



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 11:46 PM BST

PDB ID : 2KUG  
Title : Halothane binds to druggable sites in calcium-calmodulin: Solution Structure of halothane-CaM N-terminal domain  
Authors : Juranic, N.; Macura, S.; Simeonov, M.V.; Jones, K.A.; Penheiter, A.R.; Hock, T.J.; Streiff, J.H.  
Deposited on : 2010-02-17

This is a Full wwPDB NMR Structure Validation 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  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

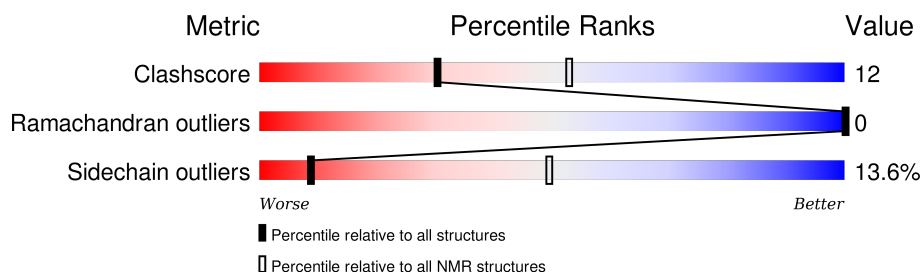
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 92%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	76	

## 2 Ensemble composition and analysis

This entry contains 5 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:4-A:73 (70)	0.26	5

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1161 atoms, of which 563 are hydrogens and 0 are deuteriums.

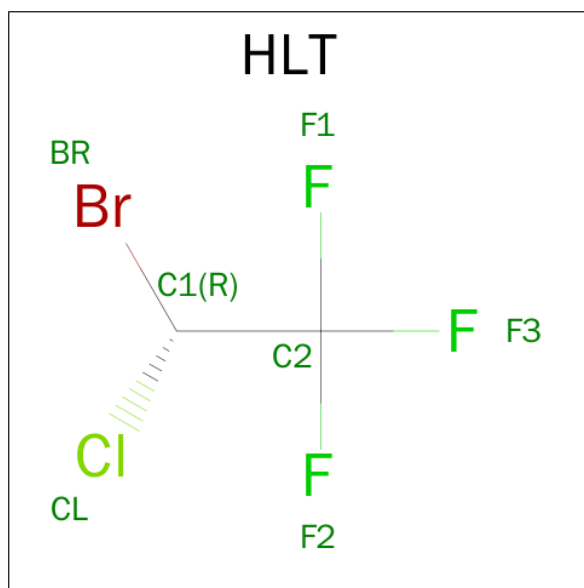
- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1151	363	562	93	128	5	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is 2-BROMO-2-CHLORO-1,1,1-TRIFLUOROETHANE (three-letter code: HLT) (formula: C<sub>2</sub>HBrClF<sub>3</sub>).



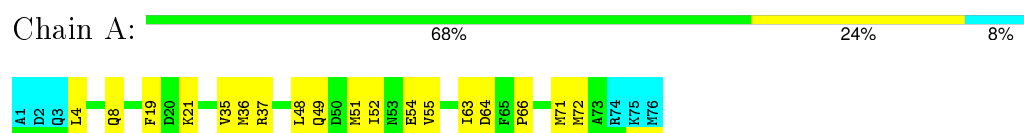
Mol	Chain	Residues	Atoms					
3	A	1	Total	Br	C	Cl	F	H
			8	1	2	1	3	1

## 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: Calmodulin

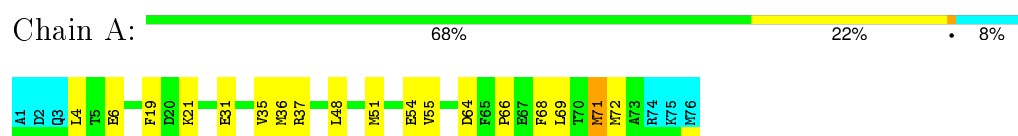


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

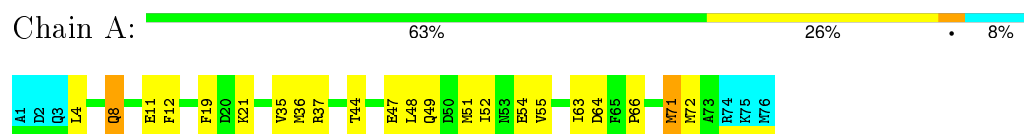
#### 4.2.1 Score per residue for model 1

- Molecule 1: Calmodulin



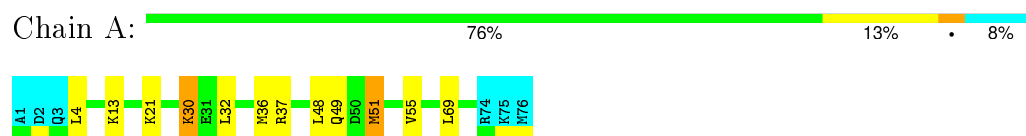
#### 4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin



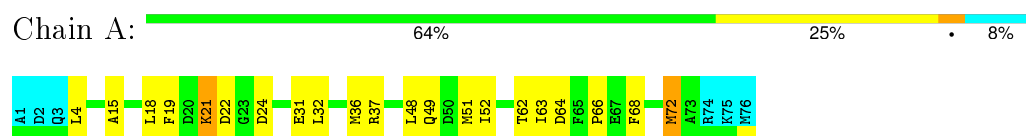
### 4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin



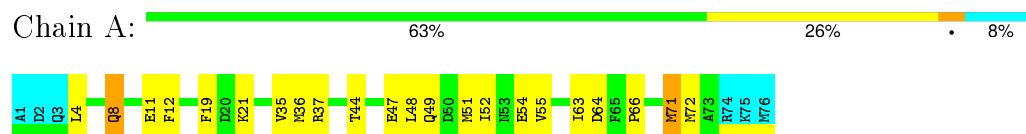
### 4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin



### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Calmodulin



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, CHARMM22 energy minimization*.

Of the 50 calculated structures, 5 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	geometry optimization	MSI XPLOR 3.843
X-PLOR	refinement	MSI XPLOR 3.843

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

Chemical shift file(s)	BMRB entry 16764
Number of chemical shift lists	1
Total number of shifts	1801
Number of shifts mapped to atoms	922
Number of unparsed shifts	2
Number of shifts with mapping errors	877
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HLT

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	538	508	508	12±3
3	A	7	1	0	6±2
All	All	2735	2545	2540	62

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:MET:CE	3:A:149:HLT:BR	1.25	2.40	1	3
1:A:71:MET:SD	3:A:149:HLT:BR	1.13	2.60	1	1
1:A:36:MET:CE	3:A:149:HLT:BR	1.10	2.54	5	4
1:A:71:MET:HE1	3:A:149:HLT:BR	1.07	2.04	1	3
1:A:36:MET:SD	3:A:149:HLT:CL	1.00	2.57	1	1
1:A:36:MET:HE1	3:A:149:HLT:BR	0.98	2.13	5	3
1:A:71:MET:HE2	3:A:149:HLT:BR	0.93	2.16	2	2
1:A:36:MET:SD	3:A:149:HLT:BR	0.82	2.92	5	4
1:A:51:MET:SD	3:A:149:HLT:CL	0.72	2.84	1	1
1:A:71:MET:HE3	3:A:149:HLT:BR	0.60	2.45	1	1
1:A:36:MET:HE1	3:A:149:HLT:F2	0.60	1.86	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:MET:HE3	3:A:149:HLT:BR	0.58	2.53	2	4
1:A:36:MET:SD	3:A:149:HLT:F2	0.58	2.51	1	1
1:A:32:LEU:HD21	3:A:149:HLT:BR	0.57	2.54	3	1
1:A:19:PHE:CD1	1:A:35:VAL:HG22	0.56	2.36	5	3
1:A:54:GLU:HG3	1:A:55:VAL:HG13	0.53	1.81	1	3
1:A:68:PHE:CE1	1:A:72:MET:SD	0.52	3.02	4	1
1:A:36:MET:CE	3:A:149:HLT:F2	0.50	2.49	1	1
1:A:12:PHE:CE1	1:A:72:MET:SD	0.49	3.05	2	2
1:A:64:ASP:CG	1:A:66:PRO:HD2	0.49	2.28	5	4
1:A:15:ALA:HA	1:A:18:LEU:HD12	0.48	1.84	4	1
1:A:51:MET:HB3	3:A:149:HLT:CL	0.47	2.46	3	1
1:A:31:GLU:O	1:A:35:VAL:HG23	0.47	2.10	1	1
1:A:30:LYS:HA	1:A:48:LEU:HD23	0.47	1.85	3	1
1:A:51:MET:O	1:A:55:VAL:HG22	0.46	2.11	1	2
1:A:71:MET:SD	1:A:72:MET:SD	0.44	3.16	1	1
1:A:8:GLN:HA	1:A:11:GLU:OE1	0.43	2.13	2	2
1:A:21:LYS:HE3	1:A:31:GLU:OE2	0.43	2.13	4	1
1:A:44:THR:HB	1:A:47:GLU:OE1	0.42	2.14	2	2
1:A:52:ILE:HG23	1:A:63:ILE:HG12	0.42	1.90	4	3
1:A:22:ASP:OD1	1:A:24:ASP:CG	0.41	2.59	4	1
1:A:19:PHE:CE2	1:A:68:PHE:CE1	0.41	3.08	4	1
1:A:19:PHE:HE2	1:A:68:PHE:CE1	0.40	2.35	1	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	70/76 (92%)	67±0 (95±1%)	3±0 (5±1%)	0±0 (0±0%)		
All	All	350/380 (92%)	333 (95%)	17 (5%)	0 (0%)		

There are no Ramachandran outliers.

### 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	59/64 (92%)	51±1 (86±1%)	8±1 (14±1%)	9	49
All	All	295/320 (92%)	255 (86%)	40 (14%)	9	49

All 15 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	37	ARG	5
1	A	21	LYS	5
1	A	4	LEU	5
1	A	51	MET	4
1	A	48	LEU	4
1	A	49	GLN	4
1	A	71	MET	3
1	A	8	GLN	2
1	A	69	LEU	2
1	A	72	MET	1
1	A	32	LEU	1
1	A	13	LYS	1
1	A	30	LYS	1
1	A	62	THR	1
1	A	6	GLU	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	HLT	A	149	-	4,6,6	1.44±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	HLT	A	149	-	3,9,9	1.14±0.00	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HLT	A	149	-	-	0±0,3,6,6	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 91% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 16764

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1801
Number of shifts mapped to atoms	922
Number of unparsed shifts	2
Number of shifts with mapping errors	877
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Chemical shift has been reported more than once. All 2 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1800	UNMAPPED	1	HAL	CA	53.60	0.10	1
1801	UNMAPPED	1	HAL	HA	6.30	0.05	1

