1583	?	166	VAL	H	8.223	0.010	1
1584	?	166	VAL	CA	66.371	0.158	1
1585	?	166	VAL	HA	3.396	0.008	1
1586	?	166	VAL	CB	31.457	0.007	1
1587	?	166	VAL	HB	2.017	0.004	1
1588	?	166	VAL	HG11	0.649	0.002	2
1589	?	166	VAL	HG12	0.649	0.002	2
1590	?	166	VAL	HG13	0.649	0.002	2
1591	?	166	VAL	HG21	0.732	0.021	2
1592	?	166	VAL	HG22	0.732	0.021	2
1593	?	166	VAL	HG23	0.732	0.021	2
1594	?	166	VAL	CG1	22.349	0.004	1
1595	?	166	VAL	CG2	22.972	0.006	1
1596	?	167	LYS	N	118.400	0.000	1
1597	?	167	LYS	H	8.447	0.013	1
1598	?	167	LYS	CA	60.848	0.011	1
1599	?	167	LYS	HA	3.585	0.006	1
1600	?	167	LYS	CB	32.480	0.028	1
1601	?	167	LYS	HB2	1.833	0.005	2
1602	?	167	LYS	HB3	1.884	0.003	2
1603	?	167	LYS	CG	26.503	0.007	1
1604	?	167	LYS	HG2	1.368	0.005	2
1605	?	167	LYS	HG3	1.582	0.002	2
1606	?	167	LYS	CD	29.702	0.023	1
1607	?	167	LYS	HD2	1.671	0.005	2
1608	?	167	LYS	HD3	1.671	0.005	2
1609	?	167	LYS	CE	42.212	0.008	1
1610	?	167	LYS	HE2	2.916	0.002	2
1611	?	167	LYS	HE3	2.916	0.002	2
1612	?	168	GLU	N	117.300	0.001	1
1613	?	168	GLU	H	7.734	0.006	1
1614	?	168	GLU	CA	59.153	0.025	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1615	?	168	GLU	HA	3.874	0.008	1
1616	?	168	GLU	CB	28.760	0.064	1
1617	?	168	GLU	HB2	1.894	0.007	2
1618	?	168	GLU	HB3	1.960	0.002	2
1619	?	168	GLU	CG	36.534	0.002	1
1620	?	168	GLU	HG2	2.068	0.007	2
1621	?	168	GLU	HG3	2.264	0.002	2
1622	?	169	ALA	N	123.785	0.065	1
1623	?	169	ALA	H	7.900	0.008	1
1624	?	169	ALA	CA	55.149	0.064	1
1625	?	169	ALA	HA	3.877	0.012	1
1626	?	169	ALA	HB1	1.325	0.007	1
1627	?	169	ALA	HB2	1.325	0.007	1
1628	?	169	ALA	HB3	1.325	0.007	1
1629	?	169	ALA	CB	18.581	0.041	1
1630	?	170	ILE	N	118.299	0.080	1
1631	?	170	ILE	H	8.093	0.013	1
1632	?	170	ILE	CA	65.948	0.036	1
1633	?	170	ILE	HA	2.981	0.010	1
1634	?	170	ILE	CB	39.039	0.024	1
1635	?	170	ILE	HB	1.126	0.009	1
1636	?	170	ILE	HG21	-0.801	0.007	1
1637	?	170	ILE	HG22	-0.801	0.007	1
1638	?	170	ILE	HG23	-0.801	0.007	1
1639	?	170	ILE	CG2	15.045	0.017	1
1640	?	170	ILE	CG1	28.509	0.010	1
1641	?	170	ILE	HG12	0.333	0.002	2
1642	?	170	ILE	HG13	1.619	0.004	2
1643	?	170	ILE	HD11	0.385	0.008	1
1644	?	170	ILE	HD12	0.385	0.008	1
1645	?	170	ILE	HD13	0.385	0.008	1
1646	?	170	ILE	CD1	14.758	0.181	1
1647	?	171	GLU	N	117.899	0.004	1
1648	?	171	GLU	H	7.839	0.008	1
1649	?	171	GLU	CA	59.407	0.015	1
1650	?	171	GLU	HA	3.452	0.011	1
1651	?	171	GLU	CB	28.717	0.051	1
1652	?	171	GLU	HB2	1.881	0.002	2
1653	?	171	GLU	HB3	1.922	0.002	2
1654	?	171	GLU	CG	36.084	0.025	1
1655	?	171	GLU	HG2	2.060	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1656	?	171	GLU	HG3	2.267	0.002	2
1657	?	172	SER	N	112.399	0.003	1
1658	?	172	SER	H	8.034	0.010	1
1659	?	172	SER	CA	60.842	0.014	1
1660	?	172	SER	HA	3.950	0.007	1
1661	?	172	SER	CB	63.090	0.008	1
1662	?	172	SER	HB2	3.795	0.002	2
1663	?	172	SER	HB3	3.795	0.002	2
1664	?	173	ALA	N	121.292	0.018	1
1665	?	173	ALA	H	7.457	0.010	1
1666	?	173	ALA	CA	54.053	0.036	1
1667	?	173	ALA	HA	4.083	0.008	1
1668	?	173	ALA	HB1	1.190	0.010	1
1669	?	173	ALA	HB2	1.190	0.010	1
1670	?	173	ALA	HB3	1.190	0.010	1
1671	?	173	ALA	CB	20.687	0.019	1
1672	?	174	ILE	N	110.000	0.001	1
1673	?	174	ILE	H	7.657	0.010	1
1674	?	174	ILE	CA	61.792	0.039	1
1675	?	174	ILE	HA	3.020	0.008	1
1676	?	174	ILE	CB	39.252	0.071	1
1677	?	174	ILE	HB	1.228	0.011	1
1678	?	174	ILE	HG21	0.159	0.002	1
1679	?	174	ILE	HG22	0.159	0.002	1
1680	?	174	ILE	HG23	0.159	0.002	1
1681	?	174	ILE	CG2	18.792	0.011	1
1682	?	174	ILE	CG1	26.322	0.012	1
1683	?	174	ILE	HG12	0.187	0.007	2
1684	?	174	ILE	HG13	0.561	0.007	2
1685	?	174	ILE	HD11	0.224	0.006	1
1686	?	174	ILE	HD12	0.224	0.006	1
1687	?	174	ILE	HD13	0.224	0.006	1
1688	?	174	ILE	CD1	13.974	0.021	1
1689	?	175	GLY	N	108.601	0.002	1
1690	?	175	GLY	H	7.334	0.008	1
1691	?	175	GLY	CA	47.499	0.016	1
1692	?	175	GLY	HA2	3.805	0.006	2
1693	?	175	GLY	HA3	3.805	0.006	2
1694	?	176	GLY	N	112.801	0.004	1
1695	?	176	GLY	H	8.865	0.052	1
1696	?	176	GLY	CA	45.058	0.022	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1697	?	176	GLY	HA2	3.975	0.012	2
1698	?	176	GLY	HA3	3.975	0.012	2
1699	?	177	ASN	N	118.507	0.025	1
1700	?	177	ASN	H	7.597	0.010	1
1701	?	177	ASN	CA	53.272	0.046	1
1702	?	177	ASN	HA	4.545	0.012	1
1703	?	177	ASN	CB	40.703	0.008	1
1704	?	177	ASN	HB2	2.009	0.006	2
1705	?	177	ASN	HB3	2.303	0.008	2
1706	?	178	ALA	N	121.309	0.015	1
1707	?	178	ALA	H	8.240	0.005	1
1708	?	178	ALA	CA	49.906	0.067	1
1709	?	178	ALA	HA	4.577	0.009	1
1710	?	178	ALA	HB1	1.403	0.009	1
1711	?	178	ALA	HB2	1.403	0.009	1
1712	?	178	ALA	HB3	1.403	0.009	1
1713	?	178	ALA	CB	20.169	0.008	1
1714	?	179	TYR	N	121.045	0.035	1
1715	?	179	TYR	H	8.687	0.014	1
1716	?	179	TYR	CA	62.433	0.044	1
1717	?	179	TYR	HA	4.050	0.009	1
1718	?	179	TYR	CB	38.698	0.018	1
1719	?	179	TYR	HB2	2.887	0.015	2
1720	?	179	TYR	HB3	3.022	0.014	2
1721	?	180	GLN	N	125.686	0.031	1
1722	?	180	GLN	H	5.502	0.013	1
1723	?	180	GLN	CA	54.825	0.005	1
1724	?	180	GLN	HA	4.232	0.007	1
1725	?	180	GLN	CB	31.901	0.002	1
1726	?	180	GLN	HB2	1.546	0.002	2
1727	?	180	GLN	HB3	1.773	0.002	2
1728	?	180	GLN	CG	33.820	0.003	1
1729	?	180	GLN	HG2	2.256	0.002	2
1730	?	180	GLN	HG3	2.348	0.001	2
1731	?	181	HIS	N	122.101	0.000	1
1732	?	181	HIS	H	8.371	0.000	1
1733	?	182	SER	CA	59.797	0.011	1
1734	?	182	SER	HA	3.806	0.006	1
1735	?	182	SER	CB	62.507	0.085	1
1736	?	182	SER	HB2	3.558	0.005	2
1737	?	182	SER	HB3	3.691	0.007	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1738	?	183	LYS	N	117.996	0.012	1
1739	?	183	LYS	H	6.530	0.021	1
1740	?	183	LYS	CA	55.415	0.005	1
1741	?	183	LYS	HA	3.949	0.012	1
1742	?	183	LYS	CB	34.043	0.005	1
1743	?	183	LYS	HB2	1.734	0.003	2
1744	?	183	LYS	HB3	1.734	0.003	2
1745	?	183	LYS	CG	24.750	0.005	1
1746	?	183	LYS	HG2	0.878	0.004	2
1747	?	183	LYS	HG3	0.878	0.004	2
1748	?	183	LYS	CD	28.781	0.002	1
1749	?	183	LYS	HD2	1.347	0.004	2
1750	?	183	LYS	HD3	1.487	0.003	2
1751	?	183	LYS	CE	42.271	0.003	1
1752	?	183	LYS	HE2	2.791	0.004	2
1753	?	183	LYS	HE3	2.791	0.004	2
1754	?	184	VAL	N	117.680	0.038	1
1755	?	184	VAL	H	6.430	0.010	1
1756	?	184	VAL	CA	64.678	0.033	1
1757	?	184	VAL	HA	3.117	0.012	1
1758	?	184	VAL	CB	30.501	0.008	1
1759	?	184	VAL	HB	1.105	0.009	1
1760	?	184	VAL	HG11	0.811	0.010	2
1761	?	184	VAL	HG12	0.811	0.010	2
1762	?	184	VAL	HG13	0.811	0.010	2
1763	?	184	VAL	HG21	0.037	0.011	2
1764	?	184	VAL	HG22	0.037	0.011	2
1765	?	184	VAL	HG23	0.037	0.011	2
1766	?	184	VAL	CG1	22.211	0.015	1
1767	?	184	VAL	CG2	18.322	0.040	1
1768	?	185	ASN	N	118.200	0.088	1
1769	?	185	ASN	H	7.835	0.008	1
1770	?	185	ASN	CA	55.696	0.008	1
1771	?	185	ASN	HA	4.430	0.009	1
1772	?	185	ASN	CB	37.472	0.009	1
1773	?	185	ASN	HB2	2.455	0.005	2
1774	?	185	ASN	HB3	2.515	0.012	2
1775	?	186	GLN	N	120.008	0.018	1
1776	?	186	GLN	H	7.423	0.009	1
1777	?	186	GLN	CA	57.807	0.005	1
1778	?	186	GLN	HA	4.000	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1779	?	186	GLN	CB	27.460	0.001	1
1780	?	186	GLN	HB2	1.948	0.004	2
1781	?	186	GLN	HB3	1.948	0.004	2
1782	?	187	TRP	H	7.398	0.006	1
1783	?	187	TRP	CA	58.520	0.006	1
1784	?	187	TRP	HA	4.458	0.006	1
1785	?	187	TRP	CB	28.481	0.035	1
1786	?	187	TRP	HB2	2.691	0.012	2
1787	?	187	TRP	HB3	3.359	0.013	2
1788	?	187	TRP	NE1	128.759	0.043	1
1789	?	187	TRP	HD1	7.117	0.001	1
1790	?	187	TRP	HE3	6.844	0.000	1
1791	?	187	TRP	CZ3	124.809	0.015	1
1792	?	187	TRP	CZ2	114.607	0.012	1
1793	?	187	TRP	HE1	9.989	0.008	1
1794	?	187	TRP	HZ3	6.923	0.002	1
1795	?	187	TRP	CH2	123.796	0.007	1
1796	?	187	TRP	HZ2	7.169	0.002	1
1797	?	187	TRP	HH2	7.433	0.009	1
1798	?	188	THR	N	109.998	0.008	1
1799	?	188	THR	H	8.485	0.011	1
1800	?	188	THR	CA	65.389	0.078	1
1801	?	188	THR	HA	3.835	0.010	1
1802	?	188	THR	CB	67.304	0.012	1
1803	?	188	THR	HB	3.961	0.011	1
1804	?	188	THR	HG21	1.223	0.006	1
1805	?	188	THR	HG22	1.223	0.006	1
1806	?	188	THR	HG23	1.223	0.006	1
1807	?	188	THR	CG2	23.069	0.017	1
1808	?	189	THR	N	117.101	0.002	1
1809	?	189	THR	H	7.076	0.015	1
1810	?	189	THR	CA	67.060	0.025	1
1811	?	189	THR	HA	3.486	0.011	1
1812	?	189	THR	CB	68.649	0.025	1
1813	?	189	THR	HB	4.135	0.011	1
1814	?	189	THR	HG21	1.096	0.009	1
1815	?	189	THR	HG22	1.096	0.009	1
1816	?	189	THR	HG23	1.096	0.009	1
1817	?	189	THR	CG2	21.604	0.008	1
1818	?	190	ASN	N	120.378	0.022	1
1819	?	190	ASN	H	8.316	0.005	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1820	?	190	ASN	CA	56.117	0.013	1
1821	?	190	ASN	HA	4.426	0.009	1
1822	?	190	ASN	CB	38.293	0.006	1
1823	?	190	ASN	HB2	2.778	0.017	2
1824	?	190	ASN	HB3	2.937	0.010	2
1825	?	191	VAL	N	119.914	0.023	1
1826	?	191	VAL	H	8.334	0.010	1
1827	?	191	VAL	CA	67.338	0.022	1
1828	?	191	VAL	HA	3.209	0.011	1
1829	?	191	VAL	CB	31.695	0.006	1
1830	?	191	VAL	HB	2.046	0.020	1
1831	?	191	VAL	HG11	0.554	0.004	2
1832	?	191	VAL	HG12	0.554	0.004	2
1833	?	191	VAL	HG13	0.554	0.004	2
1834	?	191	VAL	HG21	0.767	0.020	2
1835	?	191	VAL	HG22	0.767	0.020	2
1836	?	191	VAL	HG23	0.767	0.020	2
1837	?	191	VAL	CG1	21.999	0.004	1
1838	?	191	VAL	CG2	23.251	0.023	1
1839	?	192	VAL	N	120.000	0.097	1
1840	?	192	VAL	H	7.586	0.012	1
1841	?	192	VAL	CA	67.255	0.014	1
1842	?	192	VAL	HA	3.203	0.014	1
1843	?	192	VAL	CB	31.679	0.000	1
1844	?	192	VAL	HB	2.009	0.003	1
1845	?	192	VAL	HG11	0.638	0.011	2
1846	?	192	VAL	HG12	0.638	0.011	2
1847	?	192	VAL	HG13	0.638	0.011	2
1848	?	192	VAL	HG21	0.738	0.001	2
1849	?	192	VAL	HG22	0.738	0.001	2
1850	?	192	VAL	HG23	0.738	0.001	2
1851	?	192	VAL	CG1	21.150	0.002	1
1852	?	192	VAL	CG2	23.283	0.007	1
1853	?	193	GLU	N	118.710	0.030	1
1854	?	193	GLU	H	8.891	0.005	1
1855	?	193	GLU	CA	60.365	0.007	1
1856	?	193	GLU	HA	4.436	0.004	1
1857	?	193	GLU	CB	29.819	0.008	1
1858	?	194	GLN	N	119.000	0.000	1
1859	?	194	GLN	H	8.559	0.010	1
1860	?	194	GLN	CA	59.086	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1861	?	194	GLN	HA	3.967	0.006	1
1862	?	194	GLN	CB	28.152	0.002	1
1863	?	194	GLN	HB2	1.848	0.006	2
1864	?	194	GLN	HB3	2.102	0.002	2
1865	?	194	GLN	CG	34.011	0.001	1
1866	?	194	GLN	HG2	2.281	0.002	2
1867	?	194	GLN	HG3	2.315	0.004	2
1868	?	195	THR	N	115.406	0.012	1
1869	?	195	THR	H	7.711	0.012	1
1870	?	195	THR	CA	68.064	0.032	1
1871	?	195	THR	HA	3.337	0.008	1
1872	?	195	THR	CB	68.078	0.038	1
1873	?	195	THR	HB	3.851	0.162	1
1874	?	195	THR	HG21	0.783	0.007	1
1875	?	195	THR	HG22	0.783	0.007	1
1876	?	195	THR	HG23	0.783	0.007	1
1877	?	195	THR	CG2	22.950	0.022	1
1878	?	196	LEU	N	119.013	0.016	1
1879	?	196	LEU	H	8.088	0.009	1
1880	?	196	LEU	CA	58.518	0.022	1
1881	?	196	LEU	HA	3.567	0.007	1
1882	?	196	LEU	CB	42.223	0.059	1
1883	?	196	LEU	HB2	1.119	0.004	2
1884	?	196	LEU	HB3	1.799	0.012	2
1885	?	196	LEU	CG	26.644	0.008	1
1886	?	196	LEU	HG	0.655	0.003	1
1887	?	196	LEU	HD11	0.644	0.003	2
1888	?	196	LEU	HD12	0.644	0.003	2
1889	?	196	LEU	HD13	0.644	0.003	2
1890	?	196	LEU	HD21	0.644	0.003	2
1891	?	196	LEU	HD22	0.644	0.003	2
1892	?	196	LEU	HD23	0.644	0.003	2
1893	?	196	LEU	CD1	25.128	0.031	1
1894	?	197	SER	N	114.299	0.003	1
1895	?	197	SER	H	8.250	0.006	1
1896	?	197	SER	CA	61.723	0.011	1
1897	?	197	SER	HA	4.018	0.009	1
1898	?	197	SER	CB	62.447	0.010	1
1899	?	198	GLN	N	118.442	0.145	1
1900	?	198	GLN	H	7.875	0.013	1
1901	?	198	GLN	CA	58.328	0.005	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1902	?	198	GLN	HA	3.875	0.010	1
1903	?	198	GLN	CB	29.193	0.003	1
1904	?	198	GLN	HB2	1.808	0.002	2
1905	?	198	GLN	HB3	1.992	0.001	2
1906	?	198	GLN	CG	33.851	0.002	1
1907	?	198	GLN	HG2	2.323	0.003	2
1908	?	198	GLN	HG3	2.505	0.003	2
1909	?	199	LEU	N	119.587	0.020	1
1910	?	199	LEU	H	8.259	0.007	1
1911	?	199	LEU	CA	57.531	0.038	1
1912	?	199	LEU	HA	3.667	0.016	1
1913	?	199	LEU	CB	39.881	0.015	1
1914	?	199	LEU	HB2	-0.229	0.004	2
1915	?	199	LEU	HB3	1.128	0.006	2
1916	?	199	LEU	CG	25.632	0.018	1
1917	?	199	LEU	HG	0.109	0.005	1
1918	?	199	LEU	HD11	0.101	0.004	2
1919	?	199	LEU	HD12	0.101	0.004	2
1920	?	199	LEU	HD13	0.101	0.004	2
1921	?	199	LEU	HD21	0.338	0.006	2
1922	?	199	LEU	HD22	0.338	0.006	2
1923	?	199	LEU	HD23	0.338	0.006	2
1924	?	199	LEU	CD1	25.469	0.000	1
1925	?	199	LEU	CD2	23.216	0.022	1
1926	?	200	THR	N	110.745	0.047	1
1927	?	200	THR	H	7.962	0.010	1
1928	?	200	THR	CA	65.352	0.019	1
1929	?	200	THR	HA	3.885	0.007	1
1930	?	200	THR	CB	68.888	0.023	1
1931	?	200	THR	HB	3.748	0.010	1
1932	?	200	THR	HG21	0.366	0.006	1
1933	?	200	THR	HG22	0.366	0.006	1
1934	?	200	THR	HG23	0.366	0.006	1
1935	?	200	THR	CG2	20.546	0.004	1
1936	?	201	LYS	N	121.897	0.012	1
1937	?	201	LYS	H	7.177	0.010	1
1938	?	201	LYS	CA	58.001	0.006	1
1939	?	201	LYS	HA	3.999	0.010	1
1940	?	201	LYS	CB	32.323	0.031	1
1941	?	201	LYS	HB2	1.725	0.002	2
1942	?	201	LYS	HB3	1.854	0.002	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1943	?	201	LYS	CG	25.500	0.002	1
1944	?	201	LYS	HG2	1.343	0.002	2
1945	?	201	LYS	HG3	1.509	0.002	2
1946	?	201	LYS	CD	29.160	0.002	1
1947	?	201	LYS	HD2	1.453	0.002	2
1948	?	201	LYS	HD3	1.525	0.002	2
1949	?	201	LYS	CE	42.159	0.002	1
1950	?	201	LYS	HE2	2.802	0.005	2
1951	?	201	LYS	HE3	2.922	0.004	2
1952	?	202	LEU	N	116.504	0.014	1
1953	?	202	LEU	H	7.276	0.018	1
1954	?	202	LEU	CA	56.516	0.021	1
1955	?	202	LEU	HA	4.047	0.011	1
1956	?	202	LEU	CB	41.814	0.014	1
1957	?	202	LEU	HB2	1.267	0.005	2
1958	?	202	LEU	HB3	2.003	0.006	2
1959	?	202	LEU	CG	26.045	0.003	1
1960	?	202	LEU	HG	1.841	0.006	1
1961	?	202	LEU	HD11	0.666	0.010	2
1962	?	202	LEU	HD12	0.666	0.010	2
1963	?	202	LEU	HD13	0.666	0.010	2
1964	?	202	LEU	HD21	0.669	0.009	2
1965	?	202	LEU	HD22	0.669	0.009	2
1966	?	202	LEU	HD23	0.669	0.009	2
1967	?	202	LEU	CD1	21.800	0.008	1
1968	?	202	LEU	CD2	25.501	0.018	1
1969	?	203	GLY	N	103.900	0.001	1
1970	?	203	GLY	H	7.587	0.010	1
1971	?	203	GLY	CA	46.663	0.042	1
1972	?	203	GLY	HA2	3.875	0.014	2
1973	?	203	GLY	HA3	3.875	0.014	2
1974	?	204	LYS	N	119.837	0.044	1
1975	?	204	LYS	H	8.256	0.008	1
1976	?	204	LYS	CA	54.203	0.000	1
1977	?	204	LYS	CB	32.633	0.000	1
1978	?	205	PRO	CD	49.780	0.004	1
1979	?	205	PRO	CA	62.639	0.008	1
1980	?	205	PRO	HA	4.336	0.006	1
1981	?	205	PRO	CB	32.148	0.001	1
1982	?	205	PRO	HB2	1.747	0.001	2
1983	?	205	PRO	HB3	2.161	0.001	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1984	?	205	PRO	CG	27.169	0.003	1
1985	?	205	PRO	HG2	1.905	0.001	2
1986	?	205	PRO	HG3	1.905	0.001	2
1987	?	205	PRO	HD2	3.502	0.005	2
1988	?	205	PRO	HD3	3.502	0.005	2
1989	?	206	PHE	N	124.100	0.001	1
1990	?	206	PHE	H	8.086	0.007	1
1991	?	206	PHE	CA	57.697	0.020	1
1992	?	206	PHE	HA	4.711	0.032	1
1993	?	206	PHE	CB	42.821	0.002	1
1994	?	206	PHE	HB2	1.931	0.002	2
1995	?	206	PHE	HB3	2.177	0.001	2
1996	?	206	PHE	CD1	132.023	0.000	1
1997	?	206	PHE	HD1	6.676	0.004	1
1998	?	206	PHE	HD2	6.676	0.004	1
1999	?	207	LYS	N	116.605	0.024	1
2000	?	207	LYS	H	8.642	0.010	1
2001	?	207	LYS	CA	55.933	0.001	1
2002	?	207	LYS	HA	4.631	0.000	1
2003	?	208	TYR	N	115.600	0.001	1
2004	?	208	TYR	H	8.896	0.010	1
2005	?	208	TYR	CA	56.638	0.073	1
2006	?	208	TYR	HA	6.286	0.016	1
2007	?	208	TYR	CB	44.652	0.008	1
2008	?	208	TYR	HB2	2.448	0.009	2
2009	?	208	TYR	HB3	2.795	0.007	2
2010	?	209	ILE	N	121.323	0.027	1
2011	?	209	ILE	H	8.749	0.012	1
2012	?	209	ILE	CA	60.749	0.032	1
2013	?	209	ILE	HA	4.401	0.008	1
2014	?	209	ILE	CB	41.979	0.014	1
2015	?	209	ILE	HB	1.387	0.005	1
2016	?	209	ILE	HG21	-0.278	0.004	1
2017	?	209	ILE	HG22	-0.278	0.004	1
2018	?	209	ILE	HG23	-0.278	0.004	1
2019	?	209	ILE	CG2	16.581	0.028	1
2020	?	209	ILE	CG1	28.031	0.009	1
2021	?	209	ILE	HG12	0.892	0.004	2
2022	?	209	ILE	HG13	1.207	0.002	2
2023	?	209	ILE	HD11	0.560	0.006	1
2024	?	209	ILE	HD12	0.560	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2025	?	209	ILE	HD13	0.560	0.006	1
2026	?	209	ILE	CD1	15.545	0.491	1
2027	?	210	VAL	N	125.399	0.016	1
2028	?	210	VAL	H	8.397	0.007	1
2029	?	210	VAL	CA	60.526	0.021	1
2030	?	210	VAL	HA	5.258	0.010	1
2031	?	210	VAL	CB	35.976	0.035	1
2032	?	210	VAL	HB	1.597	0.009	1
2033	?	210	VAL	HG11	0.710	0.005	2
2034	?	210	VAL	HG12	0.710	0.005	2
2035	?	210	VAL	HG13	0.710	0.005	2
2036	?	210	VAL	HG21	0.780	0.001	2
2037	?	210	VAL	HG22	0.780	0.001	2
2038	?	210	VAL	HG23	0.780	0.001	2
2039	?	210	VAL	CG1	21.543	0.007	1
2040	?	210	VAL	CG2	22.515	0.002	1
2041	?	211	THR	N	116.302	0.008	1
2042	?	211	THR	H	9.103	0.012	1
2043	?	211	THR	CA	59.125	0.066	1
2044	?	211	THR	HA	5.175	0.011	1
2045	?	211	THR	CB	71.016	0.071	1
2046	?	211	THR	HB	4.281	0.011	1
2047	?	211	THR	HG21	1.144	0.004	1
2048	?	211	THR	HG22	1.144	0.004	1
2049	?	211	THR	HG23	1.144	0.004	1
2050	?	211	THR	CG2	20.989	0.012	1
2051	?	212	CYS	N	122.348	0.059	1
2052	?	212	CYS	H	9.162	0.084	1
2053	?	212	CYS	CA	57.261	0.055	1
2054	?	212	CYS	HA	5.173	0.010	1
2055	?	212	CYS	CB	30.475	0.149	1
2056	?	212	CYS	HB2	2.580	0.104	2
2057	?	212	CYS	HB3	2.797	0.051	2
2058	?	213	VAL	N	130.904	0.011	1
2059	?	213	VAL	H	8.965	0.008	1
2060	?	213	VAL	CA	60.733	0.053	1
2061	?	213	VAL	HA	4.882	0.015	1
2062	?	213	VAL	CB	35.229	0.022	1
2063	?	213	VAL	HB	2.125	0.024	1
2064	?	213	VAL	HG11	0.898	0.002	2
2065	?	213	VAL	HG12	0.898	0.002	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2066	?	213	VAL	HG13	0.898	0.002	2
2067	?	213	VAL	HG21	1.004	0.012	2
2068	?	213	VAL	HG22	1.004	0.012	2
2069	?	213	VAL	HG23	1.004	0.012	2
2070	?	213	VAL	CG1	21.439	0.009	1
2071	?	213	VAL	CG2	21.439	0.009	1
2072	?	214	ILE	N	125.698	0.004	1
2073	?	214	ILE	H	9.613	0.008	1
2074	?	214	ILE	CA	61.064	0.033	1
2075	?	214	ILE	HA	5.185	0.009	1
2076	?	214	ILE	CB	41.823	0.032	1
2077	?	214	ILE	HB	1.559	0.010	1
2078	?	214	ILE	HG21	1.020	0.003	1
2079	?	214	ILE	HG22	1.020	0.003	1
2080	?	214	ILE	HG23	1.020	0.003	1
2081	?	214	ILE	CG2	17.817	0.026	1
2082	?	214	ILE	CG1	29.204	0.011	1
2083	?	214	ILE	HG12	0.987	0.004	2
2084	?	214	ILE	HG13	1.692	0.002	2
2085	?	214	ILE	HD11	0.855	0.010	1
2086	?	214	ILE	HD12	0.855	0.010	1
2087	?	214	ILE	HD13	0.855	0.010	1
2088	?	214	ILE	CD1	14.021	0.028	1
2089	?	215	MET	N	126.397	0.007	1
2090	?	215	MET	H	8.807	0.003	1
2091	?	215	MET	CA	53.131	0.013	1
2092	?	215	MET	HA	5.327	0.005	1
2093	?	215	MET	CB	31.704	0.005	1
2094	?	215	MET	CG	31.543	0.000	1
2095	?	215	MET	CE	18.280	0.000	1
2096	?	216	GLN	N	127.607	0.025	1
2097	?	216	GLN	H	8.272	0.003	1
2098	?	216	GLN	CA	55.677	0.054	1
2099	?	216	GLN	HA	3.941	0.006	1
2100	?	216	GLN	CB	28.737	0.019	1
2101	?	216	GLN	HB2	1.847	0.001	2
2102	?	216	GLN	HB3	1.923	0.001	2
2103	?	216	GLN	CG	34.039	0.002	1
2104	?	216	GLN	HG2	2.209	0.003	2
2105	?	216	GLN	HG3	2.209	0.003	2
2106	?	217	LYS	N	127.268	0.044	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2107	?	217	LYS	H	8.067	0.006	1
2108	?	217	LYS	CA	57.002	0.002	1
2109	?	217	LYS	HA	4.250	0.000	1
2110	?	217	LYS	CB	33.821	0.000	1
2111	?	218	ASN	H	8.053	0.000	1
2112	?	218	ASN	CA	53.989	0.010	1
2113	?	218	ASN	HA	4.473	0.008	1
2114	?	218	ASN	CB	41.190	0.001	1
2115	?	218	ASN	HB2	2.462	0.017	2
2116	?	218	ASN	HB3	2.548	0.015	2
2117	?	219	GLY	N	105.197	0.006	1
2118	?	219	GLY	H	7.979	0.006	1
2119	?	219	GLY	CA	45.310	0.010	1
2120	?	219	GLY	HA2	3.582	0.004	2
2121	?	219	GLY	HA3	3.582	0.004	2
2122	?	220	ALA	N	123.500	0.001	1
2123	?	220	ALA	H	7.669	0.008	1
2124	?	220	ALA	CA	52.040	0.043	1
2125	?	220	ALA	HA	4.290	0.009	1
2126	?	220	ALA	HB1	1.459	0.006	1
2127	?	220	ALA	HB2	1.459	0.006	1
2128	?	220	ALA	HB3	1.459	0.006	1
2129	?	220	ALA	CB	19.532	0.007	1
2130	?	221	GLY	N	109.300	0.000	1
2131	?	221	GLY	H	8.425	0.005	1
2132	?	221	GLY	CA	45.041	0.017	1
2133	?	221	GLY	HA2	3.827	0.005	2
2134	?	221	GLY	HA3	3.827	0.005	2
2135	?	222	LEU	CA	54.264	0.060	1
2136	?	222	LEU	HA	4.924	0.014	1
2137	?	222	LEU	CB	44.995	0.008	1
2138	?	222	LEU	HB2	1.453	0.010	2
2139	?	222	LEU	HB3	1.917	0.002	2
2140	?	222	LEU	CG	27.924	0.041	1
2141	?	222	LEU	HD11	0.752	0.003	2
2142	?	222	LEU	HD12	0.752	0.003	2
2143	?	222	LEU	HD13	0.752	0.003	2
2144	?	222	LEU	HD21	0.899	0.004	2
2145	?	222	LEU	HD22	0.899	0.004	2
2146	?	222	LEU	HD23	0.899	0.004	2
2147	?	222	LEU	CD1	26.023	0.038	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2148	?	222	LEU	CD2	23.244	0.032	1
2149	?	223	HIS	N	124.868	0.043	1
2150	?	223	HIS	H	8.764	0.002	1
2151	?	223	HIS	CA	59.357	0.000	1
2152	?	224	THR	N	113.256	0.867	1
2153	?	224	THR	H	8.847	0.542	1
2154	?	224	THR	CA	59.448	0.033	1
2155	?	224	THR	HA	5.935	0.011	1
2156	?	224	THR	CB	71.886	0.083	1
2157	?	224	THR	HB	4.276	0.005	1
2158	?	224	THR	HG21	1.104	0.014	1
2159	?	224	THR	HG22	1.104	0.014	1
2160	?	224	THR	HG23	1.104	0.014	1
2161	?	224	THR	CG2	22.348	0.009	1
2162	?	225	ALA	N	122.627	0.163	1
2163	?	225	ALA	H	9.006	0.015	1
2164	?	225	ALA	CA	51.249	0.054	1
2165	?	225	ALA	HA	5.563	0.009	1
2166	?	225	ALA	HB1	1.248	0.006	1
2167	?	225	ALA	HB2	1.248	0.006	1
2168	?	225	ALA	HB3	1.248	0.006	1
2169	?	225	ALA	CB	22.716	0.014	1
2170	?	226	SER	N	112.176	0.142	1
2171	?	226	SER	H	8.630	0.024	1
2172	?	226	SER	CA	57.062	0.023	1
2173	?	226	SER	HA	5.458	0.011	1
2174	?	226	SER	CB	67.000	0.001	1
2175	?	226	SER	HB2	3.863	0.007	2
2176	?	226	SER	HB3	3.980	0.013	2
2177	?	227	SER	N	111.500	0.000	1
2178	?	227	SER	H	8.523	0.011	1
2179	?	227	SER	CA	56.853	0.019	1
2180	?	227	SER	HA	4.332	0.012	1
2181	?	227	SER	CB	63.176	0.004	1
2182	?	227	SER	HB2	3.044	0.003	2
2183	?	227	SER	HB3	4.023	0.005	2
2184	?	228	CYS	N	115.201	0.003	1
2185	?	228	CYS	H	7.801	0.006	1
2186	?	228	CYS	CA	54.392	0.116	1
2187	?	228	CYS	HA	5.271	0.010	1
2188	?	228	CYS	CB	33.183	0.025	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2189	?	228	CYS	HB2	2.123	0.008	2
2190	?	228	CYS	HB3	2.830	0.005	2
2191	?	229	PHE	N	124.294	0.020	1
2192	?	229	PHE	H	9.337	0.008	1
2193	?	229	PHE	CA	57.497	0.027	1
2194	?	229	PHE	HA	5.209	0.009	1
2195	?	229	PHE	CB	41.402	0.005	1
2196	?	229	PHE	HB2	2.939	0.004	2
2197	?	229	PHE	HB3	3.146	0.021	2
2198	?	230	TRP	N	122.505	0.012	1
2199	?	230	TRP	H	8.987	0.013	1
2200	?	230	TRP	CA	54.516	0.007	1
2201	?	230	TRP	HA	5.348	0.011	1
2202	?	230	TRP	CB	31.542	0.002	1
2203	?	230	TRP	HB2	2.844	0.002	2
2204	?	230	TRP	HB3	3.221	0.001	2
2205	?	230	TRP	NE1	127.605	0.034	1
2206	?	230	TRP	HD1	7.393	0.000	1
2207	?	230	TRP	CZ3	124.085	0.021	1
2208	?	230	TRP	CZ2	114.590	0.017	1
2209	?	230	TRP	HE1	10.017	0.014	1
2210	?	230	TRP	HZ3	7.016	0.003	1
2211	?	230	TRP	CH2	122.397	0.006	1
2212	?	230	TRP	HZ2	7.437	0.005	1
2213	?	230	TRP	HH2	7.014	0.008	1
2214	?	231	ASP	N	119.500	0.001	1
2215	?	231	ASP	H	8.577	0.005	1
2216	?	231	ASP	CA	52.307	0.094	1
2217	?	231	ASP	HA	4.998	0.005	1
2218	?	231	ASP	CB	41.355	0.047	1
2219	?	231	ASP	HB2	1.923	0.006	2
2220	?	231	ASP	HB3	2.930	0.010	2
2221	?	232	SER	N	121.024	0.041	1
2222	?	232	SER	H	8.700	0.008	1
2223	?	232	SER	CA	60.399	0.034	1
2224	?	232	SER	HA	4.693	0.010	1
2225	?	232	SER	CB	63.253	0.006	1
2226	?	232	SER	HB2	3.591	0.009	2
2227	?	232	SER	HB3	3.970	0.000	2
2228	?	233	SER	N	117.053	0.058	1
2229	?	233	SER	H	8.644	0.007	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2230	?	233	SER	CA	60.749	0.040	1
2231	?	233	SER	HA	4.315	0.008	1
2232	?	233	SER	CB	63.593	0.100	1
2233	?	233	SER	HB2	3.899	0.005	2
2234	?	233	SER	HB3	3.899	0.005	2
2235	?	234	THR	N	109.501	0.002	1
2236	?	234	THR	H	6.874	0.010	1
2237	?	234	THR	CA	62.234	0.055	1
2238	?	234	THR	HA	4.455	0.007	1
2239	?	234	THR	CB	71.447	0.025	1
2240	?	234	THR	HB	4.067	0.007	1
2241	?	234	THR	HG21	0.930	0.013	1
2242	?	234	THR	HG22	0.930	0.013	1
2243	?	234	THR	HG23	0.930	0.013	1
2244	?	234	THR	CG2	20.694	0.009	1
2245	?	235	ASP	N	124.875	0.088	1
2246	?	235	ASP	H	7.741	0.017	1
2247	?	235	ASP	CA	54.146	0.010	1
2248	?	235	ASP	HA	4.729	0.006	1
2249	?	235	ASP	CB	41.261	0.006	1
2250	?	235	ASP	HB2	2.333	0.011	2
2251	?	235	ASP	HB3	2.807	0.010	2
2252	?	236	GLY	N	105.149	0.048	1
2253	?	236	GLY	H	7.956	0.008	1
2254	?	236	GLY	CA	45.353	0.004	1
2255	?	236	GLY	HA2	4.022	0.008	2
2256	?	236	GLY	HA3	4.022	0.008	2
2257	?	237	SER	N	111.497	0.008	1
2258	?	237	SER	H	8.233	0.008	1
2259	?	237	SER	CA	56.572	0.007	1
2260	?	237	SER	HA	5.168	0.013	1
2261	?	237	SER	CB	68.249	0.092	1
2262	?	237	SER	HB2	3.365	0.007	2
2263	?	237	SER	HB3	3.848	0.003	2
2264	?	238	CYS	N	116.903	0.013	1
2265	?	238	CYS	H	8.706	0.009	1
2266	?	238	CYS	CA	57.240	0.040	1
2267	?	238	CYS	HA	4.731	0.004	1
2268	?	238	CYS	CB	30.801	0.040	1
2269	?	238	CYS	HB2	2.668	0.004	2
2270	?	238	CYS	HB3	2.825	0.006	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2271	?	239	THR	N	122.094	0.008	1
2272	?	239	THR	H	8.561	0.013	1
2273	?	239	THR	CA	62.371	0.091	1
2274	?	239	THR	HA	5.108	0.011	1
2275	?	239	THR	CB	71.331	0.028	1
2276	?	239	THR	HB	3.674	0.007	1
2277	?	239	THR	HG21	0.814	0.004	1
2278	?	239	THR	HG22	0.814	0.004	1
2279	?	239	THR	HG23	0.814	0.004	1
2280	?	239	THR	CG2	20.452	0.048	1
2281	?	240	VAL	N	129.451	0.031	1
2282	?	240	VAL	H	9.449	0.006	1
2283	?	240	VAL	CA	61.431	0.022	1
2284	?	240	VAL	HA	4.218	0.009	1
2285	?	240	VAL	CB	35.321	0.027	1
2286	?	240	VAL	HB	1.739	0.010	1
2287	?	240	VAL	HG11	0.802	0.007	2
2288	?	240	VAL	HG12	0.802	0.007	2
2289	?	240	VAL	HG13	0.802	0.007	2
2290	?	240	VAL	HG21	0.846	0.004	2
2291	?	240	VAL	HG22	0.846	0.004	2
2292	?	240	VAL	HG23	0.846	0.004	2
2293	?	240	VAL	CG1	21.497	0.002	1
2294	?	240	VAL	CG2	21.497	0.002	1
2295	?	241	ARG	N	125.494	0.013	1
2296	?	241	ARG	H	8.455	0.009	1
2297	?	241	ARG	CA	54.035	0.021	1
2298	?	241	ARG	HA	5.079	0.008	1
2299	?	241	ARG	CB	32.611	0.011	1
2300	?	241	ARG	HB2	1.718	0.001	2
2301	?	241	ARG	HB3	1.718	0.001	2
2302	?	241	ARG	CG	26.701	0.003	1
2303	?	241	ARG	HG2	1.479	0.003	2
2304	?	241	ARG	HG3	1.591	0.001	2
2305	?	241	ARG	CD	43.912	0.002	1
2306	?	241	ARG	HD2	2.930	0.004	2
2307	?	241	ARG	HD3	3.042	0.003	2
2308	?	242	TRP	N	128.068	0.045	1
2309	?	242	TRP	H	9.304	0.007	1
2310	?	242	TRP	CA	57.786	0.010	1
2311	?	242	TRP	HA	4.726	0.002	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2312	?	242	TRP	CB	34.452	0.007	1
2313	?	242	TRP	HB2	2.865	0.006	2
2314	?	242	TRP	HB3	2.951	0.014	2
2315	?	242	TRP	CE3	124.209	0.009	1
2316	?	242	TRP	NE1	130.099	0.011	1
2317	?	242	TRP	HD1	7.204	0.000	1
2318	?	242	TRP	HE3	7.431	0.007	1
2319	?	242	TRP	CZ3	124.600	0.000	1
2320	?	242	TRP	CZ2	113.896	0.006	1
2321	?	242	TRP	HE1	10.368	0.014	1
2322	?	242	TRP	HZ3	6.981	0.000	1
2323	?	242	TRP	CH2	123.904	0.006	1
2324	?	242	TRP	HZ2	7.317	0.004	1
2325	?	242	TRP	HH2	7.086	0.005	1
2326	?	243	GLU	N	123.736	0.044	1
2327	?	243	GLU	H	7.468	0.008	1
2328	?	243	GLU	CA	54.811	0.008	1
2329	?	243	GLU	HA	5.045	0.008	1
2330	?	243	GLU	CB	35.406	0.004	1
2331	?	243	GLU	HB2	1.879	0.009	2
2332	?	243	GLU	HB3	1.976	0.005	2
2333	?	244	ASN	N	122.099	0.037	1
2334	?	244	ASN	H	8.380	0.004	1
2335	?	244	ASN	CA	50.652	0.010	1
2336	?	244	ASN	HA	4.287	0.011	1
2337	?	244	ASN	CB	38.872	0.003	1
2338	?	244	ASN	HB2	2.490	0.005	2
2339	?	244	ASN	HB3	3.302	0.000	2
2340	?	245	LYS	H	8.342	0.002	1
2341	?	245	LYS	CA	60.312	0.009	1
2342	?	245	LYS	HA	3.881	0.006	1
2343	?	245	LYS	CB	32.669	0.006	1
2344	?	245	LYS	HB2	1.802	0.002	2
2345	?	245	LYS	HB3	1.848	0.001	2
2346	?	245	LYS	CG	25.483	0.006	1
2347	?	245	LYS	HG2	1.357	0.005	2
2348	?	245	LYS	HG3	1.468	0.003	2
2349	?	245	LYS	CD	29.142	0.004	1
2350	?	245	LYS	HD2	1.620	0.004	2
2351	?	245	LYS	HD3	1.620	0.004	2
2352	?	245	LYS	CE	42.261	0.004	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2353	?	245	LYS	HE2	2.909	0.001	2
2354	?	245	LYS	HE3	2.909	0.001	2
2355	?	246	THR	N	101.100	0.001	1
2356	?	246	THR	H	7.679	0.011	1
2357	?	246	THR	CA	61.688	0.007	1
2358	?	246	THR	HA	4.778	0.005	1
2359	?	246	THR	CB	72.207	0.006	1
2360	?	246	THR	HB	4.664	0.001	1
2361	?	246	THR	HG21	1.264	0.005	1
2362	?	246	THR	HG22	1.264	0.005	1
2363	?	246	THR	HG23	1.264	0.005	1
2364	?	246	THR	CG2	21.567	0.004	1
2365	?	247	MET	N	122.951	0.059	1
2366	?	247	MET	H	8.292	0.007	1
2367	?	247	MET	CA	56.176	0.028	1
2368	?	247	MET	HA	5.267	0.012	1
2369	?	247	MET	CB	39.103	0.014	1
2370	?	247	MET	HB2	1.928	0.002	2
2371	?	247	MET	HB3	2.178	0.006	2
2372	?	247	MET	CG	34.124	0.010	1
2373	?	247	MET	HG2	2.478	0.001	2
2374	?	247	MET	HG3	2.560	0.000	2
2375	?	248	TYR	N	118.100	0.000	1
2376	?	248	TYR	H	8.489	0.013	1
2377	?	248	TYR	CA	55.711	0.010	1
2378	?	248	TYR	HA	5.098	0.010	1
2379	?	249	CYS	N	123.098	0.007	1
2380	?	249	CYS	H	9.406	0.009	1
2381	?	249	CYS	CA	56.629	0.039	1
2382	?	249	CYS	HA	5.783	0.015	1
2383	?	249	CYS	CB	30.569	0.009	1
2384	?	249	CYS	HB2	2.585	0.014	2
2385	?	249	CYS	HB3	2.727	0.001	2
2386	?	250	ILE	N	126.943	0.044	1
2387	?	250	ILE	H	9.102	0.010	1
2388	?	250	ILE	CA	60.058	0.095	1
2389	?	250	ILE	HA	5.180	0.007	1
2390	?	250	ILE	CB	42.360	0.007	1
2391	?	250	ILE	HB	1.545	0.002	1
2392	?	250	ILE	HG21	0.725	0.001	1
2393	?	250	ILE	HG22	0.725	0.001	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2394	?	250	ILE	HG23	0.725	0.001	1
2395	?	250	ILE	CG2	18.096	0.003	1
2396	?	250	ILE	CG1	28.479	0.002	1
2397	?	250	ILE	HG12	0.944	0.000	2
2398	?	250	ILE	HG13	1.641	0.003	2
2399	?	250	ILE	HD11	0.833	0.002	1
2400	?	250	ILE	HD12	0.833	0.002	1
2401	?	250	ILE	HD13	0.833	0.002	1
2402	?	250	ILE	CD1	16.358	0.018	1
2403	?	251	VAL	N	129.881	0.012	1
2404	?	251	VAL	H	9.051	0.004	1
2405	?	251	VAL	CA	60.085	0.044	1
2406	?	251	VAL	HA	5.145	0.008	1
2407	?	251	VAL	CB	34.564	0.080	1
2408	?	251	VAL	HB	1.605	0.003	1
2409	?	251	VAL	HG11	0.754	0.012	2
2410	?	251	VAL	HG12	0.754	0.012	2
2411	?	251	VAL	HG13	0.754	0.012	2
2412	?	251	VAL	HG21	0.799	0.006	2
2413	?	251	VAL	HG22	0.799	0.006	2
2414	?	251	VAL	HG23	0.799	0.006	2
2415	?	251	VAL	CG1	21.507	0.007	1
2416	?	251	VAL	CG2	24.024	0.027	1
2417	?	252	SER	N	121.903	0.025	1
2418	?	252	SER	H	8.572	0.009	1
2419	?	252	SER	CA	56.795	0.036	1
2420	?	252	SER	HA	5.308	0.009	1
2421	?	252	SER	CB	65.089	0.022	1
2422	?	252	SER	HB2	3.336	0.004	2
2423	?	252	SER	HB3	3.731	0.010	2
2424	?	253	ALA	N	124.803	0.018	1
2425	?	253	ALA	H	8.646	0.006	1
2426	?	253	ALA	CA	49.635	0.029	1
2427	?	253	ALA	HA	5.406	0.011	1
2428	?	253	ALA	HB1	0.976	0.009	1
2429	?	253	ALA	HB2	0.976	0.009	1
2430	?	253	ALA	HB3	0.976	0.009	1
2431	?	253	ALA	CB	21.718	0.008	1
2432	?	254	PHE	N	119.496	0.013	1
2433	?	254	PHE	H	9.329	0.005	1
2434	?	254	PHE	CA	56.064	0.034	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2435	?	254	PHE	HA	4.952	0.011	1
2436	?	254	PHE	CB	42.618	0.007	1
2437	?	254	PHE	HB2	2.806	0.005	2
2438	?	254	PHE	HB3	2.861	0.022	2
2439	?	255	GLY	N	109.702	0.006	1
2440	?	255	GLY	H	8.954	0.009	1
2441	?	255	GLY	CA	45.208	0.006	1
2442	?	255	GLY	HA2	2.893	0.005	2
2443	?	255	GLY	HA3	2.893	0.005	2
2444	?	256	LEU	N	126.100	0.001	1
2445	?	256	LEU	H	8.927	0.007	1
2446	?	256	LEU	CA	52.470	0.010	1
2447	?	256	LEU	HA	4.768	0.010	1
2448	?	256	LEU	CB	42.493	0.044	1
2449	?	256	LEU	HB2	1.518	0.016	2
2450	?	256	LEU	HB3	1.706	0.073	2
2451	?	256	LEU	CG	28.922	0.030	1
2452	?	256	LEU	HG	1.842	0.004	1
2453	?	256	LEU	HD11	0.988	0.005	2
2454	?	256	LEU	HD12	0.988	0.005	2
2455	?	256	LEU	HD13	0.988	0.005	2
2456	?	256	LEU	HD21	1.090	0.008	2
2457	?	256	LEU	HD22	1.090	0.008	2
2458	?	256	LEU	HD23	1.090	0.008	2
2459	?	256	LEU	CD1	26.614	0.022	1
2460	?	256	LEU	CD2	24.900	0.006	1
2461	?	257	SER	N	119.998	0.005	1
2462	?	257	SER	H	9.275	0.007	1
2463	?	257	SER	CA	58.523	0.044	1
2464	?	257	SER	HA	3.618	0.007	1
2465	?	257	SER	CB	63.185	0.031	1
2466	?	257	SER	HB2	3.503	0.012	2
2467	?	257	SER	HB3	3.606	0.003	2
2468	?	258	ILE	N	122.165	0.044	1
2469	?	258	ILE	H	7.680	0.010	1
2470	?	258	ILE	CA	62.011	0.010	1
2471	?	258	ILE	HA	4.072	0.018	1
2472	?	258	ILE	CB	38.580	0.008	1
2473	?	258	ILE	HB	1.748	0.022	1
2474	?	258	ILE	HG21	0.786	0.007	1
2475	?	258	ILE	HG22	0.786	0.007	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2476	?	258	ILE	HG23	0.786	0.007	1
2477	?	258	ILE	CG2	18.215	0.022	1
2478	?	258	ILE	CG1	26.909	0.003	1
2479	?	258	ILE	HG12	1.071	0.004	2
2480	?	258	ILE	HG13	1.329	0.005	2
2481	?	258	ILE	HD11	0.768	0.005	1
2482	?	258	ILE	HD12	0.768	0.005	1
2483	?	258	ILE	HD13	0.768	0.005	1
2484	?	258	ILE	CD1	12.595	0.000	1
2485	?	259	GLY	N	110.200	0.002	1
2486	?	259	GLY	H	8.148	0.012	1
2487	?	259	GLY	CA	45.001	0.007	1
2488	?	259	GLY	HA2	3.863	0.014	2
2489	?	259	GLY	HA3	3.863	0.014	2
2490	?	260	GLY	N	108.682	0.035	1
2491	?	260	GLY	H	8.179	0.003	1
2492	?	260	GLY	CA	45.146	0.004	1
2493	?	260	GLY	HA2	3.849	0.005	2
2494	?	260	GLY	HA3	3.849	0.005	2
2495	?	261	GLY	N	108.703	0.006	1
2496	?	261	GLY	H	8.318	0.003	1
2497	?	261	GLY	CA	45.220	0.010	1
2498	?	261	GLY	HA2	3.830	0.006	2
2499	?	261	GLY	HA3	3.830	0.006	2
2500	?	262	SER	N	115.703	0.006	1
2501	?	262	SER	H	8.290	0.006	1
2502	?	262	SER	CA	58.512	0.008	1
2503	?	262	SER	HA	4.698	0.001	1
2504	?	262	SER	CB	63.727	0.002	1
2505	?	262	SER	HB2	3.750	0.001	2
2506	?	262	SER	HB3	3.793	0.001	2
2507	?	263	GLY	N	110.798	0.007	1
2508	?	263	GLY	H	8.430	0.007	1
2509	?	263	GLY	CA	45.477	0.004	1
2510	?	264	GLN	N	119.803	0.007	1
2511	?	264	GLN	H	8.039	0.006	1
2512	?	264	GLN	CA	56.000	0.004	1
2513	?	264	GLN	HA	4.259	0.012	1
2514	?	264	GLN	CB	29.113	0.010	1
2515	?	264	GLN	HB2	1.849	0.003	2
2516	?	264	GLN	HB3	2.034	0.002	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2517	?	264	GLN	CG	33.839	0.001	1
2518	?	264	GLN	HG2	2.210	0.001	2
2519	?	264	GLN	HG3	2.226	0.006	2
2520	?	265	SER	H	7.992	0.001	1
2521	?	265	SER	CA	58.271	0.008	1
2522	?	265	SER	HA	4.402	0.001	1
2523	?	265	SER	CB	63.843	0.044	1
2524	?	265	SER	HB2	3.742	0.001	2
2525	?	265	SER	HB3	3.789	0.001	2
2526	?	266	GLY	N	110.673	0.045	1
2527	?	266	GLY	H	7.948	0.008	1
2528	?	266	GLY	CA	44.376	0.004	1
2529	?	266	GLY	HA2	3.973	0.009	2
2530	?	266	GLY	HA3	4.031	0.007	2
2531	?	267	PRO	CD	49.771	0.004	1
2532	?	267	PRO	CA	62.777	0.024	1
2533	?	267	PRO	HA	4.344	0.007	1
2534	?	267	PRO	CB	31.960	0.004	1
2535	?	267	PRO	HB2	1.756	0.002	2
2536	?	267	PRO	HB3	2.161	0.004	2
2537	?	267	PRO	CG	27.162	0.005	1
2538	?	267	PRO	HG2	1.907	0.005	2
2539	?	267	PRO	HG3	1.907	0.005	2
2540	?	267	PRO	HD2	3.505	0.005	2
2541	?	267	PRO	HD3	3.505	0.005	2
2542	?	268	ILE	N	122.096	0.098	1
2543	?	268	ILE	H	8.178	0.007	1
2544	?	268	ILE	CA	61.233	0.034	1
2545	?	268	ILE	HA	3.960	0.011	1
2546	?	268	ILE	CB	38.590	0.010	1
2547	?	268	ILE	HB	1.667	0.008	1
2548	?	268	ILE	HG21	0.723	0.001	1
2549	?	268	ILE	HG22	0.723	0.001	1
2550	?	268	ILE	HG23	0.723	0.001	1
2551	?	268	ILE	CG2	17.358	0.004	1
2552	?	268	ILE	CG1	27.406	0.002	1
2553	?	268	ILE	HG12	1.029	0.002	2
2554	?	268	ILE	HG13	1.388	0.003	2
2555	?	268	ILE	HD11	0.723	0.006	1
2556	?	268	ILE	HD12	0.723	0.006	1
2557	?	268	ILE	HD13	0.723	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2558	?	268	ILE	CD1	13.496	0.006	1
2559	?	269	LYS	N	128.101	0.004	1
2560	?	269	LYS	H	8.351	0.007	1
2561	?	269	LYS	CA	55.220	0.004	1
2562	?	269	LYS	HA	4.352	0.009	1
2563	?	269	LYS	CB	32.660	0.003	1
2564	?	269	LYS	HB2	1.600	0.003	2
2565	?	269	LYS	HB3	1.733	0.006	2
2566	?	269	LYS	CG	24.511	0.002	1
2567	?	269	LYS	HG2	1.252	0.003	2
2568	?	269	LYS	HG3	1.328	0.002	2
2569	?	269	LYS	CD	29.087	0.005	1
2570	?	269	LYS	HD2	1.609	0.002	2
2571	?	269	LYS	HD3	1.609	0.002	2
2572	?	269	LYS	CE	42.157	0.004	1
2573	?	269	LYS	HE2	2.921	0.005	2
2574	?	269	LYS	HE3	2.921	0.005	2
2575	?	270	LEU	N	124.204	0.010	1
2576	?	270	LEU	H	8.003	0.009	1
2577	?	270	LEU	CA	53.071	0.047	1
2578	?	270	LEU	HA	4.531	0.008	1
2579	?	270	LEU	CB	43.054	0.019	1
2580	?	270	LEU	HB2	0.245	0.005	2
2581	?	270	LEU	HB3	1.264	0.007	2
2582	?	270	LEU	CG	26.903	0.016	1
2583	?	270	LEU	HG	1.345	0.007	1
2584	?	270	LEU	HD11	0.427	0.074	2
2585	?	270	LEU	HD12	0.427	0.074	2
2586	?	270	LEU	HD13	0.427	0.074	2
2587	?	270	LEU	HD21	0.712	0.003	2
2588	?	270	LEU	HD22	0.712	0.003	2
2589	?	270	LEU	HD23	0.712	0.003	2
2590	?	270	LEU	CD1	24.088	0.012	1
2591	?	270	LEU	CD2	26.396	0.009	1
2592	?	271	GLY	N	107.602	0.006	1
2593	?	271	GLY	H	8.713	0.006	1
2594	?	271	GLY	CA	45.075	0.007	1
2595	?	271	GLY	HA2	3.962	0.008	2
2596	?	271	GLY	HA3	4.348	0.013	2
2597	?	272	MET	N	118.699	0.002	1
2598	?	272	MET	H	8.710	0.007	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2599	?	272	MET	CA	54.607	0.005	1
2600	?	272	MET	HA	5.272	0.005	1
2601	?	272	MET	CB	33.189	0.003	1
2602	?	272	MET	HB2	2.096	0.003	2
2603	?	272	MET	HB3	2.096	0.003	2
2604	?	272	MET	CG	33.183	0.011	1
2605	?	272	MET	HG2	2.828	0.004	2
2606	?	272	MET	HG3	2.828	0.004	2
2607	?	273	ALA	N	127.483	0.045	1
2608	?	273	ALA	H	8.395	0.007	1
2609	?	273	ALA	CA	50.938	0.214	1
2610	?	273	ALA	HA	4.539	0.012	1
2611	?	273	ALA	HB1	0.986	0.006	1
2612	?	273	ALA	HB2	0.986	0.006	1
2613	?	273	ALA	HB3	0.986	0.006	1
2614	?	273	ALA	CB	20.278	0.007	1
2615	?	274	LYS	N	119.543	0.082	1
2616	?	274	LYS	H	8.242	0.005	1
2617	?	274	LYS	CA	56.390	0.021	1
2618	?	274	LYS	HA	4.258	0.006	1
2619	?	274	LYS	CB	32.611	0.004	1
2620	?	274	LYS	HB2	1.776	0.002	2
2621	?	274	LYS	HB3	1.776	0.002	2
2622	?	274	LYS	CG	24.669	0.002	1
2623	?	274	LYS	HG2	1.430	0.001	2
2624	?	274	LYS	HG3	1.471	0.002	2
2625	?	274	LYS	CD	29.431	0.004	1
2626	?	274	LYS	HD2	1.684	0.001	2
2627	?	274	LYS	HD3	1.684	0.001	2
2628	?	274	LYS	CE	42.320	0.005	1
2629	?	274	LYS	HE2	3.003	0.004	2
2630	?	274	LYS	HE3	3.003	0.004	2
2631	?	275	ILE	N	125.690	0.031	1
2632	?	275	ILE	H	8.710	0.009	1
2633	?	275	ILE	CA	60.985	0.030	1
2634	?	275	ILE	HA	4.398	0.011	1
2635	?	275	ILE	CB	37.980	0.040	1
2636	?	275	ILE	HB	1.895	0.006	1
2637	?	275	ILE	HG21	0.789	0.006	1
2638	?	275	ILE	HG22	0.789	0.006	1
2639	?	275	ILE	HG23	0.789	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2640	?	275	ILE	CG2	18.017	0.029	1
2641	?	275	ILE	CG1	27.996	0.008	1
2642	?	275	ILE	HG12	1.140	0.006	2
2643	?	275	ILE	HG13	1.608	0.009	2
2644	?	275	ILE	HD11	0.833	0.006	1
2645	?	275	ILE	HD12	0.833	0.006	1
2646	?	275	ILE	HD13	0.833	0.006	1
2647	?	275	ILE	CD1	13.419	0.023	1
2648	?	276	THR	N	121.801	0.002	1
2649	?	276	THR	H	8.120	0.008	1
2650	?	276	THR	CA	62.713	0.043	1
2651	?	276	THR	HA	4.431	0.008	1
2652	?	276	THR	CB	69.734	0.122	1
2653	?	276	THR	HB	4.002	0.013	1
2654	?	276	THR	HG21	1.053	0.004	1
2655	?	276	THR	HG22	1.053	0.004	1
2656	?	276	THR	HG23	1.053	0.004	1
2657	?	276	THR	CG2	20.751	0.007	1
2658	?	277	GLN	N	127.560	0.052	1
2659	?	277	GLN	H	8.992	0.009	1
2660	?	277	GLN	CA	54.773	0.009	1
2661	?	277	GLN	HA	5.184	0.012	1
2662	?	277	GLN	CB	33.049	0.002	1
2663	?	277	GLN	HB2	1.915	0.005	2
2664	?	277	GLN	HB3	2.017	0.002	2
2665	?	277	GLN	CG	34.929	0.003	1
2666	?	277	GLN	HG2	2.108	0.001	2
2667	?	277	GLN	HG3	2.213	0.003	2
2668	?	278	VAL	N	123.297	0.031	1
2669	?	278	VAL	H	8.198	0.005	1
2670	?	278	VAL	CA	62.589	0.005	1
2671	?	278	VAL	HA	3.953	0.006	1
2672	?	278	VAL	CB	33.443	0.004	1
2673	?	278	VAL	HB	1.971	0.001	1
2674	?	278	VAL	HG11	0.524	0.008	2
2675	?	278	VAL	HG12	0.524	0.008	2
2676	?	278	VAL	HG13	0.524	0.008	2
2677	?	278	VAL	HG21	0.630	0.008	2
2678	?	278	VAL	HG22	0.630	0.008	2
2679	?	278	VAL	HG23	0.630	0.008	2
2680	?	278	VAL	CG1	22.002	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2681	?	278	VAL	CG2	22.000	0.005	1
2682	?	279	ASP	N	126.000	0.001	1
2683	?	279	ASP	H	8.279	0.008	1
2684	?	279	ASP	CA	53.298	0.014	1
2685	?	279	ASP	HA	5.167	0.010	1
2686	?	279	ASP	CB	45.261	0.035	1
2687	?	279	ASP	HB2	2.482	0.007	2
2688	?	279	ASP	HB3	2.583	0.008	2
2689	?	280	PHE	N	125.108	0.016	1
2690	?	280	PHE	H	8.877	0.013	1
2691	?	280	PHE	CA	54.589	0.009	1
2692	?	280	PHE	HA	4.857	0.011	1
2693	?	280	PHE	CB	40.000	0.000	1
2694	?	280	PHE	HB2	2.465	0.000	2
2695	?	280	PHE	HB3	2.625	0.012	2
2696	?	283	ARG	H	8.334	0.001	1
2697	?	283	ARG	CA	55.768	0.003	1
2698	?	283	ARG	HA	4.282	0.001	1
2699	?	283	ARG	CB	32.003	0.003	1
2700	?	283	ARG	HB2	1.643	0.001	2
2701	?	283	ARG	HB3	1.740	0.001	2
2702	?	283	ARG	CG	26.610	0.001	1
2703	?	283	ARG	HG2	1.517	0.004	2
2704	?	283	ARG	HG3	1.567	0.001	2
2705	?	283	ARG	CD	43.669	0.002	1
2706	?	283	ARG	HD2	3.090	0.003	2
2707	?	283	ARG	HD3	3.090	0.003	2
2708	?	284	GLU	N	121.715	0.037	1
2709	?	284	GLU	H	8.347	0.007	1
2710	?	284	GLU	CA	56.256	0.004	1
2711	?	284	GLU	HA	4.155	0.004	1
2712	?	284	GLU	CB	30.248	0.003	1
2713	?	284	GLU	HB2	1.832	0.003	2
2714	?	284	GLU	HB3	1.935	0.002	2
2715	?	284	GLU	CG	33.873	0.004	1
2716	?	284	GLU	HG2	2.238	0.004	2
2717	?	284	GLU	HG3	2.238	0.004	2
2718	?	285	ILE	N	123.235	0.037	1
2719	?	285	ILE	H	8.222	0.006	1
2720	?	285	ILE	CA	61.094	0.096	1
2721	?	285	ILE	HA	4.076	0.011	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2722	?	285	ILE	CB	38.162	0.007	1
2723	?	285	ILE	HB	1.781	0.010	1
2724	?	285	ILE	HG21	0.782	0.005	1
2725	?	285	ILE	HG22	0.782	0.005	1
2726	?	285	ILE	HG23	0.782	0.005	1
2727	?	285	ILE	CG2	17.471	0.008	1
2728	?	285	ILE	CG1	27.166	0.011	1
2729	?	285	ILE	HG12	1.069	0.007	2
2730	?	285	ILE	HG13	1.335	0.006	2
2731	?	285	ILE	HD11	0.698	0.003	1
2732	?	285	ILE	HD12	0.698	0.003	1
2733	?	285	ILE	HD13	0.698	0.003	1
2734	?	285	ILE	CD1	12.383	0.006	1
2735	?	286	VAL	N	128.733	0.024	1
2736	?	286	VAL	H	7.591	0.006	1
2737	?	286	VAL	CA	63.391	0.021	1
2738	?	286	VAL	HA	3.968	0.008	1
2739	?	286	VAL	CB	33.328	0.015	1
2740	?	286	VAL	HB	1.977	0.003	1
2741	?	286	VAL	HG11	0.798	0.008	2
2742	?	286	VAL	HG12	0.798	0.008	2
2743	?	286	VAL	HG13	0.798	0.008	2
2744	?	286	VAL	HG21	0.798	0.008	2
2745	?	286	VAL	HG22	0.798	0.008	2
2746	?	286	VAL	HG23	0.798	0.008	2
2747	?	286	VAL	CG1	20.160	0.003	1
2748	?	286	VAL	CG2	21.631	0.003	1

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2578. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1096 (0%)	0/438 (0%)	0/440 (0%)	0/218 (0%)

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	Total	¹H	¹³C	¹⁵N
Sidechain	0/1240 (0%)	0/718 (0%)	0/476 (0%)	0/46 (0%)
Aromatic	0/242 (0%)	0/126 (0%)	0/102 (0%)	0/14 (0%)
Overall	0/2578 (0%)	0/1282 (0%)	0/1018 (0%)	0/278 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 3288. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/1414 (0%)	0/564 (0%)	0/572 (0%)	0/278 (0%)
Sidechain	0/1616 (0%)	0/942 (0%)	0/616 (0%)	0/58 (0%)
Aromatic	0/258 (0%)	0/134 (0%)	0/110 (0%)	0/14 (0%)
Overall	0/3288 (0%)	0/1640 (0%)	0/1298 (0%)	0/350 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (Tctex-IC_dimer.bmrB). RCI is only applicable to proteins.