



Full wwPDB NMR Structure Validation Report ⓘ

Dec 20, 2016 – 07:34 AM EST

PDB ID : 5KVP
Title : Solution structure of the catalytic domain of zoocin A
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Deposited on : 2016-07-15

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20028442
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

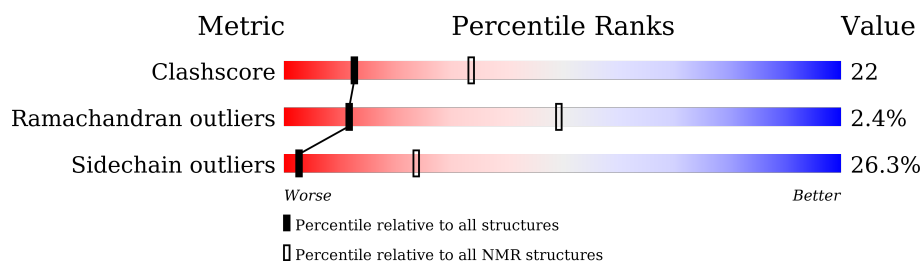
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	159	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:18-A:113, A:118-A:147 (126)	0.22	4

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 and 1 single-model cluster was found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2320 atoms, of which 1128 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zoocin A endopeptidase.

Mol	Chain	Residues	Atoms						Trace
1	A	159	Total	C	H	N	O	S	0
			2318	746	1128	219	220	5	

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O54308
A	2	ARG	-	expression tag	UNP O54308
A	3	GLY	-	expression tag	UNP O54308
A	4	SER	-	expression tag	UNP O54308
A	5	HIS	-	expression tag	UNP O54308
A	6	HIS	-	expression tag	UNP O54308
A	7	HIS	-	expression tag	UNP O54308
A	8	HIS	-	expression tag	UNP O54308
A	9	HIS	-	expression tag	UNP O54308
A	10	HIS	-	expression tag	UNP O54308
A	11	GLY	-	expression tag	UNP O54308
A	12	SER	-	expression tag	UNP O54308
A	74	ALA	CYS	engineered mutation	UNP O54308

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

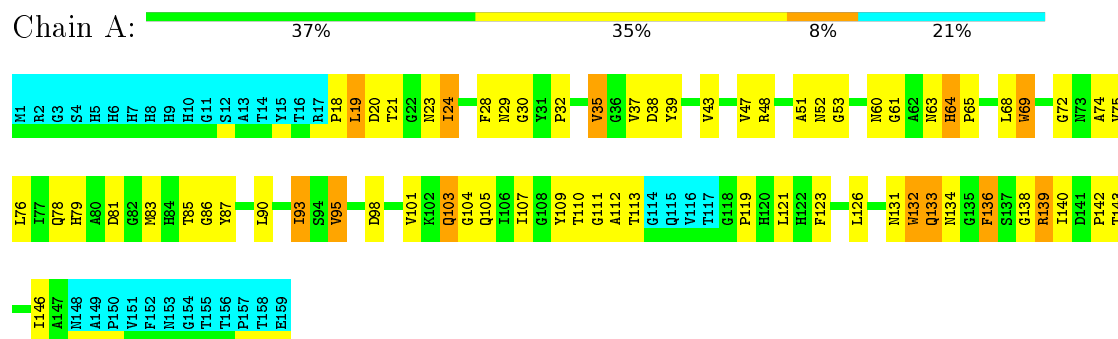
Mol	Chain	Residues	Atoms	
3	A	1	Total	O
			1	1

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: Zoocin A endopeptidase

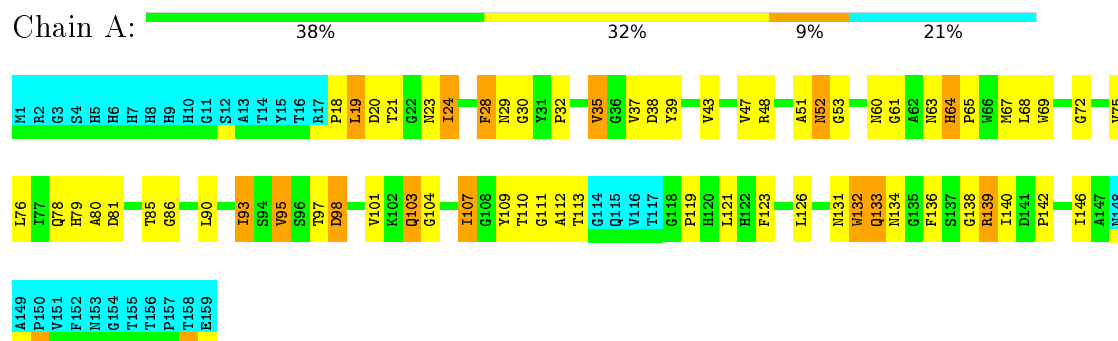


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

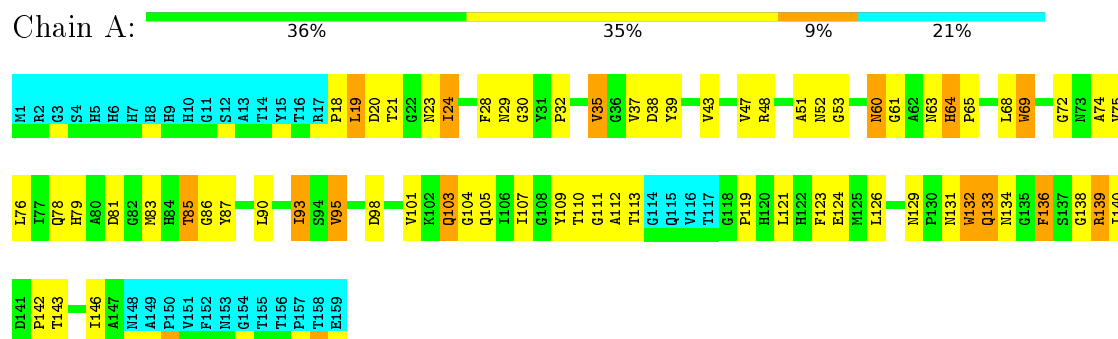
4.2.1 Score per residue for model 1

- Molecule 1: Zoocin A endopeptidase



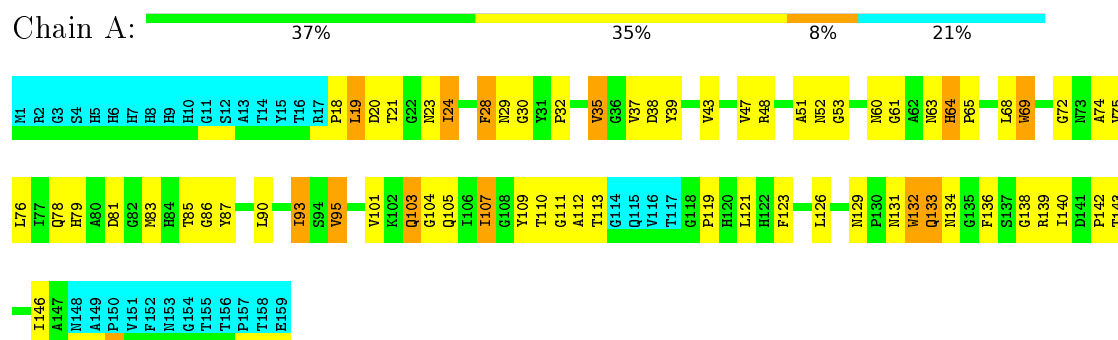
4.2.2 Score per residue for model 2

- Molecule 1: Zoocin A endopeptidase



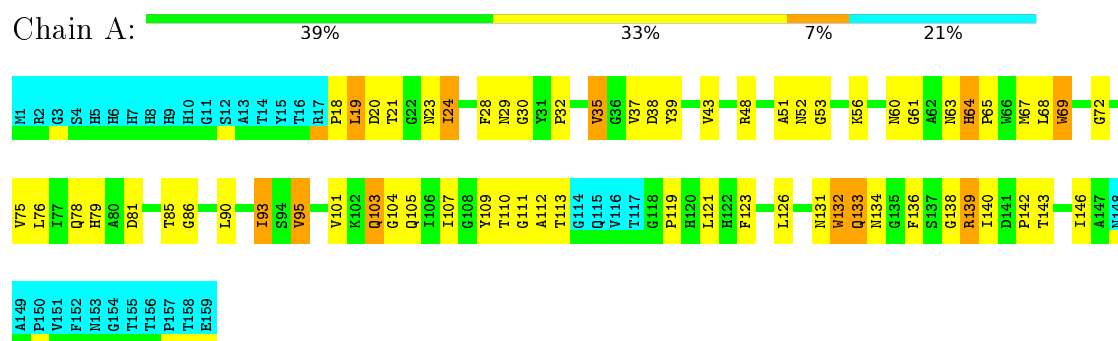
4.2.3 Score per residue for model 3

- Molecule 1: Zoocin A endopeptidase



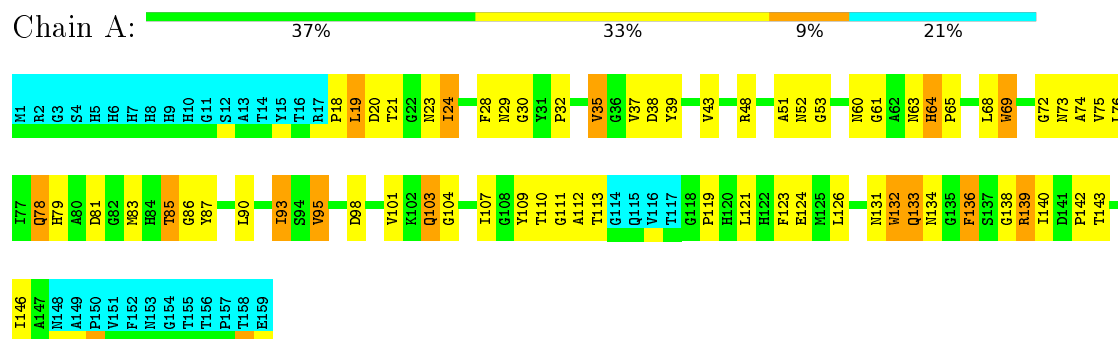
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Zoocin A endopeptidase



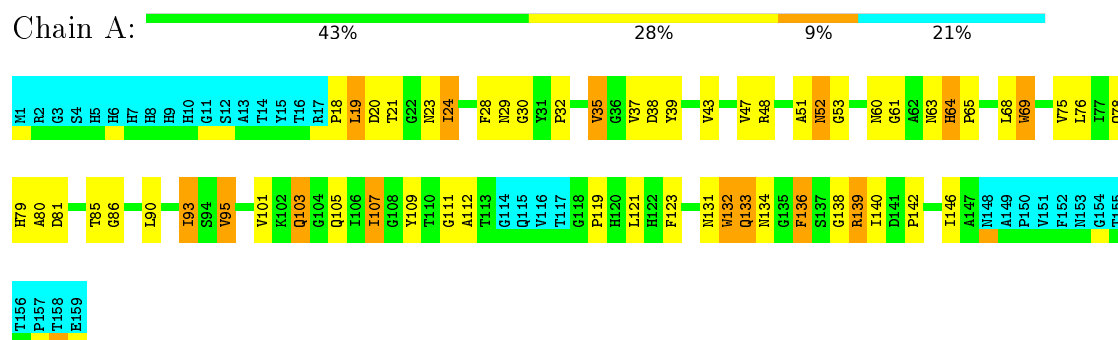
4.2.5 Score per residue for model 5

- Molecule 1: Zoocin A endopeptidase



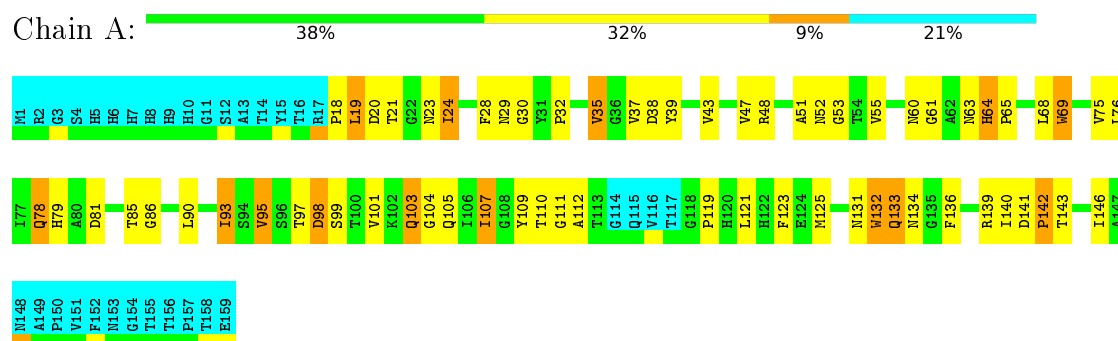
4.2.6 Score per residue for model 6

- Molecule 1: Zoocin A endopeptidase



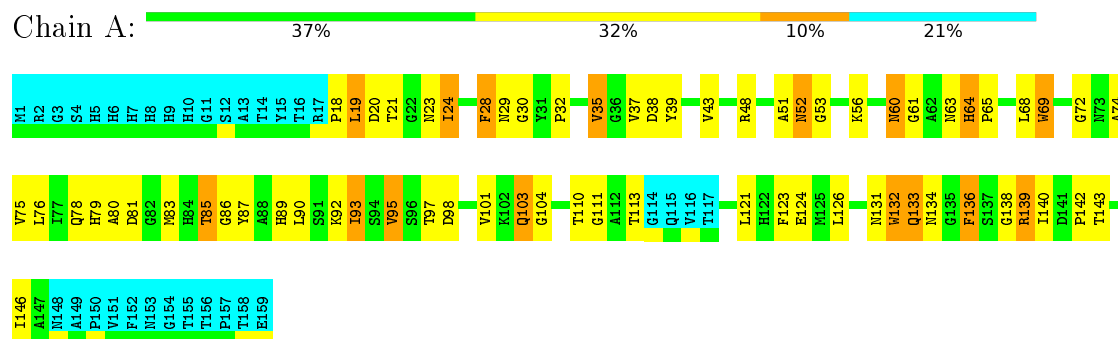
4.2.7 Score per residue for model 7

- Molecule 1: Zoocin A endopeptidase



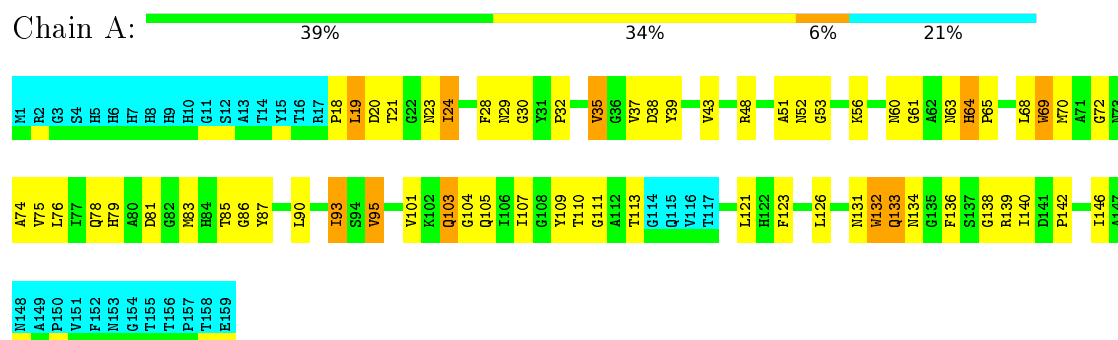
4.2.8 Score per residue for model 8

- Molecule 1: Zoocin A endopeptidase



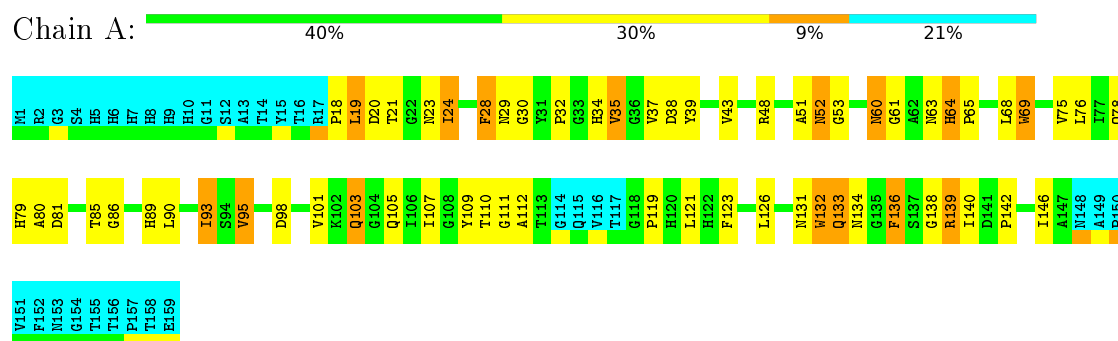
4.2.9 Score per residue for model 9

- Molecule 1: Zoocin A endopeptidase



4.2.10 Score per residue for model 10

- Molecule 1: Zoocin A endopeptidase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 100 calculated structures, 10 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
CNS	refinement	1.3
CNS	structure solution	1.3
NMRVIEW	structure solution	
NMRPIPE	structure solution	
NMRDRAW	structure solution	
TALOS+	structure solution	
TOPSPIN	structure solution	1.2
DEEPVIEW/SWISS-PDB VIEWER	structure solution	
PROCHECKNMR	structure solution	

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)	5kvp_cs.cif
Number of chemical shift lists	1
Total number of shifts	1631
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1631
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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	934	893	888	40±3
All	All	9360	8930	8880	400

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:PRO:HD2	1:A:69:TRP:NE1	0.73	1.98	2	10
1:A:19:LEU:HD12	1:A:21:THR:O	0.68	1.89	10	10
1:A:38:ASP:HA	1:A:121:LEU:O	0.68	1.89	9	10
1:A:103:GLN:C	1:A:103:GLN:HE21	0.66	1.94	10	5
1:A:103:GLN:HE21	1:A:103:GLN:C	0.66	1.94	1	5
1:A:43:VAL:HG23	1:A:111:GLY:HA2	0.62	1.69	7	10
1:A:83:MET:HB2	1:A:126:LEU:O	0.62	1.93	8	2
1:A:24:ILE:HD12	1:A:24:ILE:H	0.61	1.56	10	7
1:A:93:ILE:HG23	1:A:95:VAL:H	0.61	1.56	2	10
1:A:53:GLY:HA3	1:A:78:GLN:O	0.60	1.96	8	10
1:A:65:PRO:O	1:A:69:TRP:CD1	0.59	2.55	2	10
1:A:30:GLY:O	1:A:32:PRO:HD3	0.59	1.98	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:H	1:A:24:ILE:HD12	0.59	1.57	8	3
1:A:18:PRO:HB2	1:A:39:TYR:HB3	0.58	1.74	7	10
1:A:125:MET:SD	1:A:142:PRO:HA	0.56	2.41	7	1
1:A:51:ALA:HB3	1:A:79:HIS:ND1	0.56	2.15	8	10
1:A:75:VAL:O	1:A:86:GLY:HA2	0.55	2.02	1	10
1:A:61:GLY:HA2	1:A:64:HIS:CD2	0.55	2.37	3	7
1:A:48:ARG:HG2	1:A:104:GLY:O	0.54	2.03	7	8
1:A:126:LEU:HA	1:A:138:GLY:O	0.54	2.01	8	8
1:A:142:PRO:O	1:A:146:ILE:HG12	0.54	2.03	2	10
1:A:19:LEU:HD12	1:A:21:THR:H	0.53	1.63	8	10
1:A:112:ALA:HB2	1:A:119:PRO:HA	0.53	1.79	2	8
1:A:35:VAL:HG12	1:A:139:ARG:HG2	0.52	1.82	5	10
1:A:72:GLY:HA3	1:A:113:THR:OG1	0.52	2.04	1	7
1:A:61:GLY:HA2	1:A:64:HIS:CG	0.52	2.40	7	9
1:A:51:ALA:HB3	1:A:79:HIS:CE1	0.52	2.39	5	8
1:A:52:ASN:ND2	1:A:80:ALA:HB2	0.52	2.20	10	4
1:A:19:LEU:HB2	1:A:39:TYR:CD2	0.51	2.40	2	8
1:A:19:LEU:HB2	1:A:39:TYR:CD1	0.49	2.42	3	2
1:A:131:ASN:C	1:A:133:GLN:H	0.49	2.11	6	10
1:A:136:PHE:CE1	1:A:138:GLY:HA2	0.49	2.43	5	1
1:A:136:PHE:O	1:A:139:ARG:HG3	0.49	2.08	2	3
1:A:133:GLN:N	1:A:133:GLN:NE2	0.49	2.61	2	6
1:A:19:LEU:CD1	1:A:21:THR:O	0.49	2.61	10	9
1:A:60:ASN:N	1:A:60:ASN:HD22	0.48	2.06	10	4
1:A:133:GLN:NE2	1:A:133:GLN:N	0.48	2.62	8	4
1:A:37:VAL:HG11	1:A:142:PRO:HG3	0.48	1.86	6	1
1:A:139:ARG:HD2	1:A:139:ARG:O	0.48	2.08	7	3
1:A:60:ASN:HD22	1:A:60:ASN:N	0.47	2.06	8	6
1:A:97:THR:O	1:A:98:ASP:HB2	0.47	2.09	8	3
1:A:47:VAL:O	1:A:107:ILE:HG13	0.47	2.10	7	4
1:A:74:ALA:HA	1:A:87:TYR:O	0.47	2.10	2	5
1:A:139:ARG:O	1:A:139:ARG:HD2	0.47	2.08	9	2
1:A:90:LEU:HB3	1:A:109:TYR:O	0.47	2.10	6	9
1:A:68:LEU:HG	1:A:69:TRP:CD1	0.46	2.46	3	10
1:A:85:THR:HA	1:A:124:GLU:O	0.46	2.10	2	3
1:A:60:ASN:O	1:A:64:HIS:HB3	0.46	2.10	1	8
1:A:37:VAL:HG12	1:A:123:PHE:O	0.46	2.11	1	10
1:A:132:TRP:N	1:A:133:GLN:NE2	0.45	2.64	9	10
1:A:24:ILE:HG13	1:A:28:PHE:CD2	0.45	2.47	10	1
1:A:68:LEU:HG	1:A:69:TRP:NE1	0.45	2.27	7	10
1:A:136:PHE:CE2	1:A:138:GLY:HA2	0.45	2.47	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:TRP:N	1:A:69:TRP:CD1	0.44	2.85	4	4
1:A:51:ALA:HB3	1:A:79:HIS:CG	0.44	2.46	10	1
1:A:48:ARG:HA	1:A:105:GLN:O	0.44	2.12	7	7
1:A:69:TRP:CD1	1:A:69:TRP:N	0.44	2.86	1	5
1:A:24:ILE:N	1:A:24:ILE:HD12	0.43	2.26	10	2
1:A:125:MET:SD	1:A:141:ASP:O	0.43	2.77	7	1
1:A:90:LEU:HA	1:A:111:GLY:N	0.42	2.29	6	3
1:A:78:GLN:HA	1:A:83:MET:O	0.42	2.14	3	3
1:A:24:ILE:HG13	1:A:28:PHE:CE1	0.42	2.49	8	2
1:A:28:PHE:O	1:A:30:GLY:N	0.41	2.50	1	1
1:A:47:VAL:HG21	1:A:90:LEU:HD22	0.41	1.93	2	2
1:A:24:ILE:HG12	1:A:34:HIS:O	0.41	2.15	10	1
1:A:65:PRO:HD2	1:A:69:TRP:CD1	0.41	2.50	5	1
1:A:61:GLY:HA3	1:A:73:ASN:HD21	0.41	1.75	5	1
1:A:55:VAL:HG23	1:A:99:SER:O	0.41	2.15	7	1
1:A:52:ASN:HD21	1:A:80:ALA:HB2	0.41	1.75	10	2
1:A:65:PRO:O	1:A:69:TRP:HB2	0.41	2.15	3	2
1:A:37:VAL:HG13	1:A:39:TYR:CE1	0.41	2.51	6	2
1:A:24:ILE:HG13	1:A:28:PHE:CE2	0.41	2.50	10	1
1:A:61:GLY:HA2	1:A:64:HIS:ND1	0.40	2.31	2	1
1:A:103:GLN:NE2	1:A:103:GLN:C	0.40	2.72	8	1
1:A:24:ILE:HG13	1:A:28:PHE:CD1	0.40	2.52	8	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	126/159 (79%)	100±0 (79±0%)	23±0 (19±0%)	3±0 (2±0%)	12	49
All	All	1260/1590 (79%)	996 (79%)	234 (19%)	30 (2%)	12	49

All 3 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	29	ASN	10
1	A	132	TRP	10
1	A	134	ASN	10

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/122 (78%)	70±1 (74±1%)	25±1 (26±1%)	3	24
All	All	950/1220 (78%)	700 (74%)	250 (26%)	3	24

All 33 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	20	ASP	10
1	A	24	ILE	10
1	A	103	GLN	10
1	A	64	HIS	10
1	A	28	PHE	10
1	A	93	ILE	10
1	A	63	ASN	10
1	A	81	ASP	10
1	A	140	ILE	10
1	A	95	VAL	10
1	A	35	VAL	10
1	A	136	PHE	10
1	A	23	ASN	10
1	A	101	VAL	10
1	A	52	ASN	10
1	A	133	GLN	10
1	A	76	LEU	10
1	A	85	THR	10
1	A	19	LEU	10
1	A	69	TRP	9
1	A	110	THR	9
1	A	107	ILE	9
1	A	139	ARG	7

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Mol	Chain	Res	Type	Models (Total)
1	A	143	THR	6
1	A	98	ASP	5
1	A	60	ASN	3
1	A	56	LYS	3
1	A	129	ASN	2
1	A	78	GLN	2
1	A	67	MET	2
1	A	92	LYS	1
1	A	70	MET	1
1	A	142	PRO	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is unknown and 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: 5kvp_cs.cif

Chemical shift list name: *c74achemshifts_v2.txt*

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	1631
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1631
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- Chain not found in structure. All 1631 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	32	PRO	HD2	3.72	0.03	2
1	48	ARG	CD	43.07	0.5	1
1	137	SER	H	9.11	0.03	1
1	116	VAL	CA	62.4	0.5	1
1	73	ASN	HB2	3.2	0.03	2
1	77	ILE	CD1	14.0	0.5	1
1	84	HIS	C	177.24	0.1	1
1	24	ILE	HG12	-0.28	0.03	1
1	42	PRO	C	176.85	0.1	1
1	52	ASN	C	178.11	0.1	1
1	55	VAL	C	175.23	0.1	1
1	71	ALA	CA	53.3	0.5	1
1	101	VAL	CG1	22.59	0.5	1
1	99	SER	CB	64.65	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	76	LEU	HG	1.35	0.03	1
1	11	GLY	H	8.45	0.03	1
1	145	TYR	C	176.88	0.1	1
1	53	GLY	CA	47.38	0.5	1
1	66	TRP	HD1	6.6	0.03	1
1	77	ILE	CG2	17.8	0.5	1
1	21	THR	HG22	1.1	0.03	1
1	111	GLY	H	8.96	0.03	1
1	106	ILE	HG12	0.76	0.03	2
1	115	GLN	HA	4.18	0.03	1
1	24	ILE	HG21	0.75	0.03	1
1	19	LEU	HG	0.48	0.03	1
1	51	ALA	HB1	1.14	0.03	1
1	95	VAL	CG2	19.6	0.5	1
1	97	THR	H	8.84	0.03	1
1	150	PRO	CG	27.0	0.5	1
1	130	PRO	HB3	1.32	0.03	1
1	123	PHE	HA	5.54	0.03	1
1	90	LEU	HA	4.4	0.03	1
1	10	HIS	HB2	3.12	0.03	2
1	123	PHE	HE1	7.0	0.03	3
1	110	THR	HA	4.57	0.03	1
1	140	ILE	HG21	0.71	0.03	1
1	146	ILE	HD12	0.73	0.03	1
1	77	ILE	HA	4.7	0.03	1
1	64	HIS	HB3	1.9	0.03	1
1	70	MET	CA	53.72	0.5	1
1	144	GLY	H	9.11	0.03	1
1	132	TRP	HB3	2.89	0.03	2
1	96	SER	N	112.13	0.25	1
1	35	VAL	HG13	0.7	0.03	1
1	106	ILE	HG23	0.65	0.03	1
1	21	THR	N	109.76	0.25	1
1	117	THR	HB	4.17	0.03	1
1	139	ARG	CB	32.39	0.5	1
1	12	SER	C	173.93	0.1	1
1	107	ILE	CG2	18.87	0.5	1
1	85	THR	N	110.6	0.25	1
1	93	ILE	HG21	0.61	0.03	1
1	19	LEU	HD22	0.92	0.03	1
1	12	SER	HB3	3.78	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	52	ASN	HD22	7.0	0.03	1
1	125	MET	CE	17.5	0.5	1
1	55	VAL	CB	30.93	0.5	1
1	137	SER	CB	62.15	0.5	1
1	49	ALA	HB2	1.2	0.03	1
1	156	THR	HG21	1.2	0.03	1
1	149	ALA	HB2	1.35	0.03	1
1	157	PRO	CA	63.0	0.5	1
1	157	PRO	HA	4.51	0.03	1
1	54	THR	HB	3.87	0.03	1
1	41	VAL	N	120.23	0.25	1
1	96	SER	C	174.57	0.1	1
1	133	GLN	CB	27.53	0.5	1
1	74	ALA	CB	24.0	0.5	1
1	99	SER	H	7.86	0.03	1
1	136	PHE	CB	39.82	0.5	1
1	155	THR	HG22	1.17	0.03	1
1	101	VAL	HG23	0.57	0.03	1
1	75	VAL	CG2	19.62	0.5	1
1	93	ILE	CB	40.31	0.5	1
1	29	ASN	HB2	1.92	0.03	1
1	77	ILE	H	10.07	0.03	1
1	151	VAL	C	176.87	0.1	1
1	16	THR	HG23	1.15	0.03	1
1	35	VAL	C	175.34	0.1	1
1	93	ILE	HD11	0.73	0.03	1
1	43	VAL	H	8.56	0.03	1
1	26	THR	HB	4.05	0.03	1
1	135	GLY	H	8.53	0.03	1
1	37	VAL	HG22	0.73	0.03	1
1	148	ASN	HD21	7.55	0.03	1
1	146	ILE	C	178.04	0.1	1
1	95	VAL	H	6.87	0.03	1
1	35	VAL	CG2	22.27	0.5	1
1	103	GLN	CA	58.59	0.5	1
1	145	TYR	HB3	2.83	0.03	2
1	15	TYR	HB3	2.89	0.03	1
1	76	LEU	HB3	1.17	0.03	1
1	105	GLN	HE21	7.44	0.03	1
1	62	ALA	HB2	1.4	0.03	1
1	42	PRO	HB3	1.76	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	133	GLN	HB2	2.01	0.03	1
1	83	MET	CE	16.45	0.5	1
1	77	ILE	HG21	0.21	0.03	1
1	34	HIS	CB	27.88	0.5	1
1	78	GLN	CB	31.12	0.5	1
1	28	PHE	HE1	6.41	0.03	3
1	28	PHE	HB3	2.5	0.03	2
1	152	PHE	HB3	2.71	0.03	2
1	105	GLN	HB3	2.05	0.03	1
1	123	PHE	HZ	7.26	0.03	1
1	152	PHE	H	9.7	0.03	1
1	25	THR	HA	4.41	0.03	1
1	124	GLU	H	7.7	0.03	1
1	114	GLY	N	109.18	0.25	1
1	97	THR	HG23	1.22	0.03	1
1	21	THR	CA	59.81	0.5	1
1	83	MET	N	118.06	0.25	1
1	62	ALA	H	8.32	0.03	1
1	85	THR	CA	59.3	0.5	1
1	155	THR	N	114.13	0.25	1
1	151	VAL	CB	32.35	0.5	1
1	85	THR	HA	5.05	0.03	1
1	32	PRO	CB	31.67	0.5	1
1	102	LYS	HE2	2.97	0.03	2
1	17	ARG	HB2	1.6	0.03	2
1	34	HIS	HD2	7.19	0.03	1
1	65	PRO	HD3	3.15	0.03	1
1	104	GLY	C	172.45	0.1	1
1	68	LEU	C	174.24	0.1	1
1	101	VAL	CA	57.89	0.5	1
1	95	VAL	HG21	1.0	0.03	1
1	146	ILE	CG1	28.55	0.5	1
1	91	SER	N	115.61	0.25	1
1	22	GLY	HA3	3.86	0.03	2
1	77	ILE	CB	40.71	0.5	1
1	132	TRP	NE1	127.85	0.25	1
1	131	ASN	C	175.41	0.1	1
1	90	LEU	HD22	0.65	0.03	1
1	98	ASP	HB3	2.89	0.03	2
1	95	VAL	CB	35.27	0.5	1
1	153	ASN	N	125.29	0.25	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	29	ASN	C	176.65	0.1	1
1	140	ILE	HD13	0.68	0.03	1
1	37	VAL	HG12	0.97	0.03	1
1	90	LEU	CB	45.03	0.5	1
1	75	VAL	C	173.85	0.1	1
1	45	THR	CA	62.76	0.5	1
1	139	ARG	HA	4.89	0.03	1
1	96	SER	HA	4.82	0.03	1
1	46	PRO	CD	51.7	0.5	1
1	71	ALA	HB2	1.34	0.03	1
1	67	MET	HE2	2.07	0.03	1
1	156	THR	H	8.36	0.03	1
1	34	HIS	H	8.03	0.03	1
1	152	PHE	HA	4.12	0.03	1
1	120	HIS	HB3	3.02	0.03	2
1	41	VAL	H	7.26	0.03	1
1	108	GLY	HA2	4.24	0.03	2
1	58	ALA	H	6.88	0.03	1
1	51	ALA	CB	21.22	0.5	1
1	106	ILE	C	177.13	0.1	1
1	134	ASN	HD22	7.23	0.03	1
1	149	ALA	C	174.86	0.1	1
1	115	GLN	HB3	1.82	0.03	2
1	67	MET	H	7.97	0.03	1
1	132	TRP	HD1	7.25	0.03	1
1	134	ASN	CB	38.01	0.5	1
1	107	ILE	HD12	-0.24	0.03	1
1	100	THR	HG22	1.2	0.03	1
1	62	ALA	CB	18.9	0.5	1
1	130	PRO	CA	62.61	0.5	1
1	101	VAL	C	175.36	0.1	1
1	24	ILE	HD11	0.8	0.03	1
1	151	VAL	HA	3.98	0.03	1
1	148	ASN	HA	5.0	0.03	1
1	73	ASN	CA	53.47	0.5	1
1	119	PRO	HA	4.6	0.03	1
1	154	GLY	C	173.79	0.1	1
1	34	HIS	HB3	3.24	0.03	2
1	76	LEU	HD11	0.42	0.03	1
1	114	GLY	CA	44.11	0.5	1
1	22	GLY	N	107.1	0.25	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	76	LEU	N	128.23	0.25	1
1	40	ALA	HB2	1.49	0.03	1
1	42	PRO	CD	50.5	0.5	1
1	75	VAL	CA	60.38	0.5	1
1	52	ASN	H	9.32	0.03	1
1	67	MET	HB2	2.19	0.03	2
1	47	VAL	HG22	0.92	0.03	1
1	145	TYR	CB	38.8	0.5	1
1	64	HIS	HA	4.46	0.03	1
1	111	GLY	C	171.58	0.1	1
1	92	LYS	HE2	2.78	0.03	2
1	135	GLY	HA3	3.43	0.03	2
1	41	VAL	HG12	1.0	0.03	1
1	18	PRO	C	173.9	0.1	1
1	79	HIS	ND1	165.0	0.25	1
1	159	GLU	CB	31.07	0.5	1
1	20	ASP	C	175.71	0.1	1
1	128	ALA	N	120.24	0.25	1
1	45	THR	HG23	1.38	0.03	1
1	55	VAL	HG13	0.68	0.03	1
1	142	PRO	CA	63.17	0.5	1
1	69	TRP	N	118.22	0.25	1
1	94	SER	HB3	3.34	0.03	1
1	19	LEU	HB3	1.61	0.03	1
1	120	HIS	H	7.98	0.03	1
1	41	VAL	CB	33.79	0.5	1
1	77	ILE	HD13	0.8	0.03	1
1	51	ALA	H	7.45	0.03	1
1	63	ASN	CA	52.84	0.5	1
1	55	VAL	HG23	0.73	0.03	1
1	43	VAL	HG12	1.15	0.03	1
1	116	VAL	CB	34.64	0.5	1
1	131	ASN	HB3	2.79	0.03	1
1	106	ILE	HB	1.66	0.03	1
1	115	GLN	CG	34.1	0.5	1
1	154	GLY	CA	45.25	0.5	1
1	105	GLN	CD	179.45	0.1	1
1	143	THR	H	8.5	0.03	1
1	121	LEU	C	177.89	0.1	1
1	20	ASP	H	9.35	0.03	1
1	46	PRO	HD2	4.4	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	92	LYS	CA	55.45	0.5	1
1	24	ILE	CD1	13.3	0.5	1
1	21	THR	HG21	1.1	0.03	1
1	41	VAL	HG22	1.49	0.03	1
1	127	PRO	HG2	1.54	0.03	2
1	132	TRP	H	7.32	0.03	1
1	149	ALA	HA	4.5	0.03	1
1	84	HIS	HA	6.15	0.03	1
1	112	ALA	HB2	1.31	0.03	1
1	24	ILE	HG22	0.75	0.03	1
1	51	ALA	HB2	1.14	0.03	1
1	18	PRO	CA	63.82	0.5	1
1	150	PRO	CD	50.1	0.5	1
1	19	LEU	CG	28.17	0.5	1
1	104	GLY	H	8.11	0.03	1
1	87	TYR	HB3	2.79	0.03	2
1	110	THR	HB	4.57	0.03	1
1	60	ASN	CG	177.2	0.1	1
1	73	ASN	N	121.29	0.25	1
1	127	PRO	C	174.28	0.1	1
1	63	ASN	HB2	2.97	0.03	1
1	131	ASN	H	9.09	0.03	1
1	128	ALA	CA	55.55	0.5	1
1	129	ASN	CG	177.78	0.1	1
1	82	GLY	CA	44.55	0.5	1
1	42	PRO	HD3	3.78	0.03	2
1	53	GLY	HA2	4.34	0.03	2
1	140	ILE	HA	4.43	0.03	1
1	58	ALA	HB3	1.05	0.03	1
1	117	THR	HA	4.27	0.03	1
1	120	HIS	CB	29.62	0.5	1
1	91	SER	HB2	4.01	0.03	2
1	74	ALA	HB3	1.3	0.03	1
1	121	LEU	CA	54.99	0.5	1
1	55	VAL	CA	63.46	0.5	1
1	137	SER	HB3	4.08	0.03	2
1	106	ILE	H	8.52	0.03	1
1	18	PRO	HB2	0.63	0.03	1
1	60	ASN	HD22	7.2	0.03	1
1	49	ALA	HB1	1.2	0.03	1
1	58	ALA	C	174.68	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	12	SER	CB	64.14	0.5	1
1	149	ALA	HB1	1.35	0.03	1
1	150	PRO	HG2	2.05	0.03	2
1	69	TRP	CA	58.85	0.5	1
1	102	LYS	CG	25.19	0.5	1
1	141	ASP	C	177.28	0.1	1
1	57	PHE	N	116.51	0.25	1
1	130	PRO	HD2	3.0	0.03	2
1	64	HIS	HD2	6.6	0.03	4
1	95	VAL	N	111.64	0.25	1
1	133	GLN	CA	54.96	0.5	1
1	16	THR	CB	70.17	0.5	1
1	67	MET	CG	32.42	0.5	1
1	54	THR	H	8.56	0.03	1
1	145	TYR	N	116.13	0.25	1
1	30	GLY	H	8.28	0.03	1
1	121	LEU	CB	44.19	0.5	1
1	75	VAL	CG1	22.7	0.5	1
1	132	TRP	CB	29.22	0.5	1
1	140	ILE	CA	57.78	0.5	1
1	128	ALA	C	178.44	0.1	1
1	101	VAL	H	8.88	0.03	1
1	114	GLY	C	170.87	0.1	1
1	50	VAL	CB	31.82	0.5	1
1	31	TYR	N	113.9	0.25	1
1	93	ILE	HD12	0.73	0.03	1
1	26	THR	HA	4.44	0.03	1
1	86	GLY	N	108.95	0.25	1
1	65	PRO	HG3	1.35	0.03	2
1	68	LEU	HD11	0.1	0.03	1
1	78	GLN	HB2	1.51	0.03	1
1	48	ARG	HG2	1.05	0.03	2
1	109	TYR	HB2	2.57	0.03	2
1	148	ASN	HB3	2.5	0.03	1
1	105	GLN	HE22	7.24	0.03	1
1	56	LYS	N	132.95	0.25	1
1	76	LEU	C	175.66	0.1	1
1	134	ASN	N	118.17	0.25	1
1	60	ASN	HA	4.79	0.03	1
1	110	THR	N	116.62	0.25	1
1	107	ILE	HG13	0.4	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	77	ILE	HG22	0.21	0.03	1
1	93	ILE	HG13	0.73	0.03	2
1	102	LYS	HB3	1.52	0.03	1
1	78	GLN	CG	34.07	0.5	1
1	15	TYR	C	176.18	0.1	1
1	150	PRO	HD2	3.81	0.03	2
1	66	TRP	HZ2	7.73	0.03	1
1	82	GLY	N	109.47	0.25	1
1	156	THR	C	172.66	0.1	1
1	52	ASN	HA	4.7	0.03	1
1	152	PHE	HD1	7.2	0.03	3
1	25	THR	HB	3.65	0.03	1
1	73	ASN	HD21	7.4	0.03	1
1	55	VAL	HB	2.37	0.03	1
1	56	LYS	CE	41.42	0.5	1
1	93	ILE	HB	1.7	0.03	1
1	29	ASN	HD21	7.78	0.03	1
1	96	SER	HB3	3.76	0.03	2
1	66	TRP	HA	4.82	0.03	1
1	147	ALA	N	128.3	0.25	1
1	48	ARG	HE	9.42	0.03	1
1	69	TRP	HB2	3.15	0.03	2
1	107	ILE	HG22	0.56	0.03	1
1	32	PRO	CG	27.8	0.5	1
1	131	ASN	N	119.4	0.25	1
1	113	THR	CB	71.53	0.5	1
1	77	ILE	C	173.96	0.1	1
1	101	VAL	CB	35.45	0.5	1
1	125	MET	CA	54.87	0.5	1
1	146	ILE	CG2	18.32	0.5	1
1	125	MET	HA	5.14	0.03	1
1	139	ARG	HB2	2.09	0.03	2
1	121	LEU	HB2	1.78	0.03	1
1	25	THR	N	121.81	0.25	1
1	132	TRP	C	176.97	0.1	1
1	130	PRO	HG2	0.56	0.03	1
1	118	GLY	HA3	3.44	0.03	2
1	95	VAL	CA	58.86	0.5	1
1	45	THR	HG21	1.38	0.03	1
1	72	GLY	HA2	4.3	0.03	2
1	78	GLN	HE21	7.66	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	125	MET	HE2	1.85	0.03	1
1	37	VAL	HA	4.9	0.03	1
1	126	LEU	CD2	27.2	0.5	1
1	2	ARG	C	176.51	0.1	1
1	17	ARG	CD	44.28	0.5	1
1	59	GLY	H	8.26	0.03	1
1	28	PHE	H	9.39	0.03	1
1	94	SER	H	8.63	0.03	1
1	82	GLY	HA3	3.46	0.03	2
1	118	GLY	C	175.1	0.1	1
1	37	VAL	CG2	19.03	0.5	1
1	11	GLY	HA2	3.96	0.03	2
1	55	VAL	H	9.37	0.03	1
1	119	PRO	CG	27.38	0.5	1
1	79	HIS	HB3	3.37	0.03	2
1	66	TRP	H	10.47	0.03	1
1	85	THR	CG2	16.1	0.5	1
1	134	ASN	CA	53.52	0.5	1
1	110	THR	CA	63.28	0.5	1
1	99	SER	HB2	3.98	0.03	2
1	107	ILE	HD11	-0.24	0.03	1
1	123	PHE	CA	55.37	0.5	1
1	107	ILE	HG12	0.6	0.03	2
1	115	GLN	HE22	6.8	0.03	1
1	16	THR	HB	3.87	0.03	1
1	27	GLY	C	174.91	0.1	1
1	43	VAL	CA	64.38	0.5	1
1	130	PRO	CB	30.92	0.5	1
1	117	THR	C	173.77	0.1	1
1	138	GLY	HA2	3.53	0.03	2
1	79	HIS	N	129.62	0.25	1
1	63	ASN	ND2	111.9	0.25	1
1	133	GLN	HG2	2.92	0.03	2
1	15	TYR	HA	5.2	0.03	1
1	73	ASN	CB	37.82	0.5	1
1	104	GLY	HA3	2.05	0.03	1
1	69	TRP	NE1	131.5	0.25	1
1	50	VAL	H	7.53	0.03	1
1	80	ALA	CB	18.69	0.5	1
1	113	THR	H	7.77	0.03	1
1	138	GLY	N	103.5	0.25	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	75	VAL	HG23	1.0	0.03	1
1	85	THR	HG22	1.2	0.03	1
1	153	ASN	HD21	7.4	0.03	1
1	118	GLY	CA	44.47	0.5	1
1	96	SER	CA	56.24	0.5	1
1	101	VAL	HA	4.95	0.03	1
1	61	GLY	H	9.69	0.03	1
1	151	VAL	HG21	1.05	0.03	1
1	67	MET	N	118.26	0.25	1
1	148	ASN	H	8.64	0.03	1
1	95	VAL	HB	2.04	0.03	1
1	95	VAL	HG13	0.86	0.03	1
1	32	PRO	HB2	2.23	0.03	2
1	83	MET	HE2	1.75	0.03	1
1	41	VAL	HG11	1.0	0.03	1
1	88	ALA	CA	51.15	0.5	1
1	72	GLY	C	174.69	0.1	1
1	142	PRO	CD	50.82	0.5	1
1	79	HIS	HA	4.99	0.03	1
1	120	HIS	HA	4.57	0.03	1
1	151	VAL	CG1	22.32	0.5	1
1	57	PHE	CB	43.23	0.5	1
1	35	VAL	HA	4.06	0.03	1
1	87	TYR	H	8.47	0.03	1
1	121	LEU	HG	0.52	0.03	1
1	16	THR	N	112.24	0.25	1
1	64	HIS	CB	33.11	0.5	1
1	117	THR	CA	62.68	0.5	1
1	66	TRP	CB	29.03	0.5	1
1	17	ARG	HD2	3.2	0.03	2
1	65	PRO	CG	27.0	0.5	1
1	48	ARG	CG	28.53	0.5	1
1	14	THR	N	116.71	0.25	1
1	106	ILE	HA	4.32	0.03	1
1	14	THR	HG21	0.87	0.03	1
1	139	ARG	HE	8.3	0.03	1
1	30	GLY	HA3	3.48	0.03	2
1	29	ASN	CG	177.01	0.1	1
1	88	ALA	HB2	1.27	0.03	1
1	31	TYR	CB	37.86	0.5	1
1	129	ASN	HA	5.14	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	38	ASP	CB	44.05	0.5	1
1	56	LYS	CB	32.36	0.5	1
1	92	LYS	CD	29.36	0.5	1
1	36	GLY	CA	45.0	0.5	1
1	106	ILE	HG13	0.74	0.03	2
1	99	SER	N	115.13	0.25	1
1	140	ILE	H	7.85	0.03	1
1	154	GLY	HA3	3.7	0.03	2
1	40	ALA	H	8.45	0.03	1
1	116	VAL	HG13	1.14	0.03	2
1	102	LYS	HG3	1.48	0.03	1
1	29	ASN	CB	39.31	0.5	1
1	44	GLY	HA3	4.45	0.03	1
1	43	VAL	N	121.13	0.25	1
1	52	ASN	HB2	3.16	0.03	1
1	2	ARG	HB3	1.79	0.03	2
1	90	LEU	HG	1.3	0.03	1
1	24	ILE	HD13	0.8	0.03	1
1	13	ALA	HB2	1.29	0.03	1
1	133	GLN	HE22	6.92	0.03	1
1	47	VAL	CA	60.51	0.5	1
1	56	LYS	HA	4.45	0.03	1
1	93	ILE	CG2	19.04	0.5	1
1	77	ILE	HG13	0.71	0.03	2
1	116	VAL	HB	2.42	0.03	1
1	50	VAL	HG23	1.2	0.03	1
1	39	TYR	HB2	2.59	0.03	2
1	38	ASP	HB2	2.52	0.03	2
1	33	GLY	C	174.9	0.1	1
1	32	PRO	HA	4.54	0.03	1
1	80	ALA	C	178.04	0.1	1
1	59	GLY	CA	44.91	0.5	1
1	132	TRP	HA	4.12	0.03	1
1	126	LEU	HG	1.52	0.03	1
1	139	ARG	N	122.6	0.25	1
1	94	SER	C	173.3	0.1	1
1	147	ALA	HB1	1.44	0.03	1
1	117	THR	HG23	1.5	0.03	1
1	127	PRO	HD2	3.3	0.03	1
1	156	THR	HG22	1.2	0.03	1
1	12	SER	CA	58.32	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	157	PRO	CG	27.82	0.5	1
1	102	LYS	CD	29.12	0.5	1
1	31	TYR	H	7.2	0.03	1
1	25	THR	CB	69.2	0.5	1
1	121	LEU	HD13	1.48	0.03	1
1	135	GLY	CA	44.81	0.5	1
1	79	HIS	HD1	10.99	0.03	1
1	142	PRO	HG2	1.98	0.03	2
1	133	GLN	CD	180.65	0.1	1
1	16	THR	CA	60.14	0.5	1
1	38	ASP	H	9.0	0.03	1
1	78	GLN	HA	4.74	0.03	1
1	56	LYS	H	8.96	0.03	1
1	25	THR	HG23	0.7	0.03	1
1	107	ILE	C	175.46	0.1	1
1	14	THR	CA	63.55	0.5	1
1	70	MET	HE3	2.07	0.03	1
1	140	ILE	CB	41.4	0.5	1
1	91	SER	H	9.3	0.03	1
1	60	ASN	HB2	2.94	0.03	2
1	73	ASN	HB3	2.13	0.03	2
1	23	ASN	CG	177.08	0.1	1
1	49	ALA	C	182.82	0.1	1
1	127	PRO	HB2	1.94	0.03	1
1	26	THR	CA	63.29	0.5	1
1	68	LEU	HD12	0.1	0.03	1
1	115	GLN	C	175.91	0.1	1
1	74	ALA	CA	50.64	0.5	1
1	19	LEU	C	177.25	0.1	1
1	82	GLY	H	8.03	0.03	1
1	101	VAL	CG2	18.83	0.5	1
1	130	PRO	HA	3.6	0.03	1
1	151	VAL	CA	62.6	0.5	1
1	86	GLY	HA3	3.77	0.03	2
1	125	MET	HG2	2.29	0.03	2
1	95	VAL	CG1	22.69	0.5	1
1	19	LEU	HD11	1.02	0.03	1
1	63	ASN	HD21	7.72	0.03	1
1	133	GLN	HA	4.69	0.03	1
1	102	LYS	HA	4.77	0.03	1
1	146	ILE	HD13	0.73	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	135	GLY	C	173.79	0.1	1
1	30	GLY	N	105.73	0.25	1
1	149	ALA	H	6.99	0.03	1
1	133	GLN	NE2	111.8	0.25	1
1	65	PRO	CD	50.5	0.5	1
1	29	ASN	HD22	6.8	0.03	1
1	140	ILE	HG13	0.97	0.03	2
1	132	TRP	HB2	3.44	0.03	2
1	14	THR	C	174.05	0.1	1
1	83	MET	HB3	1.94	0.03	1
1	126	LEU	HD11	0.7	0.03	1
1	71	ALA	HA	3.8	0.03	1
1	37	VAL	CB	34.44	0.5	1
1	88	ALA	HA	5.48	0.03	1
1	73	ASN	ND2	112.5	0.25	1
1	109	TYR	CA	55.93	0.5	1
1	48	ARG	HD2	2.95	0.03	2
1	10	HIS	HA	4.61	0.03	1
1	90	LEU	CD1	23.5	0.5	1
1	93	ILE	HG22	0.61	0.03	1
1	19	LEU	HD21	0.92	0.03	1
1	12	SER	HB2	3.83	0.03	2
1	79	HIS	HE1	7.21	0.03	1
1	102	LYS	HB2	1.82	0.03	1
1	47	VAL	HG13	0.88	0.03	1
1	70	MET	C	175.11	0.1	1
1	15	TYR	H	7.75	0.03	1
1	13	ALA	HA	4.41	0.03	1
1	124	GLU	C	173.06	0.1	1
1	78	GLN	HE22	7.1	0.03	1
1	68	LEU	CA	54.72	0.5	1
1	125	MET	HB3	1.91	0.03	1
1	98	ASP	HA	4.33	0.03	1
1	64	HIS	N	121.99	0.25	1
1	62	ALA	HA	3.98	0.03	1
1	66	TRP	N	121.34	0.25	1
1	94	SER	HA	4.75	0.03	1
1	155	THR	HG23	1.17	0.03	1
1	115	GLN	N	121.51	0.25	1
1	38	ASP	HA	6.67	0.03	1
1	69	TRP	H	8.28	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	129	ASN	ND2	112.8	0.25	1
1	106	ILE	CG1	27.42	0.5	1
1	158	THR	HG23	1.2	0.03	1
1	37	VAL	HG21	0.73	0.03	1
1	155	THR	CA	62.0	0.5	1
1	134	ASN	HD21	7.66	0.03	1
1	103	GLN	CB	29.67	0.5	1
1	15	TYR	HB2	2.8	0.03	1
1	76	LEU	HB2	1.7	0.03	1
1	62	ALA	HB3	1.4	0.03	1
1	42	PRO	HB2	1.82	0.03	2
1	114	GLY	H	7.51	0.03	1
1	123	PHE	CB	42.86	0.5	1
1	78	GLN	C	175.39	0.1	1
1	112	ALA	CB	19.77	0.5	1
1	115	GLN	HE21	7.52	0.03	1
1	72	GLY	H	7.89	0.03	1
1	34	HIS	CA	56.56	0.5	1
1	75	VAL	H	8.51	0.03	1
1	37	VAL	H	8.98	0.03	1
1	130	PRO	CG	27.64	0.5	1
1	28	PHE	HB2	2.62	0.03	2
1	62	ALA	N	118.73	0.25	1
1	142	PRO	HD3	3.8	0.03	2
1	73	ASN	CG	176.3	0.1	1
1	23	ASN	HB3	2.6	0.03	2
1	89	HIS	HB2	3.76	0.03	2
1	14	THR	CG2	21.48	0.5	1
1	124	GLU	CA	52.6	0.5	1
1	130	PRO	C	174.82	0.1	1
1	48	ARG	HA	4.81	0.03	1
1	85	THR	HB	3.92	0.03	1
1	98	ASP	CB	38.8	0.5	1
1	88	ALA	CB	22.53	0.5	1
1	17	ARG	HB3	1.89	0.03	2
1	159	GLU	N	127.47	0.25	1
1	154	GLY	H	6.76	0.03	1
1	113	THR	CA	62.01	0.5	1
1	22	GLY	HA2	4.26	0.03	2
1	46	PRO	C	174.32	0.1	1
1	90	LEU	HD23	0.65	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	35	VAL	HB	2.44	0.03	1
1	98	ASP	HB2	3.14	0.03	2
1	47	VAL	CB	33.58	0.5	1
1	81	ASP	HB2	3.05	0.03	1
1	66	TRP	C	176.64	0.1	1
1	102	LYS	HD2	1.65	0.03	2
1	146	ILE	H	7.9	0.03	1
1	141	ASP	N	121.85	0.25	1
1	108	GLY	H	7.43	0.03	1
1	50	VAL	HG13	0.8	0.03	1
1	20	ASP	CA	56.33	0.5	1
1	68	LEU	HD23	0.45	0.03	1
1	143	THR	HG22	1.15	0.03	1
1	37	VAL	HG13	0.97	0.03	1
1	90	LEU	CA	55.97	0.5	1
1	150	PRO	HA	4.6	0.03	1
1	158	THR	N	114.39	0.25	1
1	123	PHE	H	9.49	0.03	1
1	28	PHE	HD1	6.69	0.03	3
1	39	TYR	N	118.4	0.25	1
1	66	TRP	HB2	3.25	0.03	2
1	46	PRO	CG	28.0	0.5	1
1	67	MET	HE3	2.07	0.03	1
1	139	ARG	HD2	3.5	0.03	2
1	131	ASN	ND2	109.7	0.25	1
1	49	ALA	H	8.11	0.03	1
1	57	PHE	HB2	3.21	0.03	2
1	104	GLY	CA	43.69	0.5	1
1	92	LYS	HG2	1.41	0.03	1
1	112	ALA	C	176.53	0.1	1
1	57	PHE	C	171.64	0.1	1
1	70	MET	HA	4.11	0.03	9
1	148	ASN	CA	51.47	0.5	1
1	14	THR	HG23	0.87	0.03	1
1	92	LYS	CG	24.86	0.5	1
1	105	GLN	HA	3.82	0.03	1
1	102	LYS	C	175.78	0.1	1
1	152	PHE	HB2	3.16	0.03	2
1	53	GLY	N	111.65	0.25	1
1	121	LEU	HD21	1.0	0.03	1
1	87	TYR	HE1	6.93	0.03	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	149	ALA	CB	17.53	0.5	1
1	119	PRO	C	176.65	0.1	1
1	100	THR	HG23	1.2	0.03	1
1	71	ALA	HB1	1.34	0.03	1
1	86	GLY	H	8.4	0.03	1
1	45	THR	C	173.14	0.1	1
1	106	ILE	HG22	0.65	0.03	1
1	42	PRO	CG	27.8	0.5	1
1	151	VAL	HB	1.96	0.03	1
1	133	GLN	HE21	7.61	0.03	1
1	34	HIS	HE1	7.35	0.03	1
1	41	VAL	CG1	23.0	0.5	1
1	88	ALA	H	9.01	0.03	1
1	43	VAL	HG21	1.09	0.03	1
1	34	HIS	HB2	3.65	0.03	2
1	124	GLU	N	122.18	0.25	1
1	110	THR	H	10.11	0.03	1
1	106	ILE	CA	61.79	0.5	1
1	40	ALA	HB3	1.49	0.03	1
1	127	PRO	HA	5.07	0.03	1
1	65	PRO	HA	4.24	0.03	1
1	158	THR	CG2	21.84	0.5	1
1	37	VAL	N	110.92	0.25	1
1	120	HIS	HD2	6.67	0.03	1
1	47	VAL	HG23	0.92	0.03	1
1	82	GLY	C	173.23	0.1	1
1	156	THR	N	120.64	0.25	1
1	121	LEU	CG	28.0	0.5	1
1	54	THR	C	173.68	0.1	1
1	50	VAL	CA	62.71	0.5	1
1	128	ALA	H	8.26	0.03	1
1	135	GLY	HA2	4.14	0.03	2
1	75	VAL	HG11	0.8	0.03	1
1	102	LYS	H	8.08	0.03	1
1	102	LYS	CA	53.4	0.5	1
1	45	THR	HG22	1.38	0.03	1
1	94	SER	HB2	3.97	0.03	1
1	79	HIS	HD2	6.47	0.03	9
1	40	ALA	C	175.38	0.1	1
1	13	ALA	H	8.45	0.03	1
1	90	LEU	HD13	0.74	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	123	PHE	HD1	6.8	0.03	3
1	55	VAL	HG22	0.73	0.03	1
1	60	ASN	ND2	111.9	0.25	1
1	128	ALA	HB1	1.34	0.03	1
1	43	VAL	HG11	1.15	0.03	1
1	111	GLY	CA	48.1	0.5	1
1	132	TRP	N	123.25	0.25	1
1	84	HIS	CA	55.38	0.5	1
1	23	ASN	CB	41.92	0.5	1
1	127	PRO	CG	27.98	0.5	1
1	61	GLY	HA2	3.85	0.03	2
1	53	GLY	C	170.5	0.1	1
1	148	ASN	N	113.42	0.25	1
1	61	GLY	N	115.64	0.25	1
1	141	ASP	H	7.93	0.03	1
1	128	ALA	HA	4.23	0.03	1
1	103	GLN	N	120.31	0.25	1
1	76	LEU	HA	5.69	0.03	1
1	134	ASN	HB3	2.88	0.03	2
1	41	VAL	HG23	1.49	0.03	1
1	100	THR	CG2	21.6	0.5	1
1	39	TYR	H	9.09	0.03	1
1	144	GLY	HA3	3.47	0.03	2
1	89	HIS	N	114.78	0.25	1
1	24	ILE	HG23	0.75	0.03	1
1	19	LEU	HA	4.72	0.03	1
1	51	ALA	HB3	1.14	0.03	1
1	18	PRO	CB	31.61	0.5	1
1	19	LEU	HD12	1.02	0.03	1
1	84	HIS	HB2	3.07	0.03	2
1	35	VAL	HG23	1.1	0.03	1
1	24	ILE	CA	62.96	0.5	1
1	128	ALA	CB	18.75	0.5	1
1	92	LYS	HA	4.58	0.03	1
1	42	PRO	HD2	3.82	0.03	2
1	16	THR	CG2	21.2	0.5	1
1	117	THR	CG2	23.1	0.5	1
1	125	MET	H	9.32	0.03	1
1	139	ARG	HG3	1.32	0.03	2
1	35	VAL	HG11	0.7	0.03	1
1	122	HIS	CA	56.49	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	12	SER	HA	4.44	0.03	1
1	37	VAL	CA	58.86	0.5	1
1	11	GLY	C	173.94	0.1	1
1	58	ALA	HB2	1.05	0.03	1
1	159	GLU	HB2	1.94	0.03	2
1	46	PRO	HA	4.1	0.03	1
1	147	ALA	CB	18.7	0.5	1
1	68	LEU	HB2	1.44	0.03	2
1	126	LEU	CA	53.55	0.5	1
1	105	GLN	NE2	110.5	0.25	1
1	50	VAL	N	115.97	0.25	1
1	159	GLU	CG	36.21	0.5	1
1	74	ALA	HB2	1.3	0.03	1
1	100	THR	C	174.48	0.1	1
1	98	ASP	N	121.5	0.25	1
1	87	TYR	CA	56.32	0.5	1
1	16	THR	HG21	1.15	0.03	1
1	35	VAL	CB	32.62	0.5	1
1	125	MET	CG	33.75	0.5	1
1	16	THR	HG22	1.15	0.03	1
1	60	ASN	HD21	7.8	0.03	1
1	89	HIS	HD2	6.44	0.03	4
1	28	PHE	HA	4.52	0.03	1
1	101	VAL	N	116.83	0.25	1
1	130	PRO	HD3	3.65	0.03	2
1	52	ASN	CG	176.26	0.1	1
1	141	ASP	CB	40.86	0.5	1
1	68	LEU	CB	43.5	0.5	1
1	144	GLY	C	174.86	0.1	1
1	76	LEU	CD1	25.8	0.5	1
1	153	ASN	CG	177.2	0.1	1
1	125	MET	C	174.72	0.1	1
1	145	TYR	HA	4.37	0.03	1
1	157	PRO	HB2	2.32	0.03	2
1	101	VAL	HG21	0.57	0.03	1
1	105	GLN	H	7.91	0.03	1
1	158	THR	CB	69.84	0.5	1
1	132	TRP	CA	57.58	0.5	1
1	48	ARG	CA	53.44	0.5	1
1	54	THR	HG23	1.09	0.03	1
1	39	TYR	CB	41.17	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	153	ASN	ND2	111.3	0.25	1
1	126	LEU	HB2	1.46	0.03	2
1	93	ILE	HD13	0.73	0.03	1
1	100	THR	H	8.7	0.03	1
1	113	THR	HG21	1.13	0.03	1
1	155	THR	CB	69.93	0.5	1
1	61	GLY	CA	47.63	0.5	1
1	65	PRO	HG2	1.65	0.03	2
1	78	GLN	HB3	2.02	0.03	1
1	63	ASN	H	8.47	0.03	1
1	55	VAL	CG2	22.5	0.5	1
1	29	ASN	HA	4.5	0.03	1
1	152	PHE	CA	60.18	0.5	1
1	14	THR	H	8.27	0.03	1
1	100	THR	N	116.17	0.25	1
1	83	MET	CG	34.77	0.5	1
1	133	GLN	C	175.63	0.1	1
1	147	ALA	H	8.94	0.03	1
1	158	THR	HA	4.32	0.03	1
1	77	ILE	HG23	0.21	0.03	1
1	96	SER	H	7.72	0.03	1
1	93	ILE	HG12	1.37	0.03	2
1	78	GLN	CD	179.81	0.1	1
1	150	PRO	HD3	4.06	0.03	2
1	22	GLY	C	173.28	0.1	1
1	138	GLY	CA	44.64	0.5	1
1	34	HIS	HA	4.49	0.03	1
1	32	PRO	C	177.44	0.1	1
1	56	LYS	HB2	1.55	0.03	2
1	65	PRO	C	177.62	0.1	1
1	74	ALA	H	9.46	0.03	1
1	85	THR	H	9.35	0.03	1
1	24	ILE	N	120.62	0.25	1
1	109	TYR	HD1	6.8	0.03	3
1	90	LEU	HB2	1.8	0.03	2
1	124	GLU	CB	33.45	0.5	1
1	122	HIS	N	126.51	0.25	1
1	76	LEU	CA	53.3	0.5	1
1	137	SER	HA	4.26	0.03	1
1	96	SER	HB2	3.81	0.03	2
1	17	ARG	HE	7.3	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	126	LEU	N	118.61	0.25	1
1	20	ASP	HB2	2.67	0.03	1
1	139	ARG	CG	26.97	0.5	1
1	98	ASP	CA	57.34	0.5	1
1	154	GLY	HA2	3.85	0.03	2
1	107	ILE	HG21	0.56	0.03	1
1	23	ASN	HD21	7.61	0.03	1
1	87	TYR	N	118.64	0.25	1
1	97	THR	HB	3.92	0.03	1
1	68	LEU	HG	0.82	0.03	1
1	139	ARG	C	177.01	0.1	1
1	3	GLY	CA	45.18	0.5	1
1	67	MET	C	174.11	0.1	1
1	21	THR	HA	4.51	0.03	1
1	95	VAL	HG23	1.0	0.03	1
1	113	THR	C	175.1	0.1	1
1	152	PHE	C	174.88	0.1	1
1	143	THR	HG23	1.15	0.03	1
1	24	ILE	HB	1.45	0.03	1
1	39	TYR	C	176.1	0.1	1
1	155	THR	H	8.06	0.03	1
1	49	ALA	HA	3.93	0.03	1
1	47	VAL	CG1	24.57	0.5	1
1	72	GLY	HA3	3.75	0.03	2
1	65	PRO	CA	64.22	0.5	1
1	143	THR	HG21	1.15	0.03	1
1	125	MET	HE3	1.85	0.03	1
1	37	VAL	HB	2.03	0.03	1
1	13	ALA	C	177.5	0.1	1
1	48	ARG	N	125.33	0.25	1
1	134	ASN	HA	4.43	0.03	1
1	46	PRO	CB	32.2	0.5	1
1	24	ILE	CG1	28.85	0.5	1
1	126	LEU	CD1	24.76	0.5	1
1	107	ILE	N	120.89	0.25	1
1	23	ASN	N	119.5	0.25	1
1	83	MET	HG2	2.56	0.03	2
1	47	VAL	HB	1.35	0.03	1
1	10	HIS	C	175.34	0.1	1
1	82	GLY	HA2	4.31	0.03	2
1	31	TYR	HD1	6.54	0.03	4

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	37	VAL	CG1	22.97	0.5	1
1	38	ASP	N	119.67	0.25	1
1	121	LEU	HD22	1.0	0.03	1
1	136	PHE	HE1	7.27	0.03	3
1	99	SER	HB3	3.93	0.03	2
1	147	ALA	C	178.61	0.1	1
1	73	ASN	C	174.18	0.1	1
1	14	THR	HA	4.0	0.03	1
1	43	VAL	CB	31.84	0.5	1
1	138	GLY	HA3	3.11	0.03	2
1	2	ARG	CA	56.34	0.5	1
1	31	TYR	HB3	2.81	0.03	2
1	136	PHE	HD1	6.96	0.03	3
1	104	GLY	HA2	2.6	0.03	1
1	60	ASN	HB3	2.92	0.03	2
1	43	VAL	HG22	1.09	0.03	1
1	129	ASN	N	112.68	0.25	1
1	23	ASN	C	174.11	0.1	1
1	89	HIS	HE1	7.34	0.03	4
1	76	LEU	HD13	0.42	0.03	1
1	31	TYR	C	172.92	0.1	1
1	66	TRP	HB3	3.3	0.03	2
1	136	PHE	HA	4.73	0.03	1
1	85	THR	HG21	1.2	0.03	1
1	74	ALA	HA	5.75	0.03	1
1	151	VAL	HG13	1.09	0.03	1
1	26	THR	CG2	20.33	0.5	1
1	42	PRO	HA	4.44	0.03	1
1	108	GLY	C	168.87	0.1	1
1	78	GLN	H	9.03	0.03	1
1	17	ARG	HG2	1.1	0.03	2
1	123	PHE	C	171.98	0.1	1
1	76	LEU	HD21	0.79	0.03	1
1	129	ASN	HB3	2.59	0.03	2
1	32	PRO	HB3	2.02	0.03	2
1	33	GLY	HA3	3.42	0.03	2
1	153	ASN	H	8.02	0.03	1
1	158	THR	HG21	1.2	0.03	1
1	83	MET	HE3	1.75	0.03	1
1	147	ALA	HB2	1.44	0.03	1
1	43	VAL	C	177.22	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	155	THR	CG2	21.77	0.5	1
1	47	VAL	H	8.25	0.03	1
1	3	GLY	N	111.14	0.1	1
1	142	PRO	C	178.02	0.1	1
1	156	THR	HG23	1.2	0.03	1
1	101	VAL	HG13	0.63	0.03	1
1	143	THR	HA	3.34	0.03	1
1	142	PRO	CG	27.54	0.5	1
1	57	PHE	HD1	7.26	0.03	4
1	57	PHE	CA	58.94	0.5	1
1	77	ILE	HD11	0.8	0.03	1
1	148	ASN	HD22	6.85	0.03	1
1	65	PRO	HB3	1.8	0.03	2
1	63	ASN	CG	177.33	0.1	1
1	86	GLY	C	171.47	0.1	1
1	138	GLY	H	7.96	0.03	1
1	117	THR	CB	69.84	0.5	1
1	87	TYR	HD1	7.1	0.03	3
1	128	ALA	HB2	1.34	0.03	1
1	17	ARG	HD3	3.3	0.03	2
1	97	THR	CG2	23.3	0.5	1
1	71	ALA	N	120.53	0.25	1
1	84	HIS	CB	31.42	0.5	1
1	140	ILE	N	109.84	0.25	1
1	81	ASP	C	176.79	0.1	1
1	23	ASN	CA	51.64	0.5	1
1	16	THR	C	174.23	0.1	1
1	88	ALA	HB3	1.27	0.03	1
1	31	TYR	CA	55.14	0.5	1
1	108	GLY	CA	45.34	0.5	1
1	38	ASP	CA	51.57	0.5	1
1	2	ARG	HG2	1.65	0.03	2
1	56	LYS	CA	55.62	0.5	1
1	55	VAL	CG1	23.3	0.5	1
1	126	LEU	HD23	0.43	0.03	1
1	120	HIS	C	174.29	0.1	1
1	116	VAL	HG12	1.14	0.03	2
1	102	LYS	HG2	1.39	0.03	1
1	123	PHE	HB2	2.83	0.03	1
1	18	PRO	CG	27.16	0.5	1
1	131	ASN	HD22	6.9	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	44	GLY	HA2	3.59	0.03	1
1	19	LEU	CA	52.2	0.5	1
1	2	ARG	HB2	1.83	0.03	2
1	139	ARG	H	7.85	0.03	1
1	60	ASN	CA	54.0	0.5	1
1	26	THR	H	7.31	0.03	1
1	13	ALA	HB3	1.29	0.03	1
1	153	ASN	HB2	2.6	0.03	2
1	80	ALA	HB1	1.52	0.03	1
1	106	ILE	HD12	0.83	0.03	1
1	151	VAL	N	120.52	0.25	1
1	134	ASN	H	7.56	0.03	1
1	105	GLN	C	175.56	0.1	1
1	77	ILE	HG12	1.76	0.03	2
1	116	VAL	HA	4.69	0.03	1
1	146	ILE	HG21	0.8	0.03	1
1	122	HIS	CB	33.76	0.5	1
1	110	THR	HG23	1.0	0.03	1
1	26	THR	HG21	1.25	0.03	1
1	140	ILE	CG1	25.62	0.5	1
1	147	ALA	CA	56.04	0.5	1
1	74	ALA	HB1	1.3	0.03	1
1	39	TYR	HA	5.24	0.03	1
1	45	THR	HA	4.57	0.03	1
1	112	ALA	HB1	1.31	0.03	1
1	133	GLN	H	7.81	0.03	1
1	117	THR	H	8.48	0.03	1
1	131	ASN	CG	177.34	0.1	1
1	69	TRP	C	176.4	0.1	1
1	127	PRO	HD3	3.57	0.03	1
1	84	HIS	H	9.58	0.03	1
1	93	ILE	H	8.86	0.03	1
1	102	LYS	CE	42.06	0.5	1
1	52	ASN	CB	38.26	0.5	1
1	25	THR	CA	62.48	0.5	1
1	121	LEU	HD12	1.48	0.03	1
1	145	TYR	H	7.27	0.03	1
1	54	THR	CG2	21.3	0.5	1
1	80	ALA	CA	55.69	0.5	1
1	133	GLN	CG	34.4	0.5	1
1	67	MET	CE	15.84	0.5	5

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	153	ASN	HD22	6.7	0.03	1
1	122	HIS	HE1	6.65	0.03	1
1	60	ASN	C	177.37	0.1	1
1	25	THR	HG22	0.7	0.03	1
1	159	GLU	H	7.97	0.03	1
1	48	ARG	CB	33.97	0.5	1
1	122	HIS	HB2	3.08	0.03	2
1	103	GLN	HE21	7.77	0.03	1
1	115	GLN	CB	29.6	0.5	1
1	105	GLN	CA	56.01	0.5	1
1	113	THR	HG22	1.13	0.03	1
1	127	PRO	HB3	2.17	0.03	1
1	26	THR	CB	70.8	0.5	1
1	68	LEU	HD13	0.1	0.03	1
1	108	GLY	N	109.55	0.25	1
1	155	THR	HB	4.15	0.03	1
1	66	TRP	HE1	10.2	0.03	1
1	79	HIS	C	176.61	0.1	1
1	152	PHE	CB	39.22	0.5	1
1	83	MET	CB	32.12	0.5	1
1	157	PRO	HD3	3.9	0.03	2
1	158	THR	HB	4.26	0.03	1
1	86	GLY	HA2	5.66	0.03	2
1	123	PHE	N	131.27	0.25	1
1	122	HIS	H	7.22	0.03	1
1	89	HIS	HA	4.72	0.03	1
1	112	ALA	N	126.03	0.25	1
1	44	GLY	CA	44.94	0.5	1
1	27	GLY	HA2	4.29	0.03	2
1	150	PRO	CA	62.0	0.5	1
1	81	ASP	HA	4.51	0.03	1
1	63	ASN	HD22	7.16	0.03	1
1	13	ALA	CB	19.7	0.5	1
1	36	GLY	HA2	4.39	0.03	2
1	81	ASP	HB3	2.58	0.03	1
1	129	ASN	CB	39.0	0.5	1
1	124	GLU	CG	36.56	0.5	1
1	111	GLY	HA3	4.08	0.03	2
1	140	ILE	HG12	0.65	0.03	2
1	106	ILE	HG21	0.65	0.03	1
1	136	PHE	HB2	3.42	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	124	GLU	HG2	2.0	0.03	2
1	83	MET	HB2	2.42	0.03	1
1	126	LEU	HD12	0.7	0.03	1
1	72	GLY	N	103.84	0.25	1
1	28	PHE	C	178.33	0.1	1
1	93	ILE	CD1	14.0	0.5	1
1	97	THR	HA	3.34	0.03	1
1	90	LEU	CD2	23.2	0.5	1
1	75	VAL	HA	4.81	0.03	1
1	54	THR	N	116.7	0.1	1
1	2	ARG	CB	30.66	0.5	1
1	90	LEU	H	8.51	0.03	1
1	57	PHE	HA	4.52	0.03	1
1	88	ALA	N	123.62	0.25	1
1	48	ARG	H	9.29	0.03	1
1	21	THR	HB	4.16	0.03	1
1	124	GLU	HA	4.9	0.03	1
1	150	PRO	HB2	2.23	0.03	2
1	115	GLN	H	7.81	0.03	1
1	24	ILE	HA	3.6	0.03	1
1	47	VAL	HG12	0.88	0.03	1
1	106	ILE	HD11	0.83	0.03	1
1	47	VAL	CG2	24.34	0.5	1
1	44	GLY	C	174.2	0.1	1
1	58	ALA	CB	21.69	0.5	1
1	157	PRO	C	176.89	0.1	1
1	59	GLY	HA3	3.7	0.03	2
1	125	MET	HB2	1.18	0.03	1
1	56	LYS	HG2	1.6	0.03	2
1	113	THR	HB	3.87	0.03	1
1	117	THR	N	114.92	0.25	1
1	83	MET	H	7.42	0.03	1
1	46	PRO	CA	64.23	0.5	1
1	24	ILE	CG2	17.0	0.5	1
1	114	GLY	HA2	4.3	0.03	2
1	12	SER	H	8.27	0.03	1
1	57	PHE	HB3	2.08	0.03	2
1	105	GLN	N	122.54	0.25	1
1	121	LEU	CD1	24.6	0.5	1
1	47	VAL	HA	4.41	0.03	1
1	29	ASN	N	126.62	0.25	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	158	THR	HG22	1.2	0.03	1
1	134	ASN	C	175.24	0.1	1
1	156	THR	HA	4.52	0.03	1
1	106	ILE	N	125.78	0.25	1
1	129	ASN	H	7.94	0.03	1
1	112	ALA	CA	50.02	0.5	1
1	44	GLY	N	113.05	0.25	1
1	149	ALA	N	124.45	0.25	1
1	14	THR	HB	3.91	0.03	1
1	148	ASN	C	174.8	0.1	1
1	130	PRO	CD	50.3	0.5	1
1	2	ARG	CD	43.45	0.5	1
1	18	PRO	HD2	3.4	0.03	2
1	142	PRO	HD2	3.57	0.03	2
1	78	GLN	HG3	2.29	0.03	1
1	136	PHE	H	8.3	0.03	1
1	23	ASN	HB2	2.77	0.03	2
1	129	ASN	HD21	7.57	0.03	1
1	141	ASP	HB2	2.32	0.03	2
1	156	THR	CA	60.48	0.5	1
1	47	VAL	N	122.38	0.25	1
1	151	VAL	H	8.32	0.03	1
1	97	THR	HG21	1.22	0.03	1
1	151	VAL	HG23	1.05	0.03	1
1	19	LEU	H	6.24	0.03	1
1	145	TYR	HD1	6.88	0.03	3
1	17	ARG	HA	4.48	0.03	1
1	60	ASN	H	9.02	0.03	1
1	59	GLY	N	111.37	0.25	1
1	21	THR	C	173.07	0.1	1
1	76	LEU	CB	47.37	0.5	1
1	137	SER	C	174.17	0.1	1
1	85	THR	C	172.84	0.1	1
1	143	THR	HB	3.92	0.03	1
1	143	THR	CB	67.98	0.5	1
1	52	ASN	N	117.35	0.25	1
1	107	ILE	CD1	12.8	0.5	1
1	135	GLY	N	110.23	0.25	1
1	109	TYR	CB	42.05	0.5	1
1	50	VAL	HG12	0.8	0.03	1
1	20	ASP	CB	40.06	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	43	VAL	CG1	22.03	0.5	1
1	81	ASP	CB	39.76	0.5	1
1	68	LEU	HD22	0.45	0.03	1
1	140	ILE	HD11	0.68	0.03	1
1	97	THR	C	174.02	0.1	1
1	40	ALA	CA	53.43	0.5	1
1	29	ASN	CA	54.57	0.5	1
1	103	GLN	HA	2.91	0.03	1
1	17	ARG	CA	55.86	0.5	1
1	83	MET	HA	4.24	0.03	1
1	92	LYS	HG3	1.33	0.03	1
1	26	THR	N	117.5	0.25	1
1	80	ALA	H	9.11	0.03	1
1	20	ASP	HA	4.49	0.03	1
1	148	ASN	CB	38.71	0.5	1
1	131	ASN	CB	37.23	0.5	1
1	14	THR	HG22	0.87	0.03	1
1	146	ILE	N	114.44	0.25	1
1	107	ILE	HA	4.34	0.03	1
1	119	PRO	CB	32.56	0.5	1
1	93	ILE	HG23	0.61	0.03	1
1	116	VAL	HG11	1.14	0.03	2
1	149	ALA	CA	50.75	0.5	1
1	18	PRO	CD	50.4	0.5	1
1	131	ASN	HD21	7.6	0.03	1
1	19	LEU	CB	46.82	0.5	1
1	99	SER	HA	4.6	0.03	1
1	94	SER	CB	64.5	0.5	1
1	60	ASN	CB	39.66	0.5	1
1	47	VAL	C	174.38	0.1	1
1	41	VAL	HB	2.0	0.03	1
1	159	GLU	C	180.85	0.1	1
1	23	ASN	ND2	113.7	0.25	1
1	41	VAL	CG2	17.64	0.5	1
1	146	ILE	HG22	0.8	0.03	1
1	106	ILE	CB	37.07	0.5	1
1	46	PRO	HB3	1.76	0.03	2
1	41	VAL	C	172.52	0.1	1
1	26	THR	HG22	1.25	0.03	1
1	97	THR	CA	66.47	0.5	1
1	24	ILE	C	177.38	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	73	ASN	H	8.17	0.03	1
1	143	THR	C	176.32	0.1	1
1	109	TYR	N	116.62	0.25	1
1	16	THR	H	8.52	0.03	1
1	50	VAL	HB	2.9	0.03	1
1	81	ASP	H	8.01	0.03	1
1	18	PRO	HB3	1.93	0.03	1
1	54	THR	CB	70.96	0.5	1
1	37	VAL	C	173.48	0.1	1
1	49	ALA	CB	18.31	0.5	1
1	75	VAL	HG12	0.8	0.03	1
1	134	ASN	ND2	111.4	0.25	1
1	35	VAL	N	121.38	0.25	1
1	126	LEU	C	173.4	0.1	1
1	84	HIS	HD2	6.54	0.03	1
1	91	SER	CA	59.23	0.5	1
1	102	LYS	CB	35.15	0.5	1
1	122	HIS	HA	6.07	0.03	1
1	52	ASN	CA	53.13	0.5	1
1	55	VAL	HG11	0.68	0.03	1
1	100	THR	CA	62.01	0.5	1
1	56	LYS	CD	28.0	0.5	1
1	10	HIS	CA	56.03	0.5	1
1	58	ALA	N	130.13	0.25	1
1	46	PRO	HG2	2.3	0.03	2
1	153	ASN	CA	52.09	0.5	1
1	21	THR	CG2	24.0	0.5	1
1	90	LEU	HD12	0.74	0.03	1
1	68	LEU	N	114.37	0.25	1
1	25	THR	HG21	0.7	0.03	1
1	55	VAL	HG21	0.73	0.03	1
1	45	THR	N	122.97	0.25	1
1	40	ALA	N	129.38	0.25	1
1	89	HIS	H	8.37	0.03	1
1	48	ARG	NE	86.5	0.25	1
1	26	THR	C	174.39	0.1	1
1	115	GLN	CA	55.46	0.5	1
1	17	ARG	N	116.83	0.25	1
1	105	GLN	CB	29.78	0.5	1
1	127	PRO	CD	50.4	0.5	1
1	57	PHE	H	7.9	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	119	PRO	HG2	1.98	0.03	2
1	146	ILE	HG12	1.28	0.03	2
1	24	ILE	HG13	-0.13	0.03	1
1	61	GLY	HA3	3.65	0.03	2
1	62	ALA	C	178.6	0.1	1
1	64	HIS	H	7.55	0.03	1
1	92	LYS	HB2	1.78	0.03	2
1	134	ASN	HB2	3.44	0.03	2
1	21	THR	HG23	1.1	0.03	1
1	144	GLY	HA2	3.71	0.03	2
1	92	LYS	C	173.71	0.1	1
1	107	ILE	H	8.72	0.03	1
1	130	PRO	HB2	-0.75	0.03	1
1	19	LEU	HD13	1.02	0.03	1
1	146	ILE	HB	1.45	0.03	1
1	10	HIS	HB3	3.01	0.03	2
1	91	SER	C	174.77	0.1	1
1	84	HIS	HB3	3.2	0.03	2
1	35	VAL	HG22	1.1	0.03	1
1	158	THR	C	173.77	0.1	1
1	146	ILE	HD11	0.73	0.03	1
1	89	HIS	C	175.38	0.1	1
1	24	ILE	CB	37.77	0.5	1
1	64	HIS	HB2	0.71	0.03	1
1	22	GLY	CA	44.3	0.5	1
1	76	LEU	CG	28.0	0.5	1
1	139	ARG	HG2	1.69	0.03	2
1	35	VAL	HG12	0.7	0.03	1
1	97	THR	N	121.64	0.25	1
1	75	VAL	N	117.31	0.25	1
1	58	ALA	HB1	1.05	0.03	1
1	159	GLU	HB3	2.06	0.03	2
1	50	VAL	HG11	0.8	0.03	1
1	115	GLN	NE2	111.3	0.25	1
1	30	GLY	C	176.32	0.1	1
1	68	LEU	HB3	1.35	0.03	2
1	126	LEU	CB	44.65	0.5	1
1	80	ALA	HA	4.13	0.03	1
1	136	PHE	HB3	2.66	0.03	2
1	109	TYR	HA	5.29	0.03	1
1	75	VAL	HB	1.68	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	87	TYR	CB	39.95	0.5	1
1	19	LEU	HD23	0.92	0.03	1
1	52	ASN	HD21	7.7	0.03	1
1	35	VAL	CA	62.78	0.5	1
1	90	LEU	CG	25.53	0.5	1
1	67	MET	CB	34.38	0.5	1
1	49	ALA	HB3	1.2	0.03	1
1	46	PRO	HG3	2.17	0.03	2
1	149	ALA	HB3	1.35	0.03	1
1	157	PRO	CB	32.3	0.5	1
1	28	PHE	CB	39.66	0.5	1
1	103	GLN	C	175.11	0.1	1
1	58	ALA	CA	50.79	0.5	1
1	122	HIS	C	171.99	0.1	1
1	63	ASN	N	112.0	0.25	1
1	141	ASP	CA	51.02	0.5	1
1	113	THR	HA	4.4	0.03	1
1	76	LEU	CD2	23.21	0.5	1
1	155	THR	HG21	1.17	0.03	1
1	101	VAL	HG22	0.57	0.03	1
1	3	GLY	H	8.65	0.03	1
1	54	THR	HG22	1.09	0.03	1
1	39	TYR	CA	55.6	0.5	1
1	154	GLY	N	107.9	0.25	1
1	29	ASN	HB3	3.32	0.03	1
1	107	ILE	CB	38.48	0.5	1
1	42	PRO	HG2	2.25	0.03	2
1	126	LEU	HB3	1.2	0.03	2
1	104	GLY	N	113.75	0.25	1
1	37	VAL	HG23	0.73	0.03	1
1	113	THR	CG2	18.8	0.5	1
1	145	TYR	HB2	2.69	0.03	2
1	71	ALA	C	176.51	0.1	1
1	24	ILE	H	8.44	0.03	1
1	62	ALA	HB1	1.4	0.03	1
1	92	LYS	N	121.53	0.25	1
1	30	GLY	CA	46.85	0.5	1
1	133	GLN	HB3	2.43	0.03	1
1	66	TRP	NE1	129.31	0.25	1
1	144	GLY	CA	46.17	0.5	1
1	153	ASN	HA	4.51	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	68	LEU	CD2	18.7	0.5	1
1	17	ARG	H	8.06	0.03	1
1	2	ARG	CG	27.38	0.5	1
1	48	ARG	C	175.71	0.1	1
1	126	LEU	H	8.36	0.03	1
1	105	GLN	HB2	1.68	0.03	1
1	129	ASN	HD22	6.9	0.03	1
1	140	ILE	HG22	0.71	0.03	1
1	53	GLY	H	8.88	0.03	1
1	97	THR	HG22	1.22	0.03	1
1	21	THR	CB	70.85	0.5	1
1	75	VAL	HG22	1.0	0.03	1
1	106	ILE	CG2	17.01	0.5	1
1	51	ALA	C	174.8	0.1	1
1	20	ASP	HB3	2.86	0.03	1
1	139	ARG	CD	39.8	0.5	1
1	121	LEU	N	119.89	0.25	1
1	147	ALA	HB3	1.44	0.03	1
1	23	ASN	HD22	7.05	0.03	1
1	32	PRO	CA	64.39	0.5	1
1	17	ARG	NE	84.8	0.25	1
1	65	PRO	HD2	1.85	0.03	1
1	55	VAL	N	127.32	0.25	1
1	95	VAL	HG22	1.0	0.03	1
1	102	LYS	N	122.93	0.5	1
1	77	ILE	CA	59.97	0.5	1
1	87	TYR	HA	5.28	0.03	1
1	65	PRO	HB2	2.15	0.03	2
1	133	GLN	N	115.92	0.25	1
1	19	LEU	CD2	25.7	0.5	1
1	43	VAL	CG2	21.1	0.5	1
1	65	PRO	CB	32.05	0.5	1
1	140	ILE	HD12	0.68	0.03	1
1	106	ILE	CD1	12.7	0.5	1
1	29	ASN	ND2	109.8	0.25	1
1	98	ASP	C	175.54	0.1	1
1	40	ALA	CB	17.71	0.5	1
1	148	ASN	CG	177.67	0.1	1
1	111	GLY	N	116.4	0.25	1
1	10	HIS	CB	30.14	0.5	1
1	84	HIS	N	120.43	0.25	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	17	ARG	CB	31.64	0.5	1
1	56	LYS	CG	24.88	0.5	1
1	109	TYR	HE1	6.6	0.03	3
1	86	GLY	CA	43.28	0.5	1
1	120	HIS	HB2	2.92	0.03	2
1	108	GLY	HA3	3.78	0.03	2
1	51	ALA	CA	51.32	0.5	1
1	15	TYR	CB	40.3	0.5	1
1	35	VAL	CG1	18.8	0.5	1
1	73	ASN	HA	5.08	0.03	1
1	39	TYR	HD1	6.7	0.03	3
1	103	GLN	CG	35.61	0.5	1
1	119	PRO	CA	63.88	0.5	1
1	121	LEU	HD23	1.0	0.03	1
1	144	GLY	N	108.91	0.25	1
1	115	GLN	HG2	2.13	0.03	2
1	107	ILE	HD13	-0.24	0.03	1
1	21	THR	H	7.53	0.03	1
1	38	ASP	C	175.17	0.1	1
1	146	ILE	CA	57.19	0.5	1
1	31	TYR	HB2	3.17	0.03	2
1	103	GLN	H	8.62	0.03	1
1	43	VAL	HG23	1.09	0.03	1
1	100	THR	HB	4.17	0.03	1
1	76	LEU	HD12	0.42	0.03	1
1	40	ALA	HB1	1.49	0.03	1
1	75	VAL	CB	36.26	0.5	1
1	63	ASN	C	173.44	0.1	1
1	25	THR	H	9.19	0.03	1
1	119	PRO	HD2	3.65	0.03	2
1	142	PRO	HB2	2.32	0.03	2
1	95	VAL	HG11	0.86	0.03	1
1	33	GLY	HA2	4.19	0.03	2
1	15	TYR	HD1	6.87	0.03	3
1	131	ASN	CA	50.27	0.5	1
1	41	VAL	HG13	1.0	0.03	1
1	27	GLY	H	9.31	0.03	1
1	52	ASN	ND2	111.7	0.25	1
1	125	MET	N	117.54	0.25	1
1	91	SER	CB	63.83	0.5	1
1	77	ILE	N	128.06	0.25	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	55	VAL	HG12	0.68	0.03	1
1	88	ALA	C	177.72	0.1	1
1	28	PHE	N	130.09	0.25	1
1	71	ALA	CB	19.3	0.5	1
1	19	LEU	HB2	1.11	0.03	1
1	67	MET	CA	55.01	0.5	1
1	77	ILE	HD12	0.8	0.03	1
1	100	THR	HG21	1.2	0.03	1
1	83	MET	C	174.91	0.1	1
1	128	ALA	HB3	1.34	0.03	1
1	43	VAL	HG13	1.15	0.03	1
1	146	ILE	CD1	14.5	0.5	1
1	157	PRO	HG2	1.98	0.03	2
1	131	ASN	HB2	2.69	0.03	1
1	115	GLN	CD	179.7	0.1	1
1	105	GLN	CG	32.85	0.5	1
1	20	ASP	N	122.95	0.25	1
1	127	PRO	CA	62.63	0.5	1
1	151	VAL	HG11	1.09	0.03	1
1	51	ALA	N	117.02	0.25	1
1	132	TRP	HE1	9.78	0.03	1
1	105	GLN	HG2	2.35	0.03	2
1	46	PRO	HD3	3.8	0.03	2
1	92	LYS	CB	36.37	0.5	1
1	126	LEU	HD22	0.43	0.03	1
1	152	PHE	N	129.33	0.25	1
1	41	VAL	HG21	1.49	0.03	1
1	50	VAL	CG1	19.62	0.5	1
1	112	ALA	HB3	1.31	0.03	1
1	29	ASN	H	8.87	0.03	1
1	123	PHE	HB3	3.08	0.03	1
1	36	GLY	C	169.64	0.1	1
1	132	TRP	HZ2	6.61	0.03	1
1	146	ILE	HA	4.82	0.03	1
1	79	HIS	CA	55.81	0.5	1
1	87	TYR	HB2	3.06	0.03	2
1	35	VAL	HG21	1.1	0.03	1
1	63	ASN	HB3	3.33	0.03	1
1	13	ALA	N	126.1	0.25	1
1	153	ASN	HB3	2.5	0.03	2
1	24	ILE	HD12	0.8	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	25	THR	CG2	16.6	0.5	1
1	80	ALA	HB2	1.52	0.03	1
1	106	ILE	HD13	0.83	0.03	1
1	13	ALA	CA	52.03	0.5	1
1	70	MET	CE	16.81	0.5	5
1	11	GLY	CA	45.22	0.5	1
1	118	GLY	N	108.72	0.25	1
1	91	SER	HA	4.56	0.03	1
1	140	ILE	HB	1.75	0.03	1
1	50	VAL	HG21	1.2	0.03	1
1	56	LYS	C	176.82	0.1	1
1	110	THR	HG22	1.0	0.03	1
1	103	GLN	HG2	1.18	0.03	2
1	44	GLY	H	8.79	0.03	1
1	42	PRO	CB	32.5	0.5	1
1	45	THR	CG2	21.53	0.5	1
1	140	ILE	CG2	18.33	0.5	1
1	120	HIS	CA	56.16	0.5	1
1	126	LEU	CG	29.4	0.5	1
1	87	TYR	C	175.06	0.1	1
1	126	LEU	HA	5.05	0.03	1
1	99	SER	C	173.32	0.1	1
1	33	GLY	CA	45.03	0.5	1
1	45	THR	HB	4.59	0.03	1
1	63	ASN	HA	4.76	0.03	1
1	140	ILE	C	174.56	0.1	1
1	80	ALA	HB3	1.52	0.03	1
1	117	THR	HG21	1.5	0.03	1
1	137	SER	HB2	4.18	0.03	2
1	69	TRP	CB	30.44	0.5	1
1	28	PHE	CA	59.52	0.5	1
1	110	THR	CG2	18.7	0.5	1
1	56	LYS	HD2	1.65	0.03	2
1	121	LEU	HD11	1.48	0.03	1
1	129	ASN	C	171.46	0.1	1
1	32	PRO	HG2	1.98	0.03	2
1	103	GLN	NE2	114.6	0.25	1
1	92	LYS	H	7.35	0.03	1
1	159	GLU	HA	4.15	0.03	1
1	70	MET	HE1	2.07	0.03	1
1	43	VAL	HB	2.03	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	27	GLY	N	114.97	0.25	1
1	54	THR	HG21	1.09	0.03	1
1	122	HIS	HB3	3.64	0.03	2
1	53	GLY	HA3	3.86	0.03	2
1	61	GLY	C	173.23	0.1	1
1	107	ILE	CA	60.54	0.5	1
1	103	GLN	HE22	6.8	0.03	1
1	113	THR	HG23	1.13	0.03	1
1	48	ARG	HG3	1.17	0.03	2
1	155	THR	HA	4.35	0.03	1
1	136	PHE	CA	57.05	0.5	1
1	148	ASN	HB2	2.94	0.03	1
1	112	ALA	H	8.97	0.03	1
1	15	TYR	N	118.11	0.25	1
1	25	THR	C	176.32	0.1	1
1	36	GLY	N	106.73	0.25	1
1	119	PRO	HB2	2.32	0.03	2
1	99	SER	CA	59.15	0.5	1
1	83	MET	CA	55.26	0.5	1
1	157	PRO	HD2	3.63	0.03	2
1	77	ILE	CG1	28.6	0.5	1
1	93	ILE	HA	4.43	0.03	1
1	68	LEU	CD1	21.0	0.5	1
1	56	LYS	HE2	2.8	0.03	2
1	69	TRP	HE1	10.37	0.03	1
1	27	GLY	HA3	3.93	0.03	2
1	150	PRO	CB	32.35	0.5	1
1	69	TRP	HD1	7.45	0.03	1
1	121	LEU	H	8.82	0.03	1
1	36	GLY	HA3	3.44	0.03	2
1	98	ASP	H	9.09	0.03	1
1	77	ILE	HB	1.92	0.03	1
1	140	ILE	CD1	14.4	0.5	1
1	11	GLY	N	110.61	0.25	1
1	93	ILE	C	176.16	0.1	1
1	129	ASN	CA	49.78	0.5	1
1	73	ASN	HD22	6.7	0.03	1
1	55	VAL	HA	3.96	0.03	1
1	111	GLY	HA2	4.64	0.03	2
1	75	VAL	HG21	1.0	0.03	1
1	131	ASN	HA	4.53	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	156	THR	CB	69.5	0.5	1
1	95	VAL	C	173.68	0.1	1
1	120	HIS	N	114.16	0.25	1
1	126	LEU	HD13	0.7	0.03	1
1	148	ASN	ND2	112.7	0.25	1
1	139	ARG	CA	57.55	0.5	1
1	33	GLY	N	113.07	0.25	1
1	40	ALA	HA	4.69	0.03	1
1	58	ALA	HA	4.79	0.03	1
1	69	TRP	HB3	3.0	0.03	2
1	3	GLY	C	173.99	0.1	1
1	107	ILE	HG23	0.56	0.03	1
1	2	ARG	HD2	3.17	0.03	2
1	141	ASP	HA	4.39	0.03	1
1	150	PRO	C	177.04	0.1	1
1	68	LEU	HA	4.74	0.03	1
1	76	LEU	HD22	0.79	0.03	1
1	67	MET	HA	4.76	0.03	1
1	136	PHE	C	175.5	0.1	1
1	109	TYR	C	176.39	0.1	1
1	156	THR	CG2	21.8	0.5	1
1	12	SER	N	115.84	0.25	1
1	125	MET	CB	38.95	0.5	1
1	137	SER	CA	58.53	0.5	1
1	121	LEU	HB3	2.17	0.03	1
1	47	VAL	HG11	0.88	0.03	1
1	143	THR	N	120.43	0.25	1
1	130	PRO	HG3	1.22	0.03	1
1	54	THR	HA	4.86	0.03	1
1	118	GLY	HA2	4.38	0.03	2
1	78	GLN	NE2	112.5	0.25	1
1	19	LEU	CD1	26.4	0.5	1
1	107	ILE	CG1	25.37	0.5	1
1	59	GLY	HA2	3.97	0.03	2
1	68	LEU	CG	25.5	0.5	1
1	18	PRO	HA	4.14	0.03	1
1	125	MET	HE1	1.85	0.03	1
1	27	GLY	CA	44.06	0.5	1
1	81	ASP	N	113.81	0.25	1
1	158	THR	CA	62.68	0.5	1
1	114	GLY	HA3	3.88	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	32	PRO	CD	50.5	0.5	1
1	112	ALA	HA	4.82	0.03	1
1	17	ARG	CG	29.39	0.5	1
1	93	ILE	CA	61.27	0.5	1
1	140	ILE	HG23	0.71	0.03	1
1	121	LEU	CD2	26.7	0.5	1
1	129	ASN	HB2	2.65	0.03	2
1	50	VAL	HA	4.17	0.03	1
1	136	PHE	N	119.53	0.25	1
1	74	ALA	N	125.93	0.25	1
1	15	TYR	CA	55.72	0.5	1
1	48	ARG	HB2	0.85	0.03	2
1	23	ASN	HA	5.06	0.03	1
1	68	LEU	H	7.42	0.03	1
1	103	GLN	CD	180.0	0.1	1
1	119	PRO	CD	50.61	0.5	1
1	31	TYR	HA	4.89	0.03	1
1	79	HIS	HB2	3.48	0.03	2
1	146	ILE	CB	45.51	0.5	1
1	110	THR	CB	70.47	0.5	1
1	16	THR	HA	4.25	0.03	1
1	78	GLN	CA	54.69	0.5	1
1	19	LEU	N	112.81	0.25	1
1	94	SER	N	122.02	0.25	1
1	18	PRO	HD3	3.15	0.03	2
1	60	ASN	N	121.01	0.25	1
1	78	GLN	HG2	1.42	0.03	1
1	34	HIS	C	177.64	0.1	1
1	51	ALA	HA	4.26	0.03	1
1	142	PRO	HA	5.07	0.03	1
1	100	THR	HA	4.87	0.03	1
1	74	ALA	C	174.9	0.1	1
1	85	THR	HG23	1.2	0.03	1
1	101	VAL	HB	1.63	0.03	1
1	96	SER	CB	66.06	0.5	1
1	158	THR	H	8.32	0.03	1
1	151	VAL	HG22	1.05	0.03	1
1	79	HIS	H	9.41	0.03	1
1	22	GLY	H	8.01	0.03	1
1	76	LEU	HD23	0.79	0.03	1
1	71	ALA	H	8.15	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	95	VAL	HA	4.77	0.03	1
1	95	VAL	HG12	0.86	0.03	1
1	85	THR	CB	71.74	0.5	1
1	45	THR	H	8.37	0.03	1
1	83	MET	HE1	1.75	0.03	1
1	101	VAL	HG12	0.63	0.03	1
1	113	THR	N	109.55	0.25	1
1	76	LEU	H	9.21	0.03	1
1	101	VAL	HG11	0.63	0.03	1
1	18	PRO	HG2	1.54	0.03	2
1	137	SER	N	113.83	0.25	1
1	49	ALA	N	119.48	0.25	1
1	23	ASN	H	8.61	0.03	1
1	143	THR	CA	69.54	0.5	1
1	138	GLY	C	174.43	0.1	1
1	151	VAL	CG2	21.1	0.5	1
1	90	LEU	HD21	0.65	0.03	1
1	33	GLY	H	8.87	0.03	1
1	2	ARG	HA	4.37	0.03	1
1	157	PRO	CD	51.25	0.5	1
1	80	ALA	N	123.06	0.25	1
1	64	HIS	CA	55.03	0.5	1
1	81	ASP	CA	53.02	0.5	1
1	66	TRP	CA	55.87	0.5	1
1	68	LEU	HD21	0.45	0.03	1
1	37	VAL	HG11	0.97	0.03	1
1	45	THR	CB	69.19	0.5	1
1	143	THR	CG2	21.1	0.5	1
1	93	ILE	N	123.94	0.25	1
1	30	GLY	HA2	3.7	0.03	2
1	67	MET	HE1	2.07	0.03	1
1	127	PRO	CB	32.51	0.5	1
1	90	LEU	C	179.4	0.1	1
1	88	ALA	HB1	1.27	0.03	1
1	151	VAL	HG12	1.09	0.03	1
1	110	THR	C	177.51	0.1	1
1	153	ASN	C	174.79	0.1	1
1	103	GLN	HB2	1.97	0.03	2
1	92	LYS	CE	42.01	0.5	1
1	126	LEU	HD21	0.43	0.03	1
1	107	ILE	HB	1.76	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	50	VAL	CG2	23.12	0.5	1
1	134	ASN	CG	178.6	0.1	1
1	118	GLY	H	7.43	0.03	1
1	59	GLY	C	171.01	0.1	1
1	34	HIS	N	118.59	0.25	1
1	78	GLN	N	124.54	0.25	1
1	52	ASN	HB3	2.86	0.03	1
1	71	ALA	HB3	1.34	0.03	1
1	94	SER	CA	58.78	0.5	1
1	79	HIS	CB	30.12	0.5	1
1	62	ALA	CA	54.43	0.5	1
1	115	GLN	HB2	1.67	0.03	2
1	109	TYR	H	8.54	0.03	1
1	41	VAL	HA	4.86	0.03	1
1	13	ALA	HB1	1.29	0.03	1
1	69	TRP	HA	4.7	0.03	1
1	116	VAL	C	176.4	0.1	1
1	93	ILE	CG1	27.49	0.5	1
1	35	VAL	H	8.29	0.03	1
1	122	HIS	HD2	6.97	0.03	1
1	146	ILE	HG23	0.8	0.03	1
1	50	VAL	HG22	1.2	0.03	1
1	39	TYR	HB3	3.07	0.03	2
1	64	HIS	C	174.67	0.1	1
1	110	THR	HG21	1.0	0.03	1
1	38	ASP	HB3	2.72	0.03	2
1	46	PRO	HB2	2.1	0.03	2
1	42	PRO	CA	61.92	0.5	1
1	26	THR	HG23	1.25	0.03	1
1	97	THR	CB	69.03	0.5	1
1	47	VAL	HG21	0.92	0.03	1
1	92	LYS	HD2	1.52	0.03	2
1	72	GLY	CA	44.74	0.5	1
1	145	TYR	CA	59.22	0.5	1
1	63	ASN	CB	39.33	0.5	1
1	139	ARG	NE	79.66	0.25	1
1	67	MET	HG2	2.32	0.03	9
1	54	THR	CA	61.02	0.5	1
1	117	THR	HG22	1.5	0.03	1
1	50	VAL	C	174.45	0.1	1
1	159	GLU	CA	58.01	0.5	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
1	49	ALA	CA	52.22	0.5	1
1	75	VAL	HG13	0.8	0.03	1
1	142	PRO	CB	33.71	0.5	1
1	100	THR	CB	70.12	0.5	1
1	147	ALA	HA	4.09	0.03	1
1	156	THR	HB	4.13	0.03	1
1	132	TRP	HE3	6.55	0.03	1
1	41	VAL	CA	58.22	0.5	1
1	153	ASN	CB	39.14	0.5	1
1	121	LEU	HA	5.2	0.03	1
1	90	LEU	HD11	0.74	0.03	1
1	36	GLY	H	5.6	0.03	1
1	90	LEU	N	115.68	0.25	1
1	124	GLU	HB2	1.92	0.03	2
1	14	THR	CB	69.51	0.5	1
1	70	MET	HE2	2.07	0.03	1
1	159	GLU	HG2	2.19	0.03	2
1	43	VAL	HA	3.77	0.03	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
$^{13}\text{C}_\alpha$	151	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	127	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	150	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	137	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 1413. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/612 (0%)	0/243 (0%)	0/252 (0%)	0/117 (0%)
Sidechain	0/635 (0%)	0/371 (0%)	0/242 (0%)	0/22 (0%)
Aromatic	0/166 (0%)	0/86 (0%)	0/65 (0%)	0/15 (0%)
Overall	0/1413 (0%)	0/700 (0%)	0/559 (0%)	0/154 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1802. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/773 (0%)	0/307 (0%)	0/318 (0%)	0/148 (0%)
Sidechain	0/798 (0%)	0/468 (0%)	0/299 (0%)	0/31 (0%)
Aromatic	0/231 (0%)	0/119 (0%)	0/85 (0%)	0/27 (0%)
Overall	0/1802 (0%)	0/894 (0%)	0/702 (0%)	0/206 (0%)

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	130	PRO	HB2	-0.75	3.82 – 0.32	-8.1
???	1	38	ASP	HA	6.67	6.15 – 3.05	6.7
???	1	64	HIS	HB2	0.71	4.91 – 1.31	-6.7
???	1	65	PRO	HD2	1.85	5.45 – 1.85	-5.0

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (c74achemshifts_v2.txt). RCI is only applicable to proteins.