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

- Residue not found in structure. All 875 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	141	PHE	CA	61.84	0.1	1
A	144	MET	N	119.0	0.1	1
A	109	MET	N	116.22	0.1	1
A	85	ILE	N	122.02	0.1	1
A	138	TYR	HD1	6.17	0.05	1
A	119	GLU	CA	59.8	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	120	GLU	CG	36.3	0.1	1
A	97	ASN	HB2	2.57	0.05	2
A	83	GLU	C	175.47	0.1	1
A	120	GLU	C	178.63	0.1	1
A	87	GLU	H	8.06	0.05	1
A	115	LYS	HB3	1.68	0.05	2
A	148	LYS	CB	33.6	0.1	1
A	117	THR	HG21	1.24	0.05	1
A	124	MET	HA	3.96	0.05	1
A	89	PHE	HB2	3.13	0.05	2
A	77	LYS	HG3	1.38	0.05	2
A	87	GLU	C	177.93	0.1	1
A	106	ARG	N	117.73	0.1	1
A	107	HIS	HD2	6.96	0.05	1
A	110	THR	HG21	1.14	0.05	1
A	119	GLU	C	175.51	0.1	1
A	122	ASP	HA	4.23	0.05	1
A	122	ASP	CA	57.6	0.1	1
A	100	ILE	HD12	0.23	0.05	1
A	83	GLU	CA	59.7	0.1	1
A	109	MET	HE2	1.95	0.05	1
A	102	ALA	HB2	1.37	0.05	1
A	92	PHE	CD2	130.3	0.1	1
A	111	ASN	ND2	111.4	0.1	1
A	96	GLY	HA2	3.72	0.05	1
A	141	PHE	N	124.67	0.1	1
A	109	MET	CA	57.7	0.1	1
A	135	GLN	CG	32.8	0.1	1
A	119	GLU	N	119.1	0.1	1
A	114	GLU	N	120.54	0.1	1
A	137	ASN	N	128.9	0.1	1
A	130	ILE	HB	1.9	0.05	1
A	89	PHE	CE1	131.3	0.1	1
A	143	GLN	H	7.38	0.05	1
A	92	PHE	CB	40.5	0.1	1
A	136	VAL	C	172.85	0.1	1
A	95	ASP	HA	4.46	0.05	1
A	120	GLU	HB2	2.33	0.05	2
A	92	PHE	CZ	130.1	0.1	1
A	112	LEU	HD12	0.72	0.05	1
A	128	ALA	CA	52.1	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	123	GLU	HB3	2.2	0.05	2
A	112	LEU	CG	26.6	0.1	1
A	112	LEU	HG	1.7	0.05	1
A	107	HIS	H	7.83	0.05	1
A	90	ARG	N	115.76	0.1	1
A	121	VAL	HG11	0.93	0.05	1
A	81	SER	HB3	3.97	0.05	2
A	122	ASP	N	119.53	0.1	1
A	140	GLU	CG	36.8	0.1	1
A	137	ASN	ND2	108.1	0.1	1
A	120	GLU	H	7.68	0.05	1
A	124	MET	C	179.26	0.1	1
A	92	PHE	HE1	6.95	0.05	1
A	104	GLU	C	179.34	0.1	1
A	100	ILE	CD1	15.4	0.1	1
A	105	LEU	C	181.48	0.1	1
A	85	ILE	CB	37.3	0.1	1
A	112	LEU	HD21	0.76	0.05	1
A	119	GLU	HB2	1.83	0.05	2
A	95	ASP	H	8.09	0.05	1
A	92	PHE	H	7.28	0.05	1
A	100	ILE	CG1	27.0	0.1	1
A	138	TYR	HE1	6.39	0.05	1
A	84	GLU	HG3	2.24	0.05	2
A	129	ASP	HB2	2.39	0.05	2
A	122	ASP	HB2	2.53	0.05	2
A	99	TYR	HB2	2.4	0.05	2
A	94	LYS	HB3	1.75	0.05	2
A	107	HIS	CB	30.8	0.1	1
A	95	ASP	HB2	2.56	0.05	2
A	114	GLU	H	7.86	0.05	1
A	139	GLU	HG2	2.22	0.05	2
A	138	TYR	CB	37.5	0.1	1
A	107	HIS	N	118.4	0.1	1
A	105	LEU	CD1	26.3	0.1	1
A	103	ALA	C	175.24	0.1	1
A	139	GLU	HB3	1.84	0.05	2
A	96	GLY	C	178.32	0.1	1
A	98	GLY	HA3	3.93	0.05	1
A	126	ARG	HD2	3.12	0.05	2
A	103	ALA	HB3	1.33	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	133	ASP	CA	53.8	0.1	1
A	104	GLU	HB3	2.23	0.05	2
A	104	GLU	CB	29.18	0.1	1
A	85	ILE	H	7.94	0.05	1
A	95	ASP	CB	39.65	0.1	1
A	145	MET	CE	17.18	0.1	1
A	141	PHE	CB	39.9	0.1	1
A	133	ASP	HB3	2.88	0.05	2
A	144	MET	CA	58.2	0.1	1
A	142	VAL	HG22	0.64	0.05	1
A	122	ASP	H	7.96	0.05	1
A	116	LEU	CB	44.8	0.1	1
A	89	PHE	HA	3.04	0.05	1
A	131	ASP	HB3	2.55	0.05	2
A	138	TYR	HD2	6.17	0.05	1
A	83	GLU	HB3	1.99	0.05	2
A	144	MET	HE2	1.81	0.05	1
A	125	ILE	HD13	0.61	0.05	1
A	119	GLU	CB	29.0	0.1	1
A	105	LEU	HA	4.05	0.05	1
A	107	HIS	HB3	3.16	0.05	2
A	143	GLN	HG2	2.31	0.05	2
A	78	ASP	HB2	2.67	0.05	2
A	114	GLU	CB	30.62	0.1	1
A	105	LEU	HB3	1.43	0.05	2
A	135	GLN	H	7.86	0.05	1
A	79	THR	CG2	21.6	0.1	1
A	146	THR	HB	4.17	0.05	1
A	138	TYR	H	8.34	0.05	1
A	101	SER	H	8.85	0.05	1
A	100	ILE	HG21	0.83	0.05	1
A	143	GLN	HE22	6.67	0.05	1
A	148	LYS	CG	24.6	0.1	1
A	94	LYS	HE3	2.72	0.05	1
A	87	GLU	CG	36.5	0.1	1
A	104	GLU	H	7.8	0.05	1
A	139	GLU	CB	28.8	0.1	1
A	107	HIS	CD2	120.4	0.1	1
A	93	ASP	HB2	2.2	0.05	2
A	148	LYS	HD3	1.56	0.05	2
A	107	HIS	HD1	6.38	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	85	ILE	CG2	19.2	0.1	1
A	123	GLU	HB2	1.93	0.05	2
A	128	ALA	HB3	1.33	0.05	1
A	133	ASP	N	120.81	0.1	1
A	94	LYS	HG3	1.34	0.05	2
A	122	ASP	CB	40.3	0.1	1
A	116	LEU	H	8.07	0.05	1
A	111	ASN	CA	55.5	0.1	1
A	131	ASP	CB	39.7	0.1	1
A	79	THR	HG23	1.11	0.05	1
A	92	PHE	CD1	130.3	0.1	1
A	77	LYS	CE	42.0	0.1	1
A	147	ALA	HB3	1.32	0.05	1
A	103	ALA	HA	3.97	0.05	1
A	127	GLU	HG2	2.26	0.05	2
A	84	GLU	C	175.12	0.1	1
A	117	THR	C	175.7	0.1	1
A	132	GLY	N	108.56	0.1	1
A	135	GLN	CB	32.6	0.1	1
A	114	GLU	C	177.23	0.1	1
A	146	THR	C	178.13	0.1	1
A	99	TYR	N	115.89	0.1	1
A	88	ALA	CA	55.1	0.1	1
A	91	VAL	N	118.21	0.1	1
A	145	MET	HA	4.2	0.05	1
A	83	GLU	HA	3.96	0.05	1
A	130	ILE	HG12	1.22	0.05	1
A	89	PHE	CE2	131.3	0.1	1
A	119	GLU	HG2	2.2	0.05	2
A	145	MET	HE1	1.72	0.05	1
A	111	ASN	HD21	6.4	0.05	2
A	97	ASN	CB	38.1	0.1	1
A	85	ILE	CD1	13.2	0.1	1
A	120	GLU	HB3	1.82	0.05	2
A	112	LEU	HD11	0.72	0.05	1
A	126	ARG	HG3	1.67	0.05	2
A	112	LEU	CB	42.1	0.1	1
A	124	MET	HG2	2.39	0.05	2
A	90	ARG	HB3	1.84	0.05	2
A	92	PHE	HA	4.12	0.05	1
A	93	ASP	CA	52.33	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	129	ASP	N	117.54	0.1	1
A	111	ASN	N	122.24	0.1	1
A	82	GLU	CG	36.2	0.1	1
A	126	ARG	CD	43.43	0.1	1
A	118	ASP	N	120.99	0.1	1
A	95	ASP	N	114.02	0.1	1
A	105	LEU	HD22	0.87	0.05	1
A	125	ILE	CB	36.4	0.1	1
A	101	SER	C	174.58	0.1	1
A	132	GLY	CA	47.55	0.1	1
A	109	MET	CE	17.5	0.1	1
A	77	LYS	HD3	1.55	0.05	2
A	116	LEU	HD13	0.7	0.05	1
A	102	ALA	CB	18.0	0.1	1
A	140	GLU	CB	29.4	0.1	1
A	146	THR	CG2	21.6	0.1	1
A	86	ARG	HG2	1.63	0.05	2
A	112	LEU	H	7.83	0.05	1
A	107	HIS	CA	59.7	0.1	1
A	79	THR	HB	4.17	0.05	1
A	115	LYS	C	174.38	0.1	1
A	80	ASP	HA	4.56	0.05	1
A	115	LYS	HG2	1.22	0.05	2
A	135	GLN	HG3	1.82	0.05	2
A	81	SER	C	174.7	0.1	1
A	98	GLY	C	177.94	0.1	1
A	105	LEU	CD2	24.4	0.1	1
A	143	GLN	CA	58.8	0.1	1
A	139	GLU	N	118.4	0.1	1
A	101	SER	HB3	3.85	0.05	2
A	111	ASN	HA	4.39	0.05	1
A	93	ASP	N	116.8	0.1	1
A	115	LYS	CG	24.6	0.1	1
A	110	THR	CG2	21.5	0.1	1
A	105	LEU	HD12	0.85	0.05	1
A	141	PHE	HB2	3.32	0.05	2
A	138	TYR	C	175.9	0.1	1
A	104	GLU	CG	36.3	0.1	1
A	146	THR	HG23	1.11	0.05	1
A	95	ASP	C	177.55	0.1	1
A	115	LYS	H	8.48	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	128	ALA	HA	4.34	0.05	1
A	140	GLU	H	8.68	0.05	1
A	116	LEU	CA	54.0	0.1	1
A	148	LYS	HA	4.04	0.05	1
A	135	GLN	HE21	5.82	0.05	1
A	143	GLN	HB3	2.04	0.05	2
A	101	SER	HA	4.73	0.05	1
A	126	ARG	H	8.13	0.05	1
A	112	LEU	HB2	1.79	0.05	2
A	77	LYS	H	7.76	0.05	1
A	141	PHE	C	180.63	0.1	1
A	119	GLU	CG	36.3	0.1	1
A	143	GLN	NE2	111.3	0.1	1
A	94	LYS	CG	24.25	0.1	1
A	135	GLN	C	177.62	0.1	1
A	124	MET	H	7.69	0.05	1
A	96	GLY	H	7.69	0.05	1
A	124	MET	HB3	1.96	0.05	2
A	106	ARG	HD2	3.13	0.05	2
A	88	ALA	H	7.86	0.05	1
A	79	THR	H	8.05	0.05	1
A	82	GLU	H	8.4	0.05	1
A	124	MET	CE	17.33	0.1	1
A	108	VAL	HG13	0.35	0.05	1
A	112	LEU	N	119.16	0.1	1
A	143	GLN	N	118.2	0.1	1
A	85	ILE	CG1	29.2	0.1	1
A	91	VAL	CG1	22.8	0.1	1
A	106	ARG	CB	30.2	0.1	1
A	137	ASN	HB2	3.15	0.05	2
A	145	MET	HG3	1.76	0.05	2
A	111	ASN	CB	38.1	0.1	1
A	83	GLU	CG	37.0	0.1	1
A	108	VAL	N	118.87	0.1	1
A	77	LYS	CB	32.9	0.1	1
A	115	LYS	HD2	1.39	0.05	2
A	93	ASP	H	7.75	0.05	1
A	106	ARG	C	179.3	0.1	1
A	127	GLU	HB3	1.94	0.05	2
A	89	PHE	HD1	7.16	0.05	1
A	78	ASP	C	176.68	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	102	ALA	N	122.87	0.1	1
A	97	ASN	HB3	3.31	0.05	2
A	88	ALA	HB1	1.7	0.05	1
A	104	GLU	HG3	2.2	0.05	2
A	108	VAL	HA	3.4	0.05	1
A	120	GLU	CB	30.55	0.1	1
A	86	ARG	HD2	2.87	0.05	2
A	148	LYS	C	174.23	0.1	1
A	145	MET	HE2	1.72	0.05	1
A	86	ARG	CA	60.0	0.1	1
A	92	PHE	N	116.0	0.1	1
A	143	GLN	HA	3.78	0.05	1
A	112	LEU	CA	55.36	0.1	1
A	112	LEU	HA	4.25	0.05	1
A	89	PHE	HB3	2.9	0.05	2
A	77	LYS	HG2	1.38	0.05	2
A	93	ASP	CB	38.4	0.1	1
A	90	ARG	CB	30.3	0.1	1
A	107	HIS	HA	4.22	0.05	1
A	145	MET	HB3	1.73	0.05	2
A	100	ILE	HD13	0.23	0.05	1
A	141	PHE	HE2	6.91	0.05	1
A	109	MET	HE3	1.95	0.05	1
A	102	ALA	HB3	1.37	0.05	1
A	96	GLY	HA3	3.75	0.05	1
A	130	ILE	C	177.9	0.1	1
A	91	VAL	CA	65.7	0.1	1
A	125	ILE	CA	63.78	0.1	1
A	86	ARG	C	179.65	0.1	1
A	85	ILE	HD12	0.7	0.05	1
A	78	ASP	N	121.8	0.1	1
A	130	ILE	CB	38.6	0.1	1
A	121	VAL	HG21	0.87	0.05	1
A	123	GLU	H	7.92	0.05	1
A	121	VAL	HG22	0.87	0.05	1
A	100	ILE	H	10.04	0.05	1
A	126	ARG	HA	3.89	0.05	1
A	86	ARG	N	121.7	0.1	1
A	79	THR	HA	4.19	0.05	1
A	123	GLU	CG	36.2	0.1	1
A	129	ASP	HA	4.38	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	147	ALA	N	126.53	0.1	1
A	89	PHE	CA	62.09	0.1	1
A	78	ASP	HA	4.56	0.05	1
A	92	PHE	HD1	7.12	0.05	1
A	128	ALA	CB	21.45	0.1	1
A	138	TYR	N	118.47	0.1	1
A	113	GLY	N	106.48	0.1	1
A	115	LYS	CD	29.2	0.1	1
A	81	SER	HB2	3.86	0.05	2
A	87	GLU	HB3	2.01	0.05	2
A	99	TYR	HD2	6.64	0.05	1
A	105	LEU	HD11	0.85	0.05	1
A	136	VAL	CA	61.8	0.1	1
A	140	GLU	HB2	1.87	0.05	2
A	130	ILE	H	8.22	0.05	1
A	108	VAL	CB	31.9	0.1	1
A	77	LYS	N	120.68	0.1	1
A	86	ARG	HB2	1.75	0.05	2
A	142	VAL	H	8.53	0.05	1
A	134	GLY	HA3	3.32	0.05	1
A	85	ILE	HG23	1.03	0.05	1
A	77	LYS	HE3	2.9	0.05	1
A	85	ILE	CA	64.7	0.1	1
A	112	LEU	HD22	0.76	0.05	1
A	119	GLU	HB3	1.96	0.05	2
A	100	ILE	CG2	17.6	0.1	1
A	143	GLN	HG3	2.31	0.05	2
A	94	LYS	CB	32.6	0.1	1
A	144	MET	H	7.73	0.05	1
A	84	GLU	HG2	2.2	0.05	2
A	126	ARG	HB3	1.75	0.05	2
A	138	TYR	CD2	132.4	0.1	1
A	122	ASP	HB3	2.67	0.05	2
A	134	GLY	N	112.85	0.1	1
A	128	ALA	H	7.19	0.05	1
A	124	MET	CB	33.1	0.1	1
A	121	VAL	CG1	22.3	0.1	1
A	143	GLN	HE21	7.4	0.05	1
A	132	GLY	HA2	3.88	0.05	1
A	94	LYS	HB2	1.75	0.05	2
A	130	ILE	CG1	28.0	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	95	ASP	HB3	2.98	0.05	2
A	107	HIS	CE1	120.0	0.1	1
A	144	MET	HG2	2.44	0.05	2
A	116	LEU	HA	4.68	0.05	1
A	142	VAL	HB	1.76	0.05	1
A	100	ILE	HG13	1.12	0.05	1
A	85	ILE	HD13	0.7	0.05	1
A	136	VAL	HG13	0.82	0.05	1
A	106	ARG	CG	27.7	0.1	1
A	94	LYS	HD2	1.53	0.05	2
A	103	ALA	HB2	1.33	0.05	1
A	136	VAL	N	125.41	0.1	1
A	140	GLU	HG3	2.3	0.05	2
A	133	ASP	CB	40.25	0.1	1
A	115	LYS	HG3	1.3	0.05	2
A	130	ILE	HD11	0.79	0.05	1
A	81	SER	CB	63.8	0.1	1
A	131	ASP	HA	4.44	0.05	1
A	144	MET	CB	32.8	0.1	1
A	116	LEU	HD23	0.72	0.05	1
A	142	VAL	HG21	0.64	0.05	1
A	101	SER	N	123.7	0.1	1
A	78	ASP	CB	41.0	0.1	1
A	135	GLN	N	115.39	0.1	1
A	127	GLU	CG	36.4	0.1	1
A	89	PHE	HD2	7.16	0.05	1
A	83	GLU	HB2	1.83	0.05	2
A	144	MET	HE1	1.81	0.05	1
A	125	ILE	HD12	0.61	0.05	1
A	120	GLU	CA	59.35	0.1	1
A	138	TYR	HB3	2.29	0.05	2
A	89	PHE	CD2	131.4	0.1	1
A	107	HIS	HB2	3.25	0.05	2
A	138	TYR	CE1	118.2	0.1	1
A	99	TYR	CB	43.0	0.1	1
A	108	VAL	HB	1.92	0.05	1
A	103	ALA	N	118.45	0.1	1
A	91	VAL	CB	31.5	0.1	1
A	114	GLU	CA	55.28	0.1	1
A	105	LEU	HB2	1.83	0.05	2
A	142	VAL	CB	31.7	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	80	ASP	C	176.76	0.1	1
A	141	PHE	HZ	7.05	0.05	1
A	146	THR	HA	4.2	0.05	1
A	100	ILE	HG22	0.83	0.05	1
A	99	TYR	HE1	6.8	0.05	1
A	148	LYS	CD	29.1	0.1	1
A	92	PHE	CE1	129.5	0.1	1
A	126	ARG	HB2	1.83	0.05	2
A	99	TYR	CE1	118.3	0.1	1
A	128	ALA	N	118.71	0.1	1
A	117	THR	HG23	1.24	0.05	1
A	138	TYR	HB2	1.99	0.05	2
A	93	ASP	HB3	1.28	0.05	2
A	90	ARG	CA	58.9	0.1	1
A	139	GLU	C	174.92	0.1	1
A	121	VAL	CA	67.0	0.1	1
A	126	ARG	HD3	3.12	0.05	2
A	79	THR	CA	62.5	0.1	1
A	132	GLY	H	7.51	0.05	1
A	97	ASN	ND2	116.4	0.1	1
A	141	PHE	HE1	6.91	0.05	1
A	82	GLU	HB2	2.02	0.05	2
A	97	ASN	HA	4.54	0.05	1
A	118	ASP	CB	39.8	0.1	1
A	116	LEU	HD21	0.72	0.05	1
A	137	ASN	H	9.39	0.05	1
A	148	LYS	HB2	1.72	0.05	2
A	91	VAL	HG11	0.91	0.05	1
A	127	GLU	HG3	2.26	0.05	2
A	135	GLN	CA	53.1	0.1	1
A	126	ARG	CG	27.75	0.1	1
A	132	GLY	C	177.97	0.1	1
A	94	LYS	N	125.83	0.1	1
A	123	GLU	C	177.3	0.1	1
A	140	GLU	HA	3.91	0.05	1
A	118	ASP	CA	58.1	0.1	1
A	144	MET	HA	4.08	0.05	1
A	130	ILE	HG13	1.59	0.05	1
A	84	GLU	CA	59.4	0.1	1
A	117	THR	CA	60.74	0.1	1
A	89	PHE	CB	39.25	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	124	MET	HB2	2.19	0.05	2
A	130	ILE	HG23	0.84	0.05	1
A	92	PHE	HD2	7.12	0.05	1
A	96	GLY	N	109.3	0.1	1
A	124	MET	N	119.5	0.1	1
A	118	ASP	H	8.83	0.05	1
A	146	THR	N	111.42	0.1	1
A	90	ARG	HB2	1.84	0.05	2
A	142	VAL	N	119.45	0.1	1
A	148	LYS	H	7.68	0.05	1
A	115	LYS	HD3	1.56	0.05	2
A	115	LYS	CA	55.7	0.1	1
A	121	VAL	HG13	0.93	0.05	1
A	99	TYR	HD1	6.64	0.05	1
A	79	THR	N	114.79	0.1	1
A	128	ALA	HB1	1.33	0.05	1
A	141	PHE	HD1	6.85	0.05	1
A	142	VAL	HG11	0.4	0.05	1
A	143	GLN	C	176.84	0.1	1
A	147	ALA	HB1	1.32	0.05	1
A	91	VAL	HA	3.37	0.05	1
A	101	SER	HB2	4.33	0.05	2
A	92	PHE	HB2	2.58	0.05	2
A	105	LEU	HD23	0.87	0.05	1
A	145	MET	N	115.0	0.1	1
A	112	LEU	CD1	22.7	0.1	1
A	134	GLY	HA2	3.94	0.05	1
A	143	GLN	HB2	2.04	0.05	2
A	112	LEU	CD2	25.8	0.1	1
A	116	LEU	HD12	0.7	0.05	1
A	85	ILE	HA	3.96	0.05	1
A	134	GLY	C	175.32	0.1	1
A	89	PHE	H	8.44	0.05	1
A	115	LYS	HE3	2.88	0.05	1
A	94	LYS	CA	59.09	0.1	1
A	138	TYR	CD1	132.4	0.1	1
A	110	THR	CB	68.8	0.1	1
A	121	VAL	CG2	23.9	0.1	1
A	82	GLU	HG3	2.3	0.05	2
A	84	GLU	N	118.9	0.1	1
A	140	GLU	C	176.14	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	98	GLY	H	10.55	0.05	1
A	120	GLU	HG3	2.31	0.05	2
A	116	LEU	CD1	24.0	0.1	1
A	146	THR	H	7.51	0.05	1
A	144	MET	HB2	1.97	0.05	2
A	143	GLN	CB	28.2	0.1	1
A	135	GLN	HA	4.77	0.05	1
A	106	ARG	CD	44.0	0.1	1
A	142	VAL	CA	67.1	0.1	1
A	108	VAL	HG23	0.78	0.05	1
A	137	ASN	HD22	7.14	0.05	2
A	113	GLY	HA3	4.13	0.05	1
A	84	GLU	HB2	2.23	0.05	2
A	81	SER	CA	59.3	0.1	1
A	87	GLU	HA	4.04	0.05	1
A	144	MET	CG	31.6	0.1	1
A	120	GLU	HG2	2.2	0.05	2
A	127	GLU	CB	29.5	0.1	1
A	110	THR	C	178.18	0.1	1
A	125	ILE	HD11	0.61	0.05	1
A	89	PHE	CD1	131.4	0.1	1
A	138	TYR	CE2	118.2	0.1	1
A	99	TYR	CA	56.0	0.1	1
A	142	VAL	C	179.49	0.1	1
A	88	ALA	N	121.84	0.1	1
A	116	LEU	C	175.43	0.1	1
A	142	VAL	HG13	0.4	0.05	1
A	106	ARG	HD3	3.04	0.05	2
A	123	GLU	N	119.47	0.1	1
A	99	TYR	HE2	6.8	0.05	1
A	92	PHE	CE2	129.5	0.1	1
A	123	GLU	HG2	2.2	0.05	2
A	141	PHE	CD2	131.9	0.1	1
A	77	LYS	HA	4.2	0.05	1
A	92	PHE	HZ	7.09	0.05	1
A	86	ARG	H	8.33	0.05	1
A	90	ARG	CD	43.53	0.1	1
A	147	ALA	HA	4.21	0.05	1
A	113	GLY	C	178.72	0.1	1
A	136	VAL	HG21	1.18	0.05	1
A	127	GLU	H	7.78	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	81	SER	HA	4.33	0.05	1
A	140	GLU	CA	58.6	0.1	1
A	91	VAL	HG12	0.91	0.05	1
A	105	LEU	CG	26.0	0.1	1
A	137	ASN	HA	5.16	0.05	1
A	130	ILE	N	127.84	0.1	1
A	127	GLU	HB2	1.61	0.05	2
A	86	ARG	HA	4.03	0.05	1
A	137	ASN	HB3	3.15	0.05	2
A	88	ALA	HB2	1.7	0.05	1
A	125	ILE	HG13	1.43	0.05	1
A	86	ARG	HD3	2.86	0.05	2
A	104	GLU	HG2	2.2	0.05	2
A	145	MET	HE3	1.72	0.05	1
A	130	ILE	HA	3.79	0.05	1
A	86	ARG	CB	29.8	0.1	1
A	147	ALA	CB	18.9	0.1	1
A	90	ARG	HA	3.77	0.05	1
A	131	ASP	CA	53.9	0.1	1
A	125	ILE	CG2	16.1	0.1	1
A	77	LYS	HB2	1.74	0.05	2
A	134	GLY	H	10.27	0.05	1
A	148	LYS	HE3	2.88	0.05	1
A	93	ASP	C	177.27	0.1	1
A	139	GLU	CG	37.1	0.1	1
A	133	ASP	HA	4.37	0.05	1
A	106	ARG	HB2	1.86	0.05	2
A	110	THR	HG23	1.14	0.05	1
A	141	PHE	HD2	6.87	0.05	1
A	145	MET	HB2	1.58	0.05	2
A	90	ARG	HG2	1.56	0.05	2
A	142	VAL	HG12	0.4	0.05	1
A	82	GLU	CA	58.6	0.1	1
A	119	GLU	H	8.57	0.05	1
A	114	GLU	HG3	2.12	0.05	2
A	99	TYR	CE2	118.3	0.1	1
A	87	GLU	HG2	2.24	0.05	2
A	109	MET	HB3	2.01	0.05	2
A	120	GLU	HA	4.0	0.05	1
A	136	VAL	H	9.02	0.05	1
A	85	ILE	HD11	0.7	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	116	LEU	HD11	0.7	0.05	1
A	130	ILE	CA	63.4	0.1	1
A	127	GLU	N	116.13	0.1	1
A	85	ILE	HB	2.09	0.05	1
A	147	ALA	H	7.67	0.05	1
A	94	LYS	HA	3.81	0.05	1
A	125	ILE	C	178.09	0.1	1
A	85	ILE	HG12	1.01	0.05	1
A	124	MET	CA	59.3	0.1	1
A	116	LEU	CD2	27.0	0.1	1
A	142	VAL	HA	3.03	0.05	1
A	112	LEU	HD13	0.72	0.05	1
A	143	GLN	CG	33.9	0.1	1
A	128	ALA	C	179.34	0.1	1
A	97	ASN	H	8.23	0.05	1
A	115	LYS	CE	42.2	0.1	1
A	141	PHE	H	8.81	0.05	1
A	126	ARG	HG2	1.53	0.05	2
A	87	GLU	HB2	1.97	0.05	2
A	91	VAL	HG22	0.53	0.05	1
A	89	PHE	C	178.64	0.1	1
A	136	VAL	CB	33.9	0.1	1
A	111	ASN	HB2	2.69	0.05	2
A	146	THR	HG21	1.11	0.05	1
A	83	GLU	N	119.5	0.1	1
A	126	ARG	CA	59.7	0.1	1
A	100	ILE	HB	1.76	0.05	1
A	108	VAL	CA	66.3	0.1	1
A	86	ARG	HB3	1.76	0.05	2
A	125	ILE	HB	2.02	0.05	1
A	89	PHE	HE2	6.5	0.05	1
A	85	ILE	HG22	1.03	0.05	1
A	77	LYS	HE2	2.9	0.05	1
A	116	LEU	CG	27.6	0.1	1
A	102	ALA	C	175.55	0.1	1
A	116	LEU	HB3	1.38	0.05	2
A	100	ILE	C	172.47	0.1	1
A	129	ASP	H	7.8	0.05	1
A	127	GLU	CA	58.63	0.1	1
A	101	SER	CB	66.7	0.1	1
A	118	ASP	HB3	2.49	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	112	LEU	HD23	0.76	0.05	1
A	148	LYS	HG3	1.3	0.05	2
A	94	LYS	CE	41.8	0.1	1
A	142	VAL	CG2	21.4	0.1	1
A	99	TYR	HA	4.96	0.05	1
A	90	ARG	HD3	3.12	0.05	2
A	114	GLU	CG	35.5	0.1	1
A	125	ILE	HG23	0.61	0.05	1
A	83	GLU	HG2	2.2	0.05	2
A	103	ALA	CB	18.5	0.1	1
A	125	ILE	CD1	10.7	0.1	1
A	132	GLY	HA3	3.72	0.05	1
A	139	GLU	H	8.03	0.05	1
A	118	ASP	C	178.09	0.1	1
A	140	GLU	HB3	1.97	0.05	2
A	126	ARG	C	179.3	0.1	1
A	102	ALA	H	9.12	0.05	1
A	125	ILE	HG12	1.22	0.05	1
A	106	ARG	HG3	1.53	0.05	2
A	109	MET	HG2	2.68	0.05	2
A	124	MET	CG	31.6	0.1	1
A	141	PHE	CD1	131.9	0.1	1
A	108	VAL	HG11	0.35	0.05	1
A	80	ASP	HB2	2.46	0.05	2
A	100	ILE	CA	60.5	0.1	1
A	100	ILE	HG12	0.22	0.05	1
A	99	TYR	CD1	133.4	0.1	1
A	82	GLU	HA	4.06	0.05	1
A	136	VAL	HG12	0.82	0.05	1
A	94	LYS	HD3	1.54	0.05	2
A	103	ALA	HB1	1.33	0.05	1
A	140	GLU	HG2	2.3	0.05	2
A	117	THR	CG2	21.8	0.1	1
A	126	ARG	N	118.27	0.1	1
A	136	VAL	HG22	1.18	0.05	1
A	147	ALA	C	177.62	0.1	1
A	139	GLU	HA	3.54	0.05	1
A	135	GLN	HB3	1.87	0.05	2
A	92	PHE	HB3	3.3	0.05	2
A	145	MET	CG	32.2	0.1	1
A	105	LEU	CB	42.0	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	103	ALA	H	8.17	0.05	1
A	78	ASP	CA	55.0	0.1	1
A	129	ASP	CB	40.4	0.1	1
A	124	MET	HE1	1.96	0.05	1
A	141	PHE	HA	3.85	0.05	1
A	146	THR	HG22	1.11	0.05	1
A	118	ASP	HA	4.11	0.05	1
A	115	LYS	HB2	1.6	0.05	2
A	86	ARG	CG	27.6	0.1	1
A	100	ILE	HG23	0.83	0.05	1
A	148	LYS	CE	42.1	0.1	1
A	147	ALA	CA	52.9	0.1	1
A	89	PHE	N	119.0	0.1	1
A	97	ASN	HD22	7.3	0.05	2
A	141	PHE	CE1	131.4	0.1	1
A	87	GLU	N	118.5	0.1	1
A	100	ILE	HA	4.68	0.05	1
A	100	ILE	N	127.36	0.1	1
A	84	GLU	H	8.05	0.05	1
A	117	THR	H	9.14	0.05	1
A	80	ASP	CA	55.2	0.1	1
A	136	VAL	HB	2.19	0.05	1
A	130	ILE	HD12	0.79	0.05	1
A	105	LEU	H	8.5	0.05	1
A	125	ILE	H	7.83	0.05	1
A	98	GLY	N	112.9	0.1	1
A	121	VAL	CB	31.5	0.1	1
A	79	THR	CB	69.9	0.1	1
A	130	ILE	CD1	12.3	0.1	1
A	121	VAL	HB	2.13	0.05	1
A	82	GLU	CB	29.5	0.1	1
A	147	ALA	HB2	1.32	0.05	1
A	82	GLU	HB3	2.26	0.05	2
A	83	GLU	CB	29.4	0.1	1
A	79	THR	HG21	1.11	0.05	1
A	77	LYS	CG	24.6	0.1	1
A	110	THR	HA	4.05	0.05	1
A	116	LEU	HD22	0.72	0.05	1
A	148	LYS	HB3	1.59	0.05	2
A	84	GLU	HA	4.04	0.05	1
A	134	GLY	CA	45.7	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	110	THR	N	115.32	0.1	1
A	94	LYS	C	177.03	0.1	1
A	84	GLU	CB	30.3	0.1	1
A	117	THR	CB	71.2	0.1	1
A	93	ASP	HA	4.44	0.05	1
A	102	ALA	HA	3.83	0.05	1
A	130	ILE	HG22	0.84	0.05	1
A	121	VAL	H	8.01	0.05	1
A	87	GLU	CA	59.06	0.1	1
A	124	MET	HE2	1.96	0.05	1
A	83	GLU	H	8.23	0.05	1
A	80	ASP	N	123.22	0.1	1
A	122	ASP	C	180.16	0.1	1
A	123	GLU	HA	3.88	0.05	1
A	115	LYS	CB	32.1	0.1	1
A	121	VAL	HG12	0.93	0.05	1
A	98	GLY	CA	45.2	0.1	1
A	119	GLU	HA	3.96	0.05	1
A	126	ARG	CB	30.1	0.1	1
A	91	VAL	HB	2.04	0.05	1
A	107	HIS	HE1	7.69	0.05	1
A	141	PHE	CZ	131.1	0.1	1
A	89	PHE	HE1	6.5	0.05	1
A	90	ARG	H	7.63	0.05	1
A	105	LEU	N	121.07	0.1	1
A	85	ILE	HG21	1.03	0.05	1
A	144	MET	HG3	2.32	0.05	2
A	109	MET	CG	33.1	0.1	1
A	101	SER	CA	56.0	0.1	1
A	145	MET	H	7.79	0.05	1
A	137	ASN	CA	51.2	0.1	1
A	120	GLU	N	120.52	0.1	1
A	115	LYS	HE2	2.84	0.05	1
A	129	ASP	HB3	2.7	0.05	2
A	103	ALA	CA	55.28	0.1	1
A	110	THR	CA	66.02	0.1	1
A	82	GLU	HG2	2.3	0.05	2
A	99	TYR	HB3	2.4	0.05	2
A	136	VAL	CG1	22.4	0.1	1
A	99	TYR	C	176.13	0.1	1
A	113	GLY	H	7.74	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	123	GLU	CB	29.4	0.1	1
A	133	ASP	C	178.32	0.1	1
A	108	VAL	CG2	23.3	0.1	1
A	129	ASP	C	177.31	0.1	1
A	116	LEU	HG	1.47	0.05	1
A	111	ASN	H	7.78	0.05	1
A	139	GLU	HG3	2.16	0.05	2
A	88	ALA	CB	17.63	0.1	1
A	125	ILE	HA	3.4	0.05	1
A	100	ILE	CB	38.8	0.1	1
A	144	MET	HB3	1.97	0.05	2
A	99	TYR	CD2	133.4	0.1	1
A	144	MET	C	179.61	0.1	1
A	98	GLY	HA2	3.32	0.05	1
A	108	VAL	HG22	0.78	0.05	1
A	81	SER	N	117.15	0.1	1
A	121	VAL	N	121.2	0.1	1
A	137	ASN	HD21	6.77	0.05	2
A	104	GLU	HB2	1.98	0.05	2
A	104	GLU	CA	59.3	0.1	1
A	115	LYS	HA	4.28	0.05	1
A	138	TYR	HA	3.32	0.05	1
A	113	GLY	HA2	3.64	0.05	1
A	90	ARG	HD2	3.12	0.05	2
A	84	GLU	HB3	1.84	0.05	2
A	80	ASP	H	8.36	0.05	1
A	130	ILE	HD13	0.79	0.05	1
A	95	ASP	CA	52.7	0.1	1
A	105	LEU	CA	58.3	0.1	1
A	89	PHE	HZ	6.9	0.05	1
A	141	PHE	HB3	3.07	0.05	2
A	142	VAL	HG23	0.64	0.05	1
A	124	MET	HE3	1.96	0.05	1
A	129	ASP	CA	54.12	0.1	1
A	121	VAL	HG23	0.87	0.05	1
A	131	ASP	HB2	2.98	0.05	2
A	144	MET	HE3	1.81	0.05	1
A	109	MET	HA	4.22	0.05	1
A	78	ASP	HB3	2.56	0.05	2
A	86	ARG	CD	43.1	0.1	1
A	117	THR	N	114.59	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	94	LYS	HE2	2.76	0.05	1
A	97	ASN	HD21	7.99	0.05	2
A	141	PHE	CE2	131.4	0.1	1
A	96	GLY	CA	47.2	0.1	1
A	123	GLU	HG3	2.2	0.05	2
A	90	ARG	C	179.31	0.1	1
A	80	ASP	CB	41.3	0.1	1
A	139	GLU	CA	60.37	0.1	1
A	148	LYS	HD2	1.4	0.05	2
A	136	VAL	HA	5.11	0.05	1
A	90	ARG	CG	27.9	0.1	1
A	115	LYS	N	124.13	0.1	1
A	117	THR	HB	4.66	0.05	1
A	121	VAL	HA	3.5	0.05	1
A	94	LYS	HG2	1.43	0.05	2
A	104	GLU	N	120.0	0.1	1
A	114	GLU	HG2	2.0	0.05	2
A	79	THR	HG22	1.11	0.05	1
A	146	THR	CA	62.6	0.1	1
A	77	LYS	CD	29.0	0.1	1
A	110	THR	HB	4.2	0.05	1
A	91	VAL	HG13	0.91	0.05	1
A	82	GLU	C	176.84	0.1	1
A	88	ALA	HA	4.11	0.05	1
A	116	LEU	N	125.02	0.1	1
A	133	ASP	H	8.24	0.05	1
A	89	PHE	CZ	131.5	0.1	1
A	81	SER	H	8.36	0.05	1
A	106	ARG	H	8.54	0.05	1
A	105	LEU	HG	1.53	0.05	1
A	88	ALA	HB3	1.7	0.05	1
A	114	GLU	HA	4.33	0.05	1
A	109	MET	H	8.21	0.05	1
A	84	GLU	CG	36.8	0.1	1
A	119	GLU	HG3	2.2	0.05	2
A	111	ASN	HD22	7.3	0.05	2
A	97	ASN	CA	52.7	0.1	1
A	133	ASP	HB2	2.4	0.05	2
A	148	LYS	CA	57.7	0.1	1
A	87	GLU	CB	29.5	0.1	1
A	87	GLU	HG3	2.24	0.05	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	130	ILE	HG21	0.84	0.05	1
A	91	VAL	H	7.38	0.05	1
A	125	ILE	CG1	28.3	0.1	1
A	77	LYS	HB3	1.74	0.05	2
A	124	MET	HG3	2.68	0.05	2
A	148	LYS	HE2	2.88	0.05	1
A	108	VAL	H	7.88	0.05	1
A	104	GLU	HA	3.94	0.05	1
A	112	LEU	C	177.74	0.1	1
A	106	ARG	HB3	1.86	0.05	2
A	110	THR	HG22	1.14	0.05	1
A	90	ARG	HG3	1.56	0.05	2
A	117	THR	HG22	1.24	0.05	1
A	100	ILE	HD11	0.23	0.05	1
A	106	ARG	HA	3.71	0.05	1
A	92	PHE	C	178.12	0.1	1
A	109	MET	HE1	1.95	0.05	1
A	102	ALA	HB1	1.37	0.05	1
A	128	ALA	HB2	1.33	0.05	1
A	105	LEU	HD21	0.87	0.05	1
A	94	LYS	H	7.64	0.05	1
A	138	TYR	CA	62.7	0.1	1
A	109	MET	HB2	2.1	0.05	2
A	109	MET	CB	31.1	0.1	1
A	107	HIS	C	177.97	0.1	1
A	88	ALA	C	179.34	0.1	1
A	137	ASN	CB	38.3	0.1	1
A	102	ALA	CA	55.97	0.1	1
A	131	ASP	C	176.06	0.1	1
A	127	GLU	C	177.23	0.1	1
A	135	GLN	NE2	108.7	0.1	1
A	86	ARG	HG3	1.47	0.05	2
A	139	GLU	HB2	1.96	0.05	2
A	136	VAL	CG2	21.8	0.1	1
A	97	ASN	N	119.6	0.1	1
A	85	ILE	HG13	1.71	0.05	1
A	123	GLU	CA	59.29	0.1	1
A	148	LYS	N	125.65	0.1	1
A	92	PHE	CA	60.06	0.1	1
A	108	VAL	CG1	20.8	0.1	1
A	130	ILE	CG2	17.4	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	135	GLN	HG2	1.88	0.05	2
A	131	ASP	N	116.53	0.1	1
A	91	VAL	HG21	0.53	0.05	1
A	108	VAL	HG21	0.78	0.05	1
A	105	LEU	HD13	0.85	0.05	1
A	125	ILE	HG21	0.61	0.05	1
A	114	GLU	HB2	1.63	0.05	2
A	111	ASN	HB3	2.7	0.05	2
A	125	ILE	HG22	0.61	0.05	1
A	78	ASP	H	8.22	0.05	1
A	145	MET	CA	55.27	0.1	1
A	125	ILE	N	118.29	0.1	1
A	144	MET	CE	17.15	0.1	1
A	92	PHE	HE2	6.95	0.05	1
A	99	TYR	H	7.53	0.05	1
A	114	GLU	HB3	1.85	0.05	2
A	116	LEU	HB2	1.49	0.05	2
A	145	MET	HG2	1.76	0.05	2
A	135	GLN	HE22	6.38	0.05	1
A	91	VAL	HG23	0.53	0.05	1
A	112	LEU	HB3	1.61	0.05	2
A	118	ASP	HB2	2.66	0.05	2
A	91	VAL	C	176.6	0.1	1
A	148	LYS	HG2	1.3	0.05	2
A	138	TYR	HE2	6.39	0.05	1
A	85	ILE	C	178.68	0.1	1
A	94	LYS	CD	28.6	0.1	1
A	142	VAL	CG1	23.05	0.1	1
A	140	GLU	N	119.87	0.1	1
A	83	GLU	HG3	2.27	0.05	2
A	127	GLU	HA	3.88	0.05	1
A	106	ARG	HG2	1.53	0.05	2
A	145	MET	C	177.97	0.1	1
A	109	MET	HG3	2.52	0.05	2
A	110	THR	H	8.11	0.05	1
A	108	VAL	HG12	0.35	0.05	1
A	80	ASP	HB3	2.58	0.05	2
A	113	GLY	CA	45.5	0.1	1
A	136	VAL	HG11	0.82	0.05	1
A	91	VAL	CG2	21.0	0.1	1
A	106	ARG	CA	59.99	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	117	THR	HA	4.35	0.05	1
A	82	GLU	N	122.46	0.1	1
A	136	VAL	HG23	1.18	0.05	1
A	131	ASP	H	8.22	0.05	1
A	146	THR	CB	70.2	0.1	1
A	77	LYS	CA	57.0	0.1	1
A	145	MET	CB	32.82	0.1	1
A	135	GLN	HB2	1.59	0.05	2

- Chain not found in structure. All 2 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HAL	HA	6.3	0.05	1
UNMAPPED	1	HAL	CA	53.6	0.1	1

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	$-0.21 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	137	$0.15 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	123	$-0.67 \pm 0.20$	Should be applied
$^{15}\text{N}$	146	$0.27 \pm 0.23$	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 92%, i.e. 739 atoms were assigned a chemical shift out of a possible 805. 8 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	331/346 (96%)	138/138 (100%)	125/140 (89%)	68/68 (100%)
Sidechain	364/414 (88%)	225/238 (95%)	133/164 (81%)	6/12 (50%)
Aromatic	44/45 (98%)	24/25 (96%)	20/20 (100%)	0/0 (—%)
Overall	739/805 (92%)	387/401 (97%)	278/324 (86%)	74/80 (92%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 91%, i.e. 810 atoms were assigned a chemical shift out of a possible 890. 8 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	359/376 (95%)	150/150 (100%)	135/152 (89%)	74/74 (100%)
Sidechain	407/469 (87%)	253/271 (93%)	147/181 (81%)	7/17 (41%)
Aromatic	44/45 (98%)	24/25 (96%)	20/20 (100%)	0/0 (—%)
Overall	810/890 (91%)	427/446 (96%)	302/353 (86%)	81/91 (89%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	107	HIS	CE1	120.00	149.70 – 125.30	-7.2

#### 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.

Random coil index (RCI) for chain A:

