Full wwPDB NMR Structure Validation Report (i)

May 29, 2020 – 07:59 am BST

PDB ID	:	5OVM
Title	:	Solution structure of lipase binding domain LID1 of foldase from Pseudomonas aeruginosa
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Deposited on	:	2017-08-29

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

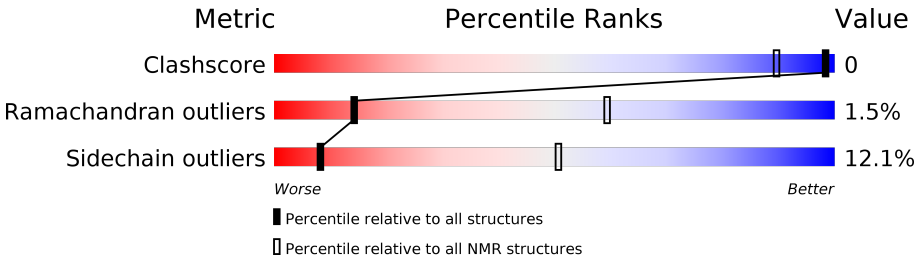
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	89	85% · · 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:67-A:146 (80)	1.09	9

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1291 atoms, of which 641 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipase chaperone.

Mol	Chain	Residues	Atoms						Trace
1	A	82	Total	C	H	N	O	S	0
			1291	411	641	112	126	1	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	MET	-	initiating methionine	UNP Q01725
A	59	GLY	-	expression tag	UNP Q01725
A	60	HIS	-	expression tag	UNP Q01725
A	61	HIS	-	expression tag	UNP Q01725
A	62	HIS	-	expression tag	UNP Q01725
A	63	HIS	-	expression tag	UNP Q01725
A	64	HIS	-	expression tag	UNP Q01725
A	65	HIS	-	expression tag	UNP Q01725

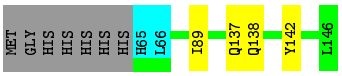
4 Residue-property plots (i)

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: Lipase chaperone

Chain A:



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

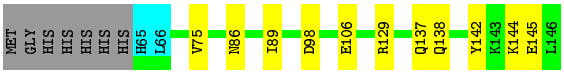
- Molecule 1: Lipase chaperone

Chain A:

4.2.2 Score per residue for model 2

- Molecule 1: Lipase chaperone

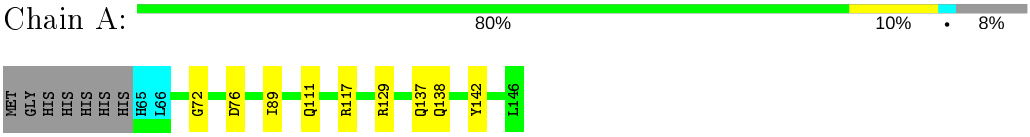
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Lipase chaperone

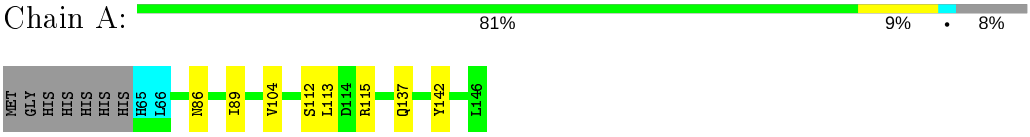
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Lipase chaperone

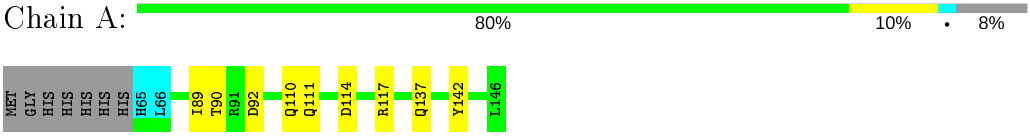
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Lipase chaperone

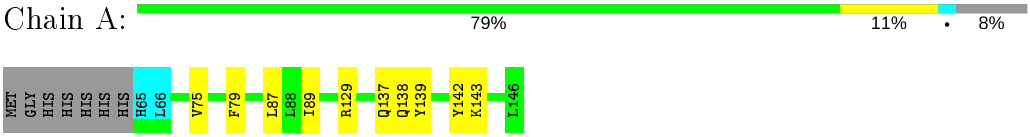
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Lipase chaperone

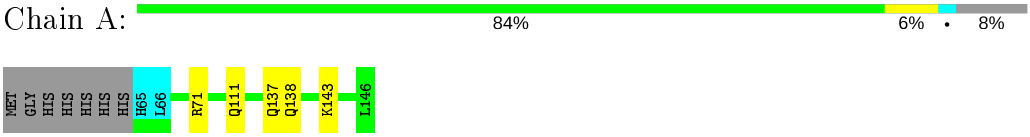
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Lipase chaperone

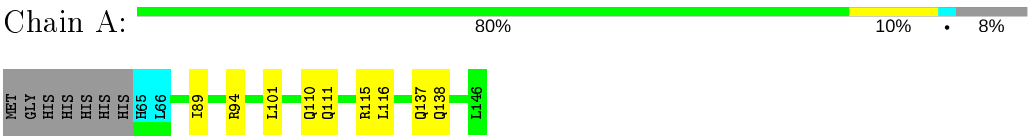
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Lipase chaperone

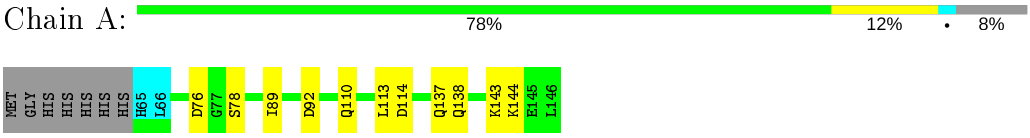
Chain A:



4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: Lipase chaperone

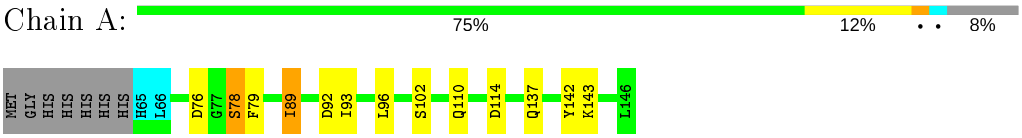
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Lipase chaperone

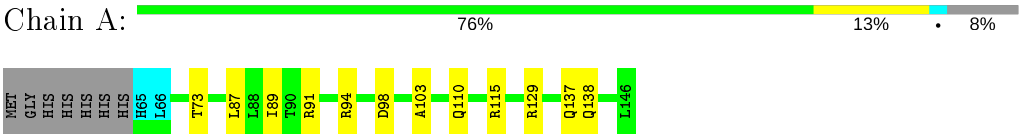
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Lipase chaperone

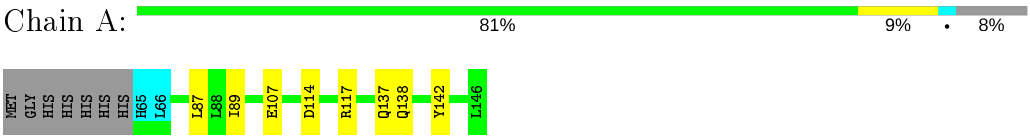
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Lipase chaperone

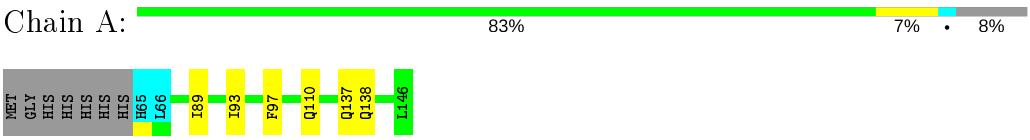
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Lipase chaperone

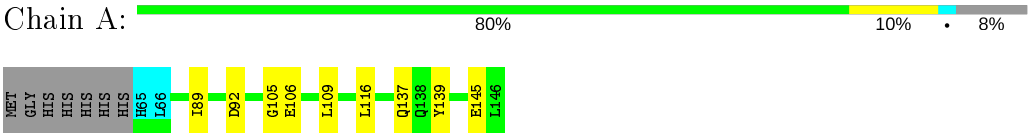
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Lipase chaperone

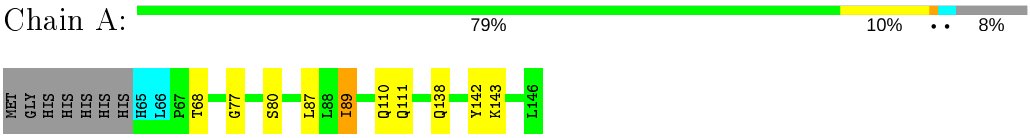
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Lipase chaperone

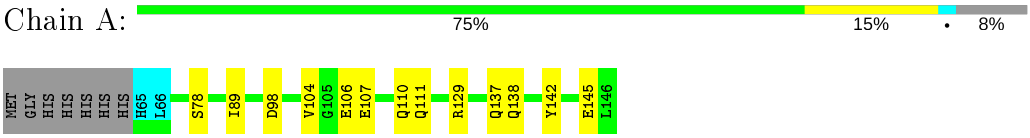
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Lipase chaperone

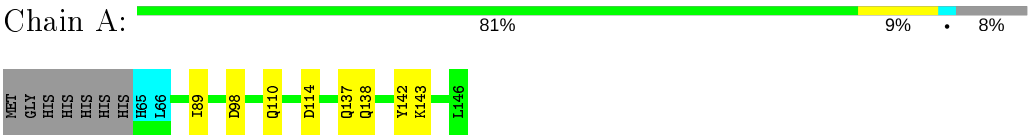
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Lipase chaperone

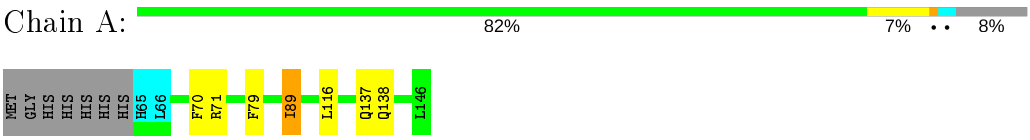
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Lipase chaperone

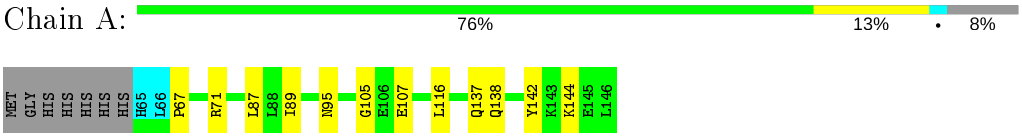
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Lipase chaperone

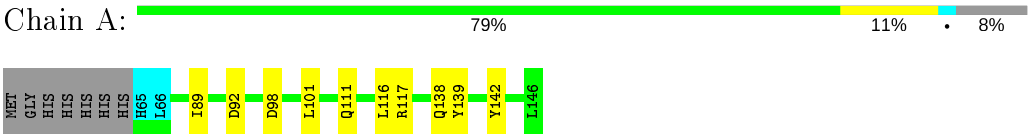
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Lipase chaperone

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 20 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
CYANA	structure calculation	
Amber	geometry optimization	
Amber	refinement	

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	929
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	929
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	632	623	623	0±1
All	All	12640	12460	12460	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ASP:OD1	1:A:117:ARG:NE	0.59	2.32	12	1
1:A:79:PHE:CE1	1:A:96:LEU:HD13	0.48	2.43	10	1
1:A:93:ILE:HA	1:A:96:LEU:HD12	0.47	1.87	10	1
1:A:93:ILE:HG22	1:A:97:PHE:CE1	0.46	2.45	13	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	79/89 (89%)	72±2 (91±3%)	6±2 (8±2%)	1±1 (2±1%)	14 59
All	All	1580/1780 (89%)	1433 (91%)	123 (8%)	24 (2%)	14 59

All 15 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	78	SER	3
1	A	89	ILE	3
1	A	105	GLY	2
1	A	75	VAL	2
1	A	106	GLU	2
1	A	104	VAL	2
1	A	70	PHE	2
1	A	67	PRO	1
1	A	77	GLY	1
1	A	80	SER	1
1	A	103	ALA	1
1	A	144	LYS	1
1	A	68	THR	1
1	A	72	GLY	1
1	A	76	ASP	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	67/75 (89%)	59±2 (88±3%)	8±2 (12±3%)	8 51
All	All	1340/1500 (89%)	1178 (88%)	162 (12%)	8 51

All 35 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	89	ILE	19
1	A	137	GLN	18
1	A	138	GLN	16

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Mol	Chain	Res	Type	Models (Total)
1	A	142	TYR	13
1	A	110	GLN	9
1	A	143	LYS	7
1	A	111	GLN	7
1	A	116	LEU	6
1	A	98	ASP	5
1	A	129	ARG	5
1	A	92	ASP	5
1	A	87	LEU	5
1	A	114	ASP	4
1	A	94	ARG	3
1	A	107	GLU	3
1	A	115	ARG	3
1	A	139	TYR	3
1	A	117	ARG	3
1	A	71	ARG	3
1	A	145	GLU	3
1	A	79	PHE	2
1	A	113	LEU	2
1	A	106	GLU	2
1	A	76	ASP	2
1	A	86	ASN	2
1	A	144	LYS	2
1	A	101	LEU	2
1	A	95	ASN	1
1	A	102	SER	1
1	A	91	ARG	1
1	A	73	THR	1
1	A	112	SER	1
1	A	90	THR	1
1	A	109	LEU	1
1	A	78	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *MD1_3.1_6.str*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	929
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	929
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Residue not found in structure. All 929 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	37	ARG	HD3	3.137	0.02	2
A	11	THR	HA	4.655	0.02	1
A	77	ALA	HA	4.275	0.02	1
A	76	LEU	HD22	0.919	0.02	2
A	52	LEU	CD1	25.353	0.3	1
A	44	LEU	HD13	0.809	0.02	2
A	24	VAL	C	176.392	0.3	1
A	42	TYR	HA	4.293	0.02	1
A	54	GLN	N	116.726	0.3	1
A	14	ARG	HD2	3.151	0.02	2
A	83	ILE	HG21	0.94	0.02	1
A	59	LEU	HD21	0.662	0.02	2
A	34	ARG	CA	57.272	0.3	1
A	18	VAL	CA	62.3	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	37	ARG	CD	43.313	0.3	1
A	76	LEU	CA	58.195	0.3	1
A	74	GLN	C	179.268	0.3	1
A	14	ARG	HG3	1.588	0.02	2
A	51	PRO	CD	50.715	0.3	1
A	9	LEU	CD2	23.42	0.3	1
A	37	ARG	CB	29.416	0.3	1
A	74	GLN	NE2	108.588	0.3	1
A	30	LEU	HG	0.797	0.02	1
A	9	LEU	H	8.154	0.02	1
A	51	PRO	CB	32.071	0.3	1
A	88	GLU	HG3	2.278	0.02	2
A	54	GLN	CG	34.51	0.3	1
A	42	TYR	HE1	7.038	0.02	1
A	42	TYR	HB3	3.127	0.02	2
A	47	VAL	HB	2.092	0.02	1
A	43	PHE	HE1	6.559	0.02	1
A	32	ILE	HG22	0.869	0.02	1
A	24	VAL	HG12	0.808	0.02	2
A	62	TYR	HB2	3.082	0.02	2
A	24	VAL	HB	1.874	0.02	1
A	24	VAL	CA	59.374	0.3	1
A	52	LEU	CB	41.846	0.3	1
A	88	GLU	HB2	1.906	0.02	2
A	44	LEU	CA	55.856	0.3	1
A	76	LEU	CG	26.784	0.3	1
A	29	ASN	HB3	2.84	0.02	2
A	67	LEU	HG	1.161	0.02	1
A	67	LEU	HA	4.71	0.02	1
A	63	ILE	HD11	0.852	0.02	1
A	36	ILE	HD12	1.091	0.02	1
A	49	GLU	N	121.045	0.3	1
A	51	PRO	HG2	1.96	0.02	2
A	32	ILE	CD1	12.08	0.3	1
A	62	TYR	C	177.197	0.3	1
A	54	GLN	HE22	6.904	0.02	2
A	18	VAL	HG12	0.719	0.02	2
A	61	ALA	HB3	1.545	0.02	1
A	69	GLU	HA	4.829	0.02	1
A	60	ARG	CA	60.616	0.3	1
A	36	ILE	HA	3.544	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	34	ARG	HG2	1.692	0.02	2
A	86	LYS	N	120.255	0.3	1
A	13	PHE	HE1	7.037	0.02	1
A	78	LEU	HD11	0.877	0.02	2
A	59	LEU	HD13	0.634	0.02	2
A	60	ARG	CB	30.121	0.3	1
A	42	TYR	CB	38.217	0.3	1
A	18	VAL	H	8.019	0.02	1
A	31	LEU	HD11	0.802	0.02	2
A	67	LEU	HD21	0.633	0.02	2
A	46	ALA	CB	19.095	0.3	1
A	55	SER	HB3	4.114	0.02	2
A	65	ALA	HB1	1.485	0.02	1
A	36	ILE	HG13	1.64	0.02	2
A	18	VAL	CB	32.423	0.3	1
A	75	ALA	CA	55.437	0.3	1
A	13	PHE	HD1	7.326	0.02	1
A	44	LEU	C	177.783	0.3	1
A	56	LEU	HB3	1.858	0.02	2
A	78	LEU	HD12	0.877	0.02	2
A	39	LEU	HD23	0.563	0.02	2
A	60	ARG	HB3	1.85	0.02	2
A	27	SER	C	174.044	0.3	1
A	85	TYR	HB3	3.125	0.02	2
A	88	GLU	C	175.521	0.3	1
A	73	GLY	H	8.958	0.02	1
A	68	GLN	N	119.921	0.3	1
A	39	LEU	HD12	0.636	0.02	2
A	85	TYR	CA	59.135	0.3	1
A	25	ASP	CB	41.595	0.3	1
A	60	ARG	CG	28.87	0.3	1
A	47	VAL	HG12	0.92	0.02	2
A	72	ARG	H	8.104	0.02	1
A	72	ARG	CB	30.447	0.3	1
A	89	LEU	N	128.156	0.3	1
A	20	GLY	CA	45.046	0.3	1
A	39	LEU	CB	41.68	0.3	1
A	30	LEU	N	121.788	0.3	1
A	63	ILE	CD1	14.47	0.3	1
A	44	LEU	CD2	23.256	0.3	1
A	54	GLN	HB2	2.161	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	55	SER	CA	61.886	0.3	1
A	59	LEU	HD23	0.662	0.02	2
A	30	LEU	CB	44.09	0.3	1
A	40	PHE	HZ	7.131	0.02	1
A	30	LEU	HD11	0.977	0.02	2
A	11	THR	HG23	1.184	0.02	1
A	82	TYR	N	120.239	0.3	1
A	89	LEU	CA	56.726	0.3	1
A	89	LEU	HB2	1.57	0.02	2
A	62	TYR	HD2	7.0	0.02	1
A	70	PRO	HB3	2.344	0.02	2
A	58	ARG	CD	43.421	0.3	1
A	40	PHE	HE1	6.926	0.02	1
A	12	SER	C	170.821	0.3	1
A	83	ILE	HB	1.99	0.02	1
A	59	LEU	C	178.126	0.3	1
A	78	LEU	HB3	1.84	0.02	2
A	19	ASP	HA	4.574	0.02	1
A	56	LEU	CD2	23.374	0.3	1
A	76	LEU	HD12	0.864	0.02	2
A	89	LEU	CB	43.389	0.3	1
A	86	LYS	HB3	1.738	0.02	2
A	89	LEU	CD2	23.502	0.3	1
A	24	VAL	HG21	0.848	0.02	2
A	76	LEU	HD11	0.864	0.02	2
A	74	GLN	CA	58.783	0.3	1
A	86	LYS	CD	28.792	0.3	1
A	18	VAL	HG23	0.641	0.02	2
A	72	ARG	C	177.061	0.3	1
A	52	LEU	HD21	0.915	0.02	2
A	33	THR	HA	4.245	0.02	1
A	66	GLU	HB3	2.066	0.02	2
A	42	TYR	HE2	7.038	0.02	1
A	40	PHE	HB2	2.691	0.02	2
A	72	ARG	CD	44.037	0.3	1
A	53	GLN	CG	33.29	0.3	1
A	13	PHE	C	175.725	0.3	1
A	32	ILE	HD11	0.843	0.02	1
A	81	GLN	C	178.141	0.3	1
A	62	TYR	HE1	6.753	0.02	1
A	26	ALA	H	8.319	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	31	LEU	HD22	0.89	0.02	2
A	13	PHE	H	8.342	0.02	1
A	56	LEU	H	8.545	0.02	1
A	58	ARG	HD2	3.362	0.02	2
A	38	ASN	HA	4.455	0.02	1
A	60	ARG	H	8.677	0.02	1
A	12	SER	HB3	3.602	0.02	2
A	41	ASP	C	178.967	0.3	1
A	68	GLN	C	177.686	0.3	1
A	89	LEU	HD11	0.869	0.02	2
A	43	PHE	HE2	6.559	0.02	1
A	19	ASP	C	173.175	0.3	1
A	63	ILE	CG2	18.896	0.3	1
A	52	LEU	HD12	0.975	0.02	2
A	9	LEU	CB	41.855	0.3	1
A	89	LEU	H	7.658	0.02	1
A	80	GLN	C	177.682	0.3	1
A	46	ALA	HB3	1.249	0.02	1
A	8	HIS	HB3	2.977	0.02	2
A	66	GLU	CG	35.95	0.3	1
A	82	TYR	HB2	3.117	0.02	2
A	9	LEU	N	124.342	0.3	1
A	89	LEU	HD13	0.869	0.02	2
A	9	LEU	HD12	0.796	0.02	2
A	9	LEU	HD21	0.784	0.02	2
A	74	GLN	HA	4.126	0.02	1
A	31	LEU	C	176.127	0.3	1
A	31	LEU	CD1	25.205	0.3	1
A	67	LEU	HD12	0.189	0.02	2
A	83	ILE	HA	3.713	0.02	1
A	64	ALA	HB2	1.42	0.02	1
A	22	PHE	HB2	2.898	0.02	2
A	66	GLU	HG2	1.726	0.02	2
A	79	MET	H	8.484	0.02	1
A	47	VAL	HG22	0.947	0.02	2
A	89	LEU	CG	26.924	0.3	1
A	75	ALA	HA	4.011	0.02	1
A	30	LEU	HB2	1.468	0.02	2
A	36	ILE	CA	64.262	0.3	1
A	86	LYS	HG2	1.284	0.02	2
A	76	LEU	HD23	0.919	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	85	TYR	C	176.819	0.3	1
A	48	GLY	HA3	4.091	0.02	2
A	81	GLN	HA	4.152	0.02	1
A	81	GLN	HE21	7.368	0.02	2
A	31	LEU	HD12	0.802	0.02	2
A	38	ASN	H	7.686	0.02	1
A	87	LYS	HE3	2.996	0.02	2
A	55	SER	C	179.073	0.3	1
A	51	PRO	CG	27.976	0.3	1
A	51	PRO	HB3	2.251	0.02	2
A	58	ARG	N	121.061	0.3	1
A	76	LEU	HD13	0.864	0.02	2
A	53	GLN	CD	177.619	0.3	1
A	45	SER	HA	4.455	0.02	1
A	61	ALA	C	180.187	0.3	1
A	79	MET	HG3	2.266	0.02	2
A	60	ARG	C	178.704	0.3	1
A	83	ILE	CD1	13.811	0.3	1
A	42	TYR	HB2	3.127	0.02	2
A	57	ASP	H	8.264	0.02	1
A	87	LYS	CA	57.029	0.3	1
A	32	ILE	HG21	0.869	0.02	1
A	24	VAL	HG13	0.808	0.02	2
A	63	ILE	C	176.896	0.3	1
A	71	ALA	HB1	1.584	0.02	1
A	44	LEU	CB	41.505	0.3	1
A	49	GLU	CA	57.451	0.3	1
A	29	ASN	HB2	2.651	0.02	2
A	39	LEU	CD2	24.348	0.3	1
A	28	GLY	HA3	4.221	0.02	2
A	56	LEU	HG	1.411	0.02	1
A	39	LEU	H	7.714	0.02	1
A	63	ILE	HD13	0.852	0.02	1
A	49	GLU	CG	36.112	0.3	1
A	51	PRO	HG3	2.039	0.02	2
A	68	GLN	HE22	6.825	0.02	2
A	22	PHE	CB	39.137	0.3	1
A	44	LEU	N	117.048	0.3	1
A	58	ARG	HG2	1.691	0.02	2
A	38	ASN	ND2	111.77	0.3	1
A	38	ASN	HD22	6.83	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	61	ALA	HB2	1.545	0.02	1
A	81	GLN	CB	28.727	0.3	1
A	36	ILE	HB	1.843	0.02	1
A	34	ARG	HG3	1.692	0.02	2
A	34	ARG	HA	4.049	0.02	1
A	13	PHE	HE2	7.037	0.02	1
A	38	ASN	HB3	2.929	0.02	2
A	81	GLN	N	117.49	0.3	1
A	63	ILE	HG22	0.847	0.02	1
A	87	LYS	CB	32.967	0.3	1
A	82	TYR	H	8.244	0.02	1
A	67	LEU	HD22	0.633	0.02	2
A	72	ARG	HA	3.436	0.02	1
A	44	LEU	CG	26.743	0.3	1
A	82	TYR	HE2	7.001	0.02	1
A	83	ILE	H	8.039	0.02	1
A	14	ARG	HB3	1.873	0.02	2
A	32	ILE	CG2	17.916	0.3	1
A	87	LYS	N	119.831	0.3	1
A	10	PRO	HD2	3.474	0.02	2
A	39	LEU	HD22	0.563	0.02	2
A	34	ARG	HB3	1.886	0.02	2
A	30	LEU	C	176.668	0.3	1
A	85	TYR	N	119.82	0.3	1
A	63	ILE	CB	38.362	0.3	1
A	83	ILE	HG13	1.297	0.02	2
A	39	LEU	HD13	0.636	0.02	2
A	49	GLU	HG3	2.253	0.02	2
A	63	ILE	N	118.832	0.3	1
A	26	ALA	CA	54.454	0.3	1
A	45	SER	N	114.293	0.3	1
A	10	PRO	CA	63.263	0.3	1
A	30	LEU	CG	26.119	0.3	1
A	59	LEU	CG	26.674	0.3	1
A	87	LYS	HA	4.157	0.02	1
A	45	SER	CB	63.835	0.3	1
A	44	LEU	CD1	25.455	0.3	1
A	54	GLN	HB3	2.223	0.02	2
A	59	LEU	HD22	0.662	0.02	2
A	54	GLN	HA	4.244	0.02	1
A	59	LEU	CA	57.658	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	79	MET	HB2	1.812	0.02	2
A	88	GLU	CB	30.26	0.3	1
A	39	LEU	C	178.767	0.3	1
A	68	GLN	CD	178.077	0.3	1
A	62	TYR	HD1	7.0	0.02	1
A	30	LEU	HD21	1.021	0.02	2
A	86	LYS	HE3	2.93	0.02	2
A	40	PHE	HE2	6.926	0.02	1
A	53	GLN	NE2	114.127	0.3	1
A	32	ILE	C	176.04	0.3	1
A	86	LYS	HG3	1.284	0.02	2
A	24	VAL	CG2	19.439	0.3	1
A	18	VAL	HG11	0.719	0.02	2
A	18	VAL	CG2	20.916	0.3	1
A	26	ALA	C	176.246	0.3	1
A	67	LEU	CA	53.441	0.3	1
A	78	LEU	N	120.311	0.3	1
A	72	ARG	HB3	1.334	0.02	2
A	52	LEU	HD22	0.915	0.02	2
A	23	SER	HB3	3.878	0.02	2
A	59	LEU	CD2	21.945	0.3	1
A	76	LEU	CD2	23.219	0.3	1
A	72	ARG	HB2	1.193	0.02	2
A	41	ASP	N	118.538	0.3	1
A	57	ASP	HB2	2.68	0.02	2
A	81	GLN	HB2	2.21	0.02	2
A	67	LEU	CB	44.547	0.3	1
A	30	LEU	CD2	23.842	0.3	1
A	86	LYS	CG	24.485	0.3	1
A	62	TYR	HE2	6.753	0.02	1
A	59	LEU	HD12	0.634	0.02	2
A	26	ALA	HA	4.186	0.02	1
A	38	ASN	N	115.866	0.3	1
A	83	ILE	CA	63.887	0.3	1
A	72	ARG	N	118.361	0.3	1
A	82	TYR	HA	4.309	0.02	1
A	34	ARG	HD3	3.204	0.02	2
A	87	LYS	H	7.825	0.02	1
A	12	SER	HB2	3.602	0.02	2
A	38	ASN	CB	37.664	0.3	1
A	38	ASN	HB2	2.797	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	72	ARG	CG	25.139	0.3	1
A	52	LEU	C	175.629	0.3	1
A	74	GLN	HB2	1.912	0.02	2
A	14	ARG	CD	43.418	0.3	1
A	63	ILE	HG23	0.847	0.02	1
A	8	HIS	CA	56.304	0.3	1
A	59	LEU	HA	3.579	0.02	1
A	8	HIS	HB2	2.977	0.02	2
A	64	ALA	HA	3.879	0.02	1
A	83	ILE	CB	37.952	0.3	1
A	83	ILE	CG2	17.64	0.3	1
A	57	ASP	HA	4.441	0.02	1
A	26	ALA	HB1	1.492	0.02	1
A	87	LYS	HB3	1.849	0.02	2
A	86	LYS	HD2	1.561	0.02	2
A	9	LEU	HD13	0.796	0.02	2
A	89	LEU	HB3	1.57	0.02	2
A	56	LEU	HD11	0.853	0.02	2
A	40	PHE	H	8.113	0.02	1
A	78	LEU	CD1	25.101	0.3	1
A	77	ALA	HB3	1.547	0.02	1
A	43	PHE	C	177.984	0.3	1
A	84	ASP	C	177.961	0.3	1
A	44	LEU	H	8.365	0.02	1
A	56	LEU	HD21	0.92	0.02	2
A	71	ALA	CA	55.668	0.3	1
A	32	ILE	N	124.151	0.3	1
A	47	VAL	HG23	0.947	0.02	2
A	77	ALA	HB1	1.547	0.02	1
A	84	ASP	HB2	2.655	0.02	2
A	14	ARG	HG2	1.588	0.02	2
A	55	SER	HB2	4.114	0.02	2
A	69	GLU	N	120.81	0.3	1
A	52	LEU	HD11	0.975	0.02	2
A	28	GLY	H	8.169	0.02	1
A	62	TYR	HA	4.256	0.02	1
A	81	GLN	NE2	110.704	0.3	1
A	83	ILE	HG12	1.662	0.02	2
A	77	ALA	H	8.044	0.02	1
A	48	GLY	HA2	3.857	0.02	2
A	34	ARG	CG	26.885	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	31	LEU	HD13	0.802	0.02	2
A	52	LEU	HA	4.235	0.02	1
A	58	ARG	CA	59.966	0.3	1
A	27	SER	H	8.194	0.02	1
A	81	GLN	H	7.852	0.02	1
A	76	LEU	HG	1.876	0.02	1
A	51	PRO	HB2	1.914	0.02	2
A	52	LEU	HG	1.747	0.02	1
A	56	LEU	N	121.267	0.3	1
A	30	LEU	HA	4.287	0.02	1
A	58	ARG	HB3	2.203	0.02	2
A	84	ASP	CA	56.628	0.3	1
A	47	VAL	CA	62.683	0.3	1
A	87	LYS	C	176.548	0.3	1
A	71	ALA	C	178.707	0.3	1
A	56	LEU	CG	26.582	0.3	1
A	63	ILE	HB	1.896	0.02	1
A	88	GLU	CA	56.669	0.3	1
A	29	ASN	HD22	6.949	0.02	2
A	65	ALA	CB	19.385	0.3	1
A	63	ILE	HG12	0.966	0.02	2
A	29	ASN	CB	39.488	0.3	1
A	80	GLN	HA	3.895	0.02	1
A	56	LEU	HD13	0.853	0.02	2
A	86	LYS	CA	56.758	0.3	1
A	52	LEU	HB3	1.854	0.02	2
A	29	ASN	N	118.014	0.3	1
A	56	LEU	HB2	1.681	0.02	2
A	68	GLN	HA	4.516	0.02	1
A	10	PRO	HA	4.474	0.02	1
A	18	VAL	HB	1.849	0.02	1
A	88	GLU	HA	4.297	0.02	1
A	39	LEU	CD1	25.39	0.3	1
A	87	LYS	CE	42.208	0.3	1
A	45	SER	H	7.722	0.02	1
A	89	LEU	HA	4.149	0.02	1
A	22	PHE	CA	57.636	0.3	1
A	31	LEU	CA	54.139	0.3	1
A	58	ARG	HG3	1.691	0.02	2
A	72	ARG	CA	59.88	0.3	1
A	61	ALA	HB1	1.545	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	47	VAL	C	176.803	0.3	1
A	82	TYR	HD1	7.049	0.02	1
A	31	LEU	CG	26.981	0.3	1
A	60	ARG	HG3	1.481	0.02	2
A	32	ILE	HA	4.036	0.02	1
A	46	ALA	HA	4.297	0.02	1
A	59	LEU	HD11	0.634	0.02	2
A	42	TYR	N	120.881	0.3	1
A	81	GLN	HG3	2.463	0.02	2
A	67	LEU	HD23	0.633	0.02	2
A	46	ALA	N	125.117	0.3	1
A	49	GLU	HG2	2.253	0.02	2
A	40	PHE	C	178.024	0.3	1
A	49	GLU	HA	4.242	0.02	1
A	74	GLN	H	7.797	0.02	1
A	81	GLN	HG2	2.463	0.02	2
A	14	ARG	HB2	1.742	0.02	2
A	56	LEU	CA	58.071	0.3	1
A	32	ILE	CG1	27.317	0.3	1
A	57	ASP	CB	40.104	0.3	1
A	10	PRO	HD3	3.719	0.02	2
A	34	ARG	HB2	1.886	0.02	2
A	73	GLY	N	107.959	0.3	1
A	63	ILE	CA	66.146	0.3	1
A	81	GLN	CG	34.188	0.3	1
A	10	PRO	CD	50.507	0.3	1
A	24	VAL	H	8.265	0.02	1
A	25	ASP	N	123.462	0.3	1
A	61	ALA	CA	54.868	0.3	1
A	78	LEU	HD22	0.811	0.02	2
A	10	PRO	CB	32.041	0.3	1
A	39	LEU	N	122.776	0.3	1
A	59	LEU	N	122.565	0.3	1
A	23	SER	CA	57.876	0.3	1
A	13	PHE	HA	4.759	0.02	1
A	71	ALA	HB2	1.584	0.02	1
A	80	GLN	N	117.934	0.3	1
A	31	LEU	H	8.662	0.02	1
A	79	MET	HB3	1.984	0.02	2
A	56	LEU	C	179.224	0.3	1
A	26	ALA	CB	18.548	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	30	LEU	HD13	0.977	0.02	2
A	65	ALA	CA	53.642	0.3	1
A	42	TYR	HD1	6.794	0.02	1
A	48	GLY	CA	45.429	0.3	1
A	33	THR	CA	62.245	0.3	1
A	30	LEU	HD22	1.021	0.02	2
A	86	LYS	HE2	2.93	0.02	2
A	24	VAL	CG1	21.56	0.3	1
A	45	SER	HB2	3.976	0.02	2
A	11	THR	CB	71.835	0.3	1
A	67	LEU	CD2	22.699	0.3	1
A	62	TYR	N	121.856	0.3	1
A	78	LEU	HA	4.177	0.02	1
A	61	ALA	N	120.375	0.3	1
A	68	GLN	CA	53.51	0.3	1
A	85	TYR	H	7.868	0.02	1
A	18	VAL	HG21	0.641	0.02	2
A	80	GLN	HB3	2.213	0.02	2
A	40	PHE	CB	36.544	0.3	1
A	52	LEU	HD23	0.915	0.02	2
A	74	GLN	HG2	2.391	0.02	2
A	23	SER	HB2	3.814	0.02	2
A	40	PHE	N	118.284	0.3	1
A	9	LEU	HB2	1.444	0.02	2
A	66	GLU	C	176.836	0.3	1
A	38	ASN	C	177.87	0.3	1
A	57	ASP	HB3	2.866	0.02	2
A	41	ASP	HB3	2.927	0.02	2
A	37	ARG	HB2	1.826	0.02	2
A	47	VAL	HG11	0.92	0.02	2
A	32	ILE	HD13	0.843	0.02	1
A	54	GLN	NE2	111.883	0.3	1
A	22	PHE	HE1	7.035	0.02	1
A	70	PRO	HA	5.254	0.02	1
A	38	ASN	CG	173.099	0.3	1
A	27	SER	N	112.974	0.3	1
A	28	GLY	N	109.305	0.3	1
A	34	ARG	HD2	3.204	0.02	2
A	48	GLY	H	8.351	0.02	1
A	14	ARG	CA	56.512	0.3	1
A	27	SER	CB	63.812	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	73	GLY	C	178.295	0.3	1
A	53	GLN	CB	28.213	0.3	1
A	68	GLN	H	8.887	0.02	1
A	14	ARG	CG	26.811	0.3	1
A	67	LEU	HD11	0.189	0.02	2
A	38	ASN	HD21	7.936	0.02	2
A	66	GLU	CA	57.036	0.3	1
A	70	PRO	CA	63.426	0.3	1
A	83	ILE	CG1	28.268	0.3	1
A	66	GLU	HA	4.175	0.02	1
A	26	ALA	HB2	1.492	0.02	1
A	87	LYS	HB2	1.849	0.02	2
A	65	ALA	H	7.595	0.02	1
A	29	ASN	H	8.407	0.02	1
A	67	LEU	HD13	0.189	0.02	2
A	71	ALA	N	128.529	0.3	1
A	32	ILE	CA	61.628	0.3	1
A	85	TYR	HA	4.437	0.02	1
A	87	LYS	HD3	1.7	0.02	2
A	56	LEU	HD22	0.92	0.02	2
A	10	PRO	HB2	1.918	0.02	2
A	41	ASP	HA	4.495	0.02	1
A	66	GLU	CB	31.861	0.3	1
A	87	LYS	HD2	1.7	0.02	2
A	31	LEU	HA	4.511	0.02	1
A	52	LEU	CD2	24.542	0.3	1
A	50	GLU	H	8.123	0.02	1
A	83	ILE	HD11	0.846	0.02	1
A	12	SER	CB	64.687	0.3	1
A	31	LEU	HG	1.481	0.02	1
A	40	PHE	HD2	6.832	0.02	1
A	76	LEU	HD21	0.919	0.02	2
A	76	LEU	N	118.341	0.3	1
A	80	GLN	CD	177.314	0.3	1
A	19	ASP	HB2	2.562	0.02	2
A	9	LEU	CD1	25.047	0.3	1
A	37	ARG	CG	27.323	0.3	1
A	68	GLN	CG	33.895	0.3	1
A	43	PHE	HB2	3.048	0.02	2
A	51	PRO	CA	63.358	0.3	1
A	83	ILE	HD12	0.846	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	54	GLN	HG3	2.448	0.02	2
A	58	ARG	HB2	2.003	0.02	2
A	36	ILE	HG23	0.601	0.02	1
A	47	VAL	CB	32.219	0.3	1
A	47	VAL	HA	4.116	0.02	1
A	66	GLU	H	7.836	0.02	1
A	48	GLY	C	174.417	0.3	1
A	8	HIS	C	174.96	0.3	1
A	89	LEU	HD12	0.869	0.02	2
A	80	GLN	HE22	6.769	0.02	2
A	63	ILE	HG13	0.966	0.02	2
A	29	ASN	CA	53.216	0.3	1
A	24	VAL	N	118.185	0.3	1
A	52	LEU	CA	58.044	0.3	1
A	24	VAL	HG11	0.808	0.02	2
A	86	LYS	CB	31.969	0.3	1
A	52	LEU	HB2	1.993	0.02	2
A	86	LYS	HA	3.997	0.02	1
A	24	VAL	CB	35.169	0.3	1
A	52	LEU	CG	26.847	0.3	1
A	36	ILE	HD11	1.091	0.02	1
A	69	GLU	HG2	1.98	0.02	2
A	56	LEU	HA	3.963	0.02	1
A	67	LEU	H	7.718	0.02	1
A	68	GLN	HG2	2.43	0.02	2
A	31	LEU	CB	42.122	0.3	1
A	25	ASP	C	178.121	0.3	1
A	88	GLU	H	8.023	0.02	1
A	43	PHE	CA	61.864	0.3	1
A	67	LEU	HB3	1.594	0.02	2
A	42	TYR	CA	61.179	0.3	1
A	60	ARG	HG2	1.481	0.02	2
A	67	LEU	N	117.679	0.3	1
A	84	ASP	CB	40.487	0.3	1
A	32	ILE	HB	1.958	0.02	1
A	83	ILE	N	118.132	0.3	1
A	53	GLN	HG2	2.455	0.02	2
A	29	ASN	C	175.14	0.3	1
A	75	ALA	CB	18.577	0.3	1
A	71	ALA	HA	4.315	0.02	1
A	75	ALA	N	123.845	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	51	PRO	HA	4.475	0.02	1
A	8	HIS	HA	4.597	0.02	1
A	87	LYS	HG2	1.5	0.02	2
A	22	PHE	HA	4.451	0.02	1
A	54	GLN	C	179.05	0.3	1
A	58	ARG	C	179.137	0.3	1
A	57	ASP	CA	57.878	0.3	1
A	85	TYR	CB	38.241	0.3	1
A	71	ALA	HB3	1.584	0.02	1
A	25	ASP	CA	52.547	0.3	1
A	74	GLN	HG3	2.516	0.02	2
A	82	TYR	CB	38.889	0.3	1
A	49	GLU	H	8.454	0.02	1
A	9	LEU	HA	4.535	0.02	1
A	88	GLU	N	120.706	0.3	1
A	55	SER	CB	62.885	0.3	1
A	20	GLY	N	109.016	0.3	1
A	64	ALA	CA	54.517	0.3	1
A	30	LEU	CA	55.454	0.3	1
A	53	GLN	HA	3.888	0.02	1
A	79	MET	C	177.262	0.3	1
A	55	SER	N	117.585	0.3	1
A	78	LEU	H	7.932	0.02	1
A	28	GLY	HA2	3.487	0.02	2
A	33	THR	HG21	1.191	0.02	1
A	43	PHE	H	8.017	0.02	1
A	44	LEU	HB2	1.676	0.02	2
A	30	LEU	HD12	0.977	0.02	2
A	82	TYR	CA	61.108	0.3	1
A	30	LEU	HD23	1.021	0.02	2
A	53	GLN	H	8.724	0.02	1
A	27	SER	HB3	3.924	0.02	2
A	77	ALA	CA	55.116	0.3	1
A	56	LEU	CD1	25.454	0.3	1
A	74	GLN	CB	27.393	0.3	1
A	89	LEU	CD1	25.462	0.3	1
A	58	ARG	CG	28.586	0.3	1
A	74	GLN	N	121.981	0.3	1
A	80	GLN	HB2	2.038	0.02	2
A	40	PHE	CA	59.169	0.3	1
A	9	LEU	C	175.067	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	32	ILE	HG12	1.202	0.02	2
A	9	LEU	HB3	1.535	0.02	2
A	41	ASP	CB	40.492	0.3	1
A	41	ASP	HB2	2.726	0.02	2
A	37	ARG	HB3	1.826	0.02	2
A	32	ILE	HG13	1.531	0.02	2
A	78	LEU	HD13	0.877	0.02	2
A	31	LEU	HD21	0.89	0.02	2
A	32	ILE	HD12	0.843	0.02	1
A	29	ASN	ND2	116.545	0.3	1
A	45	SER	HB3	3.976	0.02	2
A	68	GLN	CB	30.437	0.3	1
A	22	PHE	HE2	7.035	0.02	1
A	70	PRO	HG3	1.944	0.02	2
A	60	ARG	HD2	3.186	0.02	2
A	70	PRO	C	173.83	0.3	1
A	70	PRO	HD2	3.47	0.02	2
A	20	GLY	HA3	3.942	0.02	2
A	23	SER	C	169.734	0.3	1
A	53	GLN	CA	59.031	0.3	1
A	39	LEU	HA	4.016	0.02	1
A	75	ALA	HB3	1.362	0.02	1
A	9	LEU	CA	52.857	0.3	1
A	47	VAL	H	7.791	0.02	1
A	42	TYR	C	178.143	0.3	1
A	39	LEU	HG	1.473	0.02	1
A	45	SER	C	174.657	0.3	1
A	26	ALA	HB3	1.492	0.02	1
A	62	TYR	H	8.031	0.02	1
A	68	GLN	NE2	113.729	0.3	1
A	9	LEU	HD11	0.796	0.02	2
A	86	LYS	H	7.887	0.02	1
A	85	TYR	HD1	7.074	0.02	1
A	56	LEU	HD23	0.92	0.02	2
A	10	PRO	HB3	2.3	0.02	2
A	84	ASP	HB3	2.655	0.02	2
A	63	ILE	H	8.414	0.02	1
A	47	VAL	HG21	0.947	0.02	2
A	36	ILE	N	119.324	0.3	1
A	74	GLN	CG	34.195	0.3	1
A	43	PHE	HA	4.039	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	36	ILE	CB	37.247	0.3	1
A	40	PHE	HD1	6.832	0.02	1
A	69	GLU	CB	27.958	0.3	1
A	74	GLN	CD	176.199	0.3	1
A	73	GLY	CA	47.347	0.3	1
A	81	GLN	HE22	6.769	0.02	2
A	76	LEU	HB3	1.943	0.02	2
A	19	ASP	HB3	2.627	0.02	2
A	43	PHE	HB3	3.048	0.02	2
A	75	ALA	H	8.901	0.02	1
A	31	LEU	HB2	1.345	0.02	2
A	67	LEU	C	176.36	0.3	1
A	54	GLN	HG2	2.448	0.02	2
A	76	LEU	CD1	25.454	0.3	1
A	36	ILE	HG22	0.601	0.02	1
A	25	ASP	HB3	3.399	0.02	2
A	8	HIS	H	7.809	0.02	1
A	75	ALA	C	179.818	0.3	1
A	47	VAL	CG2	20.768	0.3	1
A	66	GLU	N	115.07	0.3	1
A	86	LYS	CE	42.075	0.3	1
A	80	GLN	HE21	7.756	0.02	2
A	65	ALA	N	117.666	0.3	1
A	68	GLN	HG3	2.43	0.02	2
A	13	PHE	HB2	2.956	0.02	2
A	85	TYR	HD2	7.074	0.02	1
A	68	GLN	HE21	7.62	0.02	2
A	25	ASP	HA	4.721	0.02	1
A	20	GLY	H	8.056	0.02	1
A	80	GLN	NE2	114.319	0.3	1
A	49	GLU	CB	29.885	0.3	1
A	47	VAL	CG1	21.446	0.3	1
A	69	GLU	HG3	2.225	0.02	2
A	87	LYS	CG	24.841	0.3	1
A	43	PHE	N	117.144	0.3	1
A	86	LYS	C	177.016	0.3	1
A	56	LEU	HD12	0.853	0.02	2
A	78	LEU	CB	42.217	0.3	1
A	60	ARG	HA	3.728	0.02	1
A	43	PHE	CB	40.617	0.3	1
A	67	LEU	HB2	1.123	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	81	GLN	CA	58.77	0.3	1
A	63	ILE	HG21	0.847	0.02	1
A	67	LEU	CG	26.275	0.3	1
A	59	LEU	HB2	1.148	0.02	2
A	53	GLN	HG3	2.455	0.02	2
A	65	ALA	HB3	1.485	0.02	1
A	69	GLU	HB3	1.694	0.02	2
A	54	GLN	CA	58.925	0.3	1
A	53	GLN	HB3	2.185	0.02	2
A	82	TYR	HE1	7.001	0.02	1
A	10	PRO	HG3	1.943	0.02	2
A	55	SER	H	7.984	0.02	1
A	39	LEU	HD21	0.563	0.02	2
A	85	TYR	HE1	6.729	0.02	1
A	57	ASP	N	119.862	0.3	1
A	68	GLN	HB3	2.319	0.02	2
A	87	LYS	HG3	1.859	0.02	2
A	72	ARG	HG2	1.389	0.02	2
A	29	ASN	HA	4.749	0.02	1
A	65	ALA	HA	4.205	0.02	1
A	89	LEU	C	182.446	0.3	1
A	36	ILE	CD1	14.137	0.3	1
A	84	ASP	H	8.146	0.02	1
A	22	PHE	HD2	6.858	0.02	1
A	64	ALA	N	117.186	0.3	1
A	41	ASP	H	8.707	0.02	1
A	45	SER	CA	59.429	0.3	1
A	53	GLN	HE22	6.844	0.02	2
A	59	LEU	H	7.957	0.02	1
A	78	LEU	CG	26.85	0.3	1
A	64	ALA	CB	18.105	0.3	1
A	88	GLU	HB3	2.118	0.02	2
A	59	LEU	CB	40.808	0.3	1
A	50	GLU	HA	4.604	0.02	1
A	78	LEU	HD21	0.811	0.02	2
A	80	GLN	CB	28.443	0.3	1
A	88	GLU	CG	36.084	0.3	1
A	33	THR	HG22	1.191	0.02	1
A	11	THR	HG21	1.184	0.02	1
A	44	LEU	HB3	1.969	0.02	2
A	19	ASP	CB	41.267	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	65	ALA	C	179.883	0.3	1
A	89	LEU	HG	1.592	0.02	1
A	78	LEU	HD23	0.811	0.02	2
A	43	PHE	HD1	7.426	0.02	1
A	78	LEU	CA	57.846	0.3	1
A	36	ILE	CG2	17.734	0.3	1
A	37	ARG	HA	3.62	0.02	1
A	37	ARG	HG3	1.669	0.02	2
A	69	GLU	CA	56.023	0.3	1
A	79	MET	HG2	1.92	0.02	2
A	27	SER	HB2	3.81	0.02	2
A	24	VAL	HG23	0.848	0.02	2
A	18	VAL	CG1	21.225	0.3	1
A	80	GLN	HG2	2.455	0.02	2
A	62	TYR	CB	38.871	0.3	1
A	59	LEU	CD1	25.933	0.3	1
A	13	PHE	HB3	2.956	0.02	2
A	54	GLN	CB	28.666	0.3	1
A	79	MET	HA	3.436	0.02	1
A	61	ALA	H	7.854	0.02	1
A	41	ASP	CA	57.631	0.3	1
A	19	ASP	CA	54.424	0.3	1
A	77	ALA	CB	17.823	0.3	1
A	30	LEU	CD1	25.338	0.3	1
A	51	PRO	HD3	3.936	0.02	2
A	87	LYS	HE2	2.996	0.02	2
A	36	ILE	H	7.496	0.02	1
A	69	GLU	H	8.931	0.02	1
A	72	ARG	HD3	3.224	0.02	2
A	70	PRO	HG2	1.627	0.02	2
A	38	ASN	CA	55.869	0.3	1
A	14	ARG	HA	4.6	0.02	1
A	77	ALA	N	123.257	0.3	1
A	60	ARG	HD3	3.186	0.02	2
A	61	ALA	HA	4.134	0.02	1
A	20	GLY	HA2	3.76	0.02	2
A	79	MET	CA	59.406	0.3	1
A	78	LEU	HG	1.538	0.02	1
A	44	LEU	HD21	0.838	0.02	2
A	79	MET	CG	31.874	0.3	1
A	8	HIS	CB	30.891	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	70	PRO	CG	24.178	0.3	1
A	9	LEU	HD23	0.784	0.02	2
A	44	LEU	HD23	0.838	0.02	2
A	74	GLN	HE21	7.321	0.02	2
A	83	ILE	C	177.94	0.3	1
A	70	PRO	HD3	3.644	0.02	2
A	71	ALA	CB	18.749	0.3	1
A	44	LEU	HD22	0.838	0.02	2
A	39	LEU	HB2	1.421	0.02	2
A	63	ILE	CG1	30.419	0.3	1
A	33	THR	CG2	21.795	0.3	1
A	11	THR	HB	4.582	0.02	1
A	69	GLU	CG	30.76	0.3	1
A	75	ALA	HB1	1.362	0.02	1
A	58	ARG	H	7.94	0.02	1
A	59	LEU	HG	1.487	0.02	1
A	14	ARG	HD3	3.151	0.02	2
A	34	ARG	CB	30.025	0.3	1
A	44	LEU	HA	4.416	0.02	1
A	76	LEU	CB	41.312	0.3	1
A	76	LEU	HB2	1.524	0.02	2
A	11	THR	CG2	21.277	0.3	1
A	34	ARG	CD	43.519	0.3	1
A	44	LEU	HG	1.88	0.02	1
A	37	ARG	CA	59.555	0.3	1
A	55	SER	HA	4.352	0.02	1
A	58	ARG	CB	30.381	0.3	1
A	74	GLN	HB3	2.495	0.02	2
A	79	MET	N	119.919	0.3	1
A	31	LEU	HB3	1.535	0.02	2
A	75	ALA	HB2	1.362	0.02	1
A	49	GLU	C	176.539	0.3	1
A	36	ILE	HG21	0.601	0.02	1
A	25	ASP	HB2	2.631	0.02	2
A	47	VAL	N	117.742	0.3	1
A	52	LEU	HD13	0.975	0.02	2
A	23	SER	HA	4.778	0.02	1
A	32	ILE	HG23	0.869	0.02	1
A	63	ILE	HA	3.232	0.02	1
A	62	TYR	HB3	3.082	0.02	2
A	46	ALA	C	177.414	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	29	ASN	HD21	8.145	0.02	2
A	24	VAL	HA	5.118	0.02	1
A	29	ASN	CG	174.176	0.3	1
A	53	GLN	C	178.083	0.3	1
A	18	VAL	HA	3.87	0.02	1
A	69	GLU	C	177.325	0.3	1
A	32	ILE	H	8.67	0.02	1
A	13	PHE	N	119.016	0.3	1
A	63	ILE	HD12	0.852	0.02	1
A	82	TYR	HB3	3.117	0.02	2
A	36	ILE	HD13	1.091	0.02	1
A	73	GLY	HA3	4.062	0.02	2
A	46	ALA	HB1	1.249	0.02	1
A	78	LEU	HB2	1.553	0.02	2
A	53	GLN	N	116.27	0.3	1
A	64	ALA	H	7.882	0.02	1
A	73	GLY	HA2	3.85	0.02	2
A	54	GLN	HE21	7.685	0.02	2
A	18	VAL	HG13	0.719	0.02	2
A	13	PHE	CB	40.829	0.3	1
A	80	GLN	H	7.8	0.02	1
A	31	LEU	N	128.473	0.3	1
A	44	LEU	HD11	0.809	0.02	2
A	83	ILE	HD13	0.846	0.02	1
A	13	PHE	CA	57.236	0.3	1
A	82	TYR	HD2	7.049	0.02	1
A	83	ILE	HG23	0.94	0.02	1
A	77	ALA	HB2	1.547	0.02	1
A	59	LEU	HB3	1.874	0.02	2
A	46	ALA	CA	52.619	0.3	1
A	37	ARG	H	7.379	0.02	1
A	65	ALA	HB2	1.485	0.02	1
A	36	ILE	HG12	1.099	0.02	2
A	69	GLU	HB2	1.694	0.02	2
A	81	GLN	HB3	2.21	0.02	2
A	13	PHE	HD2	7.326	0.02	1
A	53	GLN	HB2	2.044	0.02	2
A	12	SER	HA	4.029	0.02	1
A	10	PRO	HG2	1.943	0.02	2
A	49	GLU	HB3	2.131	0.02	2
A	56	LEU	CB	41.522	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	60	ARG	HB2	1.85	0.02	2
A	85	TYR	HB2	3.125	0.02	2
A	68	GLN	HB2	1.891	0.02	2
A	72	ARG	HG3	1.389	0.02	2
A	49	GLU	HB2	1.983	0.02	2
A	39	LEU	HD11	0.636	0.02	2
A	60	ARG	CD	43.272	0.3	1
A	86	LYS	HD3	1.561	0.02	2
A	54	GLN	CD	177.304	0.3	1
A	47	VAL	HG13	0.92	0.02	2
A	22	PHE	HD1	6.858	0.02	1
A	10	PRO	CG	27.482	0.3	1
A	39	LEU	CA	58.299	0.3	1
A	61	ALA	CB	18.229	0.3	1
A	76	LEU	C	180.098	0.3	1
A	9	LEU	HG	1.479	0.02	1
A	53	GLN	HE21	7.788	0.02	2
A	80	GLN	CG	33.549	0.3	1
A	39	LEU	CG	26.98	0.3	1
A	23	SER	CB	65.202	0.3	1
A	78	LEU	CD2	23.563	0.3	1
A	80	GLN	CA	58.682	0.3	1
A	33	THR	HG23	1.191	0.02	1
A	11	THR	HG22	1.184	0.02	1
A	84	ASP	N	120.692	0.3	1
A	27	SER	HA	4.597	0.02	1
A	42	TYR	H	8.011	0.02	1
A	58	ARG	HA	4.149	0.02	1
A	33	THR	CB	69.55	0.3	1
A	42	TYR	HD2	6.794	0.02	1
A	70	PRO	HB2	2.344	0.02	2
A	64	ALA	C	178.403	0.3	1
A	48	GLY	N	112.824	0.3	1
A	40	PHE	HA	4.453	0.02	1
A	43	PHE	HD2	7.426	0.02	1
A	36	ILE	CG1	28.871	0.3	1
A	37	ARG	HG2	1.669	0.02	2
A	76	LEU	HA	4.081	0.02	1
A	46	ALA	H	7.76	0.02	1
A	28	GLY	C	173.914	0.3	1
A	86	LYS	HB2	1.738	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	57	ASP	C	179.733	0.3	1
A	24	VAL	HG22	0.848	0.02	2
A	82	TYR	C	177.541	0.3	1
A	11	THR	CA	59.639	0.3	1
A	44	LEU	HD12	0.809	0.02	2
A	80	GLN	HG3	2.455	0.02	2
A	18	VAL	HG22	0.641	0.02	2
A	67	LEU	CD1	26.132	0.3	1
A	62	TYR	CA	61.732	0.3	1
A	37	ARG	C	175.009	0.3	1
A	83	ILE	HG22	0.94	0.02	1
A	33	THR	HB	4.216	0.02	1
A	66	GLU	HB2	1.498	0.02	2
A	40	PHE	HB3	2.951	0.02	2
A	71	ALA	H	7.672	0.02	1
A	25	ASP	H	8.836	0.02	1
A	88	GLU	HG2	2.175	0.02	2
A	77	ALA	C	180.805	0.3	1
A	64	ALA	HB3	1.42	0.02	1
A	54	GLN	H	7.611	0.02	1
A	30	LEU	H	8.852	0.02	1
A	31	LEU	HD23	0.89	0.02	2
A	51	PRO	HD2	3.594	0.02	2
A	64	ALA	HB1	1.42	0.02	1
A	58	ARG	HD3	3.362	0.02	2
A	28	GLY	CA	45.17	0.3	1
A	72	ARG	HD2	3.151	0.02	2
A	60	ARG	N	118.987	0.3	1
A	76	LEU	H	8.426	0.02	1
A	27	SER	CA	58.338	0.3	1
A	85	TYR	HE2	6.729	0.02	1
A	14	ARG	CB	30.535	0.3	1
A	79	MET	CB	32.803	0.3	1
A	87	LYS	CD	29.251	0.3	1
A	89	LEU	HD21	0.824	0.02	2
A	46	ALA	HB2	1.249	0.02	1
A	70	PRO	CB	34.072	0.3	1
A	9	LEU	CG	26.754	0.3	1
A	89	LEU	HD22	0.824	0.02	2
A	20	GLY	C	173.003	0.3	1
A	81	GLN	CD	177.301	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	70	PRO	CD	50.326	0.3	1
A	9	LEU	HD22	0.784	0.02	2
A	89	LEU	HD23	0.824	0.02	2
A	78	LEU	C	179.267	0.3	1
A	31	LEU	CD2	23.999	0.3	1
A	84	ASP	HA	4.46	0.02	1
A	22	PHE	HB3	2.898	0.02	2
A	32	ILE	CB	36.21	0.3	1
A	66	GLU	HG3	1.945	0.02	2
A	39	LEU	HB3	1.711	0.02	2
A	37	ARG	HD2	3.137	0.02	2
A	30	LEU	HB3	1.841	0.02	2
A	12	SER	CA	58.415	0.3	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	76	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	72	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	67	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	60	0.00 ± 0.00	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 990. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/394 (0%)	0/157 (0%)	0/160 (0%)	0/77 (0%)
Sidechain	0/528 (0%)	0/309 (0%)	0/191 (0%)	0/28 (0%)
Aromatic	0/68 (0%)	0/36 (0%)	0/32 (0%)	0/0 (—%)
Overall	0/990 (0%)	0/502 (0%)	0/383 (0%)	0/105 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1019. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/404 (0%)	0/161 (0%)	0/164 (0%)	0/79 (0%)
Sidechain	0/540 (0%)	0/316 (0%)	0/196 (0%)	0/28 (0%)
Aromatic	0/75 (0%)	0/40 (0%)	0/34 (0%)	0/1 (0%)
Overall	0/1019 (0%)	0/517 (0%)	0/394 (0%)	0/108 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (MD1_3.1_6.str). RCI is only applicable to proteins.