



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 22, 2024 – 02:08 PM JST

PDB ID : 8J8I  
BMRB ID : 36564  
Title : Membrane-bound structure of CD3z cytoplasmic domain  
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Deposited on : 2023-05-01

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

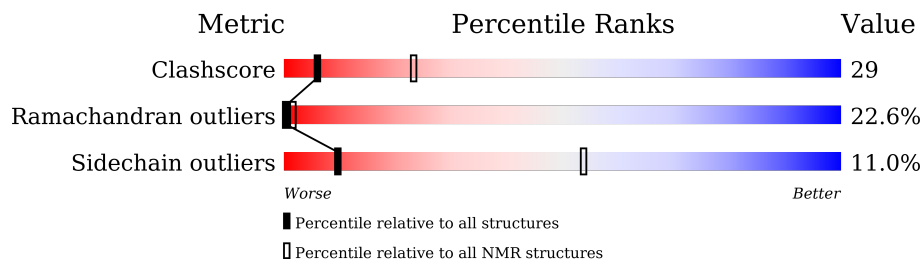
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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  $\geq 3$ , 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	140	

## 2 Ensemble composition and analysis i

This entry contains 10 models. Model 7 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:39-A:140 (102)	5.37	7

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 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 7, 9, 10
2	6, 8
Single-model clusters	1; 3

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1742 atoms, of which 858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called T-cell surface glycoprotein CD3 zeta chain.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	110	1742	539	858	172	173	0

There are 6 discrepancies between the modelled and reference sequences:

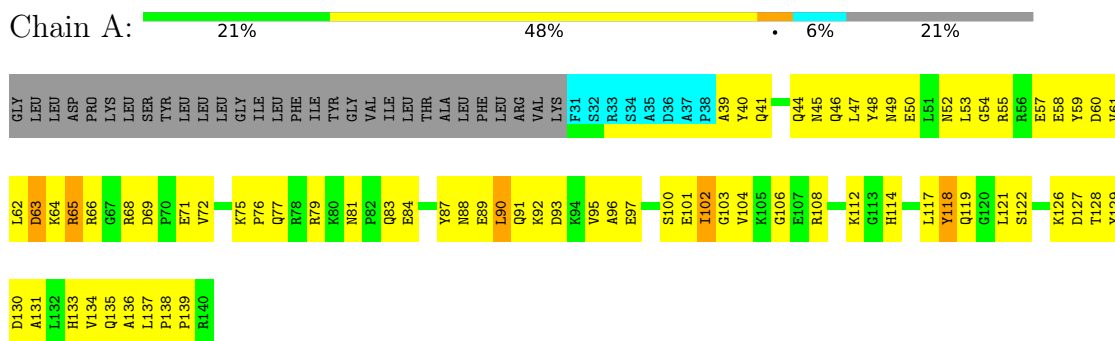
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	SER	CYS	engineered mutation	UNP P20963
A	12	LEU	ASP	engineered mutation	UNP P20963
A	72	VAL	MET	engineered mutation	UNP P20963
A	95	VAL	MET	engineered mutation	UNP P20963
A	104	VAL	MET	engineered mutation	UNP P20963
A	134	VAL	MET	engineered mutation	UNP P20963

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

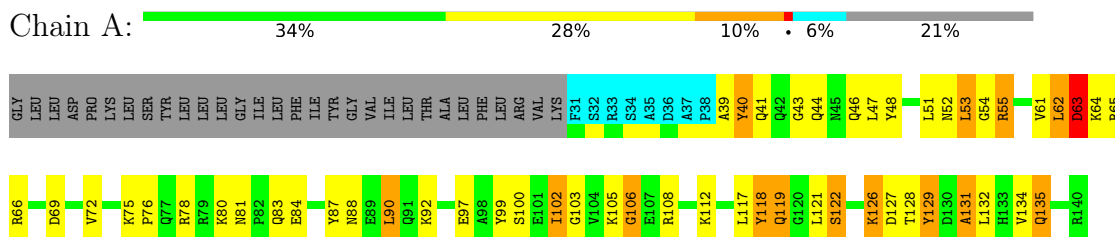
- Molecule 1: T-cell surface glycoprotein CD3 zeta chain



### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 7. Colouring as in section 4.1 above.

- Molecule 1: T-cell surface glycoprotein CD3 zeta chain



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1257
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1257
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	825	806	806	48±8
All	All	8250	8060	8060	481

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 29.

5 of 352 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ARG:H	1:A:79:ARG:NE	0.69	1.85	1	1
1:A:133:HIS:CG	1:A:134:VAL:H	0.67	2.08	1	2
1:A:137:LEU:HD12	1:A:137:LEU:O	0.67	1.90	8	2
1:A:121:LEU:HD23	1:A:121:LEU:N	0.67	2.05	9	1
1:A:102:ILE:HG22	1:A:102:ILE:O	0.67	1.89	5	2

### 6.3 Torsion angles [i](#)

#### 6.3.1 Protein backbone [i](#)

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	101/140 (72%)	39±5 (39±5%)	39±7 (38±7%)	23±3 (23±3%)	0	1
All	All	1010/1400 (72%)	394 (39%)	388 (38%)	228 (23%)	0	1

5 of 87 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	112	LYS	7
1	A	63	ASP	6
1	A	72	VAL	6
1	A	118	TYR	6
1	A	122	SER	6

### 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	84/116 (72%)	75±4 (89±4%)	9±4 (11±4%)	10	54
All	All	840/1160 (72%)	748 (89%)	92 (11%)	10	54

5 of 47 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	LEU	6
1	A	102	ILE	6
1	A	81	ASN	6
1	A	90	LEU	5
1	A	75	LYS	4

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.



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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation i

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: working\_cs.cif

Chemical shift list name: *CD3zTMCD\_20230427.str*

#### 7.1.1 Bookkeeping i

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	1257
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1257
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.

- No matching atom found in the structure. First 5 (of 1257) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	33	ARG	HB2	1.82	0.030	2
1	?	33	ARG	HB3	1.7	0.030	2
1	?	33	ARG	C	176.626	0.300	1
1	?	34	SER	N	116.662	0.300	1
1	?	34	SER	H	8.206	0.030	1
1	?	34	SER	CA	58.662	0.300	1
1	?	34	SER	HA	4.41	0.030	1
1	?	34	SER	CB	63.872	0.300	1
1	?	34	SER	HB2	3.893	0.030	2
1	?	34	SER	HB3	3.866	0.030	2
1	?	34	SER	C	174.535	0.300	1
1	?	35	ALA	N	125.662	0.300	1
1	?	35	ALA	H	8.254	0.030	1
1	?	35	ALA	CA	52.77	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	35	ALA	HA	4.287	0.030	1
1	?	35	ALA	CB	19.373	0.300	1
1	?	35	ALA	HB1	1.377	0.030	1
1	?	35	ALA	HB2	1.377	0.030	1
1	?	35	ALA	HB3	1.377	0.030	1
1	?	35	ALA	C	177.302	0.300	1
1	?	36	ASP	N	118.872	0.300	1
1	?	36	ASP	H	8.098	0.030	1
1	?	36	ASP	CA	53.71	0.300	1
1	?	36	ASP	HA	4.563	0.030	1
1	?	36	ASP	CB	41.272	0.300	1
1	?	36	ASP	HB2	2.563	0.030	2
1	?	36	ASP	HB3	2.682	0.030	2
1	?	36	ASP	C	175.475	0.300	1
1	?	37	ALA	N	124.69	0.300	1
1	?	37	ALA	H	7.96	0.030	1
1	?	37	ALA	CA	50.727	0.300	1
1	?	37	ALA	HA	4.55	0.030	1
1	?	37	ALA	CB	18.329	0.300	1
1	?	37	ALA	HB1	1.351	0.030	1
1	?	37	ALA	HB2	1.351	0.030	1
1	?	37	ALA	HB3	1.351	0.030	1
1	?	37	ALA	C	175.321	0.300	1
1	?	38	PRO	CA	63.281	0.300	1
1	?	38	PRO	HA	4.345	0.030	1
1	?	38	PRO	CB	32.044	0.300	1
1	?	38	PRO	HB2	2.218	0.030	2
1	?	38	PRO	HB3	1.724	0.030	2
1	?	38	PRO	CG	27.4	0.300	1
1	?	38	PRO	HG2	1.965	0.030	1
1	?	38	PRO	HG3	1.965	0.030	1
1	?	38	PRO	CD	50.4	0.300	1
1	?	38	PRO	HD2	3.591	0.030	2
1	?	38	PRO	HD3	3.754	0.030	2
1	?	38	PRO	C	176.839	0.300	1
1	?	39	ALA	N	123.29	0.300	1
1	?	39	ALA	H	8.247	0.030	1
1	?	39	ALA	CA	52.716	0.300	1
1	?	39	ALA	HA	4.223	0.030	1
1	?	39	ALA	CB	19.175	0.300	1
1	?	39	ALA	HB1	1.308	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	39	ALA	HB2	1.308	0.030	1
1	?	39	ALA	HB3	1.308	0.030	1
1	?	39	ALA	C	177.716	0.300	1
1	?	40	TYR	N	118.225	0.300	1
1	?	40	TYR	H	7.922	0.030	1
1	?	40	TYR	CA	57.98	0.300	1
1	?	40	TYR	HA	4.53	0.030	1
1	?	40	TYR	CB	38.74	0.300	1
1	?	40	TYR	HB2	2.983	0.030	2
1	?	40	TYR	HB3	3.022	0.030	2
1	?	40	TYR	CD1	133.158	0.300	1
1	?	40	TYR	HD1	7.091	0.030	1
1	?	40	TYR	CD2	133.158	0.300	1
1	?	40	TYR	HD2	7.091	0.030	1
1	?	40	TYR	CE1	118.262	0.300	1
1	?	40	TYR	HE1	6.8	0.030	1
1	?	40	TYR	CE2	118.262	0.300	1
1	?	40	TYR	HE2	6.8	0.030	1
1	?	40	TYR	C	175.86	0.300	1
1	?	41	GLN	N	121.489	0.300	1
1	?	41	GLN	H	8.09	0.030	1
1	?	41	GLN	CA	55.651	0.300	1
1	?	41	GLN	HA	4.26	0.030	1
1	?	41	GLN	CB	29.589	0.300	1
1	?	41	GLN	HB2	1.914	0.030	2
1	?	41	GLN	HB3	2.002	0.030	2
1	?	41	GLN	CG	33.82	0.300	1
1	?	41	GLN	HG2	2.26	0.030	1
1	?	41	GLN	HG3	2.26	0.030	1
1	?	41	GLN	NE2	111.89	0.300	1
1	?	41	GLN	HE21	7.455	0.030	2
1	?	41	GLN	HE22	6.811	0.030	2
1	?	41	GLN	C	175.723	0.300	1
1	?	42	GLN	N	121.058	0.300	1
1	?	42	GLN	H	8.254	0.030	1
1	?	42	GLN	CA	55.921	0.300	1
1	?	42	GLN	HA	4.264	0.030	1
1	?	42	GLN	CB	29.117	0.300	1
1	?	42	GLN	HB2	2.027	0.030	2
1	?	42	GLN	HB3	2.084	0.030	2
1	?	42	GLN	CG	33.914	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	42	GLN	HG2	2.334	0.030	1
1	?	42	GLN	HG3	2.334	0.030	1
1	?	42	GLN	NE2	111.89	0.300	1
1	?	42	GLN	HE21	7.455	0.030	2
1	?	42	GLN	HE22	6.811	0.030	2
1	?	42	GLN	C	176.637	0.300	1
1	?	43	GLY	N	109.768	0.300	1
1	?	43	GLY	H	8.39	0.030	1
1	?	43	GLY	CA	45.384	0.300	1
1	?	43	GLY	HA2	3.969	0.030	1
1	?	43	GLY	HA3	3.969	0.030	1
1	?	43	GLY	C	174.296	0.300	1
1	?	44	GLN	N	119.525	0.300	1
1	?	44	GLN	H	8.198	0.030	1
1	?	44	GLN	CA	55.694	0.300	1
1	?	44	GLN	HA	4.292	0.030	1
1	?	44	GLN	CB	29.29	0.300	1
1	?	44	GLN	HB2	2.084	0.030	2
1	?	44	GLN	HB3	1.968	0.030	2
1	?	44	GLN	CG	33.82	0.300	1
1	?	44	GLN	HG2	2.326	0.030	1
1	?	44	GLN	HG3	2.326	0.030	1
1	?	44	GLN	NE2	111.89	0.300	1
1	?	44	GLN	HE21	7.455	0.030	2
1	?	44	GLN	HE22	6.811	0.030	2
1	?	44	GLN	C	176.046	0.300	1
1	?	45	ASN	N	119.145	0.300	1
1	?	45	ASN	H	8.417	0.030	1
1	?	45	ASN	CA	53.303	0.300	1
1	?	45	ASN	HA	4.608	0.030	1
1	?	45	ASN	CB	38.688	0.300	1
1	?	45	ASN	HB2	2.77	0.030	2
1	?	45	ASN	HB3	2.827	0.030	2
1	?	45	ASN	ND2	112.3	0.300	1
1	?	45	ASN	HD21	6.842	0.030	2
1	?	45	ASN	HD22	7.563	0.030	2
1	?	45	ASN	C	175.303	0.300	1
1	?	46	GLN	N	120.67	0.300	1
1	?	46	GLN	H	8.318	0.030	1
1	?	46	GLN	CA	56.375	0.300	1
1	?	46	GLN	HA	4.22	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	46	GLN	CB	29.823	0.300	1
1	?	46	GLN	HB2	1.979	0.030	2
1	?	46	GLN	HB3	1.956	0.030	2
1	?	46	GLN	CG	36.208	0.300	1
1	?	46	GLN	HG2	2.255	0.030	2
1	?	46	GLN	HG3	2.14	0.030	2
1	?	46	GLN	NE2	111.89	0.300	1
1	?	46	GLN	HE21	7.455	0.030	2
1	?	46	GLN	HE22	6.811	0.030	2
1	?	46	GLN	C	176.447	0.300	1
1	?	47	LEU	N	121.921	0.300	1
1	?	47	LEU	H	8.104	0.030	1
1	?	47	LEU	CA	55.467	0.300	1
1	?	47	LEU	HA	4.232	0.030	1
1	?	47	LEU	CB	42.35	0.300	1
1	?	47	LEU	HB2	1.422	0.030	2
1	?	47	LEU	HB3	1.519	0.030	2
1	?	47	LEU	CG	27.33	0.300	1
1	?	47	LEU	HG	1.492	0.030	1
1	?	47	LEU	CD1	25.189	0.300	2
1	?	47	LEU	HD11	0.846	0.030	2
1	?	47	LEU	HD12	0.846	0.030	2
1	?	47	LEU	HD13	0.846	0.030	2
1	?	47	LEU	CD2	23.7	0.300	2
1	?	47	LEU	HD21	0.811	0.030	2
1	?	47	LEU	HD22	0.811	0.030	2
1	?	47	LEU	HD23	0.811	0.030	2
1	?	47	LEU	C	177.262	0.300	1
1	?	48	TYR	N	119.034	0.300	1
1	?	48	TYR	H	7.97	0.030	1
1	?	48	TYR	CA	58.356	0.300	1
1	?	48	TYR	HA	4.473	0.030	1
1	?	48	TYR	CB	38.439	0.300	1
1	?	48	TYR	HB2	2.988	0.030	1
1	?	48	TYR	HB3	2.988	0.030	1
1	?	48	TYR	CD1	133.158	0.300	1
1	?	48	TYR	HD1	7.091	0.030	1
1	?	48	TYR	CD2	133.158	0.300	1
1	?	48	TYR	HD2	7.091	0.030	1
1	?	48	TYR	CE1	118.262	0.300	1
1	?	48	TYR	HE1	6.8	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	48	TYR	CE2	118.262	0.300	1
1	?	48	TYR	HE2	6.8	0.030	1
1	?	48	TYR	C	175.844	0.300	1
1	?	49	ASN	N	119.397	0.300	1
1	?	49	ASN	H	8.126	0.030	1
1	?	49	ASN	CA	53.315	0.300	1
1	?	49	ASN	HA	4.626	0.030	1
1	?	49	ASN	CB	38.562	0.300	1
1	?	49	ASN	HB2	2.799	0.030	2
1	?	49	ASN	HB3	2.745	0.030	2
1	?	49	ASN	ND2	112.402	0.300	1
1	?	49	ASN	HD21	7.55	0.030	2
1	?	49	ASN	HD22	6.835	0.030	2
1	?	49	ASN	C	175.656	0.300	1
1	?	50	GLU	N	120.442	0.300	1
1	?	50	GLU	H	8.296	0.030	1
1	?	50	GLU	HB2	2.054	0.030	1
1	?	50	GLU	HB3	2.054	0.030	1
1	?	50	GLU	HG2	2.264	0.030	1
1	?	50	GLU	HG3	2.264	0.030	1
1	?	51	LEU	N	120.8	0.300	1
1	?	51	LEU	H	8.025	0.030	1
1	?	51	LEU	CA	55.204	0.300	1
1	?	51	LEU	HA	4.264	0.030	1
1	?	51	LEU	CB	41.647	0.300	1
1	?	51	LEU	HB2	1.627	0.030	2
1	?	51	LEU	HB3	1.565	0.030	2
1	?	51	LEU	CD1	25.0	0.300	2
1	?	51	LEU	HD11	0.873	0.030	2
1	?	51	LEU	HD12	0.873	0.030	2
1	?	51	LEU	HD13	0.873	0.030	2
1	?	51	LEU	CD2	23.6	0.300	2
1	?	51	LEU	HD21	0.86	0.030	2
1	?	51	LEU	HD22	0.86	0.030	2
1	?	51	LEU	HD23	0.86	0.030	2
1	?	51	LEU	C	177.137	0.300	1
1	?	52	ASN	N	118.169	0.300	1
1	?	52	ASN	H	8.18	0.030	1
1	?	52	ASN	CA	53.076	0.300	1
1	?	52	ASN	HA	4.664	0.030	1
1	?	52	ASN	CB	38.955	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	52	ASN	HB2	2.722	0.030	2
1	?	52	ASN	HB3	2.864	0.030	2
1	?	52	ASN	ND2	112.296	0.300	1
1	?	52	ASN	HD21	7.507	0.030	2
1	?	52	ASN	HD22	6.834	0.030	2
1	?	52	ASN	C	175.206	0.300	1
1	?	53	LEU	N	121.363	0.300	1
1	?	53	LEU	H	8.061	0.030	1
1	?	53	LEU	CA	55.204	0.300	1
1	?	53	LEU	HA	4.283	0.030	1
1	?	53	LEU	CB	41.623	0.300	1
1	?	53	LEU	HB2	1.627	0.030	1
1	?	53	LEU	HB3	1.627	0.030	1
1	?	53	LEU	CD1	23.42	0.300	2
1	?	53	LEU	HD11	0.855	0.030	2
1	?	53	LEU	HD12	0.855	0.030	2
1	?	53	LEU	HD13	0.855	0.030	2
1	?	53	LEU	CD2	23.42	0.300	2
1	?	53	LEU	HD21	0.855	0.030	2
1	?	53	LEU	HD22	0.855	0.030	2
1	?	53	LEU	HD23	0.855	0.030	2
1	?	53	LEU	C	177.837	0.300	1
1	?	54	GLY	N	108.364	0.300	1
1	?	54	GLY	H	8.299	0.030	1
1	?	54	GLY	CA	45.53	0.300	1
1	?	54	GLY	HA2	3.94	0.030	1
1	?	54	GLY	HA3	3.94	0.030	1
1	?	54	GLY	C	173.985	0.300	1
1	?	55	ARG	H	8.011	0.030	1
1	?	55	ARG	CA	55.969	0.300	1
1	?	55	ARG	CB	30.93	0.300	1
1	?	55	ARG	HB2	1.85	0.030	2
1	?	55	ARG	HB3	1.76	0.030	2
1	?	55	ARG	CG	27.18	0.300	1
1	?	55	ARG	HG2	1.63	0.030	1
1	?	55	ARG	HG3	1.63	0.030	1
1	?	55	ARG	CD	43.51	0.300	1
1	?	55	ARG	HD2	3.184	0.030	1
1	?	55	ARG	HD3	3.184	0.030	1
1	?	55	ARG	C	177.118	0.300	1
1	?	56	ARG	N	122.468	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	56	ARG	H	8.358	0.030	1
1	?	56	ARG	CA	55.873	0.300	1
1	?	56	ARG	CB	30.93	0.300	1
1	?	56	ARG	HB2	1.85	0.030	2
1	?	56	ARG	HB3	1.76	0.030	2
1	?	56	ARG	CG	27.18	0.300	1
1	?	56	ARG	HG2	1.631	0.030	1
1	?	56	ARG	HG3	1.631	0.030	1
1	?	56	ARG	CD	43.51	0.300	1
1	?	56	ARG	HD2	3.184	0.030	1
1	?	56	ARG	HD3	3.184	0.030	1
1	?	56	ARG	C	176.327	0.300	1
1	?	57	GLU	N	121.636	0.300	1
1	?	57	GLU	H	8.524	0.030	1
1	?	57	GLU	CA	56.351	0.300	1
1	?	57	GLU	HA	4.283	0.030	1
1	?	57	GLU	CB	30.001	0.300	1
1	?	57	GLU	HB2	1.876	0.030	2
1	?	57	GLU	HB3	1.978	0.030	2
1	?	57	GLU	CG	36.3	0.300	1
1	?	57	GLU	HG2	2.25	0.030	1
1	?	57	GLU	HG3	2.25	0.030	1
1	?	57	GLU	C	176.375	0.300	1
1	?	58	GLU	N	120.724	0.300	1
1	?	58	GLU	H	8.322	0.030	1
1	?	58	GLU	CA	56.327	0.300	1
1	?	58	GLU	HA	4.53	0.030	1
1	?	58	GLU	CB	29.852	0.300	1
1	?	58	GLU	HB2	1.922	0.030	2
1	?	58	GLU	HB3	2.1	0.030	2
1	?	58	GLU	CG	36.201	0.300	1
1	?	58	GLU	HG2	2.27	0.030	1
1	?	58	GLU	HG3	2.27	0.030	1
1	?	58	GLU	C	176.133	0.300	1
1	?	59	TYR	N	119.507	0.300	1
1	?	59	TYR	H	7.97	0.030	1
1	?	59	TYR	CA	57.427	0.300	1
1	?	59	TYR	HA	4.226	0.030	1
1	?	59	TYR	CB	38.588	0.300	1
1	?	59	TYR	HB2	3.076	0.030	2
1	?	59	TYR	HB3	2.943	0.030	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	59	TYR	CD1	133.158	0.300	1
1	?	59	TYR	HD1	7.091	0.030	1
1	?	59	TYR	CD2	133.158	0.300	1
1	?	59	TYR	HD2	7.091	0.030	1
1	?	59	TYR	CE1	118.262	0.300	1
1	?	59	TYR	HE1	6.8	0.030	1
1	?	59	TYR	CE2	118.262	0.300	1
1	?	59	TYR	HE2	6.8	0.030	1
1	?	59	TYR	C	175.464	0.300	1
1	?	60	ASP	N	121.749	0.300	1
1	?	60	ASP	H	8.277	0.030	1
1	?	60	ASP	CA	53.973	0.300	1
1	?	60	ASP	HA	4.597	0.030	1
1	?	60	ASP	CB	41.174	0.300	1
1	?	60	ASP	HB2	2.611	0.030	2
1	?	60	ASP	HB3	2.708	0.030	2
1	?	60	ASP	C	176.338	0.300	1
1	?	61	VAL	N	119.248	0.300	1
1	?	61	VAL	H	7.909	0.030	1
1	?	61	VAL	CA	62.959	0.300	1
1	?	61	VAL	HA	4.032	0.030	1
1	?	61	VAL	CB	32.1	0.300	1
1	?	61	VAL	HB	2.11	0.030	1
1	?	61	VAL	CG1	21.1	0.300	2
1	?	61	VAL	HG11	0.925	0.030	2
1	?	61	VAL	HG12	0.925	0.030	2
1	?	61	VAL	HG13	0.925	0.030	2
1	?	61	VAL	CG2	21.1	0.300	2
1	?	61	VAL	HG21	0.925	0.030	2
1	?	61	VAL	HG22	0.925	0.030	2
1	?	61	VAL	HG23	0.925	0.030	2
1	?	61	VAL	C	176.364	0.300	1
1	?	62	LEU	N	123.052	0.300	1
1	?	62	LEU	H	8.134	0.030	1
1	?	62	LEU	CA	55.192	0.300	1
1	?	62	LEU	HA	4.28	0.030	1
1	?	62	LEU	CB	41.373	0.300	1
1	?	62	LEU	HB2	1.693	0.030	2
1	?	62	LEU	HB3	1.606	0.030	2
1	?	62	LEU	CD1	25.15	0.300	2
1	?	62	LEU	HD11	0.93	0.030	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	62	LEU	HD12	0.93	0.030	2
1	?	62	LEU	HD13	0.93	0.030	2
1	?	62	LEU	CD2	23.575	0.300	2
1	?	62	LEU	HD21	0.857	0.030	2
1	?	62	LEU	HD22	0.857	0.030	2
1	?	62	LEU	HD23	0.857	0.030	2
1	?	62	LEU	C	177.265	0.300	1
1	?	63	ASP	N	120.343	0.300	1
1	?	63	ASP	H	8.07	0.030	1
1	?	63	ASP	CA	54.631	0.300	1
1	?	63	ASP	HA	4.54	0.030	1
1	?	63	ASP	CB	41.174	0.300	1
1	?	63	ASP	HB2	2.635	0.030	2
1	?	63	ASP	HB3	2.741	0.030	2
1	?	63	ASP	C	176.606	0.300	1
1	?	64	LYS	N	121.7	0.300	1
1	?	64	LYS	H	8.183	0.030	1
1	?	64	LYS	CA	56.387	0.300	1
1	?	64	LYS	HA	4.235	0.030	1
1	?	64	LYS	CB	32.67	0.300	1
1	?	64	LYS	HB2	1.883	0.030	2
1	?	64	LYS	HB3	1.772	0.030	2
1	?	64	LYS	CG	24.865	0.300	1
1	?	64	LYS	HG2	1.46	0.030	2
1	?	64	LYS	HG3	1.423	0.030	2
1	?	64	LYS	CD	29.2	0.300	1
1	?	64	LYS	HD2	1.673	0.030	1
1	?	64	LYS	HD3	1.673	0.030	1
1	?	64	LYS	CE	42.2	0.300	1
1	?	64	LYS	HE2	2.986	0.030	1
1	?	64	LYS	HE3	2.986	0.030	1
1	?	64	LYS	C	176.947	0.300	1
1	?	65	ARG	N	120.382	0.300	1
1	?	65	ARG	H	8.245	0.030	1
1	?	65	ARG	CA	56.343	0.300	1
1	?	65	ARG	HA	4.41	0.030	1
1	?	65	ARG	CB	30.93	0.300	1
1	?	65	ARG	HB2	1.81	0.030	2
1	?	65	ARG	HB3	1.76	0.030	2
1	?	65	ARG	CG	27.18	0.300	1
1	?	65	ARG	HG2	1.63	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	65	ARG	HG3	1.63	0.030	1
1	?	65	ARG	CD	43.51	0.300	1
1	?	65	ARG	HD2	3.184	0.030	1
1	?	65	ARG	HD3	3.184	0.030	1
1	?	65	ARG	C	176.663	0.300	1
1	?	66	ARG	CA	55.993	0.300	1
1	?	66	ARG	CB	30.93	0.300	1
1	?	66	ARG	HB2	1.85	0.030	2
1	?	66	ARG	HB3	1.76	0.030	2
1	?	66	ARG	CG	27.18	0.300	1
1	?	66	ARG	HG2	1.632	0.030	1
1	?	66	ARG	HG3	1.632	0.030	1
1	?	66	ARG	CD	43.51	0.300	1
1	?	66	ARG	HD2	3.184	0.030	1
1	?	66	ARG	HD3	3.184	0.030	1
1	?	66	ARG	C	176.826	0.300	1
1	?	67	GLY	N	109.596	0.300	1
1	?	67	GLY	H	8.308	0.030	1
1	?	67	GLY	CA	45.53	0.300	1
1	?	67	GLY	HA2	3.965	0.030	1
1	?	67	GLY	HA3	3.965	0.030	1
1	?	67	GLY	C	173.785	0.300	1
1	?	68	ARG	N	119.995	0.300	1
1	?	68	ARG	H	8.065	0.030	1
1	?	68	ARG	CA	55.311	0.300	1
1	?	68	ARG	HA	4.346	0.030	1
1	?	68	ARG	CB	30.682	0.300	1
1	?	68	ARG	HB2	1.827	0.030	2
1	?	68	ARG	HB3	1.76	0.030	2
1	?	68	ARG	CG	27.18	0.300	1
1	?	68	ARG	HG2	1.632	0.030	1
1	?	68	ARG	HG3	1.632	0.030	1
1	?	68	ARG	CD	43.51	0.300	1
1	?	68	ARG	HD2	3.184	0.030	1
1	?	68	ARG	HD3	3.184	0.030	1
1	?	68	ARG	C	175.841	0.300	1
1	?	69	ASP	N	123.072	0.300	1
1	?	69	ASP	H	8.318	0.030	1
1	?	69	ASP	CA	52.6	0.300	1
1	?	69	ASP	HA	4.842	0.030	1
1	?	69	ASP	CB	41.053	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	69	ASP	HB2	2.515	0.030	2
1	?	69	ASP	HB3	2.762	0.030	2
1	?	70	PRO	CA	63.74	0.300	1
1	?	70	PRO	HA	4.393	0.030	1
1	?	70	PRO	CB	32.09	0.300	1
1	?	70	PRO	HB2	1.955	0.030	2
1	?	70	PRO	HB3	2.28	0.030	2
1	?	70	PRO	CG	27.467	0.300	1
1	?	70	PRO	HG2	2.03	0.030	2
1	?	70	PRO	HG3	2.012	0.030	2
1	?	70	PRO	CD	50.732	0.300	1
1	?	70	PRO	HD2	3.85	0.030	2
1	?	70	PRO	HD3	3.774	0.030	2
1	?	70	PRO	C	177.076	0.300	1
1	?	71	GLU	N	119.988	0.300	1
1	?	71	GLU	H	8.476	0.030	1
1	?	71	GLU	CA	56.303	0.300	1
1	?	71	GLU	HA	4.269	0.030	1
1	?	71	GLU	CB	29.91	0.300	1
1	?	71	GLU	HB2	1.96	0.030	2
1	?	71	GLU	HB3	2.05	0.030	2
1	?	71	GLU	CG	36.28	0.300	1
1	?	71	GLU	HG2	2.274	0.030	1
1	?	71	GLU	HG3	2.274	0.030	1
1	?	71	GLU	C	176.819	0.300	1
1	?	72	VAL	N	119.883	0.300	1
1	?	72	VAL	H	7.955	0.030	1
1	?	72	VAL	CA	62.553	0.300	1
1	?	72	VAL	HA	4.116	0.030	1
1	?	72	VAL	CB	32.348	0.300	1
1	?	72	VAL	HB	2.093	0.030	1
1	?	72	VAL	CG1	21.1	0.300	2
1	?	72	VAL	HG11	0.93	0.030	2
1	?	72	VAL	HG12	0.93	0.030	2
1	?	72	VAL	HG13	0.93	0.030	2
1	?	72	VAL	CG2	21.1	0.300	2
1	?	72	VAL	HG21	0.93	0.030	2
1	?	72	VAL	HG22	0.93	0.030	2
1	?	72	VAL	HG23	0.93	0.030	2
1	?	72	VAL	C	176.709	0.300	1
1	?	73	GLY	N	111.88	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	73	GLY	H	8.388	0.030	1
1	?	73	GLY	CA	45.5	0.300	1
1	?	73	GLY	HA2	3.975	0.030	1
1	?	73	GLY	HA3	3.975	0.030	1
1	?	73	GLY	C	174.542	0.300	1
1	?	74	GLY	N	108.301	0.300	1
1	?	74	GLY	H	8.173	0.030	1
1	?	74	GLY	CA	45.53	0.300	1
1	?	74	GLY	HA2	3.962	0.030	1
1	?	74	GLY	HA3	3.962	0.030	1
1	?	74	GLY	C	173.648	0.300	1
1	?	75	LYS	N	121.616	0.300	1
1	?	75	LYS	H	8.133	0.030	1
1	?	75	LYS	CA	54.39	0.300	1
1	?	75	LYS	HA	4.59	0.030	1
1	?	75	LYS	CB	32.63	0.300	1
1	?	75	LYS	HB2	1.716	0.030	2
1	?	75	LYS	HB3	1.815	0.030	2
1	?	75	LYS	CG	24.81	0.300	1
1	?	75	LYS	HG2	1.46	0.030	1
1	?	75	LYS	HG3	1.46	0.030	1
1	?	75	LYS	CD	29.2	0.300	1
1	?	75	LYS	HD2	1.673	0.030	1
1	?	75	LYS	HD3	1.673	0.030	1
1	?	75	LYS	CE	42.2	0.300	1
1	?	75	LYS	HE2	2.989	0.030	1
1	?	75	LYS	HE3	2.989	0.030	1
1	?	75	LYS	C	174.649	0.300	1
1	?	76	PRO	CA	63.355	0.300	1
1	?	76	PRO	HA	4.396	0.030	1
1	?	76	PRO	CB	32.035	0.300	1
1	?	76	PRO	HB2	1.867	0.030	1
1	?	76	PRO	HB3	1.867	0.030	1
1	?	76	PRO	CG	27.467	0.300	1
1	?	76	PRO	HG2	2.021	0.030	1
1	?	76	PRO	HG3	2.021	0.030	1
1	?	76	PRO	CD	50.7	0.300	1
1	?	76	PRO	HD2	3.77	0.030	1
1	?	76	PRO	HD3	3.77	0.030	1
1	?	76	PRO	C	177.051	0.300	1
1	?	77	GLN	N	118.623	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	77	GLN	H	8.345	0.030	1
1	?	77	GLN	CA	55.742	0.300	1
1	?	77	GLN	HA	4.311	0.030	1
1	?	77	GLN	CB	28.892	0.300	1
1	?	77	GLN	HB2	2.017	0.030	2
1	?	77	GLN	HB3	2.127	0.030	2
1	?	77	GLN	CG	33.85	0.300	1
1	?	77	GLN	HG2	2.331	0.030	1
1	?	77	GLN	HG3	2.331	0.030	1
1	?	77	GLN	NE2	111.89	0.300	1
1	?	77	GLN	HE21	7.455	0.030	2
1	?	77	GLN	HE22	6.811	0.030	2
1	?	77	GLN	C	176.045	0.300	1
1	?	78	ARG	N	121.74	0.300	1
1	?	78	ARG	H	8.127	0.030	1
1	?	78	ARG	CA	56.59	0.300	1
1	?	78	ARG	HA	4.277	0.030	1
1	?	78	ARG	CB	30.93	0.300	1
1	?	78	ARG	HB2	1.76	0.030	2
1	?	78	ARG	HB3	1.85	0.030	2
1	?	78	ARG	CG	27.18	0.300	1
1	?	78	ARG	HG2	1.632	0.030	1
1	?	78	ARG	HG3	1.632	0.030	1
1	?	78	ARG	CD	43.51	0.300	1
1	?	78	ARG	HD2	3.184	0.030	1
1	?	78	ARG	HD3	3.184	0.030	1
1	?	78	ARG	C	176.951	0.300	1
1	?	79	ARG	N	120.69	0.300	1
1	?	79	ARG	H	8.118	0.030	1
1	?	79	ARG	HA	4.321	0.030	1
1	?	79	ARG	CB	30.93	0.300	1
1	?	79	ARG	HB2	1.85	0.030	2
1	?	79	ARG	HB3	1.76	0.030	2
1	?	79	ARG	CG	27.18	0.300	1
1	?	79	ARG	HG2	1.633	0.030	1
1	?	79	ARG	HG3	1.633	0.030	1
1	?	79	ARG	CD	43.51	0.300	1
1	?	79	ARG	HD2	3.184	0.030	1
1	?	79	ARG	HD3	3.184	0.030	1
1	?	80	LYS	N	122.438	0.300	1
1	?	80	LYS	H	8.325	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	80	LYS	CA	55.73	0.300	1
1	?	80	LYS	HA	4.298	0.030	1
1	?	80	LYS	CB	33.1	0.300	1
1	?	80	LYS	HB2	1.72	0.030	2
1	?	80	LYS	HB3	1.845	0.030	2
1	?	80	LYS	CG	24.865	0.300	1
1	?	80	LYS	HG2	1.398	0.030	1
1	?	80	LYS	HG3	1.398	0.030	1
1	?	80	LYS	CD	29.2	0.300	1
1	?	80	LYS	HD2	1.673	0.030	1
1	?	80	LYS	HD3	1.673	0.030	1
1	?	80	LYS	CE	42.2	0.300	1
1	?	80	LYS	HE2	2.989	0.030	1
1	?	80	LYS	HE3	2.989	0.030	1
1	?	80	LYS	C	175.933	0.300	1
1	?	81	ASN	N	120.84	0.300	1
1	?	81	ASN	H	8.493	0.030	1
1	?	81	ASN	CA	51.335	0.300	1
1	?	81	ASN	HA	4.951	0.030	1
1	?	81	ASN	CB	38.88	0.300	1
1	?	81	ASN	HB2	2.72	0.030	2
1	?	81	ASN	HB3	2.865	0.030	2
1	?	81	ASN	ND2	112.885	0.300	1
1	?	81	ASN	HD21	6.944	0.030	2
1	?	81	ASN	HD22	7.647	0.030	2
1	?	81	ASN	C	173.739	0.300	1
1	?	82	PRO	CA	63.36	0.300	1
1	?	82	PRO	HA	4.416	0.030	1
1	?	82	PRO	CB	31.793	0.300	1
1	?	82	PRO	HB2	2.02	0.030	2
1	?	82	PRO	HB3	2.288	0.030	2
1	?	82	PRO	CG	27.467	0.300	1
1	?	82	PRO	HG2	1.872	0.030	2
1	?	82	PRO	HG3	2.02	0.030	2
1	?	82	PRO	CD	50.732	0.300	1
1	?	82	PRO	HD2	3.62	0.030	2
1	?	82	PRO	HD3	3.82	0.030	2
1	?	82	PRO	C	176.857	0.300	1
1	?	83	GLN	N	120.646	0.300	1
1	?	83	GLN	H	8.444	0.030	1
1	?	83	GLN	CA	55.251	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	83	GLN	HA	4.388	0.030	1
1	?	83	GLN	CB	29.525	0.300	1
1	?	83	GLN	HB2	1.96	0.030	2
1	?	83	GLN	HB3	2.043	0.030	2
1	?	83	GLN	CG	33.85	0.300	1
1	?	83	GLN	HG2	2.388	0.030	2
1	?	83	GLN	HG3	2.271	0.030	2
1	?	83	GLN	NE2	111.89	0.300	1
1	?	83	GLN	HE21	7.455	0.030	2
1	?	83	GLN	HE22	6.811	0.030	2
1	?	83	GLN	C	175.944	0.300	1
1	?	84	GLU	N	121.252	0.300	1
1	?	84	GLU	H	8.108	0.030	1
1	?	84	GLU	CA	55.969	0.300	1
1	?	84	GLU	HA	4.272	0.030	1
1	?	84	GLU	CB	32.639	0.300	1
1	?	84	GLU	HB2	2.046	0.030	1
1	?	84	GLU	HB3	2.046	0.030	1
1	?	84	GLU	CG	36.3	0.300	1
1	?	84	GLU	HG2	2.246	0.030	1
1	?	84	GLU	HG3	2.246	0.030	1
1	?	84	GLU	C	177.163	0.300	1
1	?	85	GLY	N	109.441	0.300	1
1	?	85	GLY	H	8.325	0.030	1
1	?	85	GLY	CA	45.48	0.300	1
1	?	85	GLY	HA2	3.94	0.030	1
1	?	85	GLY	HA3	3.94	0.030	1
1	?	85	GLY	C	174.101	0.300	1
1	?	86	LEU	N	121.323	0.300	1
1	?	86	LEU	H	7.931	0.030	1
1	?	86	LEU	CA	55.228	0.300	1
1	?	86	LEU	HA	4.24	0.030	1
1	?	86	LEU	CB	42.35	0.300	1
1	?	86	LEU	HB2	1.425	0.030	2
1	?	86	LEU	HB3	1.517	0.030	2
1	?	86	LEU	CD1	23.535	0.300	2
1	?	86	LEU	HD11	0.84	0.030	2
1	?	86	LEU	HD12	0.84	0.030	2
1	?	86	LEU	HD13	0.84	0.030	2
1	?	86	LEU	CD2	24.893	0.300	2
1	?	86	LEU	HD21	0.86	0.030	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	86	LEU	HD22	0.86	0.030	2
1	?	86	LEU	HD23	0.86	0.030	2
1	?	86	LEU	C	177.197	0.300	1
1	?	87	TYR	N	119.264	0.300	1
1	?	87	TYR	H	8.105	0.030	1
1	?	87	TYR	CA	58.128	0.300	1
1	?	87	TYR	HA	4.513	0.030	1
1	?	87	TYR	CB	38.639	0.300	1
1	?	87	TYR	HB2	2.953	0.030	2
1	?	87	TYR	HB3	3.074	0.030	2
1	?	87	TYR	CD1	133.158	0.300	1
1	?	87	TYR	HD1	7.091	0.030	1
1	?	87	TYR	CD2	133.158	0.300	1
1	?	87	TYR	HD2	7.091	0.030	1
1	?	87	TYR	CE1	118.262	0.300	1
1	?	87	TYR	HE1	6.8	0.030	1
1	?	87	TYR	CE2	118.262	0.300	1
1	?	87	TYR	HE2	6.8	0.030	1
1	?	87	TYR	C	175.773	0.300	1
1	?	88	ASN	N	119.603	0.300	1
1	?	88	ASN	H	8.16	0.030	1
1	?	88	ASN	CA	53.196	0.300	1
1	?	88	ASN	HA	4.644	0.030	1
1	?	88	ASN	CB	38.96	0.300	1
1	?	88	ASN	HB2	2.75	0.030	2
1	?	88	ASN	HB3	2.799	0.030	2
1	?	88	ASN	ND2	112.398	0.300	1
1	?	88	ASN	HD21	6.836	0.030	2
1	?	88	ASN	HD22	7.566	0.030	2
1	?	88	ASN	C	175.44	0.300	1
1	?	89	GLU	N	121.5	0.300	1
1	?	89	GLU	H	8.062	0.030	1
1	?	89	GLU	CA	53.076	0.300	1
1	?	89	GLU	HA	4.273	0.030	1
1	?	89	GLU	CB	29.553	0.300	1
1	?	89	GLU	HB2	1.987	0.030	2
1	?	89	GLU	HB3	2.078	0.030	2
1	?	89	GLU	CG	36.3	0.300	1
1	?	89	GLU	HG2	2.288	0.030	1
1	?	89	GLU	HG3	2.288	0.030	1
1	?	89	GLU	C	176.663	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	90	LEU	N	121.161	0.300	1
1	?	90	LEU	H	8.047	0.030	1
1	?	90	LEU	CA	55.156	0.300	1
1	?	90	LEU	HA	4.273	0.030	1
1	?	90	LEU	CB	42.3	0.300	1
1	?	90	LEU	HB2	1.67	0.030	2
1	?	90	LEU	HB3	1.57	0.030	2
1	?	90	LEU	CD1	25.0	0.300	2
1	?	90	LEU	HD11	0.88	0.030	2
1	?	90	LEU	HD12	0.88	0.030	2
1	?	90	LEU	HD13	0.88	0.030	2
1	?	90	LEU	CD2	23.553	0.300	2
1	?	90	LEU	HD21	0.88	0.030	2
1	?	90	LEU	HD22	0.88	0.030	2
1	?	90	LEU	HD23	0.88	0.030	2
1	?	90	LEU	C	177.506	0.300	1
1	?	91	GLN	N	119.91	0.300	1
1	?	91	GLN	H	8.07	0.030	1
1	?	91	GLN	CA	55.371	0.300	1
1	?	91	GLN	HA	4.284	0.030	1
1	?	91	GLN	CB	28.879	0.300	1
1	?	91	GLN	HB2	1.995	0.030	2
1	?	91	GLN	HB3	2.123	0.030	2
1	?	91	GLN	CG	33.918	0.300	1
1	?	91	GLN	HG2	2.335	0.030	2
1	?	91	GLN	HG3	2.27	0.030	2
1	?	91	GLN	NE2	111.923	0.300	1
1	?	91	GLN	HE21	7.424	0.030	2
1	?	91	GLN	HE22	6.795	0.030	2
1	?	91	GLN	C	176.016	0.300	1
1	?	92	LYS	N	122.389	0.300	1
1	?	92	LYS	CA	56.686	0.300	1
1	?	92	LYS	HA	4.199	0.030	1
1	?	92	LYS	CB	30.93	0.300	1
1	?	92	LYS	HB2	1.796	0.030	1
1	?	92	LYS	HB3	1.796	0.030	1
1	?	92	LYS	CG	24.865	0.300	1
1	?	92	LYS	HG2	1.392	0.030	2
1	?	92	LYS	HG3	1.425	0.030	2
1	?	92	LYS	CD	29.2	0.300	1
1	?	92	LYS	HD2	1.673	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	92	LYS	HD3	1.673	0.030	1
1	?	92	LYS	CE	42.2	0.300	1
1	?	92	LYS	HE2	2.989	0.030	1
1	?	92	LYS	HE3	2.989	0.030	1
1	?	92	LYS	C	176.517	0.300	1
1	?	93	ASP	N	120.076	0.300	1
1	?	93	ASP	H	8.299	0.030	1
1	?	93	ASP	CA	54.319	0.300	1
1	?	93	ASP	HA	4.595	0.030	1
1	?	93	ASP	CB	40.95	0.300	1
1	?	93	ASP	HB2	2.674	0.030	2
1	?	93	ASP	HB3	2.711	0.030	2
1	?	93	ASP	C	176.352	0.300	1
1	?	94	LYS	N	120.791	0.300	1
1	?	94	LYS	H	8.042	0.030	1
1	?	94	LYS	CA	56.22	0.300	1
1	?	94	LYS	HA	4.283	0.030	1
1	?	94	LYS	CB	32.96	0.300	1
1	?	94	LYS	HB2	1.778	0.030	2
1	?	94	LYS	HB3	1.84	0.030	2
1	?	94	LYS	CG	24.865	0.300	1
1	?	94	LYS	HG2	1.43	0.030	1
1	?	94	LYS	HG3	1.43	0.030	1
1	?	94	LYS	CD	29.2	0.300	1
1	?	94	LYS	HD2	1.673	0.030	1
1	?	94	LYS	HD3	1.673	0.030	1
1	?	94	LYS	CE	42.209	0.300	1
1	?	94	LYS	HE2	2.988	0.030	1
1	?	94	LYS	HE3	2.988	0.030	1
1	?	94	LYS	C	176.945	0.300	1
1	?	95	VAL	N	120.646	0.300	1
1	?	95	VAL	H	7.984	0.030	1
1	?	95	VAL	CA	63.082	0.300	1
1	?	95	VAL	HA	4.01	0.030	1
1	?	95	VAL	CB	32.249	0.300	1
1	?	95	VAL	HB	2.101	0.030	1
1	?	95	VAL	CG1	21.1	0.300	2
1	?	95	VAL	HG11	0.94	0.030	2
1	?	95	VAL	HG12	0.94	0.030	2
1	?	95	VAL	HG13	0.94	0.030	2
1	?	95	VAL	CG2	21.1	0.300	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	95	VAL	HG21	0.94	0.030	2
1	?	95	VAL	HG22	0.94	0.030	2
1	?	95	VAL	HG23	0.94	0.030	2
1	?	95	VAL	C	176.12	0.300	1
1	?	96	ALA	N	126.055	0.300	1
1	?	96	ALA	H	8.195	0.030	1
1	?	96	ALA	CA	53.055	0.300	1
1	?	96	ALA	HA	4.254	0.030	1
1	?	96	ALA	CB	19.22	0.300	1
1	?	96	ALA	HB1	1.398	0.030	1
1	?	96	ALA	HB2	1.398	0.030	1
1	?	96	ALA	HB3	1.398	0.030	1
1	?	96	ALA	C	178.102	0.300	1
1	?	97	GLU	N	119.598	0.300	1
1	?	97	GLU	H	8.203	0.030	1
1	?	97	GLU	CA	56.507	0.300	1
1	?	97	GLU	HA	4.226	0.030	1
1	?	97	GLU	CB	29.678	0.300	1
1	?	97	GLU	HB2	1.978	0.030	1
1	?	97	GLU	HB3	1.978	0.030	1
1	?	97	GLU	CG	36.3	0.300	1
1	?	97	GLU	HG2	2.267	0.030	1
1	?	97	GLU	HG3	2.267	0.030	1
1	?	97	GLU	C	176.494	0.300	1
1	?	98	ALA	N	123.805	0.300	1
1	?	98	ALA	H	8.094	0.030	1
1	?	98	ALA	CA	53.053	0.300	1
1	?	98	ALA	HA	4.255	0.030	1
1	?	98	ALA	CB	19.22	0.300	1
1	?	98	ALA	HB1	1.322	0.030	1
1	?	98	ALA	HB2	1.322	0.030	1
1	?	98	ALA	HB3	1.322	0.030	1
1	?	98	ALA	C	177.669	0.300	1
1	?	99	TYR	N	118.634	0.300	1
1	?	99	TYR	H	8.05	0.030	1
1	?	99	TYR	CA	57.945	0.300	1
1	?	99	TYR	HA	4.521	0.030	1
1	?	99	TYR	CB	38.686	0.300	1
1	?	99	TYR	HB2	2.976	0.030	2
1	?	99	TYR	HB3	3.076	0.030	2
1	?	99	TYR	CD1	133.158	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	99	TYR	HD1	7.091	0.030	1
1	?	99	TYR	CD2	133.158	0.300	1
1	?	99	TYR	HD2	7.091	0.030	1
1	?	99	TYR	CE1	118.262	0.300	1
1	?	99	TYR	HE1	6.8	0.030	1
1	?	99	TYR	CE2	118.262	0.300	1
1	?	99	TYR	HE2	6.8	0.030	1
1	?	99	TYR	C	175.948	0.300	1
1	?	100	SER	N	116.634	0.300	1
1	?	100	SER	H	7.981	0.030	1
1	?	100	SER	CA	58.665	0.300	1
1	?	100	SER	HA	4.374	0.030	1
1	?	100	SER	CB	63.944	0.300	1
1	?	100	SER	HB2	3.811	0.030	2
1	?	100	SER	HB3	3.865	0.030	2
1	?	100	SER	C	174.304	0.300	1
1	?	101	GLU	N	122.355	0.300	1
1	?	101	GLU	H	8.274	0.030	1
1	?	101	GLU	CA	56.243	0.300	1
1	?	101	GLU	HA	4.34	0.030	1
1	?	101	GLU	CB	29.852	0.300	1
1	?	101	GLU	HB2	1.95	0.030	2
1	?	101	GLU	HB3	2.081	0.030	2
1	?	101	GLU	CG	36.25	0.300	1
1	?	101	GLU	HG2	2.26	0.030	1
1	?	101	GLU	HG3	2.26	0.030	1
1	?	101	GLU	C	176.428	0.300	1
1	?	102	ILE	N	120.076	0.300	1
1	?	102	ILE	H	7.954	0.030	1
1	?	102	ILE	CA	61.718	0.300	1
1	?	102	ILE	HA	4.146	0.030	1
1	?	102	ILE	CB	38.743	0.300	1
1	?	102	ILE	HB	1.875	0.030	1
1	?	102	ILE	CG1	27.5	0.300	1
1	?	102	ILE	HG12	1.497	0.030	2
1	?	102	ILE	HG13	1.195	0.030	2
1	?	102	ILE	CG2	17.615	0.300	1
1	?	102	ILE	HG21	0.91	0.030	1
1	?	102	ILE	HG22	0.91	0.030	1
1	?	102	ILE	HG23	0.91	0.030	1
1	?	102	ILE	CD1	13.161	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	102	ILE	HD11	0.856	0.030	1
1	?	102	ILE	HD12	0.856	0.030	1
1	?	102	ILE	HD13	0.856	0.030	1
1	?	102	ILE	C	176.697	0.300	1
1	?	103	GLY	N	111.727	0.300	1
1	?	103	GLY	H	8.306	0.030	1
1	?	103	GLY	CA	45.53	0.300	1
1	?	103	GLY	HA2	3.98	0.030	1
1	?	103	GLY	HA3	3.98	0.030	1
1	?	103	GLY	C	174.15	0.300	1
1	?	104	VAL	N	119.082	0.300	1
1	?	104	VAL	H	7.907	0.030	1
1	?	104	VAL	CA	62.56	0.300	1
1	?	104	VAL	HA	4.116	0.030	1
1	?	104	VAL	CB	32.647	0.300	1
1	?	104	VAL	HB	2.103	0.030	1
1	?	104	VAL	CG1	21.1	0.300	2
1	?	104	VAL	HG11	0.93	0.030	2
1	?	104	VAL	HG12	0.93	0.030	2
1	?	104	VAL	HG13	0.93	0.030	2
1	?	104	VAL	CG2	21.1	0.300	2
1	?	104	VAL	HG21	0.93	0.030	2
1	?	104	VAL	HG22	0.93	0.030	2
1	?	104	VAL	HG23	0.93	0.030	2
1	?	104	VAL	C	176.355	0.300	1
1	?	105	LYS	N	124.13	0.300	1
1	?	105	LYS	H	8.36	0.030	1
1	?	105	LYS	CA	56.243	0.300	1
1	?	105	LYS	HA	4.292	0.030	1
1	?	105	LYS	CB	30.93	0.300	1
1	?	105	LYS	HB2	1.85	0.030	2
1	?	105	LYS	HB3	1.756	0.030	2
1	?	105	LYS	CG	24.865	0.300	1
1	?	105	LYS	HG2	1.465	0.030	1
1	?	105	LYS	HG3	1.465	0.030	1
1	?	105	LYS	CD	29.2	0.300	1
1	?	105	LYS	HD2	1.663	0.030	1
1	?	105	LYS	HD3	1.663	0.030	1
1	?	105	LYS	CE	42.2	0.300	1
1	?	105	LYS	HE2	2.989	0.030	1
1	?	105	LYS	HE3	2.989	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	105	LYS	C	177.08	0.300	1
1	?	106	GLY	N	109.596	0.300	1
1	?	106	GLY	H	8.311	0.030	1
1	?	106	GLY	CA	44.937	0.300	1
1	?	106	GLY	HA2	3.953	0.030	1
1	?	106	GLY	HA3	3.953	0.030	1
1	?	106	GLY	C	174.022	0.300	1
1	?	107	GLU	N	120.61	0.300	1
1	?	107	GLU	H	8.228	0.030	1
1	?	107	GLU	CA	56.064	0.300	1
1	?	107	GLU	HA	4.283	0.030	1
1	?	107	GLU	CB	30.3	0.300	1
1	?	107	GLU	HB2	1.95	0.030	2
1	?	107	GLU	HB3	2.054	0.030	2
1	?	107	GLU	CG	36.3	0.300	1
1	?	107	GLU	HG2	2.26	0.030	1
1	?	107	GLU	HG3	2.26	0.030	1
1	?	107	GLU	C	176.519	0.300	1
1	?	108	ARG	N	122.051	0.300	1
1	?	108	ARG	H	8.358	0.030	1
1	?	108	ARG	HA	4.304	0.030	1
1	?	108	ARG	CB	30.93	0.300	1
1	?	108	ARG	HB2	1.85	0.030	2
1	?	108	ARG	HB3	1.79	0.030	2
1	?	108	ARG	CG	27.18	0.300	1
1	?	108	ARG	HG2	1.65	0.030	1
1	?	108	ARG	HG3	1.65	0.030	1
1	?	108	ARG	CD	43.5	0.300	1
1	?	108	ARG	HD2	3.184	0.030	1
1	?	108	ARG	HD3	3.184	0.030	1
1	?	108	ARG	HE	7.302	0.030	1
1	?	109	ARG	N	121.842	0.300	1
1	?	109	ARG	H	8.339	0.030	1
1	?	109	ARG	CB	30.93	0.300	1
1	?	109	ARG	HB2	1.85	0.030	2
1	?	109	ARG	HB3	1.76	0.030	2
1	?	109	ARG	CG	27.18	0.300	1
1	?	109	ARG	HG2	1.632	0.030	1
1	?	109	ARG	HG3	1.632	0.030	1
1	?	109	ARG	CD	43.51	0.300	1
1	?	109	ARG	HD2	3.184	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	109	ARG	HD3	3.184	0.030	1
1	?	110	ARG	N	121.837	0.300	1
1	?	110	ARG	H	8.319	0.030	1
1	?	110	ARG	CA	56.59	0.300	1
1	?	110	ARG	CB	30.93	0.300	1
1	?	110	ARG	HB2	1.85	0.030	2
1	?	110	ARG	HB3	1.76	0.030	2
1	?	110	ARG	CG	27.18	0.300	1
1	?	110	ARG	HG2	1.632	0.030	1
1	?	110	ARG	HG3	1.632	0.030	1
1	?	110	ARG	CD	43.51	0.300	1
1	?	110	ARG	HD2	3.184	0.030	1
1	?	110	ARG	HD3	3.184	0.030	1
1	?	110	ARG	C	176.946	0.300	1
1	?	111	GLY	N	109.405	0.300	1
1	?	111	GLY	H	8.48	0.030	1
1	?	111	GLY	CA	44.973	0.300	1
1	?	111	GLY	HA2	3.928	0.030	1
1	?	111	GLY	HA3	3.928	0.030	1
1	?	111	GLY	C	174.034	0.300	1
1	?	112	LYS	N	120.21	0.300	1
1	?	112	LYS	H	8.014	0.030	1
1	?	112	LYS	CA	55.706	0.300	1
1	?	112	LYS	HA	4.321	0.030	1
1	?	112	LYS	CB	30.93	0.300	1
1	?	112	LYS	HB2	1.85	0.030	2
1	?	112	LYS	HB3	1.756	0.030	2
1	?	112	LYS	CG	24.865	0.300	1
1	?	112	LYS	HG2	1.436	0.030	1
1	?	112	LYS	HG3	1.436	0.030	1
1	?	112	LYS	CD	29.2	0.300	1
1	?	112	LYS	HD2	1.646	0.030	1
1	?	112	LYS	HD3	1.646	0.030	1
1	?	112	LYS	CE	42.2	0.300	1
1	?	112	LYS	HE2	2.989	0.030	1
1	?	112	LYS	HE3	2.989	0.030	1
1	?	112	LYS	C	176.481	0.300	1
1	?	113	GLY	N	109.892	0.300	1
1	?	113	GLY	H	8.461	0.030	1
1	?	113	GLY	CA	44.829	0.300	1
1	?	113	GLY	HA2	3.972	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	113	GLY	HA3	3.972	0.030	1
1	?	113	GLY	C	173.93	0.300	1
1	?	114	HIS	H	8.403	0.030	1
1	?	114	HIS	CA	55.651	0.300	1
1	?	114	HIS	HA	4.713	0.030	1
1	?	114	HIS	CB	29.517	0.300	1
1	?	114	HIS	HB2	3.147	0.030	2
1	?	114	HIS	HB3	3.255	0.030	2
1	?	114	HIS	C	174.593	0.300	1
1	?	115	ASP	N	120.646	0.300	1
1	?	115	ASP	H	8.404	0.030	1
1	?	115	ASP	CA	54.821	0.300	1
1	?	115	ASP	HA	4.616	0.030	1
1	?	115	ASP	CB	41.21	0.300	1
1	?	115	ASP	HB2	2.674	0.030	1
1	?	115	ASP	HB3	2.674	0.030	1
1	?	115	ASP	C	176.826	0.300	1
1	?	116	GLY	N	108.59	0.300	1
1	?	116	GLY	H	8.42	0.030	1
1	?	116	GLY	CA	45.451	0.300	1
1	?	116	GLY	HA2	3.969	0.030	1
1	?	116	GLY	HA3	3.969	0.030	1
1	?	116	GLY	C	174.93	0.300	1
1	?	117	LEU	N	121.725	0.300	1
1	?	117	LEU	H	8.131	0.030	1
1	?	117	LEU	CA	56.231	0.300	1
1	?	117	LEU	CB	41.647	0.300	1
1	?	117	LEU	HB2	1.579	0.030	2
1	?	117	LEU	HB3	1.625	0.030	2
1	?	117	LEU	CD1	25.15	0.300	2
1	?	117	LEU	HD11	0.903	0.030	2
1	?	117	LEU	HD12	0.903	0.030	2
1	?	117	LEU	HD13	0.903	0.030	2
1	?	117	LEU	CD2	23.533	0.300	2
1	?	117	LEU	HD21	0.84	0.030	2
1	?	117	LEU	HD22	0.84	0.030	2
1	?	117	LEU	HD23	0.84	0.030	2
1	?	117	LEU	C	177.481	0.300	1
1	?	118	TYR	N	118.623	0.300	1
1	?	118	TYR	H	8.213	0.030	1
1	?	118	TYR	CA	58.909	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	118	TYR	HA	4.235	0.030	1
1	?	118	TYR	CB	38.58	0.300	1
1	?	118	TYR	HB2	3.065	0.030	1
1	?	118	TYR	HB3	3.065	0.030	1
1	?	118	TYR	CD1	133.158	0.300	1
1	?	118	TYR	HD1	7.091	0.030	1
1	?	118	TYR	CD2	133.158	0.300	1
1	?	118	TYR	HD2	7.091	0.030	1
1	?	118	TYR	CE1	118.262	0.300	1
1	?	118	TYR	HE1	6.8	0.030	1
1	?	118	TYR	CE2	118.262	0.300	1
1	?	118	TYR	HE2	6.8	0.030	1
1	?	118	TYR	C	176.996	0.300	1
1	?	119	GLN	N	121.467	0.300	1
1	?	119	GLN	H	8.088	0.030	1
1	?	119	GLN	CA	56.949	0.300	1
1	?	119	GLN	HA	4.254	0.030	1
1	?	119	GLN	CB	28.707	0.300	1
1	?	119	GLN	HB2	1.929	0.030	2
1	?	119	GLN	HB3	2.066	0.030	2
1	?	119	GLN	CG	33.826	0.300	1
1	?	119	GLN	HG2	2.263	0.030	1
1	?	119	GLN	HG3	2.263	0.030	1
1	?	119	GLN	NE2	111.894	0.300	1
1	?	119	GLN	HE21	7.435	0.030	2
1	?	119	GLN	HE22	6.81	0.030	2
1	?	119	GLN	C	177.37	0.300	1
1	?	120	GLY	N	108.64	0.300	1
1	?	120	GLY	H	7.908	0.030	1
1	?	120	GLY	CA	45.678	0.300	1
1	?	120	GLY	HA2	3.902	0.030	1
1	?	120	GLY	HA3	3.902	0.030	1
1	?	120	GLY	C	174.877	0.300	1
1	?	121	LEU	N	121.218	0.300	1
1	?	121	LEU	H	8.02	0.030	1
1	?	121	LEU	CA	56.064	0.300	1
1	?	121	LEU	HA	4.282	0.030	1
1	?	121	LEU	CB	41.522	0.300	1
1	?	121	LEU	HB2	1.72	0.030	1
1	?	121	LEU	HB3	1.72	0.030	1
1	?	121	LEU	CD1	23.7	0.300	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	121	LEU	HD11	0.86	0.030	2
1	?	121	LEU	HD12	0.86	0.030	2
1	?	121	LEU	HD13	0.86	0.030	2
1	?	121	LEU	CD2	25.3	0.300	2
1	?	121	LEU	HD21	0.894	0.030	2
1	?	121	LEU	HD22	0.894	0.030	2
1	?	121	LEU	HD23	0.894	0.030	2
1	?	121	LEU	C	178.371	0.300	1
1	?	122	SER	N	116.204	0.300	1
1	?	122	SER	H	8.375	0.030	1
1	?	122	SER	CA	59.71	0.300	1
1	?	122	SER	HA	4.295	0.030	1
1	?	122	SER	CB	63.9	0.300	1
1	?	122	SER	HB2	3.893	0.030	1
1	?	122	SER	HB3	3.893	0.030	1
1	?	122	SER	C	175.76	0.300	1
1	?	123	THR	N	116.345	0.300	1
1	?	123	THR	H	8.117	0.030	1
1	?	123	THR	CA	63.594	0.300	1
1	?	123	THR	HA	4.156	0.030	1
1	?	123	THR	CB	69.79	0.300	1
1	?	123	THR	HB	4.288	0.030	1
1	?	123	THR	CG2	21.83	0.300	1
1	?	123	THR	HG21	1.25	0.030	1
1	?	123	THR	HG22	1.25	0.030	1
1	?	123	THR	HG23	1.25	0.030	1
1	?	123	THR	C	174.988	0.300	1
1	?	124	ALA	N	124.78	0.300	1
1	?	124	ALA	H	8.006	0.030	1
1	?	124	ALA	CA	52.757	0.300	1
1	?	124	ALA	HA	4.395	0.030	1
1	?	124	ALA	CB	19.002	0.300	1
1	?	124	ALA	HB1	1.455	0.030	1
1	?	124	ALA	HB2	1.455	0.030	1
1	?	124	ALA	HB3	1.455	0.030	1
1	?	124	ALA	C	178.988	0.300	1
1	?	125	THR	N	113.622	0.300	1
1	?	125	THR	H	8.078	0.030	1
1	?	125	THR	CA	64.706	0.300	1
1	?	125	THR	HA	4.092	0.030	1
1	?	125	THR	CB	69.813	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	125	THR	HB	4.226	0.030	1
1	?	125	THR	CG2	21.893	0.300	1
1	?	125	THR	HG21	1.204	0.030	1
1	?	125	THR	HG22	1.204	0.030	1
1	?	125	THR	HG23	1.204	0.030	1
1	?	125	THR	C	175.204	0.300	1
1	?	126	LYS	N	123.683	0.300	1
1	?	126	LYS	H	8.012	0.030	1
1	?	126	LYS	CA	57.618	0.300	1
1	?	126	LYS	HA	4.283	0.030	1
1	?	126	LYS	CB	30.93	0.300	1
1	?	126	LYS	HB2	1.85	0.030	2
1	?	126	LYS	HB3	1.756	0.030	2
1	?	126	LYS	CG	24.865	0.300	1
1	?	126	LYS	HG2	1.436	0.030	1
1	?	126	LYS	HG3	1.436	0.030	1
1	?	126	LYS	CD	29.2	0.300	1
1	?	126	LYS	HD2	1.673	0.030	1
1	?	126	LYS	HD3	1.673	0.030	1
1	?	126	LYS	CE	42.2	0.300	1
1	?	126	LYS	HE2	2.989	0.030	1
1	?	126	LYS	HE3	2.989	0.030	1
1	?	127	ASP	N	119.678	0.300	1
1	?	127	ASP	H	8.469	0.030	1
1	?	127	ASP	CA	55.491	0.300	1
1	?	127	ASP	HA	4.657	0.030	1
1	?	127	ASP	CB	41.0	0.300	1
1	?	127	ASP	HB2	2.705	0.030	1
1	?	127	ASP	HB3	2.705	0.030	1
1	?	127	ASP	C	177.78	0.300	1
1	?	128	THR	N	115.656	0.300	1
1	?	128	THR	H	7.934	0.030	1
1	?	128	THR	CA	64.597	0.300	1
1	?	128	THR	HA	4.097	0.030	1
1	?	128	THR	CB	69.927	0.300	1
1	?	128	THR	HB	4.153	0.030	1
1	?	128	THR	CG2	21.83	0.300	1
1	?	128	THR	HG21	1.159	0.030	1
1	?	128	THR	HG22	1.159	0.030	1
1	?	128	THR	HG23	1.159	0.030	1
1	?	129	TYR	N	122.526	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	129	TYR	CA	59.877	0.300	1
1	?	129	TYR	CB	38.218	0.300	1
1	?	129	TYR	CD1	133.158	0.300	1
1	?	129	TYR	HD1	7.091	0.030	1
1	?	129	TYR	CD2	133.158	0.300	1
1	?	129	TYR	HD2	7.091	0.030	1
1	?	129	TYR	CE1	118.262	0.300	1
1	?	129	TYR	HE1	6.8	0.030	1
1	?	129	TYR	CE2	118.262	0.300	1
1	?	129	TYR	HE2	6.8	0.030	1
1	?	129	TYR	C	176.943	0.300	1
1	?	130	ASP	N	121.568	0.300	1
1	?	130	ASP	CA	55.466	0.300	1
1	?	130	ASP	HA	4.445	0.030	1
1	?	130	ASP	CB	40.404	0.300	1
1	?	130	ASP	HB2	2.705	0.030	1
1	?	130	ASP	HB3	2.705	0.030	1
1	?	130	ASP	C	177.279	0.300	1
1	?	131	ALA	N	122.35	0.300	1
1	?	131	ALA	H	7.927	0.030	1
1	?	131	ALA	CA	53.774	0.300	1
1	?	131	ALA	HA	4.165	0.030	1
1	?	131	ALA	CB	18.896	0.300	1
1	?	131	ALA	HB1	1.474	0.030	1
1	?	131	ALA	HB2	1.474	0.030	1
1	?	131	ALA	HB3	1.474	0.030	1
1	?	131	ALA	C	178.522	0.300	1
1	?	132	LEU	N	117.089	0.300	1
1	?	132	LEU	H	7.799	0.030	1
1	?	132	LEU	CA	55.192	0.300	1
1	?	132	LEU	HA	4.207	0.030	1
1	?	132	LEU	CB	41.696	0.300	1
1	?	132	LEU	HB2	1.698	0.030	1
1	?	132	LEU	HB3	1.698	0.030	1
1	?	132	LEU	CD1	25.144	0.300	2
1	?	132	LEU	HD11	0.911	0.030	2
1	?	132	LEU	HD12	0.911	0.030	2
1	?	132	LEU	HD13	0.911	0.030	2
1	?	132	LEU	CD2	25.3	0.300	2
1	?	132	LEU	HD21	0.865	0.030	2
1	?	132	LEU	HD22	0.865	0.030	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	132	LEU	HD23	0.865	0.030	2
1	?	132	LEU	C	177.203	0.300	1
1	?	133	HIS	N	117.145	0.300	1
1	?	133	HIS	H	7.971	0.030	1
1	?	133	HIS	CA	55.925	0.300	1
1	?	133	HIS	HA	4.567	0.030	1
1	?	133	HIS	CB	28.807	0.300	1
1	?	133	HIS	HB2	3.217	0.030	2
1	?	133	HIS	HB3	3.0	0.030	2
1	?	133	HIS	C	174.522	0.300	1
1	?	134	VAL	N	119.737	0.300	1
1	?	134	VAL	H	7.868	0.030	1
1	?	134	VAL	CA	63.052	0.300	1
1	?	134	VAL	HA	4.032	0.030	1
1	?	134	VAL	CB	32.174	0.300	1
1	?	134	VAL	HB	2.081	0.030	1
1	?	134	VAL	CG1	21.1	0.300	2
1	?	134	VAL	HG11	0.933	0.030	2
1	?	134	VAL	HG12	0.933	0.030	2
1	?	134	VAL	HG13	0.933	0.030	2
1	?	134	VAL	CG2	21.1	0.300	2
1	?	134	VAL	HG21	0.933	0.030	2
1	?	134	VAL	HG22	0.933	0.030	2
1	?	134	VAL	HG23	0.933	0.030	2
1	?	134	VAL	C	176.088	0.300	1
1	?	135	GLN	N	122.925	0.300	1
1	?	135	GLN	H	8.281	0.030	1
1	?	135	GLN	CA	55.699	0.300	1
1	?	135	GLN	HA	4.331	0.030	1
1	?	135	GLN	CB	29.365	0.300	1
1	?	135	GLN	HB2	2.065	0.030	2
1	?	135	GLN	HB3	1.98	0.030	2
1	?	135	GLN	CG	33.886	0.300	1
1	?	135	GLN	HG2	2.355	0.030	1
1	?	135	GLN	HG3	2.355	0.030	1
1	?	135	GLN	NE2	111.9	0.300	1
1	?	135	GLN	HE21	7.484	0.030	2
1	?	135	GLN	HE22	6.806	0.030	2
1	?	135	GLN	C	175.341	0.300	1
1	?	136	ALA	N	124.754	0.300	1
1	?	136	ALA	H	8.137	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	136	ALA	CA	52.313	0.300	1
1	?	136	ALA	HA	4.315	0.030	1
1	?	136	ALA	CB	19.37	0.300	1
1	?	136	ALA	HB1	1.37	0.030	1
1	?	136	ALA	HB2	1.37	0.030	1
1	?	136	ALA	HB3	1.37	0.030	1
1	?	136	ALA	C	177.089	0.300	1
1	?	137	LEU	N	122.29	0.300	1
1	?	137	LEU	H	8.043	0.030	1
1	?	137	LEU	CA	52.86	0.300	1
1	?	137	LEU	HA	4.607	0.030	1
1	?	137	LEU	CB	42.06	0.300	1
1	?	137	LEU	HB2	1.545	0.030	2
1	?	137	LEU	HB3	1.66	0.030	2
1	?	137	LEU	CD1	25.221	0.300	2
1	?	137	LEU	HD11	0.91	0.030	2
1	?	137	LEU	HD12	0.91	0.030	2
1	?	137	LEU	HD13	0.91	0.030	2
1	?	137	LEU	CD2	25.221	0.300	2
1	?	137	LEU	HD21	0.91	0.030	2
1	?	137	LEU	HD22	0.91	0.030	2
1	?	137	LEU	HD23	0.91	0.030	2
1	?	137	LEU	C	174.697	0.300	1
1	?	138	PRO	CB	32.092	0.300	1
1	?	138	PRO	HB2	2.012	0.030	1
1	?	138	PRO	HB3	2.012	0.030	1
1	?	138	PRO	CG	27.467	0.300	1
1	?	138	PRO	HG2	1.998	0.030	1
1	?	138	PRO	HG3	1.998	0.030	1
1	?	138	PRO	CD	50.454	0.300	1
1	?	138	PRO	HD2	3.608	0.030	2
1	?	138	PRO	HD3	3.842	0.030	2
1	?	139	PRO	CA	63.278	0.300	1
1	?	139	PRO	HA	4.422	0.030	1
1	?	139	PRO	CB	32.241	0.300	1
1	?	139	PRO	HB2	2.251	0.030	2
1	?	139	PRO	HB3	1.981	0.030	2
1	?	139	PRO	HG2	1.932	0.030	1
1	?	139	PRO	HG3	1.932	0.030	1
1	?	139	PRO	C	176.129	0.300	1
1	?	140	ARG	N	125.98	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	140	ARG	H	7.854	0.030	1
1	?	140	ARG	CA	56.901	0.300	1
1	?	140	ARG	HA	4.169	0.030	1
1	?	140	ARG	CB	30.93	0.300	1
1	?	140	ARG	HB2	1.85	0.030	2
1	?	140	ARG	HB3	1.76	0.030	2
1	?	140	ARG	CG	27.18	0.300	1
1	?	140	ARG	HG2	1.693	0.030	2
1	?	140	ARG	HG3	1.632	0.030	2
1	?	140	ARG	CD	43.51	0.300	1
1	?	140	ARG	HD2	3.184	0.030	1
1	?	140	ARG	HD3	3.184	0.030	1
1	?	140	ARG	C	180.978	0.300	1

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	102	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	94	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	100	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{15}\text{N}$	98	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1420. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/512 (0%)	0/211 (0%)	0/204 (0%)	0/97 (0%)
Sidechain	0/831 (0%)	0/525 (0%)	0/251 (0%)	0/55 (0%)
Aromatic	0/77 (0%)	0/36 (0%)	0/39 (0%)	0/2 (0%)
Overall	0/1420 (0%)	0/772 (0%)	0/494 (0%)	0/154 (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](#)

The image below reports *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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain ?:

