



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2020 – 02:43 PM EST

PDB ID : 2K03
Title : Structure of SDF1 in complex with the CXCR4 N-terminus containing a sulfotyrosine at position 21
Authors : Volkman, B.F.; Veldkamp, C.T.; Peterson, F.C.
Deposited on : 2008-01-24

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

<https://www.wwpdb.org/validation/2017/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	:	1.8.0 (224370), CSD as540be (2019)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.4
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

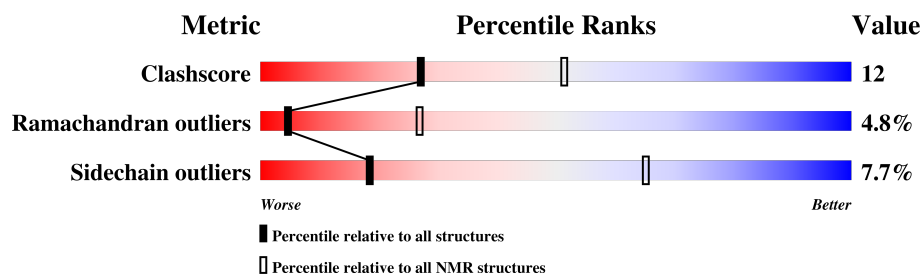
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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	70	<div> <div>53%</div> <div>27%</div> <div>•</div> <div>16%</div> <div>•</div> </div>
1	C	70	<div> <div>53%</div> <div>29%</div> <div>16%</div> <div>•</div> </div>
2	B	40	<div> <div>20%</div> <div>13%</div> <div>63%</div> <div>5%</div> </div>
2	D	40	<div> <div>23%</div> <div>15%</div> <div>58%</div> <div>5%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:43, A:47-A:67, B:114-B:120, B:122-B:127, C:208-C:243, C:247-C:267, D:312-D:320, D:322-D:327 (142)	0.59	11

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3417 atoms, of which 1686 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stromal cell-derived factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1136	353	579	106	92	6	
1	C	68	Total	C	H	N	O	S	0
			1136	353	579	106	92	6	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P48061
A	0	MET	-	expression tag	UNP P48061
A	36	CYS	LEU	ENGINEERED	UNP P48061
A	65	CYS	ALA	ENGINEERED	UNP P48061
C	199	GLY	-	expression tag	UNP P48061
C	200	MET	-	expression tag	UNP P48061
C	236	CYS	LEU	ENGINEERED	UNP P48061
C	265	CYS	ALA	ENGINEERED	UNP P48061

- Molecule 2 is a protein called C-X-C chemokine receptor type 4.

Mol	Chain	Residues	Atoms						Trace
2	B	38	Total	C	H	N	O	S	0
			572	185	264	47	72	4	
2	D	38	Total	C	H	N	O	S	0
			573	185	264	47	73	4	

There are 6 discrepancies between the modelled and reference sequences:

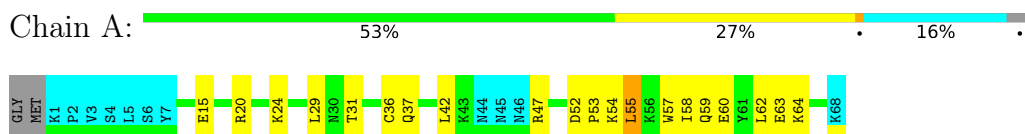
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	GLY	-	expression tag	UNP P61073
B	100	SER	-	expression tag	UNP P61073
B	128	ALA	CYS	ENGINEERED	UNP P61073
D	299	GLY	-	expression tag	UNP P61073
D	300	SER	-	expression tag	UNP P61073
D	328	ALA	CYS	ENGINEERED	UNP P61073

4 Residue-property plots [i](#)

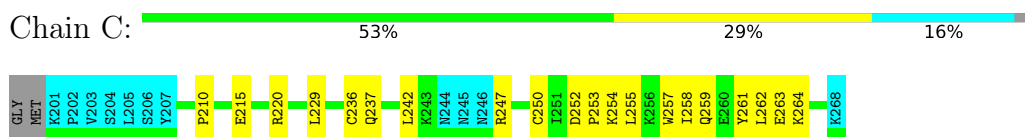
4.1 Average score per residue in the NMR ensemble

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

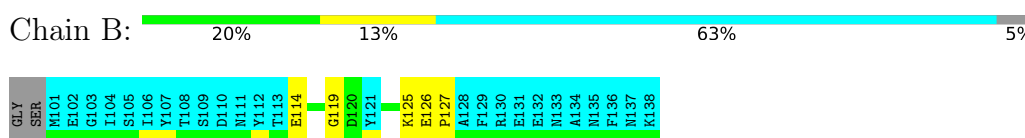
- Molecule 1: Stromal cell-derived factor 1



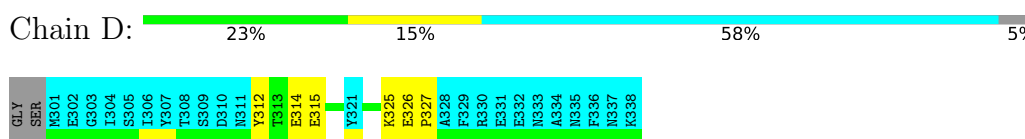
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4



- Molecule 2: C-X-C chemokine receptor type 4

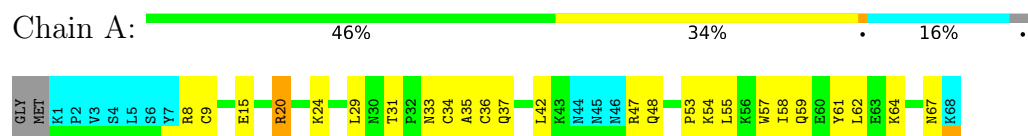


4.2 Scores per residue for each member of the ensemble

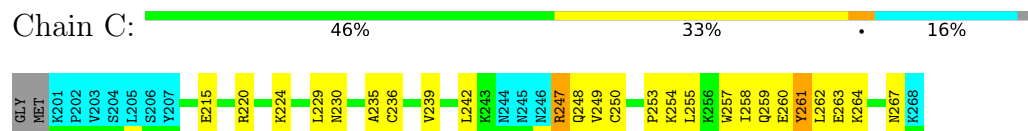
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

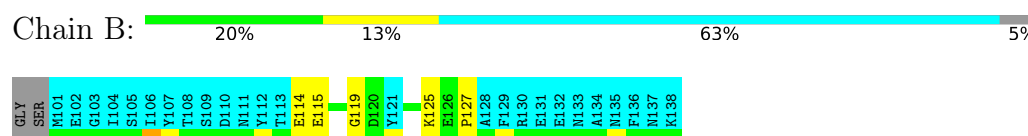
- Molecule 1: Stromal cell-derived factor 1



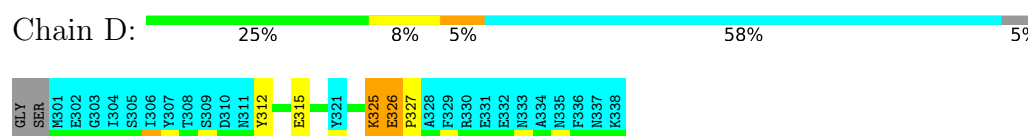
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4

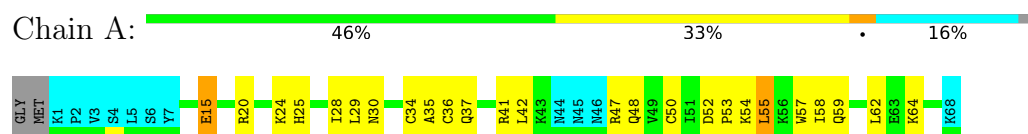


- Molecule 2: C-X-C chemokine receptor type 4

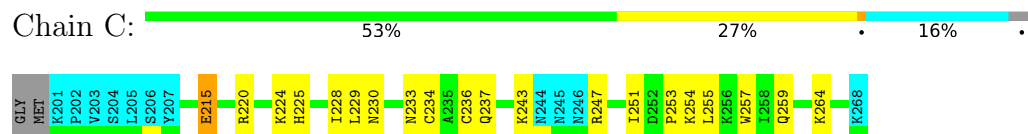


4.2.2 Score per residue for model 2

- Molecule 1: Stromal cell-derived factor 1



- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4





- Molecule 2: C-X-C chemokine receptor type 4



4.2.3 Score per residue for model 3

- Molecule 1: Stromal cell-derived factor 1



- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4



- Molecule 2: C-X-C chemokine receptor type 4



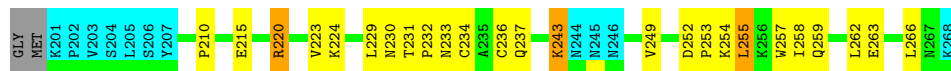
4.2.4 Score per residue for model 4

- Molecule 1: Stromal cell-derived factor 1



- Molecule 1: Stromal cell-derived factor 1

Chain C: 



- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 



- Molecule 2: C-X-C chemokine receptor type 4

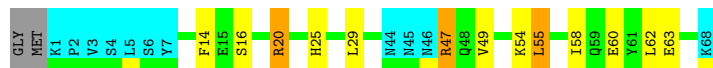
Chain D: 



4.2.5 Score per residue for model 5

- Molecule 1: Stromal cell-derived factor 1

Chain A: 



- Molecule 1: Stromal cell-derived factor 1

Chain C: 



- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 



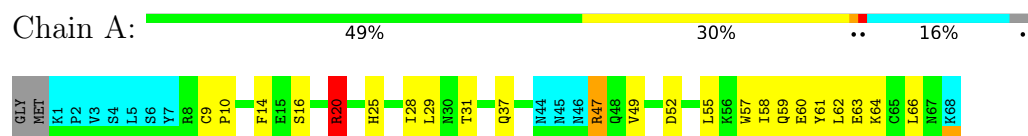
- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 

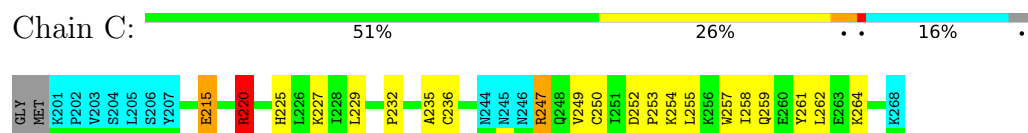


4.2.6 Score per residue for model 6

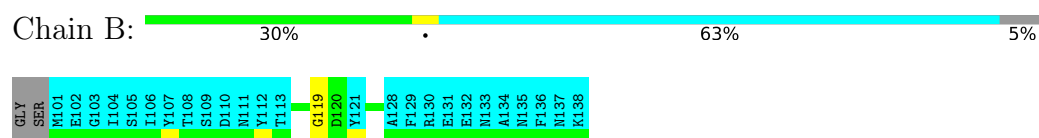
- Molecule 1: Stromal cell-derived factor 1



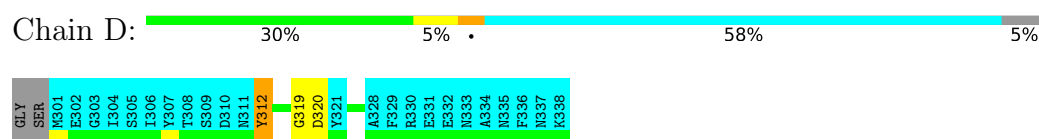
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4

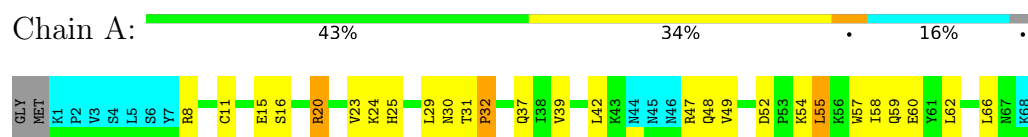


- Molecule 2: C-X-C chemokine receptor type 4

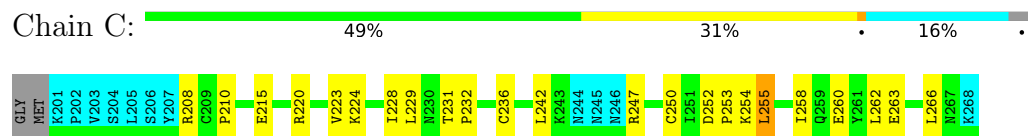


4.2.7 Score per residue for model 7

- Molecule 1: Stromal cell-derived factor 1



- Molecule 1: Stromal cell-derived factor 1



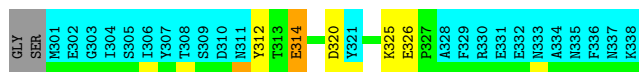
- Molecule 2: C-X-C chemokine receptor type 4





- Molecule 2: C-X-C chemokine receptor type 4

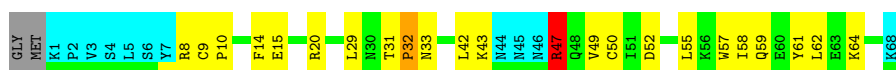
Chain D: 25% 10% 58% 5%



4.2.8 Score per residue for model 8

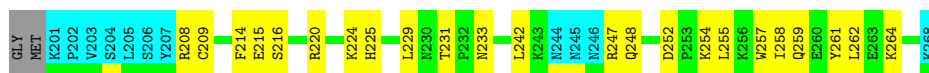
- Molecule 1: Stromal cell-derived factor 1

Chain A: 49% 30% 16%



- Molecule 1: Stromal cell-derived factor 1

Chain C: 49% 33% 16%



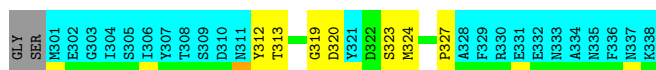
- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 23% 10% 63% 5%



- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 20% 18% 58% 5%



4.2.9 Score per residue for model 9

- Molecule 1: Stromal cell-derived factor 1

Chain A: 50% 26% 16%



- Molecule 1: Stromal cell-derived factor 1

Chain C: 



- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 



- Molecule 2: C-X-C chemokine receptor type 4

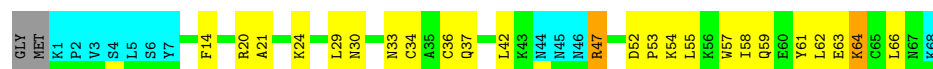
Chain D: 



4.2.10 Score per residue for model 10

- Molecule 1: Stromal cell-derived factor 1

Chain A: 



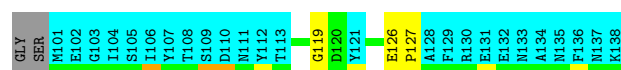
- Molecule 1: Stromal cell-derived factor 1

Chain C: 



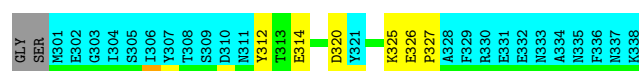
- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 



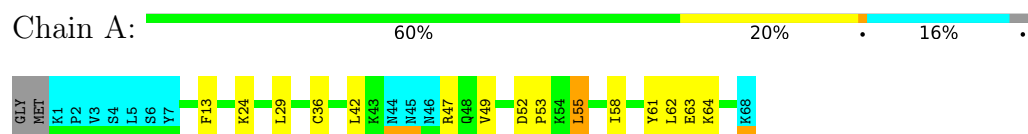
- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 

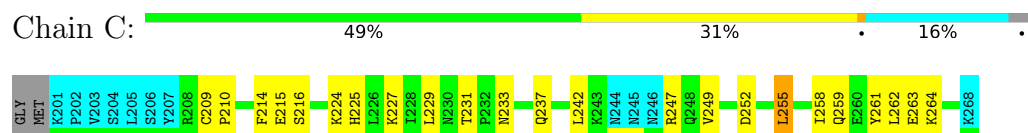


4.2.11 Score per residue for model 11 (medoid)

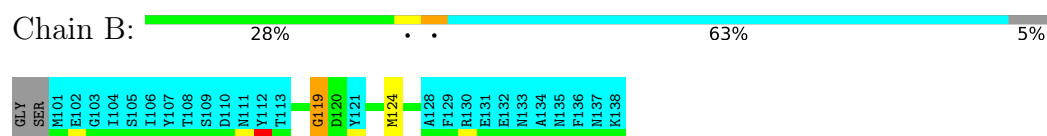
- Molecule 1: Stromal cell-derived factor 1



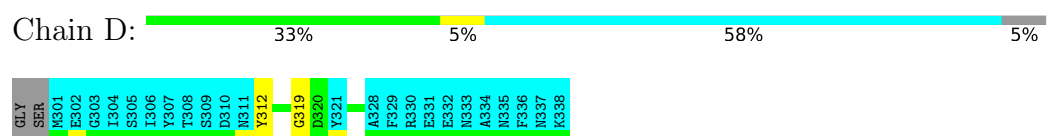
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4

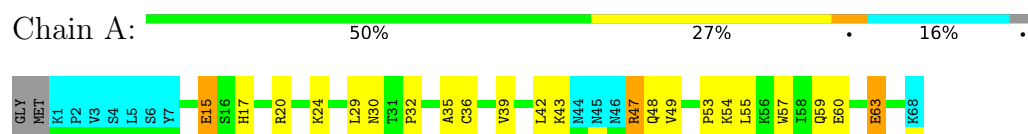


- Molecule 2: C-X-C chemokine receptor type 4

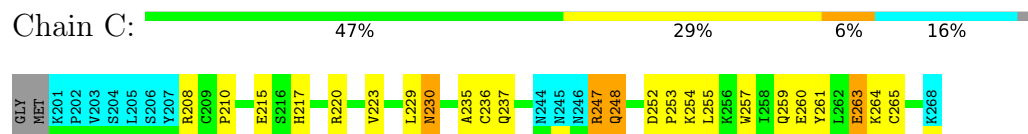


4.2.12 Score per residue for model 12

- Molecule 1: Stromal cell-derived factor 1

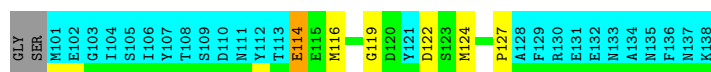


- Molecule 1: Stromal cell-derived factor 1



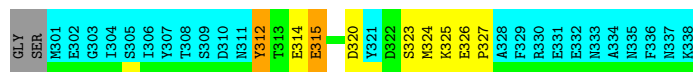
- Molecule 2: C-X-C chemokine receptor type 4





- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 15% 18% 5% 58% 5%



4.2.13 Score per residue for model 13

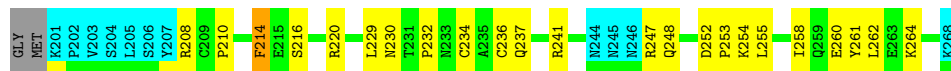
- Molecule 1: Stromal cell-derived factor 1

Chain A: 53% 26% 16%



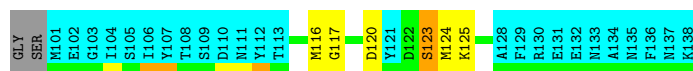
- Molecule 1: Stromal cell-derived factor 1

Chain C: 49% 31% 16%



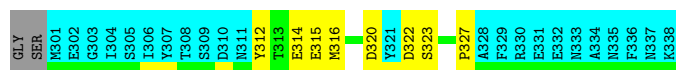
- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 18% 13% 63% 5%



- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 18% 20% 58% 5%



4.2.14 Score per residue for model 14

- Molecule 1: Stromal cell-derived factor 1

Chain A: 46% 31% 16%



- Molecule 1: Stromal cell-derived factor 1

Chain C:



- Molecule 2: C-X-C chemokine receptor type 4

Chain B:



- Molecule 2: C-X-C chemokine receptor type 4

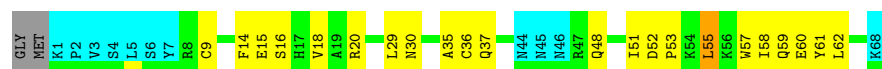
Chain D:



4.2.15 Score per residue for model 15

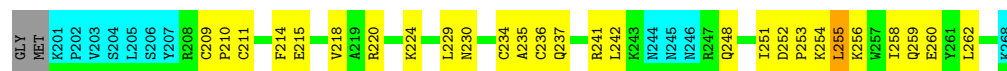
- Molecule 1: Stromal cell-derived factor 1

Chain A:



- Molecule 1: Stromal cell-derived factor 1

Chain C:



- Molecule 2: C-X-C chemokine receptor type 4

Chain B:



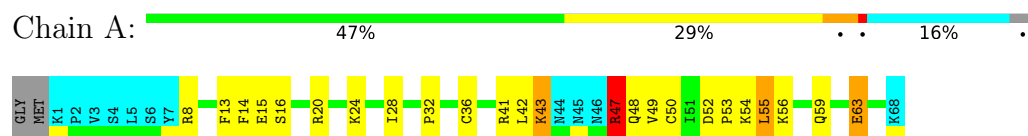
- Molecule 2: C-X-C chemokine receptor type 4

Chain D:

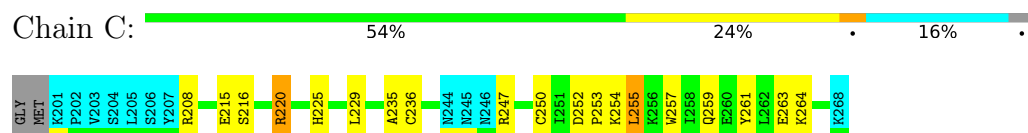


4.2.16 Score per residue for model 16

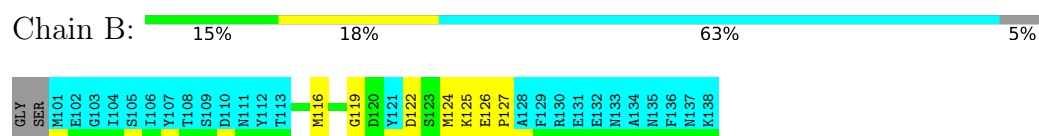
- Molecule 1: Stromal cell-derived factor 1



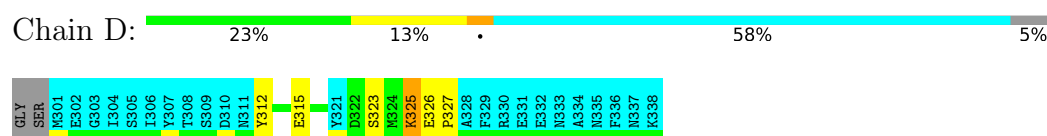
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4

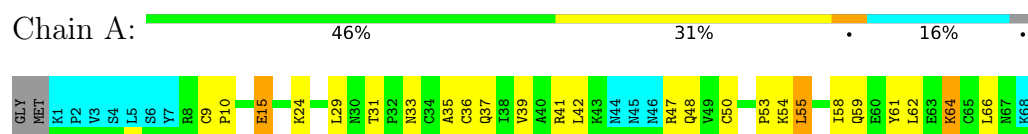


- Molecule 2: C-X-C chemokine receptor type 4

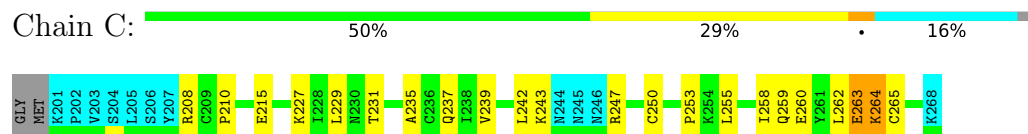


4.2.17 Score per residue for model 17

- Molecule 1: Stromal cell-derived factor 1

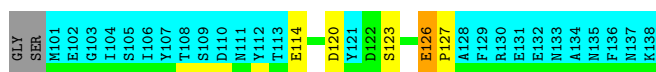


- Molecule 1: Stromal cell-derived factor 1



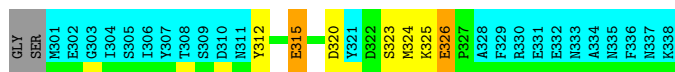
- Molecule 2: C-X-C chemokine receptor type 4





- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 20% 13% 5% 58% 5%



4.2.18 Score per residue for model 18

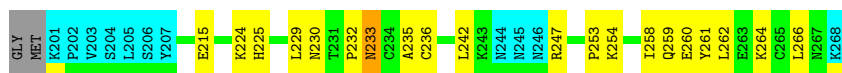
- Molecule 1: Stromal cell-derived factor 1

Chain A: 46% 34% 16%



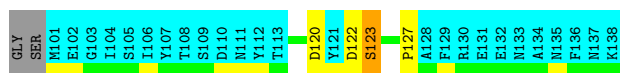
- Molecule 1: Stromal cell-derived factor 1

Chain C: 53% 27% 16%



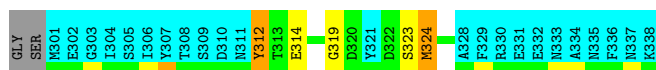
- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 23% 8% 63% 5%



- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 25% 8% 5% 58% 5%



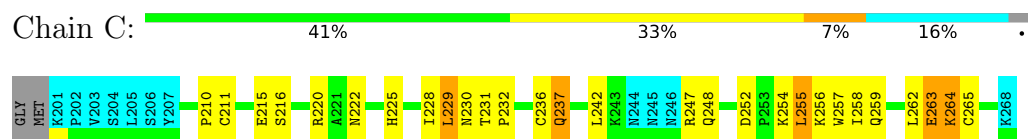
4.2.19 Score per residue for model 19

- Molecule 1: Stromal cell-derived factor 1

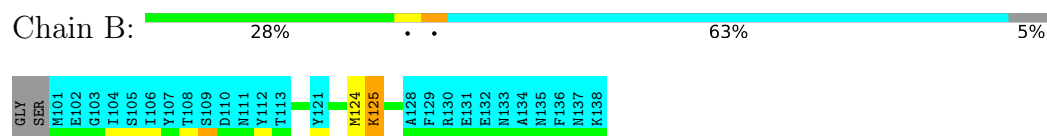
Chain A: 44% 31% 6% 16%



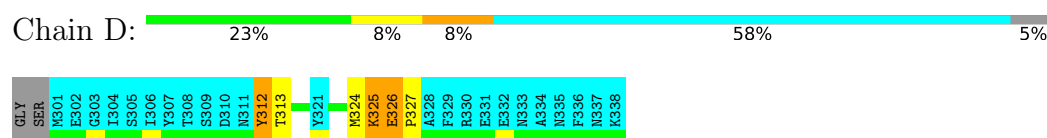
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4

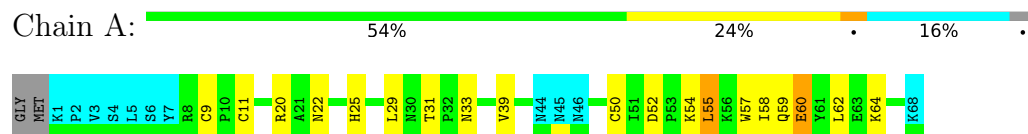


- Molecule 2: C-X-C chemokine receptor type 4

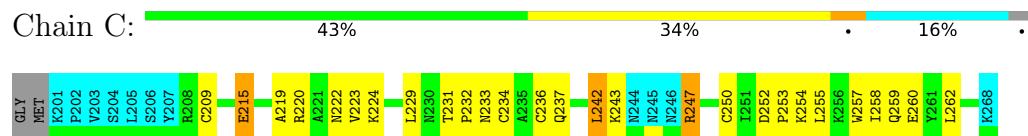


4.2.20 Score per residue for model 20

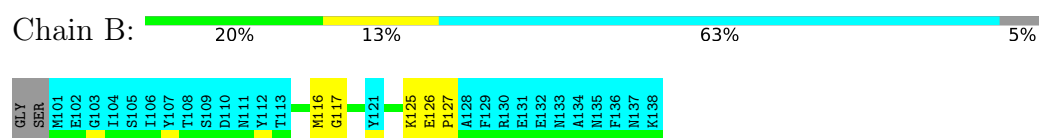
- Molecule 1: Stromal cell-derived factor 1



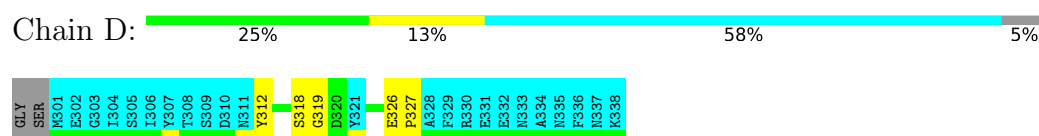
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4



- Molecule 2: C-X-C chemokine receptor type 4



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Xplor-NIH	refinement	2.9.3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	2k03_cs.cif
Number of chemical shift lists	1
Total number of shifts	4956
Number of shifts mapped to atoms	2478
Number of unparsed shifts	2478
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	469	489	487	12±3
1	C	469	489	487	14±3
2	B	95	80	80	2±1
2	D	114	96	96	4±2
All	All	22940	23080	23000	543

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:254:LYS:O	2:D:327:PRO:HA	0.75	1.81	14	9
1:C:229:LEU:HG	2:D:312:TYR:CE2	0.72	2.19	16	7
1:C:220:ARG:HG2	1:C:257:TRP:CE3	0.65	2.25	6	3
1:C:215:GLU:HG2	1:C:250:CYS:O	0.65	1.91	3	4
1:A:10:PRO:HA	2:B:114:GLU:O	0.64	1.92	8	1
1:A:9:CYS:HA	1:A:31:THR:HG21	0.64	1.70	6	1
1:A:20:ARG:HG2	1:A:57:TRP:CE3	0.64	2.28	6	4
1:C:220:ARG:HB3	1:C:257:TRP:CE3	0.64	2.28	5	5
1:A:54:LYS:O	2:B:127:PRO:HA	0.62	1.94	20	9
1:C:236:CYS:O	1:C:253:PRO:HG3	0.62	1.94	4	16
1:C:234:CYS:HB3	1:C:237:GLN:OE1	0.61	1.94	20	6
2:D:325:LYS:H	2:D:325:LYS:HE2	0.61	1.56	14	1
1:A:36:CYS:O	1:A:53:PRO:HG3	0.61	1.94	4	13
1:C:215:GLU:HB3	2:D:320:ASP:O	0.61	1.96	7	3
1:C:229:LEU:HD13	2:D:312:TYR:CD1	0.60	2.32	3	2
1:C:224:LYS:HE3	1:C:242:LEU:O	0.60	1.97	18	4
1:C:259:GLN:O	1:C:263:GLU:HB2	0.58	1.97	12	4
1:C:210:PRO:HD2	1:C:237:GLN:OE1	0.58	1.98	17	1
1:C:209:CYS:O	2:D:315:GLU:HA	0.57	1.99	14	2
1:C:229:LEU:HD22	2:D:312:TYR:CD2	0.57	2.34	5	11
1:A:9:CYS:HA	1:A:31:THR:OG1	0.57	1.98	14	4
2:B:125:LYS:HE2	2:B:125:LYS:N	0.57	2.15	14	1
1:C:252:ASP:O	1:C:255:LEU:HB2	0.56	2.00	3	10
1:C:254:LYS:HA	1:C:259:GLN:NE2	0.56	2.15	2	5
1:A:59:GLN:O	1:A:63:GLU:HB2	0.56	2.01	12	3
1:A:24:LYS:HE2	1:A:42:LEU:O	0.56	2.00	18	4
1:C:261:TYR:O	1:C:264:LYS:HG2	0.56	2.01	11	10
1:A:15:GLU:HB3	2:B:120:ASP:O	0.56	2.01	2	2
1:A:42:LEU:HD23	1:A:43:LYS:N	0.56	2.15	9	2
1:A:15:GLU:HG2	1:A:50:CYS:O	0.55	1.99	17	6
1:A:54:LYS:HA	1:A:59:GLN:NE2	0.55	2.17	12	6
1:C:255:LEU:O	1:C:259:GLN:HG2	0.55	2.00	1	15
1:A:52:ASP:O	1:A:55:LEU:HB2	0.55	2.02	16	13
1:C:220:ARG:HB3	1:C:257:TRP:CZ3	0.55	2.37	12	2
1:A:28:ILE:O	1:C:225:HIS:HB2	0.54	2.01	14	4
1:A:20:ARG:HB3	1:A:57:TRP:CE3	0.54	2.37	15	4
1:A:55:LEU:O	1:A:59:GLN:HG2	0.54	2.02	20	16
1:C:224:LYS:CG	1:C:243:LYS:HA	0.54	2.32	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:323:SER:O	2:D:324:MET:HG3	0.54	2.02	3	2
2:D:320:ASP:O	2:D:323:SER:HB2	0.54	2.03	15	5
1:A:54:LYS:HB3	2:B:127:PRO:HD3	0.54	1.80	17	1
1:A:47:ARG:NH1	1:A:49:VAL:HG12	0.53	2.18	4	4
1:A:20:ARG:HB3	1:A:57:TRP:CZ3	0.53	2.38	8	1
1:C:229:LEU:HG	2:D:312:TYR:CD2	0.53	2.38	15	5
2:D:326:GLU:OE2	2:D:327:PRO:HD2	0.53	2.04	1	1
1:A:11:CYS:HB3	1:A:37:GLN:OE1	0.53	2.04	7	1
1:C:208:ARG:O	1:C:231:THR:HB	0.53	2.03	17	1
2:B:125:LYS:H	2:B:125:LYS:HE2	0.52	1.62	14	1
1:C:215:GLU:HG2	2:D:320:ASP:N	0.52	2.19	10	1
1:A:34:CYS:HB3	1:A:37:GLN:OE1	0.52	2.05	10	4
1:C:216:SER:O	1:C:255:LEU:HD11	0.52	2.04	3	3
2:B:114:GLU:CD	2:B:114:GLU:H	0.52	2.08	12	2
1:A:20:ARG:HG2	1:A:57:TRP:CD2	0.52	2.40	6	1
1:A:20:ARG:HG3	1:A:57:TRP:CE3	0.52	2.40	2	1
1:A:15:GLU:OE1	1:A:49:VAL:HB	0.52	2.05	7	2
1:A:61:TYR:O	1:A:64:LYS:HG2	0.51	2.05	18	6
1:C:258:ILE:O	1:C:262:LEU:HG	0.51	2.05	20	17
1:C:252:ASP:OD1	1:C:254:LYS:HB2	0.51	2.05	19	6
1:A:25:HIS:HB2	1:C:228:ILE:O	0.51	2.06	19	4
1:A:47:ARG:HG2	1:A:48:GLN:H	0.51	1.66	9	1
1:C:237:GLN:HE21	1:C:237:GLN:N	0.51	2.02	19	1
1:A:59:GLN:O	1:A:63:GLU:HG3	0.51	2.04	6	1
1:C:259:GLN:O	1:C:263:GLU:HG3	0.51	2.04	1	1
1:A:58:ILE:O	1:A:62:LEU:HG	0.51	2.05	5	16
1:A:59:GLN:HA	1:A:59:GLN:HE21	0.51	1.66	18	1
1:A:60:GLU:O	1:A:64:LYS:HG2	0.51	2.05	20	1
2:B:125:LYS:HE2	2:B:125:LYS:HA	0.51	1.83	19	2
1:A:9:CYS:O	2:B:115:GLU:HA	0.50	2.06	8	1
1:A:15:GLU:HG3	2:B:120:ASP:O	0.50	2.06	8	1
1:C:214:PHE:O	2:D:323:SER:HA	0.50	2.06	9	1
1:A:25:HIS:CB	1:C:229:LEU:HG	0.50	2.36	2	5
1:A:16:SER:O	1:A:55:LEU:HD11	0.50	2.05	13	3
2:D:325:LYS:HG2	2:D:326:GLU:H	0.50	1.67	17	1
1:C:220:ARG:HG3	1:C:257:TRP:CE3	0.50	2.41	2	1
1:C:209:CYS:HA	1:C:231:THR:OG1	0.50	2.06	11	3
1:A:24:LYS:HE3	1:A:42:LEU:O	0.49	2.07	10	4
1:C:229:LEU:HD22	2:D:312:TYR:CG	0.49	2.41	13	4
2:B:126:GLU:HB2	2:B:127:PRO:CD	0.49	2.37	17	1
1:C:247:ARG:NH1	1:C:249:VAL:HA	0.49	2.22	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:210:PRO:HA	2:D:314:GLU:C	0.49	2.28	14	1
1:A:13:PHE:HB2	2:B:119:GLY:HA3	0.49	1.83	16	2
1:C:216:SER:CB	2:D:325:LYS:HB2	0.49	2.37	19	1
1:C:230:ASN:OD1	1:C:236:CYS:HA	0.49	2.08	13	1
1:C:264:LYS:HD3	1:C:265:CYS:N	0.49	2.23	17	2
1:A:11:CYS:HA	2:B:117:GLY:H	0.49	1.66	20	1
1:C:215:GLU:OE2	1:C:249:VAL:HB	0.49	2.07	1	2
1:A:47:ARG:NH1	1:A:49:VAL:HA	0.49	2.22	6	1
2:D:325:LYS:HE2	2:D:325:LYS:N	0.49	2.23	14	1
1:A:52:ASP:OD1	1:A:54:LYS:HB2	0.49	2.07	13	3
1:A:9:CYS:HA	1:A:31:THR:CG2	0.48	2.37	6	1
1:C:210:PRO:HA	2:D:314:GLU:HB2	0.48	1.85	3	1
1:C:220:ARG:O	1:C:223:VAL:HG22	0.48	2.09	14	3
1:A:67:ASN:OD1	2:D:327:PRO:HG3	0.48	2.09	19	1
2:D:312:TYR:CE2	2:D:314:GLU:HB2	0.48	2.43	18	1
1:A:57:TRP:O	1:A:61:TYR:HB2	0.48	2.09	1	4
1:C:251:ILE:CG2	1:C:255:LEU:HD12	0.48	2.38	14	2
1:A:24:LYS:HE2	1:A:43:LYS:HA	0.48	1.84	16	1
1:A:15:GLU:HG2	2:B:120:ASP:H	0.48	1.69	4	1
1:A:61:TYR:O	1:A:64:LYS:HG3	0.48	2.09	17	2
1:C:247:ARG:HG2	1:C:248:GLN:N	0.48	2.24	12	1
1:A:24:LYS:CE	1:A:43:LYS:HA	0.48	2.39	16	1
1:C:216:SER:HB3	2:D:325:LYS:HB2	0.48	1.84	19	1
1:C:222:ASN:HD21	1:C:242:LEU:HD13	0.48	1.69	19	1
1:C:219:ALA:O	1:C:222:ASN:HB3	0.48	2.09	20	1
1:C:210:PRO:HA	2:D:314:GLU:CB	0.48	2.38	3	1
1:A:10:PRO:HD3	1:A:31:THR:OG1	0.47	2.09	18	4
1:C:242:LEU:HB2	1:C:247:ARG:O	0.47	2.09	14	2
1:C:210:PRO:HD3	1:C:231:THR:OG1	0.47	2.09	10	1
1:C:252:ASP:HB3	1:C:255:LEU:HG	0.47	1.85	10	1
1:A:54:LYS:HB3	2:B:127:PRO:N	0.47	2.24	3	2
1:C:247:ARG:CZ	1:C:249:VAL:HG12	0.47	2.39	6	2
1:A:16:SER:HB3	2:B:125:LYS:CG	0.47	2.39	9	1
1:A:54:LYS:HA	1:A:59:GLN:OE1	0.47	2.09	4	1
2:B:120:ASP:O	2:B:123:SER:HB2	0.47	2.09	17	4
1:C:208:ARG:NE	1:C:208:ARG:HA	0.47	2.25	7	1
1:A:27:LYS:HG2	1:A:29:LEU:CD2	0.47	2.38	14	1
1:C:239:VAL:HG22	1:C:250:CYS:SG	0.47	2.50	1	5
1:C:220:ARG:HB3	1:C:257:TRP:CD2	0.47	2.44	4	1
1:A:8:ARG:O	1:A:31:THR:HG22	0.47	2.09	7	1
1:C:224:LYS:HE2	1:C:242:LEU:O	0.47	2.09	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:CYS:SG	2:B:117:GLY:HA3	0.47	2.49	13	1
1:A:10:PRO:HD2	1:A:37:GLN:OE1	0.47	2.08	17	1
1:C:216:SER:HA	1:C:255:LEU:HD11	0.47	1.87	5	4
1:A:36:CYS:O	1:A:53:PRO:HB3	0.47	2.08	17	1
1:A:52:ASP:CG	2:B:125:LYS:HB3	0.46	2.29	3	1
1:A:18:VAL:HG21	1:A:51:ILE:HD12	0.46	1.87	15	1
1:C:216:SER:HA	1:C:255:LEU:HG	0.46	1.86	16	1
1:C:229:LEU:HD13	2:D:312:TYR:CE1	0.46	2.45	18	2
1:A:18:VAL:HG11	1:A:51:ILE:HD12	0.46	1.86	14	2
1:A:31:THR:CG2	1:A:32:PRO:HD2	0.46	2.41	4	1
1:C:247:ARG:NH1	1:C:249:VAL:HG12	0.46	2.25	10	1
1:C:254:LYS:HB3	2:D:327:PRO:HD3	0.46	1.87	13	1
1:A:29:LEU:HG	1:C:225:HIS:CB	0.46	2.40	2	3
1:A:47:ARG:NH2	1:A:49:VAL:HA	0.46	2.26	5	1
1:A:31:THR:HG22	1:A:32:PRO:HD2	0.46	1.88	4	1
2:D:314:GLU:H	2:D:314:GLU:CD	0.46	2.14	10	1
1:C:252:ASP:OD2	1:C:254:LYS:HB2	0.46	2.11	7	3
1:C:250:CYS:SG	2:D:318:SER:HB2	0.45	2.51	20	1
2:D:325:LYS:HG2	2:D:326:GLU:N	0.45	2.26	17	1
1:C:208:ARG:HD2	2:D:315:GLU:OE2	0.45	2.11	13	1
1:A:11:CYS:HA	2:B:117:GLY:N	0.45	2.25	20	1
1:C:210:PRO:O	2:D:316:MET:HB3	0.45	2.11	15	1
2:D:325:LYS:HG3	2:D:326:GLU:OE2	0.45	2.12	19	1
1:C:214:PHE:CD1	1:C:252:ASP:HA	0.45	2.46	8	2
1:A:15:GLU:OE2	1:A:49:VAL:HB	0.44	2.13	12	1
1:A:39:VAL:HG22	1:A:50:CYS:SG	0.44	2.52	17	2
1:C:242:LEU:HD23	1:C:243:LYS:N	0.44	2.27	17	1
1:C:241:ARG:HG2	1:C:248:GLN:HB3	0.44	1.88	13	1
1:C:217:HIS:HB2	2:D:322:ASP:HB3	0.44	1.88	14	1
1:A:9:CYS:H	2:B:115:GLU:HA	0.44	1.73	1	1
1:C:215:GLU:OE1	1:C:249:VAL:HB	0.44	2.12	9	3
1:C:218:VAL:HG21	1:C:251:ILE:HD12	0.44	1.90	15	1
1:C:224:LYS:HE2	1:C:243:LYS:HA	0.44	1.88	4	1
1:C:215:GLU:HA	2:D:320:ASP:O	0.44	2.13	6	1
1:A:24:LYS:HG2	1:A:41:ARG:O	0.44	2.13	16	2
1:A:17:HIS:CD2	2:B:122:ASP:HB3	0.44	2.48	12	2
1:A:15:GLU:OE1	2:B:118:SER:HB2	0.44	2.13	7	1
1:A:42:LEU:HB2	1:A:47:ARG:O	0.44	2.12	8	2
1:A:41:ARG:HG2	1:A:48:GLN:HG2	0.43	1.89	3	2
1:C:227:LYS:O	1:C:238:ILE:HA	0.43	2.12	3	1
1:C:210:PRO:HG2	1:C:237:GLN:HG2	0.43	1.89	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:227:LYS:HG2	1:C:229:LEU:CD2	0.43	2.43	11	3
1:C:220:ARG:O	1:C:220:ARG:HD2	0.43	2.13	14	1
1:C:208:ARG:NH1	2:D:315:GLU:HB3	0.43	2.27	17	1
1:C:230:ASN:ND2	1:C:236:CYS:HA	0.43	2.28	19	1
1:C:210:PRO:HD3	1:C:231:THR:CB	0.43	2.44	7	2
1:A:9:CYS:SG	1:A:33:ASN:HB3	0.43	2.53	19	1
1:A:19:ALA:O	1:A:22:ASN:HB3	0.43	2.12	9	1
1:C:215:GLU:HA	2:D:323:SER:HA	0.43	1.91	3	1
1:A:29:LEU:HD13	1:C:225:HIS:HB3	0.43	1.90	6	1
1:A:15:GLU:HB3	1:A:50:CYS:O	0.43	2.14	8	1
1:A:20:ARG:HB3	1:A:57:TRP:CD2	0.43	2.49	7	2
1:C:210:PRO:HB3	2:D:312:TYR:HE2	0.43	1.74	13	1
2:B:125:LYS:HG2	2:B:126:GLU:H	0.43	1.73	15	1
1:A:29:LEU:HD21	1:C:225:HIS:HB3	0.43	1.90	18	1
1:C:210:PRO:HD3	1:C:231:THR:CG2	0.42	2.44	19	2
1:C:232:PRO:O	1:C:233:ASN:HB2	0.42	2.14	18	1
1:A:25:HIS:HB2	1:C:229:LEU:HG	0.42	1.90	20	1
1:C:251:ILE:HG23	1:C:255:LEU:HD12	0.42	1.90	2	1
1:A:11:CYS:SG	1:A:39:VAL:HG22	0.42	2.54	9	1
1:A:24:LYS:HG3	1:A:41:ARG:O	0.42	2.14	13	2
1:A:8:ARG:O	1:A:31:THR:HB	0.42	2.14	1	2
1:A:52:ASP:OD2	1:A:54:LYS:HB2	0.42	2.13	2	1
1:A:9:CYS:HB3	1:A:37:GLN:OE1	0.42	2.13	15	1
1:C:224:LYS:CE	1:C:241:ARG:HD2	0.42	2.43	15	1
1:A:64:LYS:HB2	1:A:64:LYS:NZ	0.42	2.28	17	1
1:A:54:LYS:HA	1:A:59:GLN:CD	0.42	2.35	4	1
2:D:314:GLU:O	2:D:315:GLU:HB2	0.42	2.13	12	1
1:C:208:ARG:HA	1:C:208:ARG:NE	0.42	2.29	12	1
1:A:37:GLN:HE21	1:A:37:GLN:N	0.42	2.13	9	1
1:A:47:ARG:CG	1:A:48:GLN:H	0.42	2.28	9	1
1:A:24:LYS:HE2	1:A:43:LYS:O	0.42	2.15	14	1
1:C:211:CYS:SG	2:D:318:SER:HB2	0.42	2.54	14	2
1:A:10:PRO:O	2:B:116:MET:HB3	0.42	2.15	14	1
1:A:16:SER:O	1:A:55:LEU:HD21	0.42	2.15	15	2
1:C:222:ASN:ND2	1:C:242:LEU:HD13	0.42	2.30	19	1
1:A:18:VAL:HG21	1:A:49:VAL:HG21	0.42	1.90	4	1
1:A:59:GLN:O	1:A:63:GLU:HG2	0.42	2.15	10	1
2:B:125:LYS:CE	2:B:125:LYS:HA	0.42	2.44	19	1
1:C:261:TYR:O	1:C:264:LYS:HG3	0.41	2.15	10	1
1:A:53:PRO:HA	1:A:58:ILE:HG21	0.41	1.92	2	1
1:C:215:GLU:HB2	1:C:250:CYS:O	0.41	2.14	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ARG:HG2	1:A:48:GLN:O	0.41	2.15	16	1
1:C:254:LYS:HD2	2:D:327:PRO:HD3	0.41	1.90	8	1
1:A:15:GLU:HG2	2:B:120:ASP:N	0.41	2.30	13	1
2:D:325:LYS:N	2:D:325:LYS:HD2	0.41	2.31	16	2
1:A:54:LYS:HD2	2:B:127:PRO:HD3	0.41	1.92	2	1
1:A:16:SER:HA	1:A:55:LEU:CD1	0.41	2.46	5	1
1:C:220:ARG:O	1:C:220:ARG:HG2	0.41	2.15	7	1
1:A:29:LEU:HG	1:C:225:HIS:HB3	0.41	1.92	8	1
1:C:215:GLU:HG3	2:D:320:ASP:C	0.41	2.35	2	1
1:A:25:HIS:HB3	1:C:229:LEU:HD13	0.41	1.91	6	1
1:A:10:PRO:CG	1:A:37:GLN:HG2	0.41	2.46	6	1
1:A:29:LEU:HG	1:C:225:HIS:HB2	0.41	1.92	11	1
1:A:15:GLU:HG3	1:A:49:VAL:HB	0.41	1.91	16	1
1:C:231:THR:CG2	2:D:314:GLU:HB2	0.41	2.46	7	1
2:D:325:LYS:HG3	2:D:326:GLU:H	0.41	1.76	12	1
1:C:208:ARG:HB3	2:D:315:GLU:HA	0.40	1.92	9	1
1:A:29:LEU:CD2	1:C:225:HIS:HB3	0.40	2.45	18	1
1:C:261:TYR:HA	1:C:264:LYS:CD	0.40	2.45	18	1
1:C:220:ARG:HG3	1:C:257:TRP:CZ3	0.40	2.52	3	1
1:A:47:ARG:CZ	1:A:49:VAL:HG12	0.40	2.46	4	1
1:A:20:ARG:O	1:A:23:VAL:HG22	0.40	2.16	7	1
1:A:54:LYS:CB	2:B:127:PRO:HD3	0.40	2.45	17	1
1:A:14:PHE:O	2:B:123:SER:HA	0.40	2.16	5	1
1:C:209:CYS:SG	1:C:210:PRO:HD2	0.40	2.56	11	1
1:A:16:SER:HB2	2:B:124:MET:O	0.40	2.17	16	1
1:A:10:PRO:HA	2:B:114:GLU:CB	0.40	2.47	3	1
1:A:15:GLU:HA	2:B:123:SER:HA	0.40	1.92	3	1
1:A:16:SER:HA	1:A:55:LEU:HD11	0.40	1.93	5	1
1:C:239:VAL:HG21	2:D:312:TYR:OH	0.40	2.16	14	1

5.2 Torsion angles ⓘ

5.2.1 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	57/70 (81%)	51±1 (90±2%)	4±1 (7±2%)	1±1 (2±2%)	10 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	57/70 (81%)	52±2 (90±3%)	4±2 (7±3%)	1±1 (2±1%)	10	46
2	B	13/40 (32%)	7±2 (55±15%)	4±2 (31±12%)	2±1 (14±7%)	1	5
2	D	15/40 (38%)	8±2 (55±10%)	5±1 (31±8%)	2±1 (15±7%)	1	4
All	All	2840/4400 (65%)	2367 (83%)	337 (12%)	136 (5%)	5	27

All 36 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	35	ALA	8
2	B	119	GLY	8
2	B	126	GLU	8
1	C	235	ALA	8
2	D	326	GLU	7
1	C	233	ASN	7
1	C	232	PRO	7
2	D	324	MET	7
2	D	319	GLY	6
1	A	33	ASN	6
1	A	32	PRO	6
2	B	116	MET	5
2	D	314	GLU	5
2	D	312	TYR	5
2	D	315	GLU	4
2	B	124	MET	4
1	A	43	LYS	4
2	B	114	GLU	4
2	B	127	PRO	3
1	C	243	LYS	3
1	A	67	ASN	2
2	D	327	PRO	2
2	D	313	THR	2
2	B	123	SER	2
2	D	322	ASP	2
2	D	318	SER	1
1	C	211	CYS	1
2	B	122	ASP	1
1	A	36	CYS	1
1	C	267	ASN	1
1	C	225	HIS	1
2	D	316	MET	1

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Mol	Chain	Res	Type	Models (Total)
2	D	317	GLY	1
2	B	115	GLU	1
2	D	323	SER	1
1	A	47	ARG	1

5.2.2 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	53/65 (82%)	48±1 (91±3%)	5±1 (9±3%)	15	61
1	C	53/65 (82%)	49±2 (92±3%)	4±2 (8±3%)	18	65
2	B	11/33 (33%)	11±1 (95±5%)	1±1 (5±5%)	34	81
2	D	13/33 (39%)	12±1 (95±5%)	1±1 (5±5%)	31	78
All	All	2600/3920 (66%)	2401 (92%)	199 (8%)	18	65

All 49 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	47	ARG	16
1	C	247	ARG	14
1	A	55	LEU	11
1	C	260	GLU	10
1	C	255	LEU	9
1	A	14	PHE	9
1	A	60	GLU	9
1	C	263	GLU	8
1	C	215	GLU	7
2	D	325	LYS	7
1	A	15	GLU	6
1	A	20	ARG	6
2	B	125	LYS	6
1	C	220	ARG	6
1	A	66	LEU	6
1	A	48	GLN	6
1	C	248	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	63	GLU	5
1	A	30	ASN	4
1	C	214	PHE	4
1	A	64	LYS	4
1	C	230	ASN	4
1	A	37	GLN	3
2	D	326	GLU	3
1	C	266	LEU	3
1	C	264	LYS	3
2	B	114	GLU	2
1	C	208	ARG	2
1	C	242	LEU	1
2	D	327	PRO	1
1	C	237	GLN	1
1	A	59	GLN	1
1	A	31	THR	1
1	A	22	ASN	1
1	A	56	LYS	1
2	B	124	MET	1
1	A	8	ARG	1
1	C	231	THR	1
2	D	316	MET	1
1	C	233	ASN	1
1	A	29	LEU	1
2	B	126	GLU	1
1	A	32	PRO	1
1	C	229	LEU	1
1	C	256	LYS	1
2	D	312	TYR	1
1	C	261	TYR	1
1	C	253	PRO	1
1	A	42	LEU	1

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics

could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	TYS	B	121	2	15,16,17	1.07±0.10	0±0 (0±0%)
2	TYS	D	321	2	15,16,17	1.08±0.12	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	TYS	B	121	2	18,22,24	1.11±0.03	0±0 (0±0%)
2	TYS	D	321	2	18,22,24	1.10±0.05	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	B	121	2	-	0±0,9,11,13	0±0,1,1,1
2	TYS	D	321	2	-	0±0,9,11,13	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 84% for the entire structure.

6.1 Chemical shift list 1

File name: 2k03_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 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	4956
Number of shifts mapped to atoms	2478
Number of unparsed shifts	2478
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.

- Chemical shift has been reported more than once. All 2478 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2479	A	1	LYS	H	8.402	0.020	1
2480	C	201	LYS	H	8.402	0.020	1
2481	A	1	LYS	N	124.577	0.1	1
2482	C	201	LYS	N	124.577	0.1	1
2483	A	2	PRO	HA	4.509	0.020	1
2484	C	202	PRO	HA	4.509	0.020	1
2485	A	2	PRO	HB2	2.309	0.020	2
2486	C	202	PRO	HB2	2.309	0.020	2
2487	A	2	PRO	HB3	1.936	0.020	2
2488	C	202	PRO	HB3	1.936	0.020	2
2489	A	2	PRO	HD2	3.885	0.020	2
2490	C	202	PRO	HD2	3.885	0.020	2
2491	A	2	PRO	HD3	3.678	0.020	2
2492	C	202	PRO	HD3	3.678	0.020	2
2493	A	2	PRO	HG2	2.054	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2494	C	202	PRO	HG2	2.054	0.020	2
2495	A	2	PRO	HG3	2.054	0.020	2
2496	C	202	PRO	HG3	2.054	0.020	2
2497	A	2	PRO	C	177.132	0.1	1
2498	C	202	PRO	C	177.132	0.1	1
2499	A	2	PRO	CA	63.529	0.1	1
2500	C	202	PRO	CA	63.529	0.1	1
2501	A	2	PRO	CB	32.476	0.1	1
2502	C	202	PRO	CB	32.476	0.1	1
2503	A	2	PRO	CD	51.064	0.1	1
2504	C	202	PRO	CD	51.064	0.1	1
2505	A	2	PRO	CG	27.775	0.1	1
2506	C	202	PRO	CG	27.775	0.1	1
2507	A	3	VAL	H	8.201	0.020	1
2508	C	203	VAL	H	8.201	0.020	1
2509	A	3	VAL	HA	4.152	0.020	1
2510	C	203	VAL	HA	4.152	0.020	1
2511	A	3	VAL	HB	2.108	0.020	1
2512	C	203	VAL	HB	2.108	0.020	1
2513	A	3	VAL	HG11	0.988	0.020	2
2514	C	203	VAL	HG11	0.988	0.020	2
2515	A	3	VAL	HG12	0.988	0.020	2
2516	C	203	VAL	HG12	0.988	0.020	2
2517	A	3	VAL	HG13	0.988	0.020	2
2518	C	203	VAL	HG13	0.988	0.020	2
2519	A	3	VAL	HG21	0.988	0.020	2
2520	C	203	VAL	HG21	0.988	0.020	2
2521	A	3	VAL	HG22	0.988	0.020	2
2522	C	203	VAL	HG22	0.988	0.020	2
2523	A	3	VAL	HG23	0.988	0.020	2
2524	C	203	VAL	HG23	0.988	0.020	2
2525	A	3	VAL	C	176.423	0.1	1
2526	C	203	VAL	C	176.423	0.1	1
2527	A	3	VAL	CA	62.873	0.1	1
2528	C	203	VAL	CA	62.873	0.1	1
2529	A	3	VAL	CB	33.455	0.1	1
2530	C	203	VAL	CB	33.455	0.1	1
2531	A	3	VAL	CG1	21.324	0.1	1
2532	C	203	VAL	CG1	21.324	0.1	1
2533	A	3	VAL	N	120.488	0.1	1
2534	C	203	VAL	N	120.488	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2535	A	4	SER	H	8.276	0.020	1
2536	C	204	SER	H	8.276	0.020	1
2537	A	4	SER	HA	4.494	0.020	1
2538	C	204	SER	HA	4.494	0.020	1
2539	A	4	SER	HB2	3.874	0.020	2
2540	C	204	SER	HB2	3.874	0.020	2
2541	A	4	SER	HB3	3.874	0.020	2
2542	C	204	SER	HB3	3.874	0.020	2
2543	A	4	SER	C	174.687	0.1	1
2544	C	204	SER	C	174.687	0.1	1
2545	A	4	SER	CA	58.375	0.1	1
2546	C	204	SER	CA	58.375	0.1	1
2547	A	4	SER	CB	64.295	0.1	1
2548	C	204	SER	CB	64.295	0.1	1
2549	A	4	SER	N	119.000	0.1	1
2550	C	204	SER	N	119.000	0.1	1
2551	A	5	LEU	H	8.238	0.020	1
2552	C	205	LEU	H	8.238	0.020	1
2553	A	5	LEU	HA	4.406	0.020	1
2554	C	205	LEU	HA	4.406	0.020	1
2555	A	5	LEU	HB2	1.605	0.020	2
2556	C	205	LEU	HB2	1.605	0.020	2
2557	A	5	LEU	HB3	1.605	0.020	2
2558	C	205	LEU	HB3	1.605	0.020	2
2559	A	5	LEU	HD11	0.943	0.020	2
2560	C	205	LEU	HD11	0.943	0.020	2
2561	A	5	LEU	HD12	0.943	0.020	2
2562	C	205	LEU	HD12	0.943	0.020	2
2563	A	5	LEU	HD13	0.943	0.020	2
2564	C	205	LEU	HD13	0.943	0.020	2
2565	A	5	LEU	C	177.406	0.1	1
2566	C	205	LEU	C	177.406	0.1	1
2567	A	5	LEU	CA	55.766	0.1	1
2568	C	205	LEU	CA	55.766	0.1	1
2569	A	5	LEU	CB	43.132	0.1	1
2570	C	205	LEU	CB	43.132	0.1	1
2571	A	5	LEU	CD1	25.588	0.1	1
2572	C	205	LEU	CD1	25.588	0.1	1
2573	A	5	LEU	N	124.704	0.1	1
2574	C	205	LEU	N	124.704	0.1	1
2575	A	6	SER	H	8.148	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2576	C	206	SER	H	8.148	0.020	1
2577	A	6	SER	HA	4.438	0.020	1
2578	C	206	SER	HA	4.438	0.020	1
2579	A	6	SER	HB2	3.829	0.020	2
2580	C	206	SER	HB2	3.829	0.020	2
2581	A	6	SER	HB3	3.829	0.020	2
2582	C	206	SER	HB3	3.829	0.020	2
2583	A	6	SER	C	174.321	0.1	1
2584	C	206	SER	C	174.321	0.1	1
2585	A	6	SER	CA	58.718	0.1	1
2586	C	206	SER	CA	58.718	0.1	1
2587	A	6	SER	CB	64.295	0.1	1
2588	C	206	SER	CB	64.295	0.1	1
2589	A	6	SER	N	115.960	0.1	1
2590	C	206	SER	N	115.960	0.1	1
2591	A	7	TYR	H	7.954	0.020	1
2592	C	207	TYR	H	7.954	0.020	1
2593	A	7	TYR	HA	4.585	0.020	1
2594	C	207	TYR	HA	4.585	0.020	1
2595	A	7	TYR	HB2	3.085	0.020	2
2596	C	207	TYR	HB2	3.085	0.020	2
2597	A	7	TYR	HB3	2.963	0.020	2
2598	C	207	TYR	HB3	2.963	0.020	2
2599	A	7	TYR	HD1	7.112	0.006	1
2600	C	207	TYR	HD1	7.112	0.006	1
2601	A	7	TYR	HD2	7.112	0.006	1
2602	C	207	TYR	HD2	7.112	0.006	1
2603	A	7	TYR	HE1	6.841	0.020	1
2604	C	207	TYR	HE1	6.841	0.020	1
2605	A	7	TYR	HE2	6.841	0.020	1
2606	C	207	TYR	HE2	6.841	0.020	1
2607	A	7	TYR	C	175.532	0.1	1
2608	C	207	TYR	C	175.532	0.1	1
2609	A	7	TYR	CA	58.335	0.1	1
2610	C	207	TYR	CA	58.335	0.1	1
2611	A	7	TYR	CB	39.474	0.1	1
2612	C	207	TYR	CB	39.474	0.1	1
2613	A	7	TYR	CD1	133.600	0.1	1
2614	C	207	TYR	CD1	133.600	0.1	1
2615	A	7	TYR	CE1	118.588	0.1	1
2616	C	207	TYR	CE1	118.588	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2617	A	7	TYR	N	121.884	0.1	1
2618	C	207	TYR	N	121.884	0.1	1
2619	A	8	ARG	H	8.117	0.020	1
2620	C	208	ARG	H	8.117	0.020	1
2621	A	8	ARG	HA	4.349	0.001	1
2622	C	208	ARG	HA	4.349	0.001	1
2623	A	8	ARG	HB2	1.837	0.020	2
2624	C	208	ARG	HB2	1.837	0.020	2
2625	A	8	ARG	HB3	1.737	0.002	2
2626	C	208	ARG	HB3	1.737	0.002	2
2627	A	8	ARG	HD2	3.182	0.020	2
2628	C	208	ARG	HD2	3.182	0.020	2
2629	A	8	ARG	HD3	3.182	0.020	2
2630	C	208	ARG	HD3	3.182	0.020	2
2631	A	8	ARG	HG2	1.557	0.005	2
2632	C	208	ARG	HG2	1.557	0.005	2
2633	A	8	ARG	HG3	1.557	0.005	2
2634	C	208	ARG	HG3	1.557	0.005	2
2635	A	8	ARG	C	175.898	0.1	1
2636	C	208	ARG	C	175.898	0.1	1
2637	A	8	ARG	CA	56.048	0.1	1
2638	C	208	ARG	CA	56.048	0.1	1
2639	A	8	ARG	CB	31.492	0.1	1
2640	C	208	ARG	CB	31.492	0.1	1
2641	A	8	ARG	CD	43.957	0.1	1
2642	C	208	ARG	CD	43.957	0.1	1
2643	A	8	ARG	CG	27.307	0.1	1
2644	C	208	ARG	CG	27.307	0.1	1
2645	A	8	ARG	N	121.977	0.1	1
2646	C	208	ARG	N	121.977	0.1	1
2647	A	9	CYS	H	8.127	0.020	1
2648	C	209	CYS	H	8.127	0.020	1
2649	A	9	CYS	HA	4.984	0.020	1
2650	C	209	CYS	HA	4.984	0.020	1
2651	A	9	CYS	HB2	3.164	0.020	2
2652	C	209	CYS	HB2	3.164	0.020	2
2653	A	9	CYS	HB3	2.737	0.020	2
2654	C	209	CYS	HB3	2.737	0.020	2
2655	A	9	CYS	C	177.771	0.1	1
2656	C	209	CYS	C	177.771	0.1	1
2657	A	9	CYS	CA	53.192	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2658	C	209	CYS	CA	53.192	0.1	1
2659	A	9	CYS	CB	40.897	0.1	1
2660	C	209	CYS	CB	40.897	0.1	1
2661	A	9	CYS	N	121.209	0.1	1
2662	C	209	CYS	N	121.209	0.1	1
2663	A	10	PRO	HA	4.321	0.020	1
2664	C	210	PRO	HA	4.321	0.020	1
2665	A	10	PRO	HB2	2.318	0.020	2
2666	C	210	PRO	HB2	2.318	0.020	2
2667	A	10	PRO	HB3	1.883	0.020	2
2668	C	210	PRO	HB3	1.883	0.020	2
2669	A	10	PRO	HD2	3.871	0.020	2
2670	C	210	PRO	HD2	3.871	0.020	2
2671	A	10	PRO	HD3	3.871	0.020	2
2672	C	210	PRO	HD3	3.871	0.020	2
2673	A	10	PRO	HG2	2.036	0.020	2
2674	C	210	PRO	HG2	2.036	0.020	2
2675	A	10	PRO	HG3	2.036	0.020	2
2676	C	210	PRO	HG3	2.036	0.020	2
2677	A	10	PRO	CA	65.478	0.1	1
2678	C	210	PRO	CA	65.478	0.1	1
2679	A	10	PRO	CB	32.904	0.1	1
2680	C	210	PRO	CB	32.904	0.1	1
2681	A	10	PRO	CD	51.251	0.1	1
2682	C	210	PRO	CD	51.251	0.1	1
2683	A	10	PRO	CG	27.900	0.1	1
2684	C	210	PRO	CG	27.900	0.1	1
2685	A	11	CYS	H	8.633	0.001	1
2686	C	211	CYS	H	8.633	0.001	1
2687	A	11	CYS	C	174.618	0.1	1
2688	C	211	CYS	C	174.618	0.1	1
2689	A	11	CYS	N	114.595	0.1	1
2690	C	211	CYS	N	114.595	0.1	1
2691	A	12	ARG	H	8.236	0.020	1
2692	C	212	ARG	H	8.236	0.020	1
2693	A	12	ARG	HA	4.067	0.020	1
2694	C	212	ARG	HA	4.067	0.020	1
2695	A	12	ARG	HB2	1.572	0.020	2
2696	C	212	ARG	HB2	1.572	0.020	2
2697	A	12	ARG	HB3	1.572	0.020	2
2698	C	212	ARG	HB3	1.572	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2699	A	12	ARG	HD2	3.062	0.020	2
2700	C	212	ARG	HD2	3.062	0.020	2
2701	A	12	ARG	HD3	3.062	0.020	2
2702	C	212	ARG	HD3	3.062	0.020	2
2703	A	12	ARG	HG2	1.331	0.020	2
2704	C	212	ARG	HG2	1.331	0.020	2
2705	A	12	ARG	HG3	1.295	0.020	2
2706	C	212	ARG	HG3	1.295	0.020	2
2707	A	12	ARG	C	175.098	0.1	1
2708	C	212	ARG	C	175.098	0.1	1
2709	A	12	ARG	CA	57.370	0.1	1
2710	C	212	ARG	CA	57.370	0.1	1
2711	A	12	ARG	CB	31.631	0.1	1
2712	C	212	ARG	CB	31.631	0.1	1
2713	A	12	ARG	CD	43.865	0.1	1
2714	C	212	ARG	CD	43.865	0.1	1
2715	A	12	ARG	CG	27.227	0.1	1
2716	C	212	ARG	CG	27.227	0.1	1
2717	A	12	ARG	N	122.779	0.1	1
2718	C	212	ARG	N	122.779	0.1	1
2719	A	13	PHE	H	7.615	0.020	1
2720	C	213	PHE	H	7.615	0.020	1
2721	A	13	PHE	HA	4.510	0.020	1
2722	C	213	PHE	HA	4.510	0.020	1
2723	A	13	PHE	HB2	3.084	0.020	2
2724	C	213	PHE	HB2	3.084	0.020	2
2725	A	13	PHE	HB3	2.807	0.020	2
2726	C	213	PHE	HB3	2.807	0.020	2
2727	A	13	PHE	HD1	7.224	0.005	1
2728	C	213	PHE	HD1	7.224	0.005	1
2729	A	13	PHE	HD2	7.224	0.005	1
2730	C	213	PHE	HD2	7.224	0.005	1
2731	A	13	PHE	HE1	7.351	0.020	1
2732	C	213	PHE	HE1	7.351	0.020	1
2733	A	13	PHE	HE2	7.351	0.020	1
2734	C	213	PHE	HE2	7.351	0.020	1
2735	A	13	PHE	C	174.162	0.1	1
2736	C	213	PHE	C	174.162	0.1	1
2737	A	13	PHE	CA	56.289	0.1	1
2738	C	213	PHE	CA	56.289	0.1	1
2739	A	13	PHE	CB	41.320	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2740	C	213	PHE	CB	41.320	0.1	1
2741	A	13	PHE	CD1	132.565	0.1	1
2742	C	213	PHE	CD1	132.565	0.1	1
2743	A	13	PHE	CE1	132.047	0.1	1
2744	C	213	PHE	CE1	132.047	0.1	1
2745	A	13	PHE	N	116.797	0.1	1
2746	C	213	PHE	N	116.797	0.1	1
2747	A	14	PHE	H	8.125	0.006	1
2748	C	214	PHE	H	8.125	0.006	1
2749	A	14	PHE	HA	4.767	0.020	1
2750	C	214	PHE	HA	4.767	0.020	1
2751	A	14	PHE	HB2	2.898	0.020	2
2752	C	214	PHE	HB2	2.898	0.020	2
2753	A	14	PHE	HB3	2.775	0.020	2
2754	C	214	PHE	HB3	2.775	0.020	2
2755	A	14	PHE	HD1	7.022	0.020	1
2756	C	214	PHE	HD1	7.022	0.020	1
2757	A	14	PHE	HD2	7.022	0.020	1
2758	C	214	PHE	HD2	7.022	0.020	1
2759	A	14	PHE	HE1	7.324	0.020	1
2760	C	214	PHE	HE1	7.324	0.020	1
2761	A	14	PHE	HE2	7.324	0.020	1
2762	C	214	PHE	HE2	7.324	0.020	1
2763	A	14	PHE	C	175.441	0.1	1
2764	C	214	PHE	C	175.441	0.1	1
2765	A	14	PHE	CA	55.767	0.1	1
2766	C	214	PHE	CA	55.767	0.1	1
2767	A	14	PHE	CB	41.320	0.1	1
2768	C	214	PHE	CB	41.320	0.1	1
2769	A	14	PHE	CD1	132.047	0.1	1
2770	C	214	PHE	CD1	132.047	0.1	1
2771	A	14	PHE	CE1	131.789	0.1	1
2772	C	214	PHE	CE1	131.789	0.1	1
2773	A	14	PHE	N	118.930	0.1	1
2774	C	214	PHE	N	118.930	0.1	1
2775	A	15	GLU	H	8.836	0.020	1
2776	C	215	GLU	H	8.836	0.020	1
2777	A	15	GLU	HA	4.579	0.020	1
2778	C	215	GLU	HA	4.579	0.020	1
2779	A	15	GLU	HB2	2.026	0.020	2
2780	C	215	GLU	HB2	2.026	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2781	A	15	GLU	HB3	2.155	0.020	2
2782	C	215	GLU	HB3	2.155	0.020	2
2783	A	15	GLU	HG2	2.392	0.020	2
2784	C	215	GLU	HG2	2.392	0.020	2
2785	A	15	GLU	HG3	2.323	0.020	2
2786	C	215	GLU	HG3	2.323	0.020	2
2787	A	15	GLU	C	176.857	0.1	1
2788	C	215	GLU	C	176.857	0.1	1
2789	A	15	GLU	CA	56.289	0.1	1
2790	C	215	GLU	CA	56.289	0.1	1
2791	A	15	GLU	CB	31.173	0.1	1
2792	C	215	GLU	CB	31.173	0.1	1
2793	A	15	GLU	CG	36.818	0.1	1
2794	C	215	GLU	CG	36.818	0.1	1
2795	A	15	GLU	N	122.929	0.1	1
2796	C	215	GLU	N	122.929	0.1	1
2797	A	16	SER	H	8.751	0.005	1
2798	C	216	SER	H	8.751	0.005	1
2799	A	16	SER	HA	4.762	0.006	1
2800	C	216	SER	HA	4.762	0.006	1
2801	A	16	SER	HB2	3.911	0.020	2
2802	C	216	SER	HB2	3.911	0.020	2
2803	A	16	SER	HB3	3.782	0.020	2
2804	C	216	SER	HB3	3.782	0.020	2
2805	A	16	SER	C	177.497	0.1	1
2806	C	216	SER	C	177.497	0.1	1
2807	A	16	SER	CA	59.328	0.1	1
2808	C	216	SER	CA	59.328	0.1	1
2809	A	16	SER	CB	64.515	0.1	1
2810	C	216	SER	CB	64.515	0.1	1
2811	A	16	SER	N	118.860	0.1	1
2812	C	216	SER	N	118.860	0.1	1
2813	A	17	HIS	H	8.761	0.020	1
2814	C	217	HIS	H	8.761	0.020	1
2815	A	17	HIS	HA	4.859	0.020	1
2816	C	217	HIS	HA	4.859	0.020	1
2817	A	17	HIS	HB2	3.248	0.020	2
2818	C	217	HIS	HB2	3.248	0.020	2
2819	A	17	HIS	HB3	3.248	0.020	2
2820	C	217	HIS	HB3	3.248	0.020	2
2821	A	17	HIS	HD2	7.175	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2822	C	217	HIS	HD2	7.175	0.006	1
2823	A	17	HIS	HE1	8.028	0.020	1
2824	C	217	HIS	HE1	8.028	0.020	1
2825	A	17	HIS	C	174.618	0.1	1
2826	C	217	HIS	C	174.618	0.1	1
2827	A	17	HIS	CA	56.449	0.1	1
2828	C	217	HIS	CA	56.449	0.1	1
2829	A	17	HIS	CB	29.870	0.1	1
2830	C	217	HIS	CB	29.870	0.1	1
2831	A	17	HIS	CD2	120.400	0.1	1
2832	C	217	HIS	CD2	120.400	0.1	1
2833	A	17	HIS	CE1	138.518	0.1	1
2834	C	217	HIS	CE1	138.518	0.1	1
2835	A	17	HIS	N	120.535	0.1	1
2836	C	217	HIS	N	120.535	0.1	1
2837	A	18	VAL	H	7.157	0.004	1
2838	C	218	VAL	H	7.157	0.004	1
2839	A	18	VAL	HA	4.181	0.020	1
2840	C	218	VAL	HA	4.181	0.020	1
2841	A	18	VAL	HB	1.953	0.020	1
2842	C	218	VAL	HB	1.953	0.020	1
2843	A	18	VAL	HG11	0.907	0.020	2
2844	C	218	VAL	HG11	0.907	0.020	2
2845	A	18	VAL	HG12	0.907	0.020	2
2846	C	218	VAL	HG12	0.907	0.020	2
2847	A	18	VAL	HG13	0.907	0.020	2
2848	C	218	VAL	HG13	0.907	0.020	2
2849	A	18	VAL	HG21	0.907	0.020	2
2850	C	218	VAL	HG21	0.907	0.020	2
2851	A	18	VAL	HG22	0.907	0.020	2
2852	C	218	VAL	HG22	0.907	0.020	2
2853	A	18	VAL	HG23	0.907	0.020	2
2854	C	218	VAL	HG23	0.907	0.020	2
2855	A	18	VAL	C	174.436	0.1	1
2856	C	218	VAL	C	174.436	0.1	1
2857	A	18	VAL	CA	62.167	0.1	1
2858	C	218	VAL	CA	62.167	0.1	1
2859	A	18	VAL	CB	34.426	0.1	1
2860	C	218	VAL	CB	34.426	0.1	1
2861	A	18	VAL	CG1	22.489	0.1	1
2862	C	218	VAL	CG1	22.489	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2863	A	18	VAL	N	120.872	0.1	1
2864	C	218	VAL	N	120.872	0.1	1
2865	A	19	ALA	H	8.521	0.001	1
2866	C	219	ALA	H	8.521	0.001	1
2867	A	19	ALA	HA	4.372	0.020	1
2868	C	219	ALA	HA	4.372	0.020	1
2869	A	19	ALA	HB1	1.362	0.020	1
2870	C	219	ALA	HB1	1.362	0.020	1
2871	A	19	ALA	HB2	1.362	0.020	1
2872	C	219	ALA	HB2	1.362	0.020	1
2873	A	19	ALA	HB3	1.362	0.020	1
2874	C	219	ALA	HB3	1.362	0.020	1
2875	A	19	ALA	C	177.657	0.1	1
2876	C	219	ALA	C	177.657	0.1	1
2877	A	19	ALA	CA	51.193	0.1	1
2878	C	219	ALA	CA	51.193	0.1	1
2879	A	19	ALA	CB	19.790	0.1	1
2880	C	219	ALA	CB	19.790	0.1	1
2881	A	19	ALA	N	131.339	0.1	1
2882	C	219	ALA	N	131.339	0.1	1
2883	A	20	ARG	H	7.790	0.001	1
2884	C	220	ARG	H	7.790	0.001	1
2885	A	20	ARG	HA	2.445	0.020	1
2886	C	220	ARG	HA	2.445	0.020	1
2887	A	20	ARG	HB2	1.062	0.020	2
2888	C	220	ARG	HB2	1.062	0.020	2
2889	A	20	ARG	HB3	0.444	0.020	2
2890	C	220	ARG	HB3	0.444	0.020	2
2891	A	20	ARG	HD2	2.897	0.002	2
2892	C	220	ARG	HD2	2.897	0.002	2
2893	A	20	ARG	HD3	2.897	0.002	2
2894	C	220	ARG	HD3	2.897	0.002	2
2895	A	20	ARG	HG2	1.194	0.001	2
2896	C	220	ARG	HG2	1.194	0.001	2
2897	A	20	ARG	HG3	0.860	0.003	2
2898	C	220	ARG	HG3	0.860	0.003	2
2899	A	20	ARG	C	178.365	0.1	1
2900	C	220	ARG	C	178.365	0.1	1
2901	A	20	ARG	CA	59.379	0.1	1
2902	C	220	ARG	CA	59.379	0.1	1
2903	A	20	ARG	CB	29.572	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2904	C	220	ARG	CB	29.572	0.1	1
2905	A	20	ARG	CD	44.132	0.1	1
2906	C	220	ARG	CD	44.132	0.1	1
2907	A	20	ARG	CG	26.984	0.1	1
2908	C	220	ARG	CG	26.984	0.1	1
2909	A	20	ARG	N	124.365	0.1	1
2910	C	220	ARG	N	124.365	0.1	1
2911	A	21	ALA	H	8.120	0.020	1
2912	C	221	ALA	H	8.120	0.020	1
2913	A	21	ALA	HA	4.060	0.020	1
2914	C	221	ALA	HA	4.060	0.020	1
2915	A	21	ALA	HB1	1.309	0.020	1
2916	C	221	ALA	HB1	1.309	0.020	1
2917	A	21	ALA	HB2	1.309	0.020	1
2918	C	221	ALA	HB2	1.309	0.020	1
2919	A	21	ALA	HB3	1.309	0.020	1
2920	C	221	ALA	HB3	1.309	0.020	1
2921	A	21	ALA	C	178.000	0.1	1
2922	C	221	ALA	C	178.000	0.1	1
2923	A	21	ALA	CA	54.100	0.1	1
2924	C	221	ALA	CA	54.100	0.1	1
2925	A	21	ALA	CB	18.713	0.1	1
2926	C	221	ALA	CB	18.713	0.1	1
2927	A	21	ALA	N	117.156	0.1	1
2928	C	221	ALA	N	117.156	0.1	1
2929	A	22	ASN	H	7.717	0.004	1
2930	C	222	ASN	H	7.717	0.004	1
2931	A	22	ASN	HA	5.010	0.003	1
2932	C	222	ASN	HA	5.010	0.003	1
2933	A	22	ASN	HB2	3.087	0.020	2
2934	C	222	ASN	HB2	3.087	0.020	2
2935	A	22	ASN	HB3	2.663	0.020	2
2936	C	222	ASN	HB3	2.663	0.020	2
2937	A	22	ASN	HD21	7.590	0.020	2
2938	C	222	ASN	HD21	7.590	0.020	2
2939	A	22	ASN	HD22	7.089	0.020	2
2940	C	222	ASN	HD22	7.089	0.020	2
2941	A	22	ASN	C	174.938	0.1	1
2942	C	222	ASN	C	174.938	0.1	1
2943	A	22	ASN	CA	52.869	0.1	1
2944	C	222	ASN	CA	52.869	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2945	A	22	ASN	CB	40.573	0.1	1
2946	C	222	ASN	CB	40.573	0.1	1
2947	A	22	ASN	N	112.819	0.1	1
2948	C	222	ASN	N	112.819	0.1	1
2949	A	22	ASN	ND2	111.993	0.019	1
2950	C	222	ASN	ND2	111.993	0.019	1
2951	A	23	VAL	H	7.489	0.005	1
2952	C	223	VAL	H	7.489	0.005	1
2953	A	23	VAL	HA	4.888	0.020	1
2954	C	223	VAL	HA	4.888	0.020	1
2955	A	23	VAL	HB	1.756	0.001	1
2956	C	223	VAL	HB	1.756	0.001	1
2957	A	23	VAL	HG11	0.899	0.020	2
2958	C	223	VAL	HG11	0.899	0.020	2
2959	A	23	VAL	HG12	0.899	0.020	2
2960	C	223	VAL	HG12	0.899	0.020	2
2961	A	23	VAL	HG13	0.899	0.020	2
2962	C	223	VAL	HG13	0.899	0.020	2
2963	A	23	VAL	HG21	0.763	0.020	2
2964	C	223	VAL	HG21	0.763	0.020	2
2965	A	23	VAL	HG22	0.763	0.020	2
2966	C	223	VAL	HG22	0.763	0.020	2
2967	A	23	VAL	HG23	0.763	0.020	2
2968	C	223	VAL	HG23	0.763	0.020	2
2969	A	23	VAL	C	175.829	0.1	1
2970	C	223	VAL	C	175.829	0.1	1
2971	A	23	VAL	CA	59.870	0.1	1
2972	C	223	VAL	CA	59.870	0.1	1
2973	A	23	VAL	CB	35.396	0.1	1
2974	C	223	VAL	CB	35.396	0.1	1
2975	A	23	VAL	CG1	22.432	0.1	1
2976	C	223	VAL	CG1	22.432	0.1	1
2977	A	23	VAL	CG2	21.807	0.1	1
2978	C	223	VAL	CG2	21.807	0.1	1
2979	A	23	VAL	N	119.721	0.1	1
2980	C	223	VAL	N	119.721	0.1	1
2981	A	24	LYS	H	9.479	0.009	1
2982	C	224	LYS	H	9.479	0.009	1
2983	A	24	LYS	HA	4.353	0.004	1
2984	C	224	LYS	HA	4.353	0.004	1
2985	A	24	LYS	HB2	1.690	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2986	C	224	LYS	HB2	1.690	0.020	2
2987	A	24	LYS	HB3	1.307	0.020	2
2988	C	224	LYS	HB3	1.307	0.020	2
2989	A	24	LYS	HD2	1.659	0.020	2
2990	C	224	LYS	HD2	1.659	0.020	2
2991	A	24	LYS	HD3	1.659	0.020	2
2992	C	224	LYS	HD3	1.659	0.020	2
2993	A	24	LYS	HE2	3.031	0.020	2
2994	C	224	LYS	HE2	3.031	0.020	2
2995	A	24	LYS	HE3	3.031	0.020	2
2996	C	224	LYS	HE3	3.031	0.020	2
2997	A	24	LYS	HG2	1.398	0.020	2
2998	C	224	LYS	HG2	1.398	0.020	2
2999	A	24	LYS	HG3	1.343	0.020	2
3000	C	224	LYS	HG3	1.343	0.020	2
3001	A	24	LYS	C	176.606	0.1	1
3002	C	224	LYS	C	176.606	0.1	1
3003	A	24	LYS	CA	58.977	0.1	1
3004	C	224	LYS	CA	58.977	0.1	1
3005	A	24	LYS	CB	34.567	0.1	1
3006	C	224	LYS	CB	34.567	0.1	1
3007	A	24	LYS	CD	30.359	0.1	1
3008	C	224	LYS	CD	30.359	0.1	1
3009	A	24	LYS	CE	42.191	0.1	1
3010	C	224	LYS	CE	42.191	0.1	1
3011	A	24	LYS	CG	25.759	0.1	1
3012	C	224	LYS	CG	25.759	0.1	1
3013	A	24	LYS	N	127.843	0.1	1
3014	C	224	LYS	N	127.843	0.1	1
3015	A	25	HIS	H	7.237	0.003	1
3016	C	225	HIS	H	7.237	0.003	1
3017	A	25	HIS	HA	4.979	0.020	1
3018	C	225	HIS	HA	4.979	0.020	1
3019	A	25	HIS	HB2	3.608	0.020	2
3020	C	225	HIS	HB2	3.608	0.020	2
3021	A	25	HIS	HB3	3.118	0.020	2
3022	C	225	HIS	HB3	3.118	0.020	2
3023	A	25	HIS	HD2	6.608	0.020	1
3024	C	225	HIS	HD2	6.608	0.020	1
3025	A	25	HIS	HE1	7.804	0.020	1
3026	C	225	HIS	HE1	7.804	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3027	A	25	HIS	C	178.434	0.1	1
3028	C	225	HIS	C	178.434	0.1	1
3029	A	25	HIS	CA	55.406	0.1	1
3030	C	225	HIS	CA	55.406	0.1	1
3031	A	25	HIS	CB	32.480	0.1	1
3032	C	225	HIS	CB	32.480	0.1	1
3033	A	25	HIS	CD2	121.435	0.1	1
3034	C	225	HIS	CD2	121.435	0.1	1
3035	A	25	HIS	CE1	138.518	0.1	1
3036	C	225	HIS	CE1	138.518	0.1	1
3037	A	25	HIS	N	109.556	0.1	1
3038	C	225	HIS	N	109.556	0.1	1
3039	A	26	LEU	H	8.189	0.002	1
3040	C	226	LEU	H	8.189	0.002	1
3041	A	26	LEU	HA	5.190	0.020	1
3042	C	226	LEU	HA	5.190	0.020	1
3043	A	26	LEU	HB2	1.708	0.020	2
3044	C	226	LEU	HB2	1.708	0.020	2
3045	A	26	LEU	HB3	1.272	0.020	2
3046	C	226	LEU	HB3	1.272	0.020	2
3047	A	26	LEU	HD11	0.578	0.003	2
3048	C	226	LEU	HD11	0.578	0.003	2
3049	A	26	LEU	HD12	0.578	0.003	2
3050	C	226	LEU	HD12	0.578	0.003	2
3051	A	26	LEU	HD13	0.578	0.003	2
3052	C	226	LEU	HD13	0.578	0.003	2
3053	A	26	LEU	HD21	0.792	0.002	2
3054	C	226	LEU	HD21	0.792	0.002	2
3055	A	26	LEU	HD22	0.792	0.002	2
3056	C	226	LEU	HD22	0.792	0.002	2
3057	A	26	LEU	HD23	0.792	0.002	2
3058	C	226	LEU	HD23	0.792	0.002	2
3059	A	26	LEU	HG	1.491	0.020	1
3060	C	226	LEU	HG	1.491	0.020	1
3061	A	26	LEU	C	175.510	0.1	1
3062	C	226	LEU	C	175.510	0.1	1
3063	A	26	LEU	CA	53.480	0.1	1
3064	C	226	LEU	CA	53.480	0.1	1
3065	A	26	LEU	CB	45.235	0.1	1
3066	C	226	LEU	CB	45.235	0.1	1
3067	A	26	LEU	CD1	26.013	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3068	C	226	LEU	CD1	26.013	0.1	1
3069	A	26	LEU	CD2	24.187	0.1	1
3070	C	226	LEU	CD2	24.187	0.1	1
3071	A	26	LEU	CG	26.653	0.1	1
3072	C	226	LEU	CG	26.653	0.1	1
3073	A	26	LEU	N	117.260	0.1	1
3074	C	226	LEU	N	117.260	0.1	1
3075	A	27	LYS	H	9.572	0.005	1
3076	C	227	LYS	H	9.572	0.005	1
3077	A	27	LYS	HA	5.372	0.020	1
3078	C	227	LYS	HA	5.372	0.020	1
3079	A	27	LYS	HB2	1.579	0.003	2
3080	C	227	LYS	HB2	1.579	0.003	2
3081	A	27	LYS	HB3	1.579	0.003	2
3082	C	227	LYS	HB3	1.579	0.003	2
3083	A	27	LYS	HD2	1.032	0.020	2
3084	C	227	LYS	HD2	1.032	0.020	2
3085	A	27	LYS	HD3	0.991	0.020	2
3086	C	227	LYS	HD3	0.991	0.020	2
3087	A	27	LYS	HE2	2.565	0.020	2
3088	C	227	LYS	HE2	2.565	0.020	2
3089	A	27	LYS	HE3	2.421	0.020	2
3090	C	227	LYS	HE3	2.421	0.020	2
3091	A	27	LYS	HG2	1.028	0.020	2
3092	C	227	LYS	HG2	1.028	0.020	2
3093	A	27	LYS	HG3	1.274	0.020	2
3094	C	227	LYS	HG3	1.274	0.020	2
3095	A	27	LYS	C	174.801	0.1	1
3096	C	227	LYS	C	174.801	0.1	1
3097	A	27	LYS	CA	55.165	0.1	1
3098	C	227	LYS	CA	55.165	0.1	1
3099	A	27	LYS	CB	35.253	0.1	1
3100	C	227	LYS	CB	35.253	0.1	1
3101	A	27	LYS	CD	29.925	0.1	1
3102	C	227	LYS	CD	29.925	0.1	1
3103	A	27	LYS	CE	41.402	0.1	1
3104	C	227	LYS	CE	41.402	0.1	1
3105	A	27	LYS	CG	25.559	0.1	1
3106	C	227	LYS	CG	25.559	0.1	1
3107	A	27	LYS	N	123.488	0.1	1
3108	C	227	LYS	N	123.488	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3109	A	28	ILE	H	9.136	0.005	1
3110	C	228	ILE	H	9.136	0.005	1
3111	A	28	ILE	HA	4.926	0.005	1
3112	C	228	ILE	HA	4.926	0.005	1
3113	A	28	ILE	HB	1.858	0.020	1
3114	C	228	ILE	HB	1.858	0.020	1
3115	A	28	ILE	HD11	0.784	0.020	1
3116	C	228	ILE	HD11	0.784	0.020	1
3117	A	28	ILE	HD12	0.784	0.020	1
3118	C	228	ILE	HD12	0.784	0.020	1
3119	A	28	ILE	HD13	0.784	0.020	1
3120	C	228	ILE	HD13	0.784	0.020	1
3121	A	28	ILE	HG12	1.513	0.020	2
3122	C	228	ILE	HG12	1.513	0.020	2
3123	A	28	ILE	HG13	1.513	0.020	2
3124	C	228	ILE	HG13	1.513	0.020	2
3125	A	28	ILE	HG21	0.962	0.020	1
3126	C	228	ILE	HG21	0.962	0.020	1
3127	A	28	ILE	HG22	0.962	0.020	1
3128	C	228	ILE	HG22	0.962	0.020	1
3129	A	28	ILE	HG23	0.962	0.020	1
3130	C	228	ILE	HG23	0.962	0.020	1
3131	A	28	ILE	C	176.949	0.1	1
3132	C	228	ILE	C	176.949	0.1	1
3133	A	28	ILE	CA	60.542	0.1	1
3134	C	228	ILE	CA	60.542	0.1	1
3135	A	28	ILE	CB	39.600	0.1	1
3136	C	228	ILE	CB	39.600	0.1	1
3137	A	28	ILE	CD1	14.041	0.1	1
3138	C	228	ILE	CD1	14.041	0.1	1
3139	A	28	ILE	CG1	27.631	0.1	1
3140	C	228	ILE	CG1	27.631	0.1	1
3141	A	28	ILE	CG2	18.698	0.1	1
3142	C	228	ILE	CG2	18.698	0.1	1
3143	A	28	ILE	N	123.846	0.1	1
3144	C	228	ILE	N	123.846	0.1	1
3145	A	29	LEU	H	8.830	0.020	1
3146	C	229	LEU	H	8.830	0.020	1
3147	A	29	LEU	HA	4.535	0.020	1
3148	C	229	LEU	HA	4.535	0.020	1
3149	A	29	LEU	HB2	2.338	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3150	C	229	LEU	HB2	2.338	0.020	2
3151	A	29	LEU	HB3	1.958	0.003	2
3152	C	229	LEU	HB3	1.958	0.003	2
3153	A	29	LEU	HD11	0.888	0.020	2
3154	C	229	LEU	HD11	0.888	0.020	2
3155	A	29	LEU	HD12	0.888	0.020	2
3156	C	229	LEU	HD12	0.888	0.020	2
3157	A	29	LEU	HD13	0.888	0.020	2
3158	C	229	LEU	HD13	0.888	0.020	2
3159	A	29	LEU	HD21	0.823	0.020	2
3160	C	229	LEU	HD21	0.823	0.020	2
3161	A	29	LEU	HD22	0.823	0.020	2
3162	C	229	LEU	HD22	0.823	0.020	2
3163	A	29	LEU	HD23	0.823	0.020	2
3164	C	229	LEU	HD23	0.823	0.020	2
3165	A	29	LEU	C	176.012	0.1	1
3166	C	229	LEU	C	176.012	0.1	1
3167	A	29	LEU	CA	55.366	0.1	1
3168	C	229	LEU	CA	55.366	0.1	1
3169	A	29	LEU	CB	43.180	0.1	1
3170	C	229	LEU	CB	43.180	0.1	1
3171	A	29	LEU	CD1	25.808	0.1	1
3172	C	229	LEU	CD1	25.808	0.1	1
3173	A	29	LEU	CD2	23.425	0.1	1
3174	C	229	LEU	CD2	23.425	0.1	1
3175	A	29	LEU	N	128.649	0.1	1
3176	C	229	LEU	N	128.649	0.1	1
3177	A	30	ASN	H	8.216	0.006	1
3178	C	230	ASN	H	8.216	0.006	1
3179	A	30	ASN	HA	5.013	0.020	1
3180	C	230	ASN	HA	5.013	0.020	1
3181	A	30	ASN	HB2	2.907	0.020	2
3182	C	230	ASN	HB2	2.907	0.020	2
3183	A	30	ASN	HB3	2.368	0.020	2
3184	C	230	ASN	HB3	2.368	0.020	2
3185	A	30	ASN	HD21	7.606	0.020	2
3186	C	230	ASN	HD21	7.606	0.020	2
3187	A	30	ASN	HD22	6.266	0.020	2
3188	C	230	ASN	HD22	6.266	0.020	2
3189	A	30	ASN	C	174.664	0.1	1
3190	C	230	ASN	C	174.664	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3191	A	30	ASN	CA	52.517	0.1	1
3192	C	230	ASN	CA	52.517	0.1	1
3193	A	30	ASN	CB	38.776	0.1	1
3194	C	230	ASN	CB	38.776	0.1	1
3195	A	30	ASN	N	120.791	0.1	1
3196	C	230	ASN	N	120.791	0.1	1
3197	A	30	ASN	ND2	111.738	0.1	1
3198	C	230	ASN	ND2	111.738	0.1	1
3199	A	31	THR	H	7.883	0.020	1
3200	C	231	THR	H	7.883	0.020	1
3201	A	31	THR	HA	4.842	0.002	1
3202	C	231	THR	HA	4.842	0.002	1
3203	A	31	THR	HB	4.196	0.002	1
3204	C	231	THR	HB	4.196	0.002	1
3205	A	31	THR	HG21	1.175	0.020	1
3206	C	231	THR	HG21	1.175	0.020	1
3207	A	31	THR	HG22	1.175	0.020	1
3208	C	231	THR	HG22	1.175	0.020	1
3209	A	31	THR	HG23	1.175	0.020	1
3210	C	231	THR	HG23	1.175	0.020	1
3211	A	31	THR	CA	58.369	0.1	1
3212	C	231	THR	CA	58.369	0.1	1
3213	A	31	THR	CB	70.018	0.1	1
3214	C	231	THR	CB	70.018	0.1	1
3215	A	31	THR	CG2	22.130	0.1	1
3216	C	231	THR	CG2	22.130	0.1	1
3217	A	31	THR	N	115.811	0.1	1
3218	C	231	THR	N	115.811	0.1	1
3219	A	32	PRO	HA	4.317	0.020	1
3220	C	232	PRO	HA	4.317	0.020	1
3221	A	32	PRO	HB2	1.866	0.020	2
3222	C	232	PRO	HB2	1.866	0.020	2
3223	A	32	PRO	HB3	2.334	0.001	2
3224	C	232	PRO	HB3	2.334	0.001	2
3225	A	32	PRO	HD2	3.777	0.004	2
3226	C	232	PRO	HD2	3.777	0.004	2
3227	A	32	PRO	HD3	3.777	0.004	2
3228	C	232	PRO	HD3	3.777	0.004	2
3229	A	32	PRO	HG2	2.020	0.020	2
3230	C	232	PRO	HG2	2.020	0.020	2
3231	A	32	PRO	HG3	2.020	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3232	C	232	PRO	HG3	2.020	0.020	2
3233	A	32	PRO	CA	65.164	0.1	1
3234	C	232	PRO	CA	65.164	0.1	1
3235	A	32	PRO	CB	32.484	0.1	1
3236	C	232	PRO	CB	32.484	0.1	1
3237	A	32	PRO	CD	51.251	0.1	1
3238	C	232	PRO	CD	51.251	0.1	1
3239	A	32	PRO	CG	27.631	0.1	1
3240	C	232	PRO	CG	27.631	0.1	1
3241	A	33	ASN	H	8.254	0.020	1
3242	C	233	ASN	H	8.254	0.020	1
3243	A	33	ASN	HA	4.651	0.020	1
3244	C	233	ASN	HA	4.651	0.020	1
3245	A	33	ASN	HB2	2.761	0.020	2
3246	C	233	ASN	HB2	2.761	0.020	2
3247	A	33	ASN	HB3	2.761	0.020	2
3248	C	233	ASN	HB3	2.761	0.020	2
3249	A	33	ASN	HD21	7.570	0.020	2
3250	C	233	ASN	HD21	7.570	0.020	2
3251	A	33	ASN	HD22	6.892	0.020	2
3252	C	233	ASN	HD22	6.892	0.020	2
3253	A	33	ASN	C	174.710	0.1	1
3254	C	233	ASN	C	174.710	0.1	1
3255	A	33	ASN	CA	54.532	0.1	1
3256	C	233	ASN	CA	54.532	0.1	1
3257	A	33	ASN	CB	39.167	0.1	1
3258	C	233	ASN	CB	39.167	0.1	1
3259	A	33	ASN	N	120.081	0.1	1
3260	C	233	ASN	N	120.081	0.1	1
3261	A	33	ASN	ND2	112.472	0.1	1
3262	C	233	ASN	ND2	112.472	0.1	1
3263	A	34	CYS	H	7.548	0.020	1
3264	C	234	CYS	H	7.548	0.020	1
3265	A	34	CYS	HA	4.694	0.007	1
3266	C	234	CYS	HA	4.694	0.007	1
3267	A	34	CYS	HB2	3.119	0.020	2
3268	C	234	CYS	HB2	3.119	0.020	2
3269	A	34	CYS	HB3	3.006	0.020	2
3270	C	234	CYS	HB3	3.006	0.020	2
3271	A	34	CYS	C	173.865	0.1	1
3272	C	234	CYS	C	173.865	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3273	A	34	CYS	CA	55.447	0.1	1
3274	C	234	CYS	CA	55.447	0.1	1
3275	A	34	CYS	CB	45.228	0.1	1
3276	C	234	CYS	CB	45.228	0.1	1
3277	A	34	CYS	N	117.076	0.1	1
3278	C	234	CYS	N	117.076	0.1	1
3279	A	35	ALA	H	8.472	0.020	1
3280	C	235	ALA	H	8.472	0.020	1
3281	A	35	ALA	HA	4.236	0.020	1
3282	C	235	ALA	HA	4.236	0.020	1
3283	A	35	ALA	HB1	1.449	0.020	1
3284	C	235	ALA	HB1	1.449	0.020	1
3285	A	35	ALA	HB2	1.449	0.020	1
3286	C	235	ALA	HB2	1.449	0.020	1
3287	A	35	ALA	HB3	1.449	0.020	1
3288	C	235	ALA	HB3	1.449	0.020	1
3289	A	35	ALA	C	176.423	0.1	1
3290	C	235	ALA	C	176.423	0.1	1
3291	A	35	ALA	CA	53.537	0.1	1
3292	C	235	ALA	CA	53.537	0.1	1
3293	A	35	ALA	CB	19.202	0.1	1
3294	C	235	ALA	CB	19.202	0.1	1
3295	A	35	ALA	N	125.153	0.1	1
3296	C	235	ALA	N	125.153	0.1	1
3297	A	36	CYS	H	8.316	0.002	1
3298	C	236	CYS	H	8.316	0.002	1
3299	A	36	CYS	HA	4.196	0.020	1
3300	C	236	CYS	HA	4.196	0.020	1
3301	A	36	CYS	HB2	3.462	0.020	2
3302	C	236	CYS	HB2	3.462	0.020	2
3303	A	36	CYS	HB3	2.659	0.003	2
3304	C	236	CYS	HB3	2.659	0.003	2
3305	A	36	CYS	C	173.705	0.1	1
3306	C	236	CYS	C	173.705	0.1	1
3307	A	36	CYS	CA	58.616	0.1	1
3308	C	236	CYS	CA	58.616	0.1	1
3309	A	36	CYS	CB	45.705	0.1	1
3310	C	236	CYS	CB	45.705	0.1	1
3311	A	36	CYS	N	118.837	0.1	1
3312	C	236	CYS	N	118.837	0.1	1
3313	A	37	GLN	H	8.921	0.009	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3314	C	237	GLN	H	8.921	0.009	1
3315	A	37	GLN	HA	4.609	0.020	1
3316	C	237	GLN	HA	4.609	0.020	1
3317	A	37	GLN	HB2	2.328	0.020	2
3318	C	237	GLN	HB2	2.328	0.020	2
3319	A	37	GLN	HB3	2.328	0.020	2
3320	C	237	GLN	HB3	2.328	0.020	2
3321	A	37	GLN	HE21	7.264	0.010	2
3322	C	237	GLN	HE21	7.264	0.010	2
3323	A	37	GLN	HE22	6.891	0.013	2
3324	C	237	GLN	HE22	6.891	0.013	2
3325	A	37	GLN	HG2	2.557	0.020	2
3326	C	237	GLN	HG2	2.557	0.020	2
3327	A	37	GLN	HG3	2.557	0.020	2
3328	C	237	GLN	HG3	2.557	0.020	2
3329	A	37	GLN	C	173.636	0.1	1
3330	C	237	GLN	C	173.636	0.1	1
3331	A	37	GLN	CA	54.603	0.1	1
3332	C	237	GLN	CA	54.603	0.1	1
3333	A	37	GLN	CB	31.761	0.1	1
3334	C	237	GLN	CB	31.761	0.1	1
3335	A	37	GLN	CG	34.722	0.1	1
3336	C	237	GLN	CG	34.722	0.1	1
3337	A	37	GLN	N	128.567	0.1	1
3338	C	237	GLN	N	128.567	0.1	1
3339	A	37	GLN	NE2	112.756	0.006	1
3340	C	237	GLN	NE2	112.756	0.006	1
3341	A	38	ILE	H	8.893	0.003	1
3342	C	238	ILE	H	8.893	0.003	1
3343	A	38	ILE	HA	5.068	0.020	1
3344	C	238	ILE	HA	5.068	0.020	1
3345	A	38	ILE	HB	1.790	0.020	1
3346	C	238	ILE	HB	1.790	0.020	1
3347	A	38	ILE	HD11	0.722	0.020	1
3348	C	238	ILE	HD11	0.722	0.020	1
3349	A	38	ILE	HD12	0.722	0.020	1
3350	C	238	ILE	HD12	0.722	0.020	1
3351	A	38	ILE	HD13	0.722	0.020	1
3352	C	238	ILE	HD13	0.722	0.020	1
3353	A	38	ILE	HG12	1.814	0.020	2
3354	C	238	ILE	HG12	1.814	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3355	A	38	ILE	HG13	1.814	0.020	2
3356	C	238	ILE	HG13	1.814	0.020	2
3357	A	38	ILE	HG21	0.755	0.020	1
3358	C	238	ILE	HG21	0.755	0.020	1
3359	A	38	ILE	HG22	0.755	0.020	1
3360	C	238	ILE	HG22	0.755	0.020	1
3361	A	38	ILE	HG23	0.755	0.020	1
3362	C	238	ILE	HG23	0.755	0.020	1
3363	A	38	ILE	C	174.390	0.1	1
3364	C	238	ILE	C	174.390	0.1	1
3365	A	38	ILE	CA	60.582	0.1	1
3366	C	238	ILE	CA	60.582	0.1	1
3367	A	38	ILE	CB	40.048	0.1	1
3368	C	238	ILE	CB	40.048	0.1	1
3369	A	38	ILE	CD1	14.371	0.1	1
3370	C	238	ILE	CD1	14.371	0.1	1
3371	A	38	ILE	CG1	28.278	0.1	1
3372	C	238	ILE	CG1	28.278	0.1	1
3373	A	38	ILE	CG2	19.218	0.1	1
3374	C	238	ILE	CG2	19.218	0.1	1
3375	A	38	ILE	N	123.962	0.1	1
3376	C	238	ILE	N	123.962	0.1	1
3377	A	39	VAL	H	9.120	0.005	1
3378	C	239	VAL	H	9.120	0.005	1
3379	A	39	VAL	HA	4.845	0.020	1
3380	C	239	VAL	HA	4.845	0.020	1
3381	A	39	VAL	HB	2.177	0.020	1
3382	C	239	VAL	HB	2.177	0.020	1
3383	A	39	VAL	HG11	0.896	0.020	2
3384	C	239	VAL	HG11	0.896	0.020	2
3385	A	39	VAL	HG12	0.896	0.020	2
3386	C	239	VAL	HG12	0.896	0.020	2
3387	A	39	VAL	HG13	0.896	0.020	2
3388	C	239	VAL	HG13	0.896	0.020	2
3389	A	39	VAL	HG21	0.950	0.020	2
3390	C	239	VAL	HG21	0.950	0.020	2
3391	A	39	VAL	HG22	0.950	0.020	2
3392	C	239	VAL	HG22	0.950	0.020	2
3393	A	39	VAL	HG23	0.950	0.020	2
3394	C	239	VAL	HG23	0.950	0.020	2
3395	A	39	VAL	C	175.487	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3396	C	239	VAL	C	175.487	0.1	1
3397	A	39	VAL	CA	59.980	0.1	1
3398	C	239	VAL	CA	59.980	0.1	1
3399	A	39	VAL	CB	35.868	0.1	1
3400	C	239	VAL	CB	35.868	0.1	1
3401	A	39	VAL	CG1	21.807	0.1	1
3402	C	239	VAL	CG1	21.807	0.1	1
3403	A	39	VAL	CG2	21.745	0.1	1
3404	C	239	VAL	CG2	21.745	0.1	1
3405	A	39	VAL	N	126.354	0.1	1
3406	C	239	VAL	N	126.354	0.1	1
3407	A	40	ALA	H	9.513	0.020	1
3408	C	240	ALA	H	9.513	0.020	1
3409	A	40	ALA	HA	5.154	0.001	1
3410	C	240	ALA	HA	5.154	0.001	1
3411	A	40	ALA	HB1	1.342	0.003	1
3412	C	240	ALA	HB1	1.342	0.003	1
3413	A	40	ALA	HB2	1.342	0.003	1
3414	C	240	ALA	HB2	1.342	0.003	1
3415	A	40	ALA	HB3	1.342	0.003	1
3416	C	240	ALA	HB3	1.342	0.003	1
3417	A	40	ALA	C	175.944	0.1	1
3418	C	240	ALA	C	175.944	0.1	1
3419	A	40	ALA	CA	50.591	0.1	1
3420	C	240	ALA	CA	50.591	0.1	1
3421	A	40	ALA	CB	22.432	0.1	1
3422	C	240	ALA	CB	22.432	0.1	1
3423	A	40	ALA	N	128.406	0.1	1
3424	C	240	ALA	N	128.406	0.1	1
3425	A	41	ARG	H	7.717	0.005	1
3426	C	241	ARG	H	7.717	0.005	1
3427	A	41	ARG	HA	4.979	0.005	1
3428	C	241	ARG	HA	4.979	0.005	1
3429	A	41	ARG	HB2	1.454	0.020	2
3430	C	241	ARG	HB2	1.454	0.020	2
3431	A	41	ARG	HB3	1.454	0.020	2
3432	C	241	ARG	HB3	1.454	0.020	2
3433	A	41	ARG	HD2	3.097	0.020	2
3434	C	241	ARG	HD2	3.097	0.020	2
3435	A	41	ARG	HD3	3.097	0.020	2
3436	C	241	ARG	HD3	3.097	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3437	A	41	ARG	HG2	1.379	0.020	2
3438	C	241	ARG	HG2	1.379	0.020	2
3439	A	41	ARG	HG3	1.379	0.020	2
3440	C	241	ARG	HG3	1.379	0.020	2
3441	A	41	ARG	C	175.510	0.1	1
3442	C	241	ARG	C	175.510	0.1	1
3443	A	41	ARG	CA	54.162	0.1	1
3444	C	241	ARG	CA	54.162	0.1	1
3445	A	41	ARG	CB	31.200	0.1	1
3446	C	241	ARG	CB	31.200	0.1	1
3447	A	41	ARG	CD	42.649	0.1	1
3448	C	241	ARG	CD	42.649	0.1	1
3449	A	41	ARG	CG	27.631	0.1	1
3450	C	241	ARG	CG	27.631	0.1	1
3451	A	41	ARG	N	121.663	0.1	1
3452	C	241	ARG	N	121.663	0.1	1
3453	A	42	LEU	H	9.163	0.002	1
3454	C	242	LEU	H	9.163	0.002	1
3455	A	42	LEU	HA	5.033	0.020	1
3456	C	242	LEU	HA	5.033	0.020	1
3457	A	42	LEU	HB2	1.770	0.020	2
3458	C	242	LEU	HB2	1.770	0.020	2
3459	A	42	LEU	HB3	2.207	0.020	2
3460	C	242	LEU	HB3	2.207	0.020	2
3461	A	42	LEU	HD11	1.018	0.020	2
3462	C	242	LEU	HD11	1.018	0.020	2
3463	A	42	LEU	HD12	1.018	0.020	2
3464	C	242	LEU	HD12	1.018	0.020	2
3465	A	42	LEU	HD13	1.018	0.020	2
3466	C	242	LEU	HD13	1.018	0.020	2
3467	A	42	LEU	HD21	0.809	0.020	2
3468	C	242	LEU	HD21	0.809	0.020	2
3469	A	42	LEU	HD22	0.809	0.020	2
3470	C	242	LEU	HD22	0.809	0.020	2
3471	A	42	LEU	HD23	0.809	0.020	2
3472	C	242	LEU	HD23	0.809	0.020	2
3473	A	42	LEU	HG	1.814	0.001	1
3474	C	242	LEU	HG	1.814	0.001	1
3475	A	42	LEU	C	177.840	0.1	1
3476	C	242	LEU	C	177.840	0.1	1
3477	A	42	LEU	CA	54.724	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3478	C	242	LEU	CA	54.724	0.1	1
3479	A	42	LEU	CB	41.712	0.1	1
3480	C	242	LEU	CB	41.712	0.1	1
3481	A	42	LEU	CD1	25.759	0.1	1
3482	C	242	LEU	CD1	25.759	0.1	1
3483	A	42	LEU	CD2	23.452	0.1	1
3484	C	242	LEU	CD2	23.452	0.1	1
3485	A	42	LEU	CG	27.815	0.1	1
3486	C	242	LEU	CG	27.815	0.1	1
3487	A	42	LEU	N	129.087	0.1	1
3488	C	242	LEU	N	129.087	0.1	1
3489	A	43	LYS	H	8.417	0.005	1
3490	C	243	LYS	H	8.417	0.005	1
3491	A	43	LYS	HA	3.950	0.020	1
3492	C	243	LYS	HA	3.950	0.020	1
3493	A	43	LYS	HB2	1.900	0.020	2
3494	C	243	LYS	HB2	1.900	0.020	2
3495	A	43	LYS	HB3	1.708	0.002	2
3496	C	243	LYS	HB3	1.708	0.002	2
3497	A	43	LYS	HD2	1.656	0.020	2
3498	C	243	LYS	HD2	1.656	0.020	2
3499	A	43	LYS	HD3	1.740	0.020	2
3500	C	243	LYS	HD3	1.740	0.020	2
3501	A	43	LYS	HE2	3.054	0.005	2
3502	C	243	LYS	HE2	3.054	0.005	2
3503	A	43	LYS	HE3	3.054	0.005	2
3504	C	243	LYS	HE3	3.054	0.005	2
3505	A	43	LYS	HG2	1.335	0.020	2
3506	C	243	LYS	HG2	1.335	0.020	2
3507	A	43	LYS	HG3	1.234	0.020	2
3508	C	243	LYS	HG3	1.234	0.020	2
3509	A	43	LYS	CA	59.016	0.1	1
3510	C	243	LYS	CA	59.016	0.1	1
3511	A	43	LYS	CB	34.102	0.1	1
3512	C	243	LYS	CB	34.102	0.1	1
3513	A	43	LYS	CD	29.896	0.1	1
3514	C	243	LYS	CD	29.896	0.1	1
3515	A	43	LYS	CG	26.660	0.1	1
3516	C	243	LYS	CG	26.660	0.1	1
3517	A	43	LYS	N	119.674	0.1	1
3518	C	243	LYS	N	119.674	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3519	A	46	ASN	HA	4.723	0.020	1
3520	C	246	ASN	HA	4.723	0.020	1
3521	A	46	ASN	HB2	3.124	0.020	2
3522	C	246	ASN	HB2	3.124	0.020	2
3523	A	46	ASN	HB3	2.773	0.020	2
3524	C	246	ASN	HB3	2.773	0.020	2
3525	A	46	ASN	HD21	7.572	0.001	2
3526	C	246	ASN	HD21	7.572	0.001	2
3527	A	46	ASN	HD22	6.911	0.020	2
3528	C	246	ASN	HD22	6.911	0.020	2
3529	A	46	ASN	C	175.098	0.1	1
3530	C	246	ASN	C	175.098	0.1	1
3531	A	46	ASN	CA	54.764	0.1	1
3532	C	246	ASN	CA	54.764	0.1	1
3533	A	46	ASN	CB	39.265	0.1	1
3534	C	246	ASN	CB	39.265	0.1	1
3535	A	46	ASN	ND2	113.190	0.1	1
3536	C	246	ASN	ND2	113.190	0.1	1
3537	A	47	ARG	H	7.919	0.005	1
3538	C	247	ARG	H	7.919	0.005	1
3539	A	47	ARG	HA	4.353	0.003	1
3540	C	247	ARG	HA	4.353	0.003	1
3541	A	47	ARG	HB2	1.798	0.003	2
3542	C	247	ARG	HB2	1.798	0.003	2
3543	A	47	ARG	HB3	1.798	0.003	2
3544	C	247	ARG	HB3	1.798	0.003	2
3545	A	47	ARG	HD2	3.214	0.020	2
3546	C	247	ARG	HD2	3.214	0.020	2
3547	A	47	ARG	HD3	3.149	0.020	2
3548	C	247	ARG	HD3	3.149	0.020	2
3549	A	47	ARG	HG2	1.663	0.002	2
3550	C	247	ARG	HG2	1.663	0.002	2
3551	A	47	ARG	HG3	1.589	0.020	2
3552	C	247	ARG	HG3	1.589	0.020	2
3553	A	47	ARG	C	175.601	0.1	1
3554	C	247	ARG	C	175.601	0.1	1
3555	A	47	ARG	CA	57.051	0.1	1
3556	C	247	ARG	CA	57.051	0.1	1
3557	A	47	ARG	CB	32.121	0.1	1
3558	C	247	ARG	CB	32.121	0.1	1
3559	A	47	ARG	CD	43.788	0.021	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3560	C	247	ARG	CD	43.788	0.021	1
3561	A	47	ARG	CG	28.500	0.1	1
3562	C	247	ARG	CG	28.500	0.1	1
3563	A	47	ARG	N	119.826	0.1	1
3564	C	247	ARG	N	119.826	0.1	1
3565	A	48	GLN	H	8.547	0.006	1
3566	C	248	GLN	H	8.547	0.006	1
3567	A	48	GLN	HA	5.456	0.020	1
3568	C	248	GLN	HA	5.456	0.020	1
3569	A	48	GLN	HB2	1.988	0.020	2
3570	C	248	GLN	HB2	1.988	0.020	2
3571	A	48	GLN	HB3	1.873	0.020	2
3572	C	248	GLN	HB3	1.873	0.020	2
3573	A	48	GLN	HE21	7.615	0.020	2
3574	C	248	GLN	HE21	7.615	0.020	2
3575	A	48	GLN	HE22	7.082	0.020	2
3576	C	248	GLN	HE22	7.082	0.020	2
3577	A	48	GLN	HG2	2.435	0.001	2
3578	C	248	GLN	HG2	2.435	0.001	2
3579	A	48	GLN	HG3	2.435	0.001	2
3580	C	248	GLN	HG3	2.435	0.001	2
3581	A	48	GLN	C	175.578	0.1	1
3582	C	248	GLN	C	175.578	0.1	1
3583	A	48	GLN	CA	55.125	0.1	1
3584	C	248	GLN	CA	55.125	0.1	1
3585	A	48	GLN	CB	32.121	0.1	1
3586	C	248	GLN	CB	32.121	0.1	1
3587	A	48	GLN	CG	36.035	0.1	1
3588	C	248	GLN	CG	36.035	0.1	1
3589	A	48	GLN	N	120.767	0.1	1
3590	C	248	GLN	N	120.767	0.1	1
3591	A	48	GLN	NE2	111.045	0.1	1
3592	C	248	GLN	NE2	111.045	0.1	1
3593	A	49	VAL	H	8.630	0.003	1
3594	C	249	VAL	H	8.630	0.003	1
3595	A	49	VAL	HA	4.826	0.020	1
3596	C	249	VAL	HA	4.826	0.020	1
3597	A	49	VAL	HB	2.172	0.020	1
3598	C	249	VAL	HB	2.172	0.020	1
3599	A	49	VAL	HG11	0.756	0.020	2
3600	C	249	VAL	HG11	0.756	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3601	A	49	VAL	HG12	0.756	0.020	2
3602	C	249	VAL	HG12	0.756	0.020	2
3603	A	49	VAL	HG13	0.756	0.020	2
3604	C	249	VAL	HG13	0.756	0.020	2
3605	A	49	VAL	HG21	0.921	0.020	2
3606	C	249	VAL	HG21	0.921	0.020	2
3607	A	49	VAL	HG22	0.921	0.020	2
3608	C	249	VAL	HG22	0.921	0.020	2
3609	A	49	VAL	HG23	0.921	0.020	2
3610	C	249	VAL	HG23	0.921	0.020	2
3611	A	49	VAL	C	175.258	0.1	1
3612	C	249	VAL	C	175.258	0.1	1
3613	A	49	VAL	CA	59.338	0.1	1
3614	C	249	VAL	CA	59.338	0.1	1
3615	A	49	VAL	CB	36.155	0.1	1
3616	C	249	VAL	CB	36.155	0.1	1
3617	A	49	VAL	CG1	22.145	0.1	1
3618	C	249	VAL	CG1	22.145	0.1	1
3619	A	49	VAL	CG2	19.918	0.1	1
3620	C	249	VAL	CG2	19.918	0.1	1
3621	A	49	VAL	N	116.678	0.1	1
3622	C	249	VAL	N	116.678	0.1	1
3623	A	50	CYS	H	9.100	0.003	1
3624	C	250	CYS	H	9.100	0.003	1
3625	A	50	CYS	HA	5.301	0.020	1
3626	C	250	CYS	HA	5.301	0.020	1
3627	A	50	CYS	HB2	3.700	0.005	2
3628	C	250	CYS	HB2	3.700	0.005	2
3629	A	50	CYS	HB3	2.932	0.020	2
3630	C	250	CYS	HB3	2.932	0.020	2
3631	A	50	CYS	C	174.527	0.1	1
3632	C	250	CYS	C	174.527	0.1	1
3633	A	50	CYS	CA	58.054	0.1	1
3634	C	250	CYS	CA	58.054	0.1	1
3635	A	50	CYS	CB	43.375	0.1	1
3636	C	250	CYS	CB	43.375	0.1	1
3637	A	50	CYS	N	124.549	0.1	1
3638	C	250	CYS	N	124.549	0.1	1
3639	A	51	ILE	H	8.485	0.009	1
3640	C	251	ILE	H	8.485	0.009	1
3641	A	51	ILE	HA	4.964	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3642	C	251	ILE	HA	4.964	0.020	1
3643	A	51	ILE	HB	1.563	0.020	1
3644	C	251	ILE	HB	1.563	0.020	1
3645	A	51	ILE	HD11	0.746	0.020	1
3646	C	251	ILE	HD11	0.746	0.020	1
3647	A	51	ILE	HD12	0.746	0.020	1
3648	C	251	ILE	HD12	0.746	0.020	1
3649	A	51	ILE	HD13	0.746	0.020	1
3650	C	251	ILE	HD13	0.746	0.020	1
3651	A	51	ILE	HG12	1.372	0.020	2
3652	C	251	ILE	HG12	1.372	0.020	2
3653	A	51	ILE	HG13	1.181	0.020	2
3654	C	251	ILE	HG13	1.181	0.020	2
3655	A	51	ILE	HG21	0.756	0.020	1
3656	C	251	ILE	HG21	0.756	0.020	1
3657	A	51	ILE	HG22	0.756	0.020	1
3658	C	251	ILE	HG22	0.756	0.020	1
3659	A	51	ILE	HG23	0.756	0.020	1
3660	C	251	ILE	HG23	0.756	0.020	1
3661	A	51	ILE	C	173.019	0.1	1
3662	C	251	ILE	C	173.019	0.1	1
3663	A	51	ILE	CA	58.897	0.1	1
3664	C	251	ILE	CA	58.897	0.1	1
3665	A	51	ILE	CB	42.201	0.1	1
3666	C	251	ILE	CB	42.201	0.1	1
3667	A	51	ILE	CD1	14.665	0.1	1
3668	C	251	ILE	CD1	14.665	0.1	1
3669	A	51	ILE	CG1	27.986	0.028	1
3670	C	251	ILE	CG1	27.986	0.028	1
3671	A	51	ILE	CG2	18.126	0.1	1
3672	C	251	ILE	CG2	18.126	0.1	1
3673	A	51	ILE	N	122.581	0.1	1
3674	C	251	ILE	N	122.581	0.1	1
3675	A	52	ASP	H	7.661	0.006	1
3676	C	252	ASP	H	7.661	0.006	1
3677	A	52	ASP	HA	3.642	0.020	1
3678	C	252	ASP	HA	3.642	0.020	1
3679	A	52	ASP	HB2	2.702	0.020	2
3680	C	252	ASP	HB2	2.702	0.020	2
3681	A	52	ASP	HB3	2.238	0.020	2
3682	C	252	ASP	HB3	2.238	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3683	A	52	ASP	CA	51.574	0.1	1
3684	C	252	ASP	CA	51.574	0.1	1
3685	A	52	ASP	CB	42.515	0.1	1
3686	C	252	ASP	CB	42.515	0.1	1
3687	A	52	ASP	N	125.772	0.1	1
3688	C	252	ASP	N	125.772	0.1	1
3689	A	53	PRO	HA	4.025	0.004	1
3690	C	253	PRO	HA	4.025	0.004	1
3691	A	53	PRO	HB2	1.905	0.005	2
3692	C	253	PRO	HB2	1.905	0.005	2
3693	A	53	PRO	HB3	2.178	0.020	2
3694	C	253	PRO	HB3	2.178	0.020	2
3695	A	53	PRO	HD2	3.434	0.020	2
3696	C	253	PRO	HD2	3.434	0.020	2
3697	A	53	PRO	HD3	3.434	0.020	2
3698	C	253	PRO	HD3	3.434	0.020	2
3699	A	53	PRO	HG2	1.892	0.020	2
3700	C	253	PRO	HG2	1.892	0.020	2
3701	A	53	PRO	HG3	1.814	0.020	2
3702	C	253	PRO	HG3	1.814	0.020	2
3703	A	53	PRO	C	176.126	0.1	1
3704	C	253	PRO	C	176.126	0.1	1
3705	A	53	PRO	CA	63.993	0.1	1
3706	C	253	PRO	CA	63.993	0.1	1
3707	A	53	PRO	CB	33.002	0.1	1
3708	C	253	PRO	CB	33.002	0.1	1
3709	A	53	PRO	CD	51.251	0.1	1
3710	C	253	PRO	CD	51.251	0.1	1
3711	A	53	PRO	CG	27.631	0.1	1
3712	C	253	PRO	CG	27.631	0.1	1
3713	A	54	LYS	H	7.931	0.005	1
3714	C	254	LYS	H	7.931	0.005	1
3715	A	54	LYS	HA	3.988	0.020	1
3716	C	254	LYS	HA	3.988	0.020	1
3717	A	54	LYS	HB2	1.787	0.003	2
3718	C	254	LYS	HB2	1.787	0.003	2
3719	A	54	LYS	HB3	1.747	0.020	2
3720	C	254	LYS	HB3	1.747	0.020	2
3721	A	54	LYS	HD2	1.691	0.020	2
3722	C	254	LYS	HD2	1.691	0.020	2
3723	A	54	LYS	HD3	1.691	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3724	C	254	LYS	HD3	1.691	0.020	2
3725	A	54	LYS	HE2	3.026	0.020	2
3726	C	254	LYS	HE2	3.026	0.020	2
3727	A	54	LYS	HE3	3.026	0.020	2
3728	C	254	LYS	HE3	3.026	0.020	2
3729	A	54	LYS	HG2	1.418	0.001	2
3730	C	254	LYS	HG2	1.418	0.001	2
3731	A	54	LYS	HG3	1.361	0.020	2
3732	C	254	LYS	HG3	1.361	0.020	2
3733	A	54	LYS	C	177.931	0.1	1
3734	C	254	LYS	C	177.931	0.1	1
3735	A	54	LYS	CA	56.770	0.1	1
3736	C	254	LYS	CA	56.770	0.1	1
3737	A	54	LYS	CB	32.023	0.1	1
3738	C	254	LYS	CB	32.023	0.1	1
3739	A	54	LYS	CD	28.925	0.1	1
3740	C	254	LYS	CD	28.925	0.1	1
3741	A	54	LYS	CE	41.868	0.1	1
3742	C	254	LYS	CE	41.868	0.1	1
3743	A	54	LYS	CG	25.270	0.1	1
3744	C	254	LYS	CG	25.270	0.1	1
3745	A	54	LYS	N	112.924	0.1	1
3746	C	254	LYS	N	112.924	0.1	1
3747	A	55	LEU	H	7.162	0.003	1
3748	C	255	LEU	H	7.162	0.003	1
3749	A	55	LEU	HA	4.059	0.020	1
3750	C	255	LEU	HA	4.059	0.020	1
3751	A	55	LEU	HB2	1.257	0.020	2
3752	C	255	LEU	HB2	1.257	0.020	2
3753	A	55	LEU	HB3	1.054	0.020	2
3754	C	255	LEU	HB3	1.054	0.020	2
3755	A	55	LEU	HD11	1.083	0.020	2
3756	C	255	LEU	HD11	1.083	0.020	2
3757	A	55	LEU	HD12	1.083	0.020	2
3758	C	255	LEU	HD12	1.083	0.020	2
3759	A	55	LEU	HD13	1.083	0.020	2
3760	C	255	LEU	HD13	1.083	0.020	2
3761	A	55	LEU	HD21	1.081	0.020	2
3762	C	255	LEU	HD21	1.081	0.020	2
3763	A	55	LEU	HD22	1.081	0.020	2
3764	C	255	LEU	HD22	1.081	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3765	A	55	LEU	HD23	1.081	0.020	2
3766	C	255	LEU	HD23	1.081	0.020	2
3767	A	55	LEU	HG	1.900	0.020	1
3768	C	255	LEU	HG	1.900	0.020	1
3769	A	55	LEU	C	179.416	0.1	1
3770	C	255	LEU	C	179.416	0.1	1
3771	A	55	LEU	CA	56.088	0.1	1
3772	C	255	LEU	CA	56.088	0.1	1
3773	A	55	LEU	CB	42.191	0.1	1
3774	C	255	LEU	CB	42.191	0.1	1
3775	A	55	LEU	CD1	26.013	0.1	1
3776	C	255	LEU	CD1	26.013	0.1	1
3777	A	55	LEU	CD2	23.425	0.1	1
3778	C	255	LEU	CD2	23.425	0.1	1
3779	A	55	LEU	CG	27.631	0.1	1
3780	C	255	LEU	CG	27.631	0.1	1
3781	A	55	LEU	N	120.593	0.1	1
3782	C	255	LEU	N	120.593	0.1	1
3783	A	56	LYS	H	8.720	0.001	1
3784	C	256	LYS	H	8.720	0.001	1
3785	A	56	LYS	HA	3.920	0.020	1
3786	C	256	LYS	HA	3.920	0.020	1
3787	A	56	LYS	HB2	2.030	0.020	2
3788	C	256	LYS	HB2	2.030	0.020	2
3789	A	56	LYS	HB3	2.030	0.020	2
3790	C	256	LYS	HB3	2.030	0.020	2
3791	A	56	LYS	HD2	1.833	0.020	2
3792	C	256	LYS	HD2	1.833	0.020	2
3793	A	56	LYS	HD3	1.799	0.006	2
3794	C	256	LYS	HD3	1.799	0.006	2
3795	A	56	LYS	HE2	3.060	0.020	2
3796	C	256	LYS	HE2	3.060	0.020	2
3797	A	56	LYS	HE3	3.060	0.020	2
3798	C	256	LYS	HE3	3.060	0.020	2
3799	A	56	LYS	HG2	1.615	0.004	2
3800	C	256	LYS	HG2	1.615	0.004	2
3801	A	56	LYS	HG3	1.571	0.003	2
3802	C	256	LYS	HG3	1.571	0.003	2
3803	A	56	LYS	C	178.937	0.1	1
3804	C	256	LYS	C	178.937	0.1	1
3805	A	56	LYS	CA	60.301	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3806	C	256	LYS	CA	60.301	0.1	1
3807	A	56	LYS	CB	32.121	0.1	1
3808	C	256	LYS	CB	32.121	0.1	1
3809	A	56	LYS	CD	29.576	0.1	1
3810	C	256	LYS	CD	29.576	0.1	1
3811	A	56	LYS	CE	42.495	0.1	1
3812	C	256	LYS	CE	42.495	0.1	1
3813	A	56	LYS	CG	25.074	0.1	1
3814	C	256	LYS	CG	25.074	0.1	1
3815	A	56	LYS	N	125.479	0.1	1
3816	C	256	LYS	N	125.479	0.1	1
3817	A	57	TRP	H	7.811	0.020	1
3818	C	257	TRP	H	7.811	0.020	1
3819	A	57	TRP	HA	4.664	0.003	1
3820	C	257	TRP	HA	4.664	0.003	1
3821	A	57	TRP	HB2	3.635	0.005	2
3822	C	257	TRP	HB2	3.635	0.005	2
3823	A	57	TRP	HB3	3.316	0.002	2
3824	C	257	TRP	HB3	3.316	0.002	2
3825	A	57	TRP	HD1	7.743	0.009	1
3826	C	257	TRP	HD1	7.743	0.009	1
3827	A	57	TRP	HE1	10.309	0.003	1
3828	C	257	TRP	HE1	10.309	0.003	1
3829	A	57	TRP	HE3	7.363	0.006	1
3830	C	257	TRP	HE3	7.363	0.006	1
3831	A	57	TRP	HH2	6.722	0.005	1
3832	C	257	TRP	HH2	6.722	0.005	1
3833	A	57	TRP	HZ2	7.032	0.008	1
3834	C	257	TRP	HZ2	7.032	0.008	1
3835	A	57	TRP	HZ3	6.631	0.020	1
3836	C	257	TRP	HZ3	6.631	0.020	1
3837	A	57	TRP	C	178.868	0.1	1
3838	C	257	TRP	C	178.868	0.1	1
3839	A	57	TRP	CA	58.897	0.1	1
3840	C	257	TRP	CA	58.897	0.1	1
3841	A	57	TRP	CB	28.036	0.1	1
3842	C	257	TRP	CB	28.036	0.1	1
3843	A	57	TRP	CD1	128.682	0.1	1
3844	C	257	TRP	CD1	128.682	0.1	1
3845	A	57	TRP	CE3	121.176	0.1	1
3846	C	257	TRP	CE3	121.176	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3847	A	57	TRP	CH2	124.023	0.1	1
3848	C	257	TRP	CH2	124.023	0.1	1
3849	A	57	TRP	CZ2	113.929	0.1	1
3850	C	257	TRP	CZ2	113.929	0.1	1
3851	A	57	TRP	CZ3	121.176	0.1	1
3852	C	257	TRP	CZ3	121.176	0.1	1
3853	A	57	TRP	N	113.433	0.1	1
3854	C	257	TRP	N	113.433	0.1	1
3855	A	57	TRP	NE1	130.751	0.1	1
3856	C	257	TRP	NE1	130.751	0.1	1
3857	A	58	ILE	H	6.467	0.005	1
3858	C	258	ILE	H	6.467	0.005	1
3859	A	58	ILE	HA	3.325	0.020	1
3860	C	258	ILE	HA	3.325	0.020	1
3861	A	58	ILE	HB	1.757	0.020	1
3862	C	258	ILE	HB	1.757	0.020	1
3863	A	58	ILE	HD11	0.548	0.020	1
3864	C	258	ILE	HD11	0.548	0.020	1
3865	A	58	ILE	HD12	0.548	0.020	1
3866	C	258	ILE	HD12	0.548	0.020	1
3867	A	58	ILE	HD13	0.548	0.020	1
3868	C	258	ILE	HD13	0.548	0.020	1
3869	A	58	ILE	HG12	-0.380	0.020	2
3870	C	258	ILE	HG12	-0.380	0.020	2
3871	A	58	ILE	HG13	0.144	0.020	2
3872	C	258	ILE	HG13	0.144	0.020	2
3873	A	58	ILE	HG21	0.544	0.020	1
3874	C	258	ILE	HG21	0.544	0.020	1
3875	A	58	ILE	HG22	0.544	0.020	1
3876	C	258	ILE	HG22	0.544	0.020	1
3877	A	58	ILE	HG23	0.544	0.020	1
3878	C	258	ILE	HG23	0.544	0.020	1
3879	A	58	ILE	C	177.726	0.1	1
3880	C	258	ILE	C	177.726	0.1	1
3881	A	58	ILE	CA	64.314	0.1	1
3882	C	258	ILE	CA	64.314	0.1	1
3883	A	58	ILE	CB	35.897	0.1	1
3884	C	258	ILE	CB	35.897	0.1	1
3885	A	58	ILE	CD1	16.953	0.1	1
3886	C	258	ILE	CD1	16.953	0.1	1
3887	A	58	ILE	CG1	26.986	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3888	C	258	ILE	CG1	26.986	0.1	1
3889	A	58	ILE	CG2	17.277	0.1	1
3890	C	258	ILE	CG2	17.277	0.1	1
3891	A	58	ILE	N	124.379	0.1	1
3892	C	258	ILE	N	124.379	0.1	1
3893	A	59	GLN	H	7.624	0.004	1
3894	C	259	GLN	H	7.624	0.004	1
3895	A	59	GLN	HA	3.755	0.020	1
3896	C	259	GLN	HA	3.755	0.020	1
3897	A	59	GLN	HB2	2.264	0.020	2
3898	C	259	GLN	HB2	2.264	0.020	2
3899	A	59	GLN	HB3	2.220	0.020	2
3900	C	259	GLN	HB3	2.220	0.020	2
3901	A	59	GLN	HE21	7.078	0.020	2
3902	C	259	GLN	HE21	7.078	0.020	2
3903	A	59	GLN	HE22	7.925	0.004	2
3904	C	259	GLN	HE22	7.925	0.004	2
3905	A	59	GLN	HG2	2.389	0.020	2
3906	C	259	GLN	HG2	2.389	0.020	2
3907	A	59	GLN	HG3	2.389	0.020	2
3908	C	259	GLN	HG3	2.389	0.020	2
3909	A	59	GLN	C	178.434	0.1	1
3910	C	259	GLN	C	178.434	0.1	1
3911	A	59	GLN	CA	59.379	0.1	1
3912	C	259	GLN	CA	59.379	0.1	1
3913	A	59	GLN	CB	28.602	0.1	1
3914	C	259	GLN	CB	28.602	0.1	1
3915	A	59	GLN	CG	34.102	0.1	1
3916	C	259	GLN	CG	34.102	0.1	1
3917	A	59	GLN	N	119.070	0.1	1
3918	C	259	GLN	N	119.070	0.1	1
3919	A	59	GLN	NE2	115.396	0.005	1
3920	C	259	GLN	NE2	115.396	0.005	1
3921	A	60	GLU	H	8.064	0.001	1
3922	C	260	GLU	H	8.064	0.001	1
3923	A	60	GLU	HA	4.087	0.020	1
3924	C	260	GLU	HA	4.087	0.020	1
3925	A	60	GLU	HB2	2.120	0.020	2
3926	C	260	GLU	HB2	2.120	0.020	2
3927	A	60	GLU	HB3	2.257	0.020	2
3928	C	260	GLU	HB3	2.257	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3929	A	60	GLU	HG2	2.540	0.020	2
3930	C	260	GLU	HG2	2.540	0.020	2
3931	A	60	GLU	HG3	2.299	0.020	2
3932	C	260	GLU	HG3	2.299	0.020	2
3933	A	60	GLU	C	179.051	0.1	1
3934	C	260	GLU	C	179.051	0.1	1
3935	A	60	GLU	CA	59.659	0.1	1
3936	C	260	GLU	CA	59.659	0.1	1
3937	A	60	GLU	CB	30.457	0.1	1
3938	C	260	GLU	CB	30.457	0.1	1
3939	A	60	GLU	CG	37.308	0.1	1
3940	C	260	GLU	CG	37.308	0.1	1
3941	A	60	GLU	N	117.166	0.1	1
3942	C	260	GLU	N	117.166	0.1	1
3943	A	61	TYR	H	7.924	0.006	1
3944	C	261	TYR	H	7.924	0.006	1
3945	A	61	TYR	HA	4.254	0.020	1
3946	C	261	TYR	HA	4.254	0.020	1
3947	A	61	TYR	HB2	3.313	0.020	2
3948	C	261	TYR	HB2	3.313	0.020	2
3949	A	61	TYR	HB3	3.445	0.001	2
3950	C	261	TYR	HB3	3.445	0.001	2
3951	A	61	TYR	HD1	7.173	0.006	1
3952	C	261	TYR	HD1	7.173	0.006	1
3953	A	61	TYR	HD2	7.173	0.006	1
3954	C	261	TYR	HD2	7.173	0.006	1
3955	A	61	TYR	HE1	6.831	0.020	1
3956	C	261	TYR	HE1	6.831	0.020	1
3957	A	61	TYR	HE2	6.831	0.020	1
3958	C	261	TYR	HE2	6.831	0.020	1
3959	A	61	TYR	C	178.617	0.1	1
3960	C	261	TYR	C	178.617	0.1	1
3961	A	61	TYR	CA	61.184	0.1	1
3962	C	261	TYR	CA	61.184	0.1	1
3963	A	61	TYR	CB	39.461	0.1	1
3964	C	261	TYR	CB	39.461	0.1	1
3965	A	61	TYR	CD1	133.083	0.1	1
3966	C	261	TYR	CD1	133.083	0.1	1
3967	A	61	TYR	CE1	118.070	0.1	1
3968	C	261	TYR	CE1	118.070	0.1	1
3969	A	61	TYR	N	121.271	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3970	C	261	TYR	N	121.271	0.1	1
3971	A	62	LEU	H	8.260	0.005	1
3972	C	262	LEU	H	8.260	0.005	1
3973	A	62	LEU	HA	3.966	0.020	1
3974	C	262	LEU	HA	3.966	0.020	1
3975	A	62	LEU	HB2	1.964	0.020	2
3976	C	262	LEU	HB2	1.964	0.020	2
3977	A	62	LEU	HB3	1.231	0.020	2
3978	C	262	LEU	HB3	1.231	0.020	2
3979	A	62	LEU	HD11	0.710	0.020	2
3980	C	262	LEU	HD11	0.710	0.020	2
3981	A	62	LEU	HD12	0.710	0.020	2
3982	C	262	LEU	HD12	0.710	0.020	2
3983	A	62	LEU	HD13	0.710	0.020	2
3984	C	262	LEU	HD13	0.710	0.020	2
3985	A	62	LEU	HD21	0.763	0.020	2
3986	C	262	LEU	HD21	0.763	0.020	2
3987	A	62	LEU	HD22	0.763	0.020	2
3988	C	262	LEU	HD22	0.763	0.020	2
3989	A	62	LEU	HD23	0.763	0.020	2
3990	C	262	LEU	HD23	0.763	0.020	2
3991	A	62	LEU	HG	1.942	0.020	1
3992	C	262	LEU	HG	1.942	0.020	1
3993	A	62	LEU	C	179.553	0.1	1
3994	C	262	LEU	C	179.553	0.1	1
3995	A	62	LEU	CA	58.014	0.1	1
3996	C	262	LEU	CA	58.014	0.1	1
3997	A	62	LEU	CB	42.397	0.1	1
3998	C	262	LEU	CB	42.397	0.1	1
3999	A	62	LEU	CD1	26.604	0.1	1
4000	C	262	LEU	CD1	26.604	0.1	1
4001	A	62	LEU	CD2	23.313	0.1	1
4002	C	262	LEU	CD2	23.313	0.1	1
4003	A	62	LEU	CG	26.984	0.1	1
4004	C	262	LEU	CG	26.984	0.1	1
4005	A	62	LEU	N	116.299	0.1	1
4006	C	262	LEU	N	116.299	0.1	1
4007	A	63	GLU	H	8.454	0.002	1
4008	C	263	GLU	H	8.454	0.002	1
4009	A	63	GLU	HA	3.854	0.002	1
4010	C	263	GLU	HA	3.854	0.002	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4011	A	63	GLU	HB2	2.252	0.020	2
4012	C	263	GLU	HB2	2.252	0.020	2
4013	A	63	GLU	HB3	2.092	0.020	2
4014	C	263	GLU	HB3	2.092	0.020	2
4015	A	63	GLU	HG2	2.483	0.020	2
4016	C	263	GLU	HG2	2.483	0.020	2
4017	A	63	GLU	HG3	2.268	0.004	2
4018	C	263	GLU	HG3	2.268	0.004	2
4019	A	63	GLU	C	179.279	0.1	1
4020	C	263	GLU	C	179.279	0.1	1
4021	A	63	GLU	CA	60.301	0.1	1
4022	C	263	GLU	CA	60.301	0.1	1
4023	A	63	GLU	CB	29.870	0.1	1
4024	C	263	GLU	CB	29.870	0.1	1
4025	A	63	GLU	CG	37.406	0.1	1
4026	C	263	GLU	CG	37.406	0.1	1
4027	A	63	GLU	N	118.616	0.1	1
4028	C	263	GLU	N	118.616	0.1	1
4029	A	64	LYS	H	7.575	0.020	1
4030	C	264	LYS	H	7.575	0.020	1
4031	A	64	LYS	HA	4.225	0.002	1
4032	C	264	LYS	HA	4.225	0.002	1
4033	A	64	LYS	HB2	1.944	0.020	2
4034	C	264	LYS	HB2	1.944	0.020	2
4035	A	64	LYS	HB3	2.017	0.001	2
4036	C	264	LYS	HB3	2.017	0.001	2
4037	A	64	LYS	HD2	1.697	0.020	2
4038	C	264	LYS	HD2	1.697	0.020	2
4039	A	64	LYS	HD3	1.697	0.020	2
4040	C	264	LYS	HD3	1.697	0.020	2
4041	A	64	LYS	HE2	3.006	0.004	2
4042	C	264	LYS	HE2	3.006	0.004	2
4043	A	64	LYS	HE3	3.006	0.004	2
4044	C	264	LYS	HE3	3.006	0.004	2
4045	A	64	LYS	HG2	1.641	0.020	2
4046	C	264	LYS	HG2	1.641	0.020	2
4047	A	64	LYS	HG3	1.600	0.020	2
4048	C	264	LYS	HG3	1.600	0.020	2
4049	A	64	LYS	C	178.457	0.1	1
4050	C	264	LYS	C	178.457	0.1	1
4051	A	64	LYS	CA	58.496	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4052	C	264	LYS	CA	58.496	0.1	1
4053	A	64	LYS	CB	32.400	0.1	1
4054	C	264	LYS	CB	32.400	0.1	1
4055	A	64	LYS	CD	29.249	0.1	1
4056	C	264	LYS	CD	29.249	0.1	1
4057	A	64	LYS	CE	42.838	0.1	1
4058	C	264	LYS	CE	42.838	0.1	1
4059	A	64	LYS	CG	25.336	0.1	1
4060	C	264	LYS	CG	25.336	0.1	1
4061	A	64	LYS	N	117.166	0.1	1
4062	C	264	LYS	N	117.166	0.1	1
4063	A	65	CYS	H	7.918	0.005	1
4064	C	265	CYS	H	7.918	0.005	1
4065	A	65	CYS	HA	4.526	0.020	1
4066	C	265	CYS	HA	4.526	0.020	1
4067	A	65	CYS	HB2	3.100	0.002	2
4068	C	265	CYS	HB2	3.100	0.002	2
4069	A	65	CYS	HB3	3.001	0.020	2
4070	C	265	CYS	HB3	3.001	0.020	2
4071	A	65	CYS	C	174.893	0.1	1
4072	C	265	CYS	C	174.893	0.1	1
4073	A	65	CYS	CA	56.329	0.1	1
4074	C	265	CYS	CA	56.329	0.1	1
4075	A	65	CYS	CB	45.235	0.1	1
4076	C	265	CYS	CB	45.235	0.1	1
4077	A	65	CYS	N	115.330	0.1	1
4078	C	265	CYS	N	115.330	0.1	1
4079	A	66	LEU	H	7.559	0.002	1
4080	C	266	LEU	H	7.559	0.002	1
4081	A	66	LEU	HA	4.491	0.001	1
4082	C	266	LEU	HA	4.491	0.001	1
4083	A	66	LEU	HB2	1.742	0.020	2
4084	C	266	LEU	HB2	1.742	0.020	2
4085	A	66	LEU	HB3	1.595	0.020	2
4086	C	266	LEU	HB3	1.595	0.020	2
4087	A	66	LEU	HD11	0.873	0.020	2
4088	C	266	LEU	HD11	0.873	0.020	2
4089	A	66	LEU	HD12	0.873	0.020	2
4090	C	266	LEU	HD12	0.873	0.020	2
4091	A	66	LEU	HD13	0.873	0.020	2
4092	C	266	LEU	HD13	0.873	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4093	A	66	LEU	HD21	0.867	0.020	2
4094	C	266	LEU	HD21	0.867	0.020	2
4095	A	66	LEU	HD22	0.867	0.020	2
4096	C	266	LEU	HD22	0.867	0.020	2
4097	A	66	LEU	HD23	0.867	0.020	2
4098	C	266	LEU	HD23	0.867	0.020	2
4099	A	66	LEU	HG	1.700	0.020	1
4100	C	266	LEU	HG	1.700	0.020	1
4101	A	66	LEU	C	176.812	0.1	1
4102	C	266	LEU	C	176.812	0.1	1
4103	A	66	LEU	CA	55.366	0.1	1
4104	C	266	LEU	CA	55.366	0.1	1
4105	A	66	LEU	CB	43.278	0.1	1
4106	C	266	LEU	CB	43.278	0.1	1
4107	A	66	LEU	CD1	26.013	0.1	1
4108	C	266	LEU	CD1	26.013	0.1	1
4109	A	66	LEU	CD2	23.998	0.1	1
4110	C	266	LEU	CD2	23.998	0.1	1
4111	A	66	LEU	CG	27.307	0.1	1
4112	C	266	LEU	CG	27.307	0.1	1
4113	A	66	LEU	N	120.930	0.1	1
4114	C	266	LEU	N	120.930	0.1	1
4115	A	67	ASN	H	8.265	0.001	1
4116	C	267	ASN	H	8.265	0.001	1
4117	A	67	ASN	HA	4.669	0.020	1
4118	C	267	ASN	HA	4.669	0.020	1
4119	A	67	ASN	HB2	2.859	0.020	2
4120	C	267	ASN	HB2	2.859	0.020	2
4121	A	67	ASN	HB3	2.609	0.020	2
4122	C	267	ASN	HB3	2.609	0.020	2
4123	A	67	ASN	HD21	7.554	0.020	2
4124	C	267	ASN	HD21	7.554	0.020	2
4125	A	67	ASN	HD22	6.813	0.020	2
4126	C	267	ASN	HD22	6.813	0.020	2
4127	A	67	ASN	CA	53.761	0.1	1
4128	C	267	ASN	CA	53.761	0.1	1
4129	A	67	ASN	CB	39.069	0.1	1
4130	C	267	ASN	CB	39.069	0.1	1
4131	A	67	ASN	N	120.279	0.1	1
4132	C	267	ASN	N	120.279	0.1	1
4133	A	67	ASN	ND2	111.986	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4134	C	267	ASN	ND2	111.986	0.1	1
4135	A	68	LYS	H	7.841	0.004	1
4136	C	268	LYS	H	7.841	0.004	1
4137	A	68	LYS	HA	4.175	0.020	1
4138	C	268	LYS	HA	4.175	0.020	1
4139	A	68	LYS	HB2	1.849	0.020	2
4140	C	268	LYS	HB2	1.849	0.020	2
4141	A	68	LYS	HB3	1.704	0.020	2
4142	C	268	LYS	HB3	1.704	0.020	2
4143	A	68	LYS	HD2	1.689	0.020	2
4144	C	268	LYS	HD2	1.689	0.020	2
4145	A	68	LYS	HD3	1.689	0.020	2
4146	C	268	LYS	HD3	1.689	0.020	2
4147	A	68	LYS	HE2	3.035	0.003	2
4148	C	268	LYS	HE2	3.035	0.003	2
4149	A	68	LYS	HE3	3.035	0.003	2
4150	C	268	LYS	HE3	3.035	0.003	2
4151	A	68	LYS	HG2	1.400	0.020	2
4152	C	268	LYS	HG2	1.400	0.020	2
4153	A	68	LYS	HG3	1.400	0.020	2
4154	C	268	LYS	HG3	1.400	0.020	2
4155	A	68	LYS	CA	57.722	0.1	1
4156	C	268	LYS	CA	57.722	0.1	1
4157	A	68	LYS	CB	34.102	0.1	1
4158	C	268	LYS	CB	34.102	0.1	1
4159	A	68	LYS	CD	29.572	0.1	1
4160	C	268	LYS	CD	29.572	0.1	1
4161	A	68	LYS	CG	25.042	0.1	1
4162	C	268	LYS	CG	25.042	0.1	1
4163	A	68	LYS	N	127.034	0.1	1
4164	C	268	LYS	N	127.034	0.1	1
4165	B	101	MET	HA	4.492	0.020	1
4166	D	301	MET	HA	4.492	0.020	1
4167	B	101	MET	HB2	2.157	0.020	2
4168	D	301	MET	HB2	2.157	0.020	2
4169	B	101	MET	HB3	2.047	0.020	2
4170	D	301	MET	HB3	2.047	0.020	2
4171	B	101	MET	HG2	2.656	0.002	2
4172	D	301	MET	HG2	2.656	0.002	2
4173	B	101	MET	HG3	2.575	0.020	2
4174	D	301	MET	HG3	2.575	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4175	B	101	MET	C	176.332	0.1	1
4176	D	301	MET	C	176.332	0.1	1
4177	B	101	MET	CA	55.902	0.1	1
4178	D	301	MET	CA	55.902	0.1	1
4179	B	101	MET	CB	33.026	0.1	1
4180	D	301	MET	CB	33.026	0.1	1
4181	B	102	GLU	H	8.342	0.020	1
4182	D	302	GLU	H	8.342	0.020	1
4183	B	102	GLU	HA	4.282	0.020	1
4184	D	302	GLU	HA	4.282	0.020	1
4185	B	102	GLU	HB2	2.088	0.020	2
4186	D	302	GLU	HB2	2.088	0.020	2
4187	B	102	GLU	HB3	1.986	0.003	2
4188	D	302	GLU	HB3	1.986	0.003	2
4189	B	102	GLU	HG2	2.293	0.001	2
4190	D	302	GLU	HG2	2.293	0.001	2
4191	B	102	GLU	HG3	2.293	0.001	2
4192	D	302	GLU	HG3	2.293	0.001	2
4193	B	102	GLU	C	177.132	0.1	1
4194	D	302	GLU	C	177.132	0.1	1
4195	B	102	GLU	CA	57.410	0.1	1
4196	D	302	GLU	CA	57.410	0.1	1
4197	B	102	GLU	CG	36.797	0.1	1
4198	D	302	GLU	CG	36.797	0.1	1
4199	B	102	GLU	N	121.884	0.1	1
4200	D	302	GLU	N	121.884	0.1	1
4201	B	103	GLY	H	8.331	0.003	1
4202	D	303	GLY	H	8.331	0.003	1
4203	B	103	GLY	HA2	3.960	0.020	2
4204	D	303	GLY	HA2	3.960	0.020	2
4205	B	103	GLY	HA3	3.960	0.020	2
4206	D	303	GLY	HA3	3.960	0.020	2
4207	B	103	GLY	C	174.207	0.1	1
4208	D	303	GLY	C	174.207	0.1	1
4209	B	103	GLY	CA	45.731	0.1	1
4210	D	303	GLY	CA	45.731	0.1	1
4211	B	103	GLY	N	110.055	0.1	1
4212	D	303	GLY	N	110.055	0.1	1
4213	B	104	ILE	H	7.831	0.002	1
4214	D	304	ILE	H	7.831	0.002	1
4215	B	104	ILE	HA	4.286	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4216	D	304	ILE	HA	4.286	0.020	1
4217	B	104	ILE	HB	1.912	0.020	1
4218	D	304	ILE	HB	1.912	0.020	1
4219	B	104	ILE	HD11	0.867	0.020	1
4220	D	304	ILE	HD11	0.867	0.020	1
4221	B	104	ILE	HD12	0.867	0.020	1
4222	D	304	ILE	HD12	0.867	0.020	1
4223	B	104	ILE	HD13	0.867	0.020	1
4224	D	304	ILE	HD13	0.867	0.020	1
4225	B	104	ILE	HG12	1.455	0.020	2
4226	D	304	ILE	HG12	1.455	0.020	2
4227	B	104	ILE	HG13	1.191	0.020	2
4228	D	304	ILE	HG13	1.191	0.020	2
4229	B	104	ILE	HG21	0.923	0.020	1
4230	D	304	ILE	HG21	0.923	0.020	1
4231	B	104	ILE	HG22	0.923	0.020	1
4232	D	304	ILE	HG22	0.923	0.020	1
4233	B	104	ILE	HG23	0.923	0.020	1
4234	D	304	ILE	HG23	0.923	0.020	1
4235	B	104	ILE	C	176.401	0.1	1
4236	D	304	ILE	C	176.401	0.1	1
4237	B	104	ILE	CA	61.558	0.1	1
4238	D	304	ILE	CA	61.558	0.1	1
4239	B	104	ILE	CB	39.436	0.1	1
4240	D	304	ILE	CB	39.436	0.1	1
4241	B	104	ILE	CD1	13.418	0.1	1
4242	D	304	ILE	CD1	13.418	0.1	1
4243	B	104	ILE	CG1	27.496	0.1	1
4244	D	304	ILE	CG1	27.496	0.1	1
4245	B	104	ILE	CG2	18.069	0.1	1
4246	D	304	ILE	CG2	18.069	0.1	1
4247	B	104	ILE	N	119.606	0.1	1
4248	D	304	ILE	N	119.606	0.1	1
4249	B	105	SER	H	8.350	0.020	1
4250	D	305	SER	H	8.350	0.020	1
4251	B	105	SER	HA	4.545	0.020	1
4252	D	305	SER	HA	4.545	0.020	1
4253	B	105	SER	HB2	3.877	0.020	2
4254	D	305	SER	HB2	3.877	0.020	2
4255	B	105	SER	HB3	3.836	0.020	2
4256	D	305	SER	HB3	3.836	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4257	B	105	SER	C	174.550	0.1	1
4258	D	305	SER	C	174.550	0.1	1
4259	B	105	SER	CA	58.667	0.1	1
4260	D	305	SER	CA	58.667	0.1	1
4261	B	105	SER	CB	64.072	0.1	1
4262	D	305	SER	CB	64.072	0.1	1
4263	B	105	SER	N	119.853	0.1	1
4264	D	305	SER	N	119.853	0.1	1
4265	B	106	ILE	H	7.921	0.002	1
4266	D	306	ILE	H	7.921	0.002	1
4267	B	106	ILE	HA	4.205	0.020	1
4268	D	306	ILE	HA	4.205	0.020	1
4269	B	106	ILE	HB	1.805	0.020	1
4270	D	306	ILE	HB	1.805	0.020	1
4271	B	106	ILE	HD11	0.798	0.020	1
4272	D	306	ILE	HD11	0.798	0.020	1
4273	B	106	ILE	HD12	0.798	0.020	1
4274	D	306	ILE	HD12	0.798	0.020	1
4275	B	106	ILE	HD13	0.798	0.020	1
4276	D	306	ILE	HD13	0.798	0.020	1
4277	B	106	ILE	HG12	1.220	0.020	2
4278	D	306	ILE	HG12	1.220	0.020	2
4279	B	106	ILE	HG13	1.077	0.020	2
4280	D	306	ILE	HG13	1.077	0.020	2
4281	B	106	ILE	HG21	0.804	0.020	1
4282	D	306	ILE	HG21	0.804	0.020	1
4283	B	106	ILE	HG22	0.804	0.020	1
4284	D	306	ILE	HG22	0.804	0.020	1
4285	B	106	ILE	HG23	0.804	0.020	1
4286	D	306	ILE	HG23	0.804	0.020	1
4287	B	106	ILE	C	175.921	0.1	1
4288	D	306	ILE	C	175.921	0.1	1
4289	B	106	ILE	CA	61.935	0.1	1
4290	D	306	ILE	CA	61.935	0.1	1
4291	B	106	ILE	CB	39.436	0.1	1
4292	D	306	ILE	CB	39.436	0.1	1
4293	B	106	ILE	CD1	13.418	0.1	1
4294	D	306	ILE	CD1	13.418	0.1	1
4295	B	106	ILE	CG1	27.370	0.1	1
4296	D	306	ILE	CG1	27.370	0.1	1
4297	B	106	ILE	CG2	18.069	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4298	D	306	ILE	CG2	18.069	0.1	1
4299	B	106	ILE	N	121.730	0.1	1
4300	D	306	ILE	N	121.730	0.1	1
4301	B	107	TYR	H	8.166	0.009	1
4302	D	307	TYR	H	8.166	0.009	1
4303	B	107	TYR	HA	4.713	0.020	1
4304	D	307	TYR	HA	4.713	0.020	1
4305	B	107	TYR	HB2	2.920	0.020	2
4306	D	307	TYR	HB2	2.920	0.020	2
4307	B	107	TYR	HB3	3.089	0.020	2
4308	D	307	TYR	HB3	3.089	0.020	2
4309	B	107	TYR	HD1	7.114	0.014	1
4310	D	307	TYR	HD1	7.114	0.014	1
4311	B	107	TYR	HD2	7.114	0.014	1
4312	D	307	TYR	HD2	7.114	0.014	1
4313	B	107	TYR	HE1	6.824	0.020	1
4314	D	307	TYR	HE1	6.824	0.020	1
4315	B	107	TYR	HE2	6.824	0.020	1
4316	D	307	TYR	HE2	6.824	0.020	1
4317	B	107	TYR	C	176.058	0.1	1
4318	D	307	TYR	C	176.058	0.1	1
4319	B	107	TYR	CA	58.165	0.1	1
4320	D	307	TYR	CA	58.165	0.1	1
4321	B	107	TYR	CB	39.436	0.1	1
4322	D	307	TYR	CB	39.436	0.1	1
4323	B	107	TYR	CD1	133.344	0.1	1
4324	D	307	TYR	CD1	133.344	0.1	1
4325	B	107	TYR	CE1	118.588	0.1	1
4326	D	307	TYR	CE1	118.588	0.1	1
4327	B	107	TYR	N	123.598	0.1	1
4328	D	307	TYR	N	123.598	0.1	1
4329	B	108	THR	H	7.961	0.020	1
4330	D	308	THR	H	7.961	0.020	1
4331	B	108	THR	HA	4.433	0.020	1
4332	D	308	THR	HA	4.433	0.020	1
4333	B	108	THR	HB	4.283	0.020	1
4334	D	308	THR	HB	4.283	0.020	1
4335	B	108	THR	HG21	1.205	0.020	1
4336	D	308	THR	HG21	1.205	0.020	1
4337	B	108	THR	HG22	1.205	0.020	1
4338	D	308	THR	HG22	1.205	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4339	B	108	THR	HG23	1.205	0.020	1
4340	D	308	THR	HG23	1.205	0.020	1
4341	B	108	THR	C	174.459	0.1	1
4342	D	308	THR	C	174.459	0.1	1
4343	B	108	THR	CA	62.061	0.1	1
4344	D	308	THR	CA	62.061	0.1	1
4345	B	108	THR	CB	70.608	0.1	1
4346	D	308	THR	CB	70.608	0.1	1
4347	B	108	THR	CG2	21.965	0.1	1
4348	D	308	THR	CG2	21.965	0.1	1
4349	B	108	THR	N	115.642	0.1	1
4350	D	308	THR	N	115.642	0.1	1
4351	B	109	SER	H	8.211	0.020	1
4352	D	309	SER	H	8.211	0.020	1
4353	B	109	SER	HA	4.507	0.020	1
4354	D	309	SER	HA	4.507	0.020	1
4355	B	109	SER	HB2	3.953	0.020	2
4356	D	309	SER	HB2	3.953	0.020	2
4357	B	109	SER	HB3	3.909	0.020	2
4358	D	309	SER	HB3	3.909	0.020	2
4359	B	109	SER	C	174.504	0.1	1
4360	D	309	SER	C	174.504	0.1	1
4361	B	109	SER	CA	58.919	0.1	1
4362	D	309	SER	CA	58.919	0.1	1
4363	B	109	SER	CB	64.198	0.1	1
4364	D	309	SER	CB	64.198	0.1	1
4365	B	109	SER	N	117.260	0.1	1
4366	D	309	SER	N	117.260	0.1	1
4367	B	110	ASP	H	8.351	0.020	1
4368	D	310	ASP	H	8.351	0.020	1
4369	B	110	ASP	HA	4.631	0.020	1
4370	D	310	ASP	HA	4.631	0.020	1
4371	B	110	ASP	HB2	2.704	0.020	2
4372	D	310	ASP	HB2	2.704	0.020	2
4373	B	110	ASP	HB3	2.657	0.020	2
4374	D	310	ASP	HB3	2.657	0.020	2
4375	B	110	ASP	C	176.058	0.1	1
4376	D	310	ASP	C	176.058	0.1	1
4377	B	110	ASP	CA	55.022	0.1	1
4378	D	310	ASP	CA	55.022	0.1	1
4379	B	110	ASP	CB	41.825	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4380	D	310	ASP	CB	41.825	0.1	1
4381	B	110	ASP	N	122.020	0.1	1
4382	D	310	ASP	N	122.020	0.1	1
4383	B	111	ASN	H	8.230	0.020	1
4384	D	311	ASN	H	8.230	0.020	1
4385	B	111	ASN	HA	4.726	0.020	1
4386	D	311	ASN	HA	4.726	0.020	1
4387	B	111	ASN	HB2	2.842	0.020	2
4388	D	311	ASN	HB2	2.842	0.020	2
4389	B	111	ASN	HB3	2.707	0.020	2
4390	D	311	ASN	HB3	2.707	0.020	2
4391	B	111	ASN	C	175.030	0.1	1
4392	D	311	ASN	C	175.030	0.1	1
4393	B	111	ASN	CA	53.765	0.1	1
4394	D	311	ASN	CA	53.765	0.1	1
4395	B	111	ASN	CB	39.562	0.1	1
4396	D	311	ASN	CB	39.562	0.1	1
4397	B	111	ASN	N	118.317	0.1	1
4398	D	311	ASN	N	118.317	0.1	1
4399	B	112	TYR	H	8.101	0.020	1
4400	D	312	TYR	H	8.101	0.020	1
4401	B	112	TYR	HA	4.638	0.020	1
4402	D	312	TYR	HA	4.638	0.020	1
4403	B	112	TYR	HB2	3.038	0.020	2
4404	D	312	TYR	HB2	3.038	0.020	2
4405	B	112	TYR	HB3	3.062	0.020	2
4406	D	312	TYR	HB3	3.062	0.020	2
4407	B	112	TYR	HD1	7.110	0.012	1
4408	D	312	TYR	HD1	7.110	0.012	1
4409	B	112	TYR	HD2	7.110	0.012	1
4410	D	312	TYR	HD2	7.110	0.012	1
4411	B	112	TYR	HE1	6.820	0.009	1
4412	D	312	TYR	HE1	6.820	0.009	1
4413	B	112	TYR	HE2	6.820	0.009	1
4414	D	312	TYR	HE2	6.820	0.009	1
4415	B	112	TYR	C	176.081	0.1	1
4416	D	312	TYR	C	176.081	0.1	1
4417	B	112	TYR	CA	58.793	0.1	1
4418	D	312	TYR	CA	58.793	0.1	1
4419	B	112	TYR	CB	39.436	0.1	1
4420	D	312	TYR	CB	39.436	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4421	B	112	TYR	CD1	133.344	0.1	1
4422	D	312	TYR	CD1	133.344	0.1	1
4423	B	112	TYR	CE1	118.588	0.1	1
4424	D	312	TYR	CE1	118.588	0.1	1
4425	B	112	TYR	N	120.850	0.1	1
4426	D	312	TYR	N	120.850	0.1	1
4427	B	113	THR	H	7.879	0.020	1
4428	D	313	THR	H	7.879	0.020	1
4429	B	113	THR	HA	4.284	0.020	1
4430	D	313	THR	HA	4.284	0.020	1
4431	B	113	THR	HB	4.218	0.020	1
4432	D	313	THR	HB	4.218	0.020	1
4433	B	113	THR	HG21	1.177	0.020	1
4434	D	313	THR	HG21	1.177	0.020	1
4435	B	113	THR	HG22	1.177	0.020	1
4436	D	313	THR	HG22	1.177	0.020	1
4437	B	113	THR	HG23	1.177	0.020	1
4438	D	313	THR	HG23	1.177	0.020	1
4439	B	113	THR	C	174.413	0.1	1
4440	D	313	THR	C	174.413	0.1	1
4441	B	113	THR	CA	62.187	0.1	1
4442	D	313	THR	CA	62.187	0.1	1
4443	B	113	THR	CB	70.341	0.1	1
4444	D	313	THR	CB	70.341	0.1	1
4445	B	113	THR	CG2	21.965	0.1	1
4446	D	313	THR	CG2	21.965	0.1	1
4447	B	113	THR	N	116.126	0.1	1
4448	D	313	THR	N	116.126	0.1	1
4449	B	114	GLU	H	8.253	0.020	1
4450	D	314	GLU	H	8.253	0.020	1
4451	B	114	GLU	HA	4.256	0.020	1
4452	D	314	GLU	HA	4.256	0.020	1
4453	B	114	GLU	HB2	2.065	0.020	2
4454	D	314	GLU	HB2	2.065	0.020	2
4455	B	114	GLU	HB3	1.977	0.020	2
4456	D	314	GLU	HB3	1.977	0.020	2
4457	B	114	GLU	HG2	2.312	0.020	2
4458	D	314	GLU	HG2	2.312	0.020	2
4459	B	114	GLU	HG3	2.312	0.020	2
4460	D	314	GLU	HG3	2.312	0.020	2
4461	B	114	GLU	C	176.766	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4462	D	314	GLU	C	176.766	0.1	1
4463	B	114	GLU	CA	57.410	0.1	1
4464	D	314	GLU	CA	57.410	0.1	1
4465	B	114	GLU	CB	30.620	0.1	1
4466	D	314	GLU	CB	30.620	0.1	1
4467	B	114	GLU	CG	36.923	0.1	1
4468	D	314	GLU	CG	36.923	0.1	1
4469	B	114	GLU	N	123.052	0.1	1
4470	D	314	GLU	N	123.052	0.1	1
4471	B	115	GLU	H	8.331	0.020	1
4472	D	315	GLU	H	8.331	0.020	1
4473	B	115	GLU	HA	4.292	0.020	1
4474	D	315	GLU	HA	4.292	0.020	1
4475	B	115	GLU	HB2	2.085	0.020	2
4476	D	315	GLU	HB2	2.085	0.020	2
4477	B	115	GLU	HB3	1.979	0.020	2
4478	D	315	GLU	HB3	1.979	0.020	2
4479	B	115	GLU	HG2	2.295	0.020	2
4480	D	315	GLU	HG2	2.295	0.020	2
4481	B	115	GLU	HG3	2.295	0.020	2
4482	D	315	GLU	HG3	2.295	0.020	2
4483	B	115	GLU	C	176.880	0.1	1
4484	D	315	GLU	C	176.880	0.1	1
4485	B	115	GLU	CA	57.410	0.1	1
4486	D	315	GLU	CA	57.410	0.1	1
4487	B	115	GLU	CB	30.525	0.1	1
4488	D	315	GLU	CB	30.525	0.1	1
4489	B	115	GLU	CG	36.923	0.1	1
4490	D	315	GLU	CG	36.923	0.1	1
4491	B	115	GLU	N	121.688	0.1	1
4492	D	315	GLU	N	121.688	0.1	1
4493	B	116	MET	H	8.317	0.020	1
4494	D	316	MET	H	8.317	0.020	1
4495	B	116	MET	HA	4.490	0.020	1
4496	D	316	MET	HA	4.490	0.020	1
4497	B	116	MET	HB2	2.127	0.020	2
4498	D	316	MET	HB2	2.127	0.020	2
4499	B	116	MET	HB3	2.046	0.020	2
4500	D	316	MET	HB3	2.046	0.020	2
4501	B	116	MET	HG2	2.633	0.001	2
4502	D	316	MET	HG2	2.633	0.001	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4503	B	116	MET	HG3	2.546	0.020	2
4504	D	316	MET	HG3	2.546	0.020	2
4505	B	116	MET	C	177.086	0.1	1
4506	D	316	MET	C	177.086	0.1	1
4507	B	116	MET	CA	56.279	0.1	1
4508	D	316	MET	CA	56.279	0.1	1
4509	B	116	MET	CB	33.026	0.1	1
4510	D	316	MET	CB	33.026	0.1	1
4511	B	116	MET	N	121.270	0.1	1
4512	D	316	MET	N	121.270	0.1	1
4513	B	117	GLY	H	8.320	0.020	1
4514	D	317	GLY	H	8.320	0.020	1
4515	B	117	GLY	HA2	4.054	0.020	2
4516	D	317	GLY	HA2	4.054	0.020	2
4517	B	117	GLY	HA3	4.054	0.020	2
4518	D	317	GLY	HA3	4.054	0.020	2
4519	B	117	GLY	C	174.481	0.1	1
4520	D	317	GLY	C	174.481	0.1	1
4521	B	117	GLY	CA	45.847	0.1	1
4522	D	317	GLY	CA	45.847	0.1	1
4523	B	117	GLY	N	110.055	0.1	1
4524	D	317	GLY	N	110.055	0.1	1
4525	B	118	SER	H	8.230	0.020	1
4526	D	318	SER	H	8.230	0.020	1
4527	B	118	SER	HA	4.476	0.020	1
4528	D	318	SER	HA	4.476	0.020	1
4529	B	118	SER	HB2	3.952	0.020	2
4530	D	318	SER	HB2	3.952	0.020	2
4531	B	118	SER	HB3	3.893	0.020	2
4532	D	318	SER	HB3	3.893	0.020	2
4533	B	118	SER	C	175.327	0.1	1
4534	D	318	SER	C	175.327	0.1	1
4535	B	118	SER	CA	58.919	0.1	1
4536	D	318	SER	CA	58.919	0.1	1
4537	B	118	SER	CB	64.575	0.1	1
4538	D	318	SER	CB	64.575	0.1	1
4539	B	118	SER	N	115.664	0.1	1
4540	D	318	SER	N	115.664	0.1	1
4541	B	119	GLY	H	8.371	0.020	1
4542	D	319	GLY	H	8.371	0.020	1
4543	B	119	GLY	HA2	3.951	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4544	D	319	GLY	HA2	3.951	0.020	2
4545	B	119	GLY	HA3	3.951	0.020	2
4546	D	319	GLY	HA3	3.951	0.020	2
4547	B	119	GLY	C	174.002	0.1	1
4548	D	319	GLY	C	174.002	0.1	1
4549	B	119	GLY	CA	45.721	0.1	1
4550	D	319	GLY	CA	45.721	0.1	1
4551	B	119	GLY	N	110.872	0.1	1
4552	D	319	GLY	N	110.872	0.1	1
4553	B	120	ASP	H	8.072	0.014	1
4554	D	320	ASP	H	8.072	0.014	1
4555	B	120	ASP	HA	4.629	0.020	1
4556	D	320	ASP	HA	4.629	0.020	1
4557	B	120	ASP	HB2	2.659	0.001	2
4558	D	320	ASP	HB2	2.659	0.001	2
4559	B	120	ASP	HB3	2.537	0.002	2
4560	D	320	ASP	HB3	2.537	0.002	2
4561	B	120	ASP	C	176.355	0.1	1
4562	D	320	ASP	C	176.355	0.1	1
4563	B	120	ASP	CA	54.771	0.1	1
4564	D	320	ASP	CA	54.771	0.1	1
4565	B	120	ASP	CB	41.699	0.1	1
4566	D	320	ASP	CB	41.699	0.1	1
4567	B	120	ASP	N	120.530	0.1	1
4568	D	320	ASP	N	120.530	0.1	1
4569	B	121	TYS	H	8.180	0.020	1
4570	D	321	TYS	H	8.180	0.020	1
4571	B	121	TYS	HA	4.628	0.020	1
4572	D	321	TYS	HA	4.628	0.020	1
4573	B	121	TYS	HB2	3.049	0.020	2
4574	D	321	TYS	HB2	3.049	0.020	2
4575	B	121	TYS	HB3	3.219	0.020	2
4576	D	321	TYS	HB3	3.219	0.020	2
4577	B	121	TYS	HD1	7.261	0.020	1
4578	D	321	TYS	HD1	7.261	0.020	1
4579	B	121	TYS	HD2	7.261	0.020	1
4580	D	321	TYS	HD2	7.261	0.020	1
4581	B	121	TYS	HE1	7.260	0.020	1
4582	D	321	TYS	HE1	7.260	0.020	1
4583	B	121	TYS	HE2	7.260	0.020	1
4584	D	321	TYS	HE2	7.260	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4585	B	121	TYS	C	176.058	0.1	1
4586	D	321	TYS	C	176.058	0.1	1
4587	B	121	TYS	CA	58.667	0.1	1
4588	D	321	TYS	CA	58.667	0.1	1
4589	B	121	TYS	CB	39.311	0.1	1
4590	D	321	TYS	CB	39.311	0.1	1
4591	B	121	TYS	CD1	133.344	0.1	1
4592	D	321	TYS	CD1	133.344	0.1	1
4593	B	121	TYS	CE1	124.540	0.1	1
4594	D	321	TYS	CE1	124.540	0.1	1
4595	B	121	TYS	N	120.283	0.1	1
4596	D	321	TYS	N	120.283	0.1	1
4597	B	122	ASP	H	8.322	0.020	1
4598	D	322	ASP	H	8.322	0.020	1
4599	B	122	ASP	HA	4.602	0.020	1
4600	D	322	ASP	HA	4.602	0.020	1
4601	B	122	ASP	HB2	2.665	0.020	2
4602	D	322	ASP	HB2	2.665	0.020	2
4603	B	122	ASP	HB3	2.658	0.020	2
4604	D	322	ASP	HB3	2.658	0.020	2
4605	B	122	ASP	C	176.835	0.1	1
4606	D	322	ASP	C	176.835	0.1	1
4607	B	122	ASP	CA	55.022	0.1	1
4608	D	322	ASP	CA	55.022	0.1	1
4609	B	122	ASP	CB	41.825	0.1	1
4610	D	322	ASP	CB	41.825	0.1	1
4611	B	122	ASP	N	121.417	0.1	1
4612	D	322	ASP	N	121.417	0.1	1
4613	B	123	SER	H	8.155	0.020	1
4614	D	323	SER	H	8.155	0.020	1
4615	B	123	SER	HA	4.404	0.020	1
4616	D	323	SER	HA	4.404	0.020	1
4617	B	123	SER	HB2	3.956	0.001	2
4618	D	323	SER	HB2	3.956	0.001	2
4619	B	123	SER	HB3	3.925	0.002	2
4620	D	323	SER	HB3	3.925	0.002	2
4621	B	123	SER	C	175.075	0.1	1
4622	D	323	SER	C	175.075	0.1	1
4623	B	123	SER	CA	59.347	0.1	1
4624	D	323	SER	CA	59.347	0.1	1
4625	B	123	SER	CB	63.879	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4626	D	323	SER	CB	63.879	0.1	1
4627	B	123	SER	N	116.126	0.1	1
4628	D	323	SER	N	116.126	0.1	1
4629	B	124	MET	H	8.221	0.020	1
4630	D	324	MET	H	8.221	0.020	1
4631	B	124	MET	HA	4.482	0.020	1
4632	D	324	MET	HA	4.482	0.020	1
4633	B	124	MET	HB2	2.137	0.002	2
4634	D	324	MET	HB2	2.137	0.002	2
4635	B	124	MET	HB3	2.063	0.001	2
4636	D	324	MET	HB3	2.063	0.001	2
4637	B	124	MET	HG2	2.626	0.005	2
4638	D	324	MET	HG2	2.626	0.005	2
4639	B	124	MET	HG3	2.553	0.006	2
4640	D	324	MET	HG3	2.553	0.006	2
4641	B	124	MET	C	176.355	0.1	1
4642	D	324	MET	C	176.355	0.1	1
4643	B	124	MET	CA	56.279	0.1	1
4644	D	324	MET	CA	56.279	0.1	1
4645	B	124	MET	CB	32.900	0.1	1
4646	D	324	MET	CB	32.900	0.1	1
4647	B	124	MET	CG	32.900	0.1	1
4648	D	324	MET	CG	32.900	0.1	1
4649	B	124	MET	N	121.210	0.1	1
4650	D	324	MET	N	121.210	0.1	1
4651	B	125	LYS	H	8.036	0.020	1
4652	D	325	LYS	H	8.036	0.020	1
4653	B	125	LYS	HA	4.333	0.020	1
4654	D	325	LYS	HA	4.333	0.020	1
4655	B	125	LYS	HB2	1.855	0.020	2
4656	D	325	LYS	HB2	1.855	0.020	2
4657	B	125	LYS	HB3	1.767	0.020	2
4658	D	325	LYS	HB3	1.767	0.020	2
4659	B	125	LYS	HD2	1.682	0.020	2
4660	D	325	LYS	HD2	1.682	0.020	2
4661	B	125	LYS	HD3	1.682	0.020	2
4662	D	325	LYS	HD3	1.682	0.020	2
4663	B	125	LYS	HE2	3.012	0.020	2
4664	D	325	LYS	HE2	3.012	0.020	2
4665	B	125	LYS	HE3	3.012	0.020	2
4666	D	325	LYS	HE3	3.012	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4667	B	125	LYS	HG2	1.420	0.020	2
4668	D	325	LYS	HG2	1.420	0.020	2
4669	B	125	LYS	HG3	1.420	0.020	2
4670	D	325	LYS	HG3	1.420	0.020	2
4671	B	125	LYS	C	176.355	0.1	1
4672	D	325	LYS	C	176.355	0.1	1
4673	B	125	LYS	CA	56.656	0.1	1
4674	D	325	LYS	CA	56.656	0.1	1
4675	B	125	LYS	CB	33.529	0.1	1
4676	D	325	LYS	CB	33.529	0.1	1
4677	B	125	LYS	CD	29.632	0.1	1
4678	D	325	LYS	CD	29.632	0.1	1
4679	B	125	LYS	CE	42.579	0.1	1
4680	D	325	LYS	CE	42.579	0.1	1
4681	B	125	LYS	CG	25.107	0.1	1
4682	D	325	LYS	CG	25.107	0.1	1
4683	B	125	LYS	N	121.457	0.1	1
4684	D	325	LYS	N	121.457	0.1	1
4685	B	126	GLU	H	8.205	0.020	1
4686	D	326	GLU	H	8.205	0.020	1
4687	B	126	GLU	N	122.740	0.1	1
4688	D	326	GLU	N	122.740	0.1	1
4689	B	127	PRO	HA	4.377	0.020	1
4690	D	327	PRO	HA	4.377	0.020	1
4691	B	127	PRO	HB2	2.243	0.020	2
4692	D	327	PRO	HB2	2.243	0.020	2
4693	B	127	PRO	HB3	1.832	0.020	2
4694	D	327	PRO	HB3	1.832	0.020	2
4695	B	127	PRO	HD2	3.791	0.020	2
4696	D	327	PRO	HD2	3.791	0.020	2
4697	B	127	PRO	HD3	3.692	0.020	2
4698	D	327	PRO	HD3	3.692	0.020	2
4699	B	127	PRO	HG2	2.022	0.020	2
4700	D	327	PRO	HG2	2.022	0.020	2
4701	B	127	PRO	HG3	2.022	0.020	2
4702	D	327	PRO	HG3	2.022	0.020	2
4703	B	127	PRO	C	176.812	0.1	1
4704	D	327	PRO	C	176.812	0.1	1
4705	B	127	PRO	CA	63.821	0.1	1
4706	D	327	PRO	CA	63.821	0.1	1
4707	B	127	PRO	CB	32.272	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4708	D	327	PRO	CB	32.272	0.1	1
4709	B	127	PRO	CD	51.000	0.1	1
4710	D	327	PRO	CD	51.000	0.1	1
4711	B	127	PRO	CG	27.873	0.1	1
4712	D	327	PRO	CG	27.873	0.1	1
4713	B	128	ALA	H	8.273	0.020	1
4714	D	328	ALA	H	8.273	0.020	1
4715	B	128	ALA	HA	4.287	0.020	1
4716	D	328	ALA	HA	4.287	0.020	1
4717	B	128	ALA	HB1	1.322	0.020	1
4718	D	328	ALA	HB1	1.322	0.020	1
4719	B	128	ALA	HB2	1.322	0.020	1
4720	D	328	ALA	HB2	1.322	0.020	1
4721	B	128	ALA	HB3	1.322	0.020	1
4722	D	328	ALA	HB3	1.322	0.020	1
4723	B	128	ALA	C	177.589	0.1	1
4724	D	328	ALA	C	177.589	0.1	1
4725	B	128	ALA	CA	52.873	0.1	1
4726	D	328	ALA	CA	52.873	0.1	1
4727	B	128	ALA	CB	19.703	0.1	1
4728	D	328	ALA	CB	19.703	0.1	1
4729	B	128	ALA	N	123.577	0.1	1
4730	D	328	ALA	N	123.577	0.1	1
4731	B	129	PHE	H	8.019	0.020	1
4732	D	329	PHE	H	8.019	0.020	1
4733	B	129	PHE	HA	4.621	0.020	1
4734	D	329	PHE	HA	4.621	0.020	1
4735	B	129	PHE	HB2	3.148	0.020	2
4736	D	329	PHE	HB2	3.148	0.020	2
4737	B	129	PHE	HB3	3.062	0.020	2
4738	D	329	PHE	HB3	3.062	0.020	2
4739	B	129	PHE	HD1	7.261	0.020	1
4740	D	329	PHE	HD1	7.261	0.020	1
4741	B	129	PHE	HD2	7.261	0.020	1
4742	D	329	PHE	HD2	7.261	0.020	1
4743	B	129	PHE	HE1	7.345	0.020	1
4744	D	329	PHE	HE1	7.345	0.020	1
4745	B	129	PHE	HE2	7.345	0.020	1
4746	D	329	PHE	HE2	7.345	0.020	1
4747	B	129	PHE	C	175.624	0.1	1
4748	D	329	PHE	C	175.624	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4749	B	129	PHE	CA	58.039	0.1	1
4750	D	329	PHE	CA	58.039	0.1	1
4751	B	129	PHE	CB	40.055	0.1	1
4752	D	329	PHE	CB	40.055	0.1	1
4753	B	129	PHE	CD1	132.047	0.1	1
4754	D	329	PHE	CD1	132.047	0.1	1
4755	B	129	PHE	CE1	132.047	0.1	1
4756	D	329	PHE	CE1	132.047	0.1	1
4757	B	129	PHE	N	118.994	0.1	1
4758	D	329	PHE	N	118.994	0.1	1
4759	B	130	ARG	H	8.042	0.020	1
4760	D	330	ARG	H	8.042	0.020	1
4761	B	130	ARG	HA	4.332	0.020	1
4762	D	330	ARG	HA	4.332	0.020	1
4763	B	130	ARG	HB2	1.823	0.020	2
4764	D	330	ARG	HB2	1.823	0.020	2
4765	B	130	ARG	HB3	1.720	0.020	2
4766	D	330	ARG	HB3	1.720	0.020	2
4767	B	130	ARG	HD2	3.192	0.020	2
4768	D	330	ARG	HD2	3.192	0.020	2
4769	B	130	ARG	HD3	3.192	0.020	2
4770	D	330	ARG	HD3	3.192	0.020	2
4771	B	130	ARG	HG2	1.576	0.001	2
4772	D	330	ARG	HG2	1.576	0.001	2
4773	B	130	ARG	HG3	1.576	0.001	2
4774	D	330	ARG	HG3	1.576	0.001	2
4775	B	130	ARG	C	175.875	0.1	1
4776	D	330	ARG	C	175.875	0.1	1
4777	B	130	ARG	CA	56.154	0.1	1
4778	D	330	ARG	CA	56.154	0.1	1
4779	B	130	ARG	CB	31.643	0.1	1
4780	D	330	ARG	CB	31.643	0.1	1
4781	B	130	ARG	CD	43.961	0.1	1
4782	D	330	ARG	CD	43.961	0.1	1
4783	B	130	ARG	CG	27.300	0.1	1
4784	D	330	ARG	CG	27.300	0.1	1
4785	B	130	ARG	N	122.929	0.1	1
4786	D	330	ARG	N	122.929	0.1	1
4787	B	131	GLU	H	8.389	0.020	1
4788	D	331	GLU	H	8.389	0.020	1
4789	B	131	GLU	HA	4.276	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4790	D	331	GLU	HA	4.276	0.020	1
4791	B	131	GLU	HB2	2.084	0.020	2
4792	D	331	GLU	HB2	2.084	0.020	2
4793	B	131	GLU	HB3	1.988	0.020	2
4794	D	331	GLU	HB3	1.988	0.020	2
4795	B	131	GLU	HG2	2.303	0.020	2
4796	D	331	GLU	HG2	2.303	0.020	2
4797	B	131	GLU	HG3	2.303	0.020	2
4798	D	331	GLU	HG3	2.303	0.020	2
4799	B	131	GLU	C	176.766	0.1	1
4800	D	331	GLU	C	176.766	0.1	1
4801	B	131	GLU	CA	57.285	0.1	1
4802	D	331	GLU	CA	57.285	0.1	1
4803	B	131	GLU	CB	30.512	0.1	1
4804	D	331	GLU	CB	30.512	0.1	1
4805	B	131	GLU	CG	36.797	0.1	1
4806	D	331	GLU	CG	36.797	0.1	1
4807	B	131	GLU	N	122.719	0.1	1
4808	D	331	GLU	N	122.719	0.1	1
4809	B	132	GLU	H	8.502	0.020	1
4810	D	332	GLU	H	8.502	0.020	1
4811	B	132	GLU	HA	4.275	0.020	1
4812	D	332	GLU	HA	4.275	0.020	1
4813	B	132	GLU	HB2	2.079	0.020	2
4814	D	332	GLU	HB2	2.079	0.020	2
4815	B	132	GLU	HB3	1.974	0.020	2
4816	D	332	GLU	HB3	1.974	0.020	2
4817	B	132	GLU	HG2	2.290	0.002	2
4818	D	332	GLU	HG2	2.290	0.002	2
4819	B	132	GLU	HG3	2.290	0.002	2
4820	D	332	GLU	HG3	2.290	0.002	2
4821	B	132	GLU	C	176.560	0.1	1
4822	D	332	GLU	C	176.560	0.1	1
4823	B	132	GLU	CA	57.400	0.1	1
4824	D	332	GLU	CA	57.400	0.1	1
4825	B	132	GLU	CB	30.526	0.040	1
4826	D	332	GLU	CB	30.526	0.040	1
4827	B	132	GLU	CG	36.797	0.1	1
4828	D	332	GLU	CG	36.797	0.1	1
4829	B	132	GLU	N	122.122	0.1	1
4830	D	332	GLU	N	122.122	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4831	B	133	ASN	H	8.362	0.020	1
4832	D	333	ASN	H	8.362	0.020	1
4833	B	133	ASN	HA	4.693	0.020	1
4834	D	333	ASN	HA	4.693	0.020	1
4835	B	133	ASN	HB2	2.846	0.020	2
4836	D	333	ASN	HB2	2.846	0.020	2
4837	B	133	ASN	HB3	2.776	0.020	2
4838	D	333	ASN	HB3	2.776	0.020	2
4839	B	133	ASN	C	175.258	0.1	1
4840	D	333	ASN	C	175.258	0.1	1
4841	B	133	ASN	CA	53.765	0.1	1
4842	D	333	ASN	CA	53.765	0.1	1
4843	B	133	ASN	CB	39.562	0.1	1
4844	D	333	ASN	CB	39.562	0.1	1
4845	B	133	ASN	N	119.552	0.1	1
4846	D	333	ASN	N	119.552	0.1	1
4847	B	134	ALA	H	8.155	0.020	1
4848	D	334	ALA	H	8.155	0.020	1
4849	B	134	ALA	HA	4.289	0.020	1
4850	D	334	ALA	HA	4.289	0.020	1
4851	B	134	ALA	HB1	1.326	0.020	1
4852	D	334	ALA	HB1	1.326	0.020	1
4853	B	134	ALA	HB2	1.326	0.020	1
4854	D	334	ALA	HB2	1.326	0.020	1
4855	B	134	ALA	HB3	1.326	0.020	1
4856	D	334	ALA	HB3	1.326	0.020	1
4857	B	134	ALA	C	177.520	0.1	1
4858	D	334	ALA	C	177.520	0.1	1
4859	B	134	ALA	CA	52.873	0.1	1
4860	D	334	ALA	CA	52.873	0.1	1
4861	B	134	ALA	CB	19.703	0.1	1
4862	D	334	ALA	CB	19.703	0.1	1
4863	B	134	ALA	N	124.376	0.1	1
4864	D	334	ALA	N	124.376	0.1	1
4865	B	135	ASN	H	8.210	0.020	1
4866	D	335	ASN	H	8.210	0.020	1
4867	B	135	ASN	HA	4.694	0.020	1
4868	D	335	ASN	HA	4.694	0.020	1
4869	B	135	ASN	HB2	2.773	0.020	2
4870	D	335	ASN	HB2	2.773	0.020	2
4871	B	135	ASN	HB3	2.706	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4872	D	335	ASN	HB3	2.706	0.020	2
4873	B	135	ASN	C	175.144	0.1	1
4874	D	335	ASN	C	175.144	0.1	1
4875	B	135	ASN	CA	53.640	0.1	1
4876	D	335	ASN	CA	53.640	0.1	1
4877	B	135	ASN	CB	39.311	0.1	1
4878	D	335	ASN	CB	39.311	0.1	1
4879	B	135	ASN	N	117.103	0.1	1
4880	D	335	ASN	N	117.103	0.1	1
4881	B	136	PHE	H	7.997	0.020	1
4882	D	336	PHE	H	7.997	0.020	1
4883	B	136	PHE	HA	4.659	0.020	1
4884	D	336	PHE	HA	4.659	0.020	1
4885	B	136	PHE	HB2	3.219	0.020	2
4886	D	336	PHE	HB2	3.219	0.020	2
4887	B	136	PHE	HB3	3.055	0.020	2
4888	D	336	PHE	HB3	3.055	0.020	2
4889	B	136	PHE	HD1	7.267	0.020	1
4890	D	336	PHE	HD1	7.267	0.020	1
4891	B	136	PHE	HD2	7.267	0.020	1
4892	D	336	PHE	HD2	7.267	0.020	1
4893	B	136	PHE	HE1	7.379	0.020	1
4894	D	336	PHE	HE1	7.379	0.020	1
4895	B	136	PHE	HE2	7.379	0.020	1
4896	D	336	PHE	HE2	7.379	0.020	1
4897	B	136	PHE	C	175.601	0.1	1
4898	D	336	PHE	C	175.601	0.1	1
4899	B	136	PHE	CA	58.165	0.1	1
4900	D	336	PHE	CA	58.165	0.1	1
4901	B	136	PHE	CB	39.939	0.1	1
4902	D	336	PHE	CB	39.939	0.1	1
4903	B	136	PHE	CD1	132.047	0.1	1
4904	D	336	PHE	CD1	132.047	0.1	1
4905	B	136	PHE	CE1	132.047	0.1	1
4906	D	336	PHE	CE1	132.047	0.1	1
4907	B	136	PHE	N	120.229	0.1	1
4908	D	336	PHE	N	120.229	0.1	1
4909	B	137	ASN	H	8.272	0.020	1
4910	D	337	ASN	H	8.272	0.020	1
4911	B	137	ASN	HA	4.733	0.020	1
4912	D	337	ASN	HA	4.733	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4913	B	137	ASN	HB2	2.846	0.020	2
4914	D	337	ASN	HB2	2.846	0.020	2
4915	B	137	ASN	HB3	2.709	0.020	2
4916	D	337	ASN	HB3	2.709	0.020	2
4917	B	137	ASN	C	174.047	0.1	1
4918	D	337	ASN	C	174.047	0.1	1
4919	B	137	ASN	CA	53.891	0.1	1
4920	D	337	ASN	CA	53.891	0.1	1
4921	B	137	ASN	CB	39.688	0.1	1
4922	D	337	ASN	CB	39.688	0.1	1
4923	B	137	ASN	N	120.594	0.1	1
4924	D	337	ASN	N	120.594	0.1	1
4925	B	138	LYS	H	7.697	0.020	1
4926	D	338	LYS	H	7.697	0.020	1
4927	B	138	LYS	HA	4.174	0.020	1
4928	D	338	LYS	HA	4.174	0.020	1
4929	B	138	LYS	HB2	1.856	0.020	2
4930	D	338	LYS	HB2	1.856	0.020	2
4931	B	138	LYS	HB3	1.726	0.020	2
4932	D	338	LYS	HB3	1.726	0.020	2
4933	B	138	LYS	HD2	1.705	0.020	2
4934	D	338	LYS	HD2	1.705	0.020	2
4935	B	138	LYS	HD3	1.705	0.020	2
4936	D	338	LYS	HD3	1.705	0.020	2
4937	B	138	LYS	HE2	3.020	0.020	2
4938	D	338	LYS	HE2	3.020	0.020	2
4939	B	138	LYS	HE3	3.020	0.020	2
4940	D	338	LYS	HE3	3.020	0.020	2
4941	B	138	LYS	HG2	1.413	0.020	2
4942	D	338	LYS	HG2	1.413	0.020	2
4943	B	138	LYS	HG3	1.413	0.020	2
4944	D	338	LYS	HG3	1.413	0.020	2
4945	B	138	LYS	CA	58.046	0.1	1
4946	D	338	LYS	CA	58.046	0.1	1
4947	B	138	LYS	CB	34.102	0.1	1
4948	D	338	LYS	CB	34.102	0.1	1
4949	B	138	LYS	CD	29.896	0.1	1
4950	D	338	LYS	CD	29.896	0.1	1
4951	B	138	LYS	CE	42.838	0.1	1
4952	D	338	LYS	CE	42.838	0.1	1
4953	B	138	LYS	CG	25.042	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4954	D	338	LYS	CG	25.042	0.1	1
4955	B	138	LYS	N	126.523	0.1	1
4956	D	338	LYS	N	126.523	0.1	1

6.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	202	-0.47 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	194	-0.42 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	188	-0.27 ± 0.08	None needed (< 0.5 ppm)
^{15}N	194	-0.51 ± 0.45	None needed (imprecise)

6.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1615 atoms were assigned a chemical shift out of a possible 1849. 18 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	672/694 (97%)	272/276 (99%)	266/284 (94%)	134/134 (100%)
Sidechain	861/1039 (83%)	547/618 (89%)	300/363 (83%)	14/58 (24%)
Aromatic	82/116 (71%)	48/60 (80%)	32/46 (70%)	2/10 (20%)
Overall	1615/1849 (87%)	867/954 (91%)	598/693 (86%)	150/202 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 2256 atoms were assigned a chemical shift out of a possible 2694. 18 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	970/1030 (94%)	392/410 (96%)	386/420 (92%)	192/200 (96%)
Sidechain	1150/1472 (78%)	736/874 (84%)	398/514 (77%)	16/84 (19%)
Aromatic	136/192 (71%)	84/100 (84%)	50/82 (61%)	2/10 (20%)
Overall	2256/2694 (84%)	1212/1384 (88%)	834/1016 (82%)	210/294 (71%)

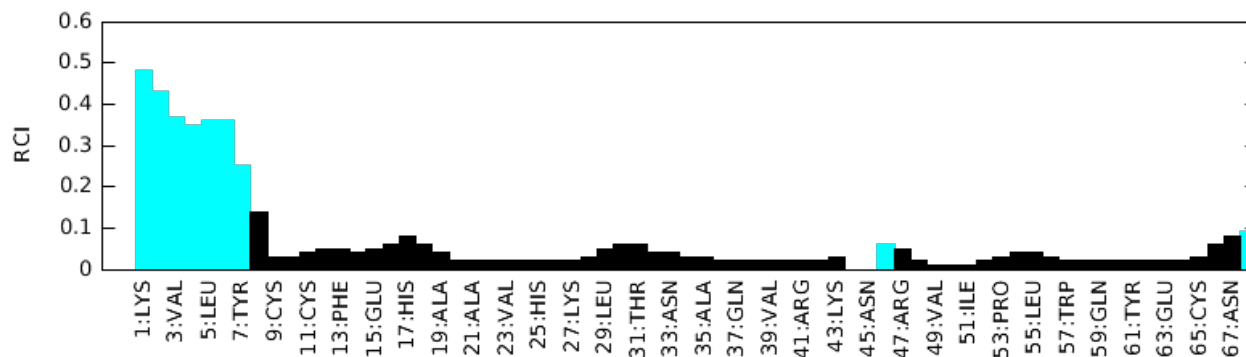
6.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

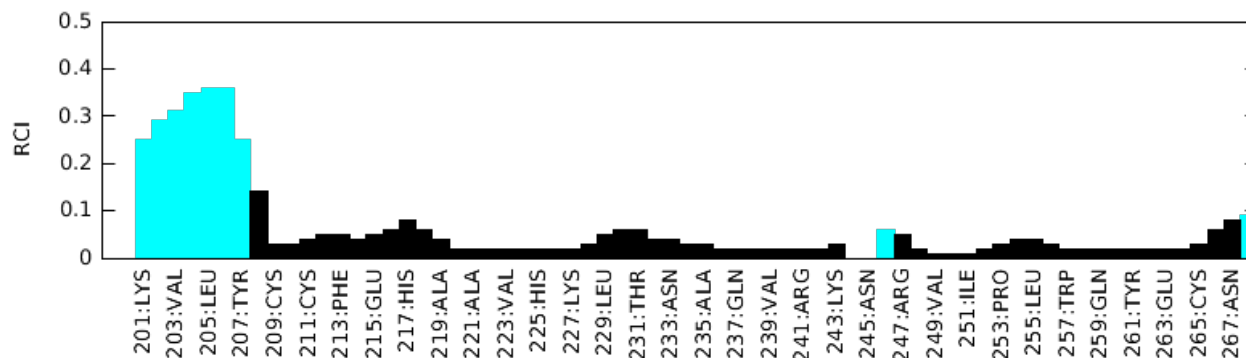
6.1.5 Random Coil Index (RCI) plots [i](#)

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

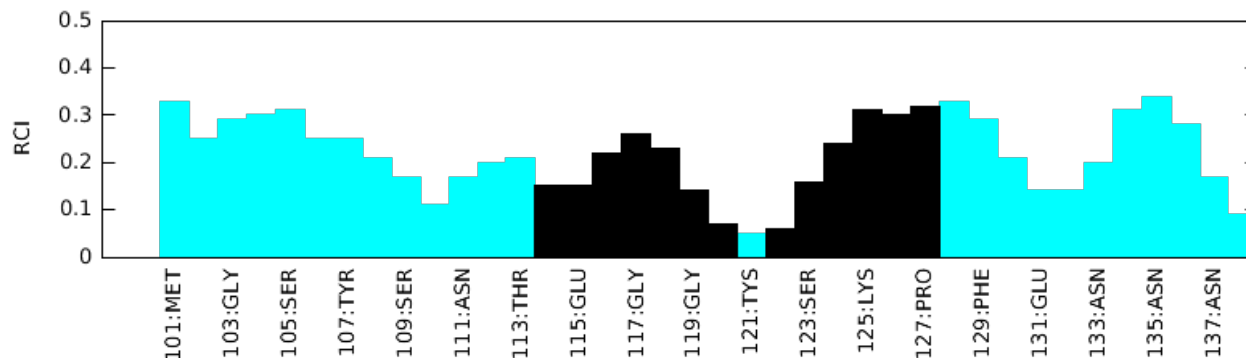
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain D:

