W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB NMR Structure Validation Summary Report (i)

Apr 29, 2016 – 03:48 AM EDT

PDB ID : 2MLX
Title : NMR structure of E. coli Trigger Factor in complex with unfolded PhoA220-310
Authors : Saio, T.; Guan, X.; Rossi, P.; Economou, A.; Kalodimos, C.G.
Deposited on : 2014-03-05

The following versions of software and data (see references (i)) were used in the production of this report:
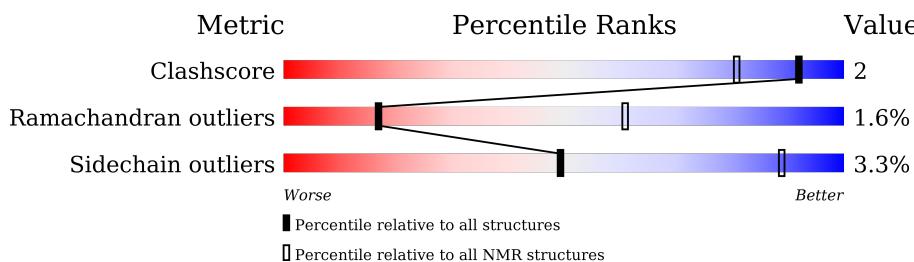
|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
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 33%.

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		1.6%
Sidechain outliers		3.3%

Worse — *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	443	93% ··
2	B	93	32% 9% 57% ·

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:431,　　B:233-B:241, B:275-B:303 (469)	1.00	8

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

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

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

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8128 atoms, of which 4067 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	432	6789	2119	3403	582	674	11	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP U6N325
A	-9	ASN	-	EXPRESSION TAG	UNP U6N325
A	-8	HIS	-	EXPRESSION TAG	UNP U6N325
A	-7	LYS	-	EXPRESSION TAG	UNP U6N325
A	-6	VAL	-	EXPRESSION TAG	UNP U6N325
A	-5	HIS	-	EXPRESSION TAG	UNP U6N325
A	-4	HIS	-	EXPRESSION TAG	UNP U6N325
A	-3	HIS	-	EXPRESSION TAG	UNP U6N325
A	-2	HIS	-	EXPRESSION TAG	UNP U6N325
A	-1	HIS	-	EXPRESSION TAG	UNP U6N325
A	0	HIS	-	EXPRESSION TAG	UNP U6N325

- Molecule 2 is a protein called Alkaline phosphatase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	91	1339	419	664	122	132	2	0

There are 2 discrepancies between the modelled and reference sequences:
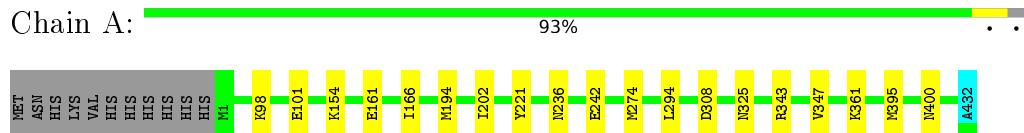
| Chain	Residue	Modelled	Actual	Comment	Reference
B	218	HIS	-	EXPRESSION TAG	UNP U6N3P1
B	219	MET	-	EXPRESSION TAG	UNP U6N3P1

4 Residue-property plots ⓘ
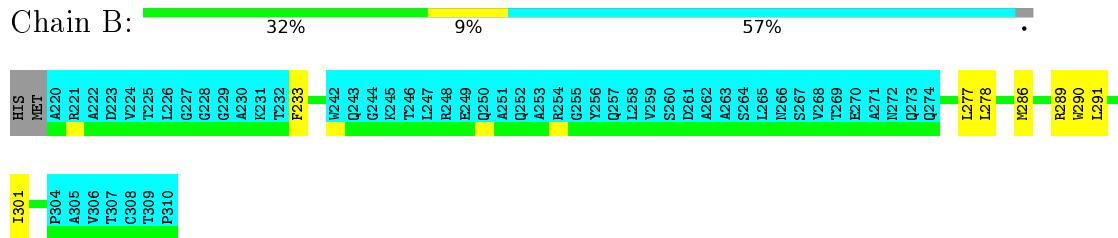
4.1 Average score per residue in the NMR ensemble

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: Trigger factor
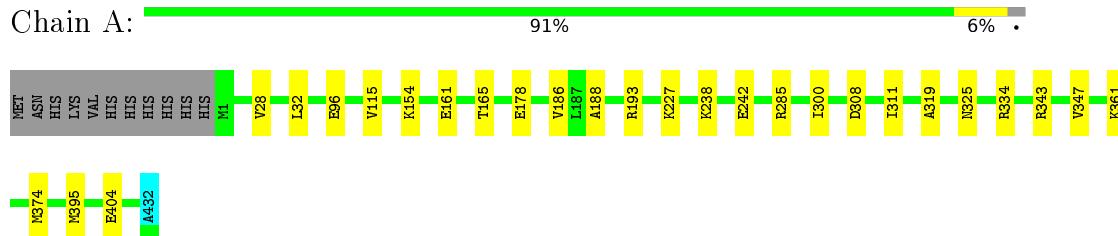
- Molecule 2: Alkaline phosphatase

4.2 Residue scores for the representative (medoid) model from the NMR ensemble
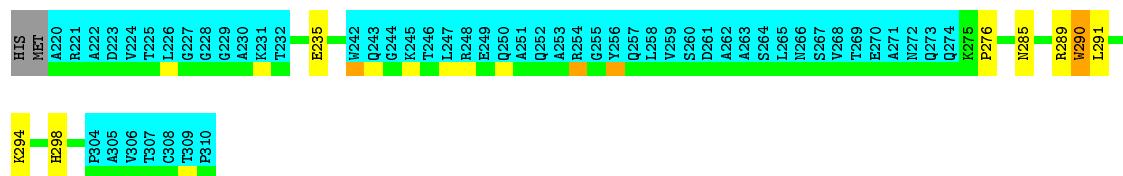
The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Trigger factor

- Molecule 2: Alkaline phosphatase

5   Refinement protocol and experimental data overview (i)

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

Of the 1000 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	
CYANA	structure solution	3.0
X-PLOR NIH	structure solution	
TALOSN	geometry optimization	

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)	2mlx_cs.cif
Number of chemical shift lists	3
Total number of shifts	3237
Number of shifts mapped to atoms	3237
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%

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

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.85±0.01	0±0/3421 (0.0±0.0%)	0.62±0.01	0±0/4601 (0.0±0.0%)
2	B	1.00±0.03	0±0/297 (0.0±0.0%)	0.75±0.06	0±0/405 (0.0±0.0%)
All	All	0.86	0/37180 (0.0%)	0.63	2/50060 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
2	B	0.0±0.0	0.2±0.4
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	285	ARG	NE-CZ-NH1	6.79	123.69	120.30	9	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	B	289	ARG	Peptide	2
1	A	166	ILE	Peptide	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	3380	3398	3398	13±3
2	B	288	284	283	3±1
All	All	36680	36820	36810	139

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 2.

5 of 99 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:154:LYS:HD3	1:A:242:GLU:HB2	0.60	1.73	4	6
1:A:377:ALA:HB1	2:B:286:MET:SD	0.59	2.37	6	1
1:A:325:ASN:HB3	1:A:328:GLN:HB3	0.57	1.75	4	4
1:A:283:ARG:HH21	1:A:405:GLU:HB3	0.57	1.59	10	1
1:A:19:ILE:HD13	1:A:70:LEU:HB3	0.55	1.79	2	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/443 (97%)	396±4 (92±1%)	33±4 (8±1%)	1±1 (0±0%)	50	83
2	B	38/93 (41%)	20±3 (52±8%)	12±3 (32±8%)	6±1 (16±3%)	1	4
All	All	4680/5360 (87%)	4156 (89%)	451 (10%)	73 (2%)	17	61

5 of 36 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	290	TRP	7

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Mol	Chain	Res	Type	Models (Total)
2	B	291	LEU	4
2	B	288	VAL	4
1	A	10	GLY	4
2	B	289	ARG	4

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	359/370 (97%)	349±2 (97±1%)	10±2 (3±1%)	54	91
2	B	28/69 (41%)	26±1 (92±3%)	2±1 (8±3%)	20	65
All	All	3870/4390 (88%)	3744 (97%)	126 (3%)	49	89

5 of 51 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	400	ASN	7
1	A	361	LYS	7
1	A	236	ASN	6
1	A	395	MET	6
1	A	161	GLU	6

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)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 31% for the entire structure.

7.1 Chemical shift list 1

File name: 2mlx_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	2240
Number of shifts mapped to atoms	2240
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	861

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	86	-0.03 ± 0.25	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	100	0.01 ± 0.25	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	395	0.14 ± 0.29	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 31%, i.e. 1785 atoms were assigned a chemical shift out of a possible 5764. 0 out of 78 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	960/2315 (41%)	480/923 (52%)	86/938 (9%)	394/454 (87%)
Sidechain	740/3158 (23%)	413/1834 (23%)	327/1171 (28%)	0/153 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	85/291 (29%)	46/155 (30%)	38/128 (30%)	1/8 (12%)
Overall	1785/5764 (31%)	939/2912 (32%)	451/2237 (20%)	395/615 (64%)

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	432	ALA	H	131.62	11.19 − 5.19	205.7
1	A	363	ASP	H	125.16	11.17 − 5.47	205.0
1	A	421	GLU	H	130.90	11.34 − 5.34	204.3
1	A	301	ASP	H	124.12	11.17 − 5.47	203.2
1	A	127	LYS	H	131.42	11.24 − 5.14	202.0
1	A	299	ASP	H	122.93	11.17 − 5.47	201.1
1	A	304	ALA	H	128.66	11.19 − 5.19	200.8
1	A	126	GLU	H	128.15	11.34 − 5.34	199.7
1	A	364	GLU	H	127.93	11.34 − 5.34	199.3
1	A	136	ASP	H	121.66	11.17 − 5.47	198.8
1	A	124	GLU	H	127.44	11.34 − 5.34	198.5
1	A	259	GLU	H	127.17	11.34 − 5.34	198.0
1	A	134	ASP	H	121.11	11.17 − 5.47	197.9
1	A	362	ALA	H	126.88	11.19 − 5.19	197.8
1	A	396	ASP	H	120.99	11.17 − 5.47	197.7
1	A	116	GLU	H	126.84	11.34 − 5.34	197.5
1	A	138	ASP	H	120.66	11.17 − 5.47	197.1
1	A	308	ASP	H	120.45	11.17 − 5.47	196.7
1	A	407	ALA	H	125.63	11.19 − 5.19	195.7
1	A	131	GLU	H	125.77	11.34 − 5.34	195.7
1	A	281	ALA	H	125.43	11.19 − 5.19	195.4
1	A	392	LYS	H	127.16	11.24 − 5.14	195.0
1	A	142	ASP	H	119.40	11.17 − 5.47	194.9
1	A	312	ASP	H	119.38	11.17 − 5.47	194.8
1	A	118	GLN	H	122.90	11.17 − 5.27	194.4
1	A	290	ALA	H	124.39	11.19 − 5.19	193.7
1	A	419	GLU	H	124.47	11.34 − 5.34	193.6
1	A	149	ALA	H	123.98	11.19 − 5.19	193.0
1	A	310	GLU	H	124.08	11.34 − 5.34	192.9
1	A	140	MET	H	123.97	11.26 − 5.26	192.9
1	A	250	ALA	H	123.77	11.19 − 5.19	192.6
1	A	353	GLU	H	123.88	11.34 − 5.34	192.6

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	410	ALA	H	123.45	11.19 − 5.19	192.1
1	A	431	GLN	H	121.47	11.17 − 5.27	192.0
1	A	402	ALA	H	123.15	11.19 − 5.19	191.6
1	A	318	ALA	H	123.12	11.19 − 5.19	191.6
1	A	340	GLN	H	121.11	11.17 − 5.27	191.3
1	A	329	ALA	H	122.97	11.19 − 5.19	191.3
1	A	377	ALA	H	122.87	11.19 − 5.19	191.1
1	A	380	ASP	H	117.25	11.17 − 5.47	191.1
1	A	420	LYS	H	124.59	11.24 − 5.14	190.8
1	A	260	ASP	H	116.94	11.17 − 5.47	190.6
1	A	341	ALA	H	122.22	11.19 − 5.19	190.1
1	A	415	ALA	H	121.75	11.19 − 5.19	189.3
1	A	326	GLU	H	121.83	11.34 − 5.34	189.1
1	A	430	GLN	H	119.81	11.17 − 5.27	189.1
1	A	135	ALA	H	121.61	11.19 − 5.19	189.0
1	A	406	GLN	H	119.75	11.17 − 5.27	189.0
1	A	271	ARG	H	123.43	11.29 − 5.19	188.8
1	A	374	MET	H	121.54	11.26 − 5.26	188.8
1	A	285	ARG	H	123.39	11.29 − 5.19	188.8
1	A	289	GLN	H	119.50	11.17 − 5.27	188.6
1	A	334	ARG	H	123.17	11.29 − 5.19	188.4
1	A	264	GLU	H	121.38	11.34 − 5.34	188.4
1	A	375	ALA	H	120.99	11.19 − 5.19	188.0
1	A	269	GLU	H	121.10	11.34 − 5.34	187.9
1	A	386	GLU	H	120.82	11.34 − 5.34	187.5
1	A	147	GLN	H	118.69	11.17 − 5.27	187.2
1	A	148	GLN	H	118.63	11.17 − 5.27	187.1
1	A	418	THR	H	124.18	11.34 − 5.14	187.0
1	A	122	ALA	H	120.33	11.19 − 5.19	186.9
1	A	277	GLU	H	120.43	11.34 − 5.34	186.8
1	A	372	GLU	H	120.41	11.34 − 5.34	186.8
1	A	328	GLN	H	118.35	11.17 − 5.27	186.7
1	A	315	ARG	H	122.04	11.29 − 5.19	186.6
1	A	319	ALA	H	120.07	11.19 − 5.19	186.5
1	A	339	GLU	H	120.15	11.34 − 5.34	186.3
1	A	404	GLU	H	120.03	11.34 − 5.34	186.2
1	A	338	GLU	H	120.02	11.34 − 5.34	186.1
1	A	268	ALA	H	119.86	11.19 − 5.19	186.1
1	A	133	THR	H	123.41	11.34 − 5.14	185.8
1	A	416	LYS	H	121.41	11.24 − 5.14	185.6
1	A	373	GLU	H	119.68	11.34 − 5.34	185.6
1	A	292	GLU	H	119.56	11.34 − 5.34	185.4

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	383	GLU	H	119.55	11.34 − 5.34	185.4
1	A	320	GLN	H	117.53	11.17 − 5.27	185.3
1	A	395	MET	H	119.32	11.26 − 5.26	185.1
1	A	361	LYS	H	121.03	11.24 − 5.14	185.0
1	A	398	MET	H	119.25	11.26 − 5.26	185.0
1	A	409	GLU	H	119.30	11.34 − 5.34	184.9
1	A	399	ARG	H	120.99	11.29 − 5.19	184.8
1	A	287	LYS	H	120.71	11.24 − 5.14	184.5
1	A	359	GLU	H	118.94	11.34 − 5.34	184.3
1	A	426	GLU	H	118.92	11.34 − 5.34	184.3
1	A	413	ALA	H	118.51	11.19 − 5.19	183.9
1	A	393	GLU	H	118.46	11.34 − 5.34	183.5
1	A	327	LYS	H	120.07	11.24 − 5.14	183.4
1	A	391	ASN	H	121.66	11.45 − 5.25	182.8
1	A	335	GLU	H	117.94	11.34 − 5.34	182.7
1	A	305	ALA	H	117.60	11.19 − 5.19	182.3
1	A	145	ARG	H	119.43	11.29 − 5.19	182.3
1	A	262	SER	H	115.80	11.23 − 5.33	182.2
1	A	146	LYS	H	119.32	11.24 − 5.14	182.2
1	A	331	GLU	H	117.62	11.34 − 5.34	182.1
1	A	356	ARG	H	119.30	11.29 − 5.19	182.1
1	A	283	ARG	H	119.16	11.29 − 5.19	181.8
1	A	279	LYS	H	119.06	11.24 − 5.14	181.7
1	A	296	LYS	H	119.01	11.24 − 5.14	181.7
1	A	321	ARG	H	118.99	11.29 − 5.19	181.6
1	A	297	ALA	H	117.05	11.19 − 5.19	181.4
1	A	422	THR	H	120.71	11.34 − 5.14	181.4
1	A	267	ARG	H	118.79	11.29 − 5.19	181.2
1	A	251	GLU	H	117.06	11.34 − 5.34	181.2
1	A	368	LYS	H	118.69	11.24 − 5.14	181.2
1	A	390	LYS	H	118.55	11.24 − 5.14	180.9
1	A	117	LEU	H	125.36	11.47 − 4.97	180.2
1	A	309	SER	H	114.50	11.23 − 5.33	180.0
1	A	314	LEU	H	125.15	11.47 − 4.97	179.9
1	A	343	ARG	H	117.92	11.29 − 5.19	179.8
1	A	280	SER	H	114.32	11.23 − 5.33	179.7
1	A	344	ARG	H	117.63	11.29 − 5.19	179.3
1	A	342	LYS	H	117.54	11.24 − 5.14	179.3
1	A	325	ASN	H	119.49	11.45 − 5.25	179.3
1	A	266	LEU	H	124.73	11.47 − 4.97	179.3
1	A	397	ASN	H	119.47	11.45 − 5.25	179.2
1	A	370	LEU	H	124.55	11.47 − 4.97	179.0

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	417	VAL	H	129.55	11.69 − 4.89	178.3
1	A	428	MET	H	115.03	11.26 − 5.26	177.9
1	A	298	ASN	H	118.41	11.45 − 5.25	177.5
1	A	143	THR	H	118.18	11.34 − 5.14	177.3
1	A	349	LEU	H	123.31	11.47 − 4.97	177.1
1	A	288	SER	H	112.59	11.23 − 5.33	176.8
1	A	400	ASN	H	117.91	11.45 − 5.25	176.7
1	A	382	LYS	H	115.81	11.24 − 5.14	176.4
1	A	429	ASN	H	117.62	11.45 − 5.25	176.2
1	A	284	ASN	H	117.50	11.45 − 5.25	176.0
1	A	278	LEU	H	122.60	11.47 − 4.97	176.0
1	A	414	LYS	H	115.41	11.24 − 5.14	175.8
1	A	144	LEU	H	122.45	11.47 − 4.97	175.7
1	A	121	GLU	H	113.50	11.34 − 5.34	175.3
1	A	358	ASN	H	116.63	11.45 − 5.25	174.6
1	A	120	LEU	H	121.60	11.47 − 4.97	174.4
1	A	141	LEU	H	121.55	11.47 − 4.97	174.4
1	A	425	ASN	H	116.07	11.45 − 5.25	173.7
1	A	389	SER	H	110.69	11.23 − 5.33	173.6
1	A	130	VAL	H	126.20	11.69 − 4.89	173.4
1	A	394	LEU	H	120.51	11.47 − 4.97	172.8
1	A	350	LEU	H	120.47	11.47 − 4.97	172.7
1	A	427	LEU	H	120.09	11.47 − 4.97	172.1
1	A	412	LEU	H	120.04	11.47 − 4.97	172.0
1	A	354	VAL	H	125.20	11.69 − 4.89	171.9
1	A	249	THR	H	114.27	11.34 − 5.14	171.0
1	A	336	LEU	H	119.29	11.47 − 4.97	170.9
1	A	403	LEU	H	118.86	11.47 − 4.97	170.2
1	A	263	VAL	H	123.72	11.69 − 4.89	169.7
1	A	115	VAL	H	123.60	11.69 − 4.89	169.6
1	A	401	VAL	H	123.54	11.69 − 4.89	169.5
1	A	351	LEU	H	118.33	11.47 − 4.97	169.4
1	A	125	VAL	H	123.45	11.69 − 4.89	169.3
1	A	129	ILE	H	125.13	11.73 − 4.83	169.3
1	A	137	VAL	H	123.14	11.69 − 4.89	168.9
1	A	423	THR	H	112.74	11.34 − 5.14	168.5
1	A	357	THR	H	112.44	11.34 − 5.14	168.1
1	A	302	VAL	H	122.08	11.69 − 4.89	167.3
1	A	132	VAL	H	122.04	11.69 − 4.89	167.3
1	A	330	LEU	H	116.66	11.47 − 4.97	166.8
1	A	313	VAL	H	121.34	11.69 − 4.89	166.3
1	A	360	LEU	H	116.26	11.47 − 4.97	166.2

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	384	VAL	H	121.26	11.69 − 4.89	166.1
1	A	346	VAL	H	121.24	11.69 − 4.89	166.1
1	A	123	ILE	H	122.86	11.73 − 4.83	166.1
1	A	367	VAL	H	120.67	11.69 − 4.89	165.3
1	A	411	VAL	H	120.58	11.69 − 4.89	165.1
1	A	306	LEU	H	115.48	11.47 − 4.97	165.0
1	A	258	VAL	H	120.48	11.69 − 4.89	165.0
1	A	286	VAL	H	120.17	11.69 − 4.89	164.5
1	A	355	ILE	H	121.73	11.73 − 4.83	164.4
1	A	347	VAL	H	120.05	11.69 − 4.89	164.3
1	A	345	VAL	H	119.99	11.69 − 4.89	164.3
1	A	371	ILE	H	121.56	11.73 − 4.83	164.2
1	A	270	VAL	H	119.89	11.69 − 4.89	164.1
1	A	311	ILE	H	121.49	11.73 − 4.83	164.1
1	A	307	ILE	H	121.08	11.73 − 4.83	163.5
1	A	295	VAL	H	119.42	11.69 − 4.89	163.4
1	A	385	ILE	H	120.97	11.73 − 4.83	163.3
1	A	408	VAL	H	119.19	11.69 − 4.89	163.1
1	A	282	ILE	H	120.78	11.73 − 4.83	163.1
1	A	253	ILE	H	120.64	11.73 − 4.83	162.8
1	A	300	ILE	H	120.28	11.73 − 4.83	162.3
1	A	424	PHE	H	124.76	11.96 − 4.76	161.7
1	A	252	PHE	H	121.87	11.96 − 4.76	157.7
1	A	291	ILE	H	116.53	11.73 − 4.83	156.9
1	A	387	PHE	H	121.13	11.96 − 4.76	156.6
1	A	323	GLY	H	110.69	11.63 − 5.03	155.1
1	A	265	GLY	H	110.39	11.63 − 5.03	154.6
1	A	324	GLY	H	108.59	11.63 − 5.03	151.9
1	A	261	GLY	H	108.32	11.63 − 5.03	151.5
1	A	139	GLY	H	107.80	11.63 − 5.03	150.7
1	A	322	PHE	H	116.85	11.96 − 4.76	150.7
1	A	388	TYR	H	119.60	12.02 − 4.62	150.4
1	A	352	GLY	H	107.01	11.63 − 5.03	149.5
1	A	369	GLY	H	106.89	11.63 − 5.03	149.3
1	A	378	TYR	H	118.45	12.02 − 4.62	148.8
1	A	257	GLY	H	105.52	11.63 − 5.03	147.3
1	A	337	PHE	H	114.26	11.96 − 4.76	147.1
1	A	119	GLY	H	105.40	11.63 − 5.03	147.1
1	A	348	GLY	H	105.22	11.63 − 5.03	146.8
1	A	293	GLY	H	105.17	11.63 − 5.03	146.7
1	A	347	VAL	HG12	25.98	2.13 − -0.47	96.7
1	A	347	VAL	HG11	25.98	2.13 − -0.47	96.7

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	347	VAL	HG13	25.98	2.13 − -0.47	96.7
1	A	411	VAL	HG13	25.82	2.13 − -0.47	96.1
1	A	411	VAL	HG12	25.82	2.13 − -0.47	96.1
1	A	411	VAL	HG11	25.82	2.13 − -0.47	96.1
1	A	278	LEU	HD12	26.67	2.16 − -0.64	92.5
1	A	278	LEU	HD13	26.67	2.16 − -0.64	92.5
1	A	278	LEU	HD11	26.67	2.16 − -0.64	92.5
1	A	132	VAL	HG11	24.88	2.13 − -0.47	92.5
1	A	132	VAL	HG13	24.88	2.13 − -0.47	92.5
1	A	132	VAL	HG12	24.88	2.13 − -0.47	92.5
1	A	314	LEU	HD23	26.57	2.14 − -0.66	92.2
1	A	314	LEU	HD22	26.57	2.14 − -0.66	92.2
1	A	314	LEU	HD21	26.57	2.14 − -0.66	92.2
1	A	332	LEU	HD11	26.46	2.16 − -0.64	91.8
1	A	332	LEU	HD13	26.46	2.16 − -0.64	91.8
1	A	332	LEU	HD12	26.46	2.16 − -0.64	91.8
1	A	144	LEU	HD13	26.44	2.16 − -0.64	91.7
1	A	144	LEU	HD12	26.44	2.16 − -0.64	91.7
1	A	349	LEU	HD13	26.44	2.16 − -0.64	91.7
1	A	427	LEU	HD13	26.44	2.16 − -0.64	91.7
1	A	349	LEU	HD11	26.44	2.16 − -0.64	91.7
1	A	427	LEU	HD11	26.44	2.16 − -0.64	91.7
1	A	427	LEU	HD12	26.44	2.16 − -0.64	91.7
1	A	144	LEU	HD11	26.44	2.16 − -0.64	91.7
1	A	349	LEU	HD12	26.44	2.16 − -0.64	91.7
1	A	266	LEU	HD21	26.14	2.14 − -0.66	90.7
1	A	266	LEU	HD22	26.14	2.14 − -0.66	90.7
1	A	266	LEU	HD23	26.14	2.14 − -0.66	90.7
1	A	370	LEU	HD13	26.05	2.16 − -0.64	90.3
1	A	370	LEU	HD12	26.05	2.16 − -0.64	90.3
1	A	370	LEU	HD11	26.05	2.16 − -0.64	90.3
1	A	117	LEU	HD11	25.99	2.16 − -0.64	90.1
1	A	117	LEU	HD12	25.99	2.16 − -0.64	90.1
1	A	117	LEU	HD13	25.99	2.16 − -0.64	90.1
1	A	367	VAL	HG11	23.97	2.13 − -0.47	89.0
1	A	367	VAL	HG12	23.97	2.13 − -0.47	89.0
1	A	367	VAL	HG13	23.97	2.13 − -0.47	89.0
1	A	412	LEU	HD11	25.67	2.16 − -0.64	89.0
1	A	412	LEU	HD12	25.67	2.16 − -0.64	89.0
1	A	412	LEU	HD13	25.67	2.16 − -0.64	89.0
1	A	302	VAL	HG11	23.93	2.13 − -0.47	88.9
1	A	302	VAL	HG12	23.93	2.13 − -0.47	88.9

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	302	VAL	HG13	23.93	2.13 − -0.47	88.9
1	A	248	LEU	HD12	25.41	2.16 − -0.64	88.0
1	A	248	LEU	HD13	25.41	2.16 − -0.64	88.0
1	A	248	LEU	HD11	25.41	2.16 − -0.64	88.0
1	A	141	LEU	HD11	25.40	2.16 − -0.64	88.0
1	A	141	LEU	HD13	25.40	2.16 − -0.64	88.0
1	A	141	LEU	HD12	25.40	2.16 − -0.64	88.0
1	A	120	LEU	HD12	25.30	2.16 − -0.64	87.6
1	A	120	LEU	HD13	25.30	2.16 − -0.64	87.6
1	A	120	LEU	HD11	25.30	2.16 − -0.64	87.6
1	A	360	LEU	HD11	25.21	2.16 − -0.64	87.3
1	A	360	LEU	HD12	25.21	2.16 − -0.64	87.3
1	A	360	LEU	HD13	25.21	2.16 − -0.64	87.3
1	A	336	LEU	HD22	25.05	2.14 − -0.66	86.8
1	A	336	LEU	HD23	25.05	2.14 − -0.66	86.8
1	A	336	LEU	HD21	25.05	2.14 − -0.66	86.8
1	A	306	LEU	HD13	25.02	2.16 − -0.64	86.7
1	A	306	LEU	HD11	25.02	2.16 − -0.64	86.7
1	A	306	LEU	HD12	25.02	2.16 − -0.64	86.7
1	A	394	LEU	HD11	24.98	2.16 − -0.64	86.5
1	A	394	LEU	HD13	24.98	2.16 − -0.64	86.5
1	A	394	LEU	HD12	24.98	2.16 − -0.64	86.5
1	A	330	LEU	HD13	24.88	2.16 − -0.64	86.1
1	A	330	LEU	HD12	24.88	2.16 − -0.64	86.1
1	A	330	LEU	HD11	24.88	2.16 − -0.64	86.1
1	A	408	VAL	HG13	23.18	2.13 − -0.47	86.0
1	A	408	VAL	HG12	23.18	2.13 − -0.47	86.0
1	A	408	VAL	HG11	23.18	2.13 − -0.47	86.0
1	A	345	VAL	HG12	22.91	2.13 − -0.47	84.9
1	A	345	VAL	HG11	22.91	2.13 − -0.47	84.9
1	A	345	VAL	HG13	22.91	2.13 − -0.47	84.9
1	A	403	LEU	HD23	24.51	2.14 − -0.66	84.9
1	A	403	LEU	HD22	24.51	2.14 − -0.66	84.9
1	A	403	LEU	HD21	24.51	2.14 − -0.66	84.9
1	A	403	LEU	HD12	24.37	2.16 − -0.64	84.3
1	A	403	LEU	HD13	24.37	2.16 − -0.64	84.3
1	A	403	LEU	HD11	24.37	2.16 − -0.64	84.3
1	A	270	VAL	HG12	22.69	2.13 − -0.47	84.1
1	A	270	VAL	HG13	22.69	2.13 − -0.47	84.1
1	A	270	VAL	HG11	22.69	2.13 − -0.47	84.1
1	A	427	LEU	HD21	24.25	2.14 − -0.66	84.0
1	A	427	LEU	HD23	24.25	2.14 − -0.66	84.0

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	427	LEU	HD22	24.25	2.14 − -0.66	84.0
1	A	294	LEU	HD21	24.15	2.14 − -0.66	83.6
1	A	294	LEU	HD23	24.15	2.14 − -0.66	83.6
1	A	294	LEU	HD22	24.15	2.14 − -0.66	83.6
1	A	412	LEU	HD22	24.06	2.14 − -0.66	83.3
1	A	412	LEU	HD23	24.06	2.14 − -0.66	83.3
1	A	412	LEU	HD21	24.06	2.14 − -0.66	83.3
1	A	278	LEU	HD21	24.05	2.14 − -0.66	83.2
1	A	141	LEU	HD21	24.05	2.14 − -0.66	83.2
1	A	278	LEU	HD23	24.05	2.14 − -0.66	83.2
1	A	141	LEU	HD22	24.05	2.14 − -0.66	83.2
1	A	278	LEU	HD22	24.05	2.14 − -0.66	83.2
1	A	141	LEU	HD23	24.05	2.14 − -0.66	83.2
1	A	120	LEU	HD21	23.95	2.14 − -0.66	82.9
1	A	120	LEU	HD23	23.95	2.14 − -0.66	82.9
1	A	120	LEU	HD22	23.95	2.14 − -0.66	82.9
1	A	401	VAL	HG13	22.29	2.13 − -0.47	82.5
1	A	401	VAL	HG11	22.29	2.13 − -0.47	82.5
1	A	401	VAL	HG12	22.29	2.13 − -0.47	82.5
1	A	354	VAL	HG13	22.28	2.13 − -0.47	82.5
1	A	354	VAL	HG12	22.28	2.13 − -0.47	82.5
1	A	354	VAL	HG11	22.28	2.13 − -0.47	82.5
1	A	117	LEU	HD22	23.84	2.14 − -0.66	82.5
1	A	117	LEU	HD21	23.84	2.14 − -0.66	82.5
1	A	117	LEU	HD23	23.84	2.14 − -0.66	82.5
1	A	294	LEU	HD11	23.84	2.16 − -0.64	82.4
1	A	294	LEU	HD12	23.84	2.16 − -0.64	82.4
1	A	294	LEU	HD13	23.84	2.16 − -0.64	82.4
1	A	351	LEU	HD11	23.78	2.16 − -0.64	82.2
1	A	351	LEU	HD12	23.78	2.16 − -0.64	82.2
1	A	351	LEU	HD13	23.78	2.16 − -0.64	82.2
1	A	286	VAL	HG11	22.17	2.13 − -0.47	82.1
1	A	286	VAL	HG13	22.17	2.13 − -0.47	82.1
1	A	286	VAL	HG12	22.17	2.13 − -0.47	82.1
1	A	411	VAL	HG23	23.29	2.20 − -0.60	80.3
1	A	411	VAL	HG22	23.29	2.20 − -0.60	80.3
1	A	411	VAL	HG21	23.29	2.20 − -0.60	80.3
1	A	132	VAL	HG22	23.25	2.20 − -0.60	80.2
1	A	132	VAL	HG23	23.25	2.20 − -0.60	80.2
1	A	132	VAL	HG21	23.25	2.20 − -0.60	80.2
1	A	345	VAL	HG23	23.02	2.20 − -0.60	79.3
1	A	345	VAL	HG21	23.02	2.20 − -0.60	79.3

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	345	VAL	HG22	23.02	2.20 − -0.60	79.3
1	A	248	LEU	HD22	22.91	2.14 − -0.66	79.2
1	A	248	LEU	HD23	22.91	2.14 − -0.66	79.2
1	A	248	LEU	HD21	22.91	2.14 − -0.66	79.2
1	A	370	LEU	HD23	22.87	2.14 − -0.66	79.0
1	A	370	LEU	HD22	22.87	2.14 − -0.66	79.0
1	A	370	LEU	HD21	22.87	2.14 − -0.66	79.0
1	A	349	LEU	HD21	22.82	2.14 − -0.66	78.9
1	A	349	LEU	HD22	22.82	2.14 − -0.66	78.9
1	A	349	LEU	HD23	22.82	2.14 − -0.66	78.9
1	A	332	LEU	HD21	22.65	2.14 − -0.66	78.2
1	A	332	LEU	HD22	22.65	2.14 − -0.66	78.2
1	A	332	LEU	HD23	22.65	2.14 − -0.66	78.2
1	A	330	LEU	HD23	22.63	2.14 − -0.66	78.2
1	A	330	LEU	HD21	22.63	2.14 − -0.66	78.2
1	A	330	LEU	HD22	22.63	2.14 − -0.66	78.2
1	A	258	VAL	HG13	21.14	2.13 − -0.47	78.1
1	A	258	VAL	HG12	21.14	2.13 − -0.47	78.1
1	A	258	VAL	HG11	21.14	2.13 − -0.47	78.1
1	A	263	VAL	HG12	21.13	2.13 − -0.47	78.1
1	A	263	VAL	HG13	21.13	2.13 − -0.47	78.1
1	A	263	VAL	HG11	21.13	2.13 − -0.47	78.1
1	A	394	LEU	HD22	22.60	2.14 − -0.66	78.1
1	A	394	LEU	HD23	22.60	2.14 − -0.66	78.1
1	A	394	LEU	HD21	22.60	2.14 − -0.66	78.1
1	A	336	LEU	HD11	22.60	2.16 − -0.64	78.0
1	A	336	LEU	HD13	22.60	2.16 − -0.64	78.0
1	A	336	LEU	HD12	22.60	2.16 − -0.64	78.0
1	A	306	LEU	HD21	22.55	2.14 − -0.66	77.9
1	A	306	LEU	HD23	22.55	2.14 − -0.66	77.9
1	A	306	LEU	HD22	22.55	2.14 − -0.66	77.9
1	A	137	VAL	HG22	22.60	2.20 − -0.60	77.8
1	A	137	VAL	HG21	22.60	2.20 − -0.60	77.8
1	A	137	VAL	HG23	22.60	2.20 − -0.60	77.8
1	A	125	VAL	HG12	21.07	2.13 − -0.47	77.8
1	A	125	VAL	HG11	21.07	2.13 − -0.47	77.8
1	A	125	VAL	HG13	21.07	2.13 − -0.47	77.8
1	A	417	VAL	HG12	21.02	2.13 − -0.47	77.7
1	A	384	VAL	HG11	21.02	2.13 − -0.47	77.7
1	A	115	VAL	HG11	21.02	2.13 − -0.47	77.7
1	A	115	VAL	HG13	21.02	2.13 − -0.47	77.7
1	A	417	VAL	HG11	21.02	2.13 − -0.47	77.7

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	115	VAL	HG12	21.02	2.13 − -0.47	77.7
1	A	384	VAL	HG13	21.02	2.13 − -0.47	77.7
1	A	417	VAL	HG13	21.02	2.13 − -0.47	77.7
1	A	384	VAL	HG12	21.02	2.13 − -0.47	77.7
1	A	144	LEU	HD23	22.46	2.14 − -0.66	77.6
1	A	144	LEU	HD22	22.46	2.14 − -0.66	77.6
1	A	144	LEU	HD21	22.46	2.14 − -0.66	77.6
1	A	360	LEU	HD21	22.34	2.14 − -0.66	77.1
1	A	360	LEU	HD23	22.34	2.14 − -0.66	77.1
1	A	360	LEU	HD22	22.34	2.14 − -0.66	77.1
1	A	270	VAL	HG21	22.22	2.20 − -0.60	76.5
1	A	270	VAL	HG23	22.22	2.20 − -0.60	76.5
1	A	270	VAL	HG22	22.22	2.20 − -0.60	76.5
1	A	263	VAL	HG22	22.18	2.20 − -0.60	76.3
1	A	263	VAL	HG21	22.18	2.20 − -0.60	76.3
1	A	263	VAL	HG23	22.18	2.20 − -0.60	76.3
1	A	341	ALA	HB1	20.40	2.61 − 0.11	76.1
1	A	341	ALA	HB2	20.40	2.61 − 0.11	76.1
1	A	341	ALA	HB3	20.40	2.61 − 0.11	76.1
1	A	297	ALA	HB3	20.37	2.61 − 0.11	76.0
1	A	297	ALA	HB2	20.37	2.61 − 0.11	76.0
1	A	297	ALA	HB1	20.37	2.61 − 0.11	76.0
1	A	130	VAL	HG13	20.39	2.13 − -0.47	75.2
1	A	130	VAL	HG11	20.39	2.13 − -0.47	75.2
1	A	130	VAL	HG12	20.39	2.13 − -0.47	75.2
1	A	314	LEU	HD11	21.79	2.16 − -0.64	75.1
1	A	314	LEU	HD13	21.79	2.16 − -0.64	75.1
1	A	314	LEU	HD12	21.79	2.16 − -0.64	75.1
1	A	401	VAL	HG21	21.78	2.20 − -0.60	74.9
1	A	401	VAL	HG23	21.78	2.20 − -0.60	74.9
1	A	401	VAL	HG22	21.78	2.20 − -0.60	74.9
1	A	417	VAL	HG21	21.76	2.20 − -0.60	74.8
1	A	417	VAL	HG22	21.76	2.20 − -0.60	74.8
1	A	417	VAL	HG23	21.76	2.20 − -0.60	74.8
1	A	384	VAL	HG23	21.65	2.20 − -0.60	74.5
1	A	384	VAL	HG22	21.65	2.20 − -0.60	74.5
1	A	384	VAL	HG21	21.65	2.20 − -0.60	74.5
1	A	367	VAL	HG21	21.64	2.20 − -0.60	74.4
1	A	367	VAL	HG23	21.64	2.20 − -0.60	74.4
1	A	367	VAL	HG22	21.64	2.20 − -0.60	74.4
1	A	432	ALA	HB2	19.95	2.61 − 0.11	74.4
1	A	432	ALA	HB3	19.95	2.61 − 0.11	74.4

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	432	ALA	HB1	19.95	2.61 − 0.11	74.4
1	A	347	VAL	HG21	21.59	2.20 − -0.60	74.2
1	A	347	VAL	HG22	21.59	2.20 − -0.60	74.2
1	A	347	VAL	HG23	21.59	2.20 − -0.60	74.2
1	A	130	VAL	HG21	21.58	2.20 − -0.60	74.2
1	A	130	VAL	HG22	21.58	2.20 − -0.60	74.2
1	A	130	VAL	HG23	21.58	2.20 − -0.60	74.2
1	A	351	LEU	HD21	21.35	2.14 − -0.66	73.6
1	A	351	LEU	HD23	21.35	2.14 − -0.66	73.6
1	A	351	LEU	HD22	21.35	2.14 − -0.66	73.6
1	A	415	ALA	HB3	19.71	2.61 − 0.11	73.4
1	A	415	ALA	HB2	19.71	2.61 − 0.11	73.4
1	A	415	ALA	HB1	19.71	2.61 − 0.11	73.4
1	A	408	VAL	HG22	21.28	2.20 − -0.60	73.1
1	A	408	VAL	HG23	21.28	2.20 − -0.60	73.1
1	A	408	VAL	HG21	21.28	2.20 − -0.60	73.1
1	A	302	VAL	HG23	21.21	2.20 − -0.60	72.9
1	A	302	VAL	HG22	21.21	2.20 − -0.60	72.9
1	A	302	VAL	HG21	21.21	2.20 − -0.60	72.9
1	A	115	VAL	HG23	20.87	2.20 − -0.60	71.7
1	A	115	VAL	HG22	20.87	2.20 − -0.60	71.7
1	A	115	VAL	HG21	20.87	2.20 − -0.60	71.7
1	A	375	ALA	HB3	19.18	2.61 − 0.11	71.3
1	A	375	ALA	HB2	19.18	2.61 − 0.11	71.3
1	A	375	ALA	HB1	19.18	2.61 − 0.11	71.3
1	A	377	ALA	HB3	19.08	2.61 − 0.11	70.9
1	A	377	ALA	HB1	19.08	2.61 − 0.11	70.9
1	A	377	ALA	HB2	19.08	2.61 − 0.11	70.9
1	A	122	ALA	HB3	19.07	2.61 − 0.11	70.8
1	A	122	ALA	HB1	19.07	2.61 − 0.11	70.8
1	A	122	ALA	HB2	19.07	2.61 − 0.11	70.8
1	A	125	VAL	HG21	20.33	2.20 − -0.60	69.8
1	A	125	VAL	HG22	20.33	2.20 − -0.60	69.8
1	A	125	VAL	HG23	20.33	2.20 − -0.60	69.8
1	A	281	ALA	HB2	18.77	2.61 − 0.11	69.6
1	A	281	ALA	HB3	18.77	2.61 − 0.11	69.6
1	A	281	ALA	HB1	18.77	2.61 − 0.11	69.6
1	A	149	ALA	HB2	18.74	2.61 − 0.11	69.5
1	A	149	ALA	HB1	18.74	2.61 − 0.11	69.5
1	A	149	ALA	HB3	18.74	2.61 − 0.11	69.5
1	A	258	VAL	HG22	20.27	2.20 − -0.60	69.5
1	A	258	VAL	HG21	20.27	2.20 − -0.60	69.5

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	258	VAL	HG23	20.27	2.20 − -0.60	69.5
1	A	407	ALA	HB1	18.47	2.61 − 0.11	68.5
1	A	407	ALA	HB2	18.47	2.61 − 0.11	68.5
1	A	407	ALA	HB3	18.47	2.61 − 0.11	68.5
1	A	329	ALA	HB3	18.45	2.61 − 0.11	68.4
1	A	329	ALA	HB1	18.45	2.61 − 0.11	68.4
1	A	329	ALA	HB2	18.45	2.61 − 0.11	68.4
1	A	305	ALA	HB1	18.40	2.61 − 0.11	68.2
1	A	305	ALA	HB3	18.40	2.61 − 0.11	68.2
1	A	305	ALA	HB2	18.40	2.61 − 0.11	68.2
1	A	413	ALA	HB1	18.34	2.61 − 0.11	67.9
1	A	413	ALA	HB2	18.34	2.61 − 0.11	67.9
1	A	413	ALA	HB3	18.34	2.61 − 0.11	67.9
1	A	362	ALA	HB3	18.31	2.61 − 0.11	67.8
1	A	362	ALA	HB1	18.31	2.61 − 0.11	67.8
1	A	362	ALA	HB2	18.31	2.61 − 0.11	67.8
1	A	250	ALA	HB1	18.30	2.61 − 0.11	67.8
1	A	250	ALA	HB2	18.30	2.61 − 0.11	67.8
1	A	250	ALA	HB3	18.30	2.61 − 0.11	67.8
1	A	304	ALA	HB1	18.29	2.61 − 0.11	67.7
1	A	304	ALA	HB2	18.29	2.61 − 0.11	67.7
1	A	304	ALA	HB3	18.29	2.61 − 0.11	67.7
1	A	402	ALA	HB3	18.11	2.61 − 0.11	67.0
1	A	402	ALA	HB2	18.11	2.61 − 0.11	67.0
1	A	402	ALA	HB1	18.11	2.61 − 0.11	67.0
1	A	318	ALA	HB1	18.07	2.61 − 0.11	66.8
1	A	318	ALA	HB2	18.07	2.61 − 0.11	66.8
1	A	318	ALA	HB3	18.07	2.61 − 0.11	66.8
1	A	268	ALA	HB3	18.02	2.61 − 0.11	66.7
1	A	268	ALA	HB2	18.02	2.61 − 0.11	66.7
1	A	268	ALA	HB1	18.02	2.61 − 0.11	66.7
1	A	319	ALA	HB1	17.96	2.61 − 0.11	66.4
1	A	319	ALA	HB2	17.96	2.61 − 0.11	66.4
1	A	319	ALA	HB3	17.96	2.61 − 0.11	66.4
1	A	135	ALA	HB3	17.81	2.61 − 0.11	65.8
1	A	135	ALA	HB2	17.81	2.61 − 0.11	65.8
1	A	135	ALA	HB1	17.81	2.61 − 0.11	65.8
1	A	290	ALA	HB1	17.65	2.61 − 0.11	65.2
1	A	290	ALA	HB2	17.65	2.61 − 0.11	65.2
1	A	290	ALA	HB3	17.65	2.61 − 0.11	65.2
1	A	410	ALA	HB2	17.21	2.61 − 0.11	63.4
1	A	410	ALA	HB3	17.21	2.61 − 0.11	63.4

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	410	ALA	HB1	17.21	2.61 − 0.11	63.4
1	A	300	ILE	HD11	14.22	2.13 − -0.77	46.7
1	A	300	ILE	HD12	14.22	2.13 − -0.77	46.7
1	A	300	ILE	HD13	14.22	2.13 − -0.77	46.7
1	A	371	ILE	HD11	14.18	2.13 − -0.77	46.5
1	A	371	ILE	HD12	14.18	2.13 − -0.77	46.5
1	A	371	ILE	HD13	14.18	2.13 − -0.77	46.5
1	A	311	ILE	HD11	14.14	2.13 − -0.77	46.4
1	A	311	ILE	HD12	14.14	2.13 − -0.77	46.4
1	A	311	ILE	HD13	14.14	2.13 − -0.77	46.4
1	A	282	ILE	HD13	14.10	2.13 − -0.77	46.3
1	A	282	ILE	HD12	14.10	2.13 − -0.77	46.3
1	A	282	ILE	HD11	14.10	2.13 − -0.77	46.3
1	A	123	ILE	HD11	13.84	2.13 − -0.77	45.4
1	A	123	ILE	HD13	13.84	2.13 − -0.77	45.4
1	A	123	ILE	HD12	13.84	2.13 − -0.77	45.4
1	A	355	ILE	HD11	13.83	2.13 − -0.77	45.3
1	A	355	ILE	HD12	13.83	2.13 − -0.77	45.3
1	A	355	ILE	HD13	13.83	2.13 − -0.77	45.3
1	A	385	ILE	HD13	13.55	2.13 − -0.77	44.4
1	A	385	ILE	HD12	13.55	2.13 − -0.77	44.4
1	A	385	ILE	HD11	13.55	2.13 − -0.77	44.4
1	A	253	ILE	HD11	13.06	2.13 − -0.77	42.7
1	A	253	ILE	HD13	13.06	2.13 − -0.77	42.7
1	A	253	ILE	HD12	13.06	2.13 − -0.77	42.7
1	A	307	ILE	HD13	12.89	2.13 − -0.77	42.1
1	A	307	ILE	HD12	12.89	2.13 − -0.77	42.1
1	A	307	ILE	HD11	12.89	2.13 − -0.77	42.1
1	A	291	ILE	HD11	12.09	2.13 − -0.77	39.4
1	A	291	ILE	HD13	12.09	2.13 − -0.77	39.4
1	A	291	ILE	HD12	12.09	2.13 − -0.77	39.4
1	A	129	ILE	HD11	10.84	2.13 − -0.77	35.0
1	A	129	ILE	HD13	10.84	2.13 − -0.77	35.0
1	A	129	ILE	HD12	10.84	2.13 − -0.77	35.0
1	A	415	ALA	N	7.11	141.07 − 105.37	-32.5
1	A	297	ALA	N	7.16	141.07 − 105.37	-32.5
1	A	122	ALA	N	7.26	141.07 − 105.37	-32.5
1	A	377	ALA	N	7.36	141.07 − 105.37	-32.5
1	A	398	MET	HE2	17.44	4.28 − -0.52	32.4
1	A	398	MET	HE1	17.44	4.28 − -0.52	32.4
1	A	398	MET	HE3	17.44	4.28 − -0.52	32.4
1	A	413	ALA	N	7.57	141.07 − 105.37	-32.4

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	268	ALA	N	7.67	141.07 − 105.37	-32.4
1	A	410	ALA	N	7.83	141.07 − 105.37	-32.3
1	A	432	ALA	N	7.87	141.07 − 105.37	-32.3
1	A	338	GLU	N	7.33	138.24 − 103.14	-32.3
1	A	329	ALA	N	7.96	141.07 − 105.37	-32.3
1	A	318	ALA	N	7.98	141.07 − 105.37	-32.3
1	A	149	ALA	N	7.99	141.07 − 105.37	-32.3
1	A	319	ALA	N	8.01	141.07 − 105.37	-32.3
1	A	135	ALA	N	8.03	141.07 − 105.37	-32.3
1	A	383	GLU	N	7.46	138.24 − 103.14	-32.3
1	A	310	GLU	N	7.49	138.24 − 103.14	-32.3
1	A	281	ALA	N	8.10	141.07 − 105.37	-32.2
1	A	331	GLU	N	7.52	138.24 − 103.14	-32.2
1	A	402	ALA	N	8.14	141.07 − 105.37	-32.2
1	A	290	ALA	N	8.18	141.07 − 105.37	-32.2
1	A	426	GLU	N	7.62	138.24 − 103.14	-32.2
1	A	274	MET	HE2	17.34	4.28 − -0.52	32.2
1	A	274	MET	HE1	17.34	4.28 − -0.52	32.2
1	A	274	MET	HE3	17.34	4.28 − -0.52	32.2
1	A	359	GLU	N	7.67	138.24 − 103.14	-32.2
1	A	353	GLU	N	7.67	138.24 − 103.14	-32.2
1	A	375	ALA	N	8.39	141.07 − 105.37	-32.2
1	A	269	GLU	N	7.87	138.24 − 103.14	-32.1
1	A	386	GLU	N	7.91	138.24 − 103.14	-32.1
1	A	404	GLU	N	7.96	138.24 − 103.14	-32.1
1	A	250	ALA	N	8.58	141.07 − 105.37	-32.1
1	A	409	GLU	N	8.03	138.24 − 103.14	-32.1
1	A	341	ALA	N	8.64	141.07 − 105.37	-32.1
1	A	373	GLU	N	8.04	138.24 − 103.14	-32.1
1	A	304	ALA	N	8.66	141.07 − 105.37	-32.1
1	A	305	ALA	N	8.74	141.07 − 105.37	-32.1
1	A	277	GLU	N	8.16	138.24 − 103.14	-32.1
1	A	407	ALA	N	8.79	141.07 − 105.37	-32.1
1	A	372	GLU	N	8.22	138.24 − 103.14	-32.0
1	A	292	GLU	N	8.23	138.24 − 103.14	-32.0
1	A	393	GLU	N	8.25	138.24 − 103.14	-32.0
1	A	124	GLU	N	8.27	138.24 − 103.14	-32.0
1	A	251	GLU	N	8.29	138.24 − 103.14	-32.0
1	A	362	ALA	N	8.90	141.07 − 105.37	-32.0
1	A	116	GLU	N	8.32	138.24 − 103.14	-32.0
1	A	131	GLU	N	8.53	138.24 − 103.14	-32.0
1	A	326	GLU	N	8.53	138.24 − 103.14	-32.0

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	259	GLU	N	8.54	138.24 − 103.14	-32.0
1	A	339	GLU	N	8.63	138.24 − 103.14	-31.9
1	A	121	GLU	N	8.64	138.24 − 103.14	-31.9
1	A	419	GLU	N	8.72	138.24 − 103.14	-31.9
1	A	264	GLU	N	8.75	138.24 − 103.14	-31.9
1	A	364	GLU	N	8.98	138.24 − 103.14	-31.8
1	A	421	GLU	N	9.11	138.24 − 103.14	-31.8
1	A	126	GLU	N	9.11	138.24 − 103.14	-31.8
1	A	335	GLU	N	9.49	138.24 − 103.14	-31.7
1	A	140	MET	HE2	17.09	4.28 − -0.52	31.7
1	A	140	MET	HE1	17.09	4.28 − -0.52	31.7
1	A	140	MET	HE3	17.09	4.28 − -0.52	31.7
1	A	140	MET	N	7.69	137.94 − 102.24	-31.5
1	A	374	MET	N	7.84	137.94 − 102.24	-31.4
1	A	428	MET	N	7.93	137.94 − 102.24	-31.4
1	A	395	MET	N	8.06	137.94 − 102.24	-31.4
1	A	398	MET	N	8.13	137.94 − 102.24	-31.4
1	A	289	GLN	N	7.37	138.01 − 101.71	-31.0
1	A	320	GLN	N	7.67	138.01 − 101.71	-30.9
1	A	428	MET	HE1	16.71	4.28 − -0.52	30.9
1	A	428	MET	HE2	16.71	4.28 − -0.52	30.9
1	A	428	MET	HE3	16.71	4.28 − -0.52	30.9
1	A	148	GLN	N	7.74	138.01 − 101.71	-30.9
1	A	430	GLN	N	7.75	138.01 − 101.71	-30.9
1	A	147	GLN	N	7.84	138.01 − 101.71	-30.9
1	A	328	GLN	N	7.88	138.01 − 101.71	-30.8
1	A	431	GLN	N	8.08	138.01 − 101.71	-30.8
1	A	406	GLN	N	8.55	138.01 − 101.71	-30.7
1	A	340	GLN	N	8.57	138.01 − 101.71	-30.7
1	A	374	MET	HE2	16.53	4.28 − -0.52	30.5
1	A	374	MET	HE3	16.53	4.28 − -0.52	30.5
1	A	374	MET	HE1	16.53	4.28 − -0.52	30.5
1	A	321	ARG	N	7.52	139.40 − 102.20	-30.5
1	A	118	GLN	N	9.38	138.01 − 101.71	-30.4
1	A	271	ARG	N	7.61	139.40 − 102.20	-30.4
1	A	283	ARG	N	7.62	139.40 − 102.20	-30.4
1	A	343	ARG	N	7.63	139.40 − 102.20	-30.4
1	A	344	ARG	N	7.91	139.40 − 102.20	-30.3
1	A	356	ARG	N	8.03	139.40 − 102.20	-30.3
1	A	280	SER	N	7.55	134.24 − 98.34	-30.3
1	A	309	SER	N	7.62	134.24 − 98.34	-30.3
1	A	285	ARG	N	8.20	139.40 − 102.20	-30.3

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	145	ARG	N	8.21	139.40 − 102.20	-30.3
1	A	389	SER	N	7.88	134.24 − 98.34	-30.2
1	A	267	ARG	N	8.48	139.40 − 102.20	-30.2
1	A	399	ARG	N	8.56	139.40 − 102.20	-30.2
1	A	315	ARG	N	8.64	139.40 − 102.20	-30.2
1	A	334	ARG	N	8.69	139.40 − 102.20	-30.1
1	A	262	SER	N	8.14	134.24 − 98.34	-30.1
1	A	288	SER	N	8.30	134.24 − 98.34	-30.1
1	A	414	LYS	N	7.09	140.01 − 102.11	-30.1
1	A	390	LYS	N	7.16	140.01 − 102.11	-30.1
1	A	368	LYS	N	7.70	140.01 − 102.11	-29.9
1	A	146	LYS	N	7.85	140.01 − 102.11	-29.9
1	A	382	LYS	N	7.85	140.01 − 102.11	-29.9
1	A	279	LYS	N	7.96	140.01 − 102.11	-29.8
1	A	327	LYS	N	8.01	140.01 − 102.11	-29.8
1	A	296	LYS	N	8.18	140.01 − 102.11	-29.8
1	A	342	LYS	N	8.23	140.01 − 102.11	-29.8
1	A	420	LYS	N	8.23	140.01 − 102.11	-29.8
1	A	287	LYS	N	8.27	140.01 − 102.11	-29.8
1	A	361	LYS	N	8.28	140.01 − 102.11	-29.8
1	A	392	LYS	N	8.48	140.01 − 102.11	-29.7
1	A	416	LYS	N	8.64	140.01 − 102.11	-29.7
1	A	127	LYS	N	9.22	140.01 − 102.11	-29.5
1	A	395	MET	HE3	15.86	4.28 − -0.52	29.1
1	A	395	MET	HE2	15.86	4.28 − -0.52	29.1
1	A	395	MET	HE1	15.86	4.28 − -0.52	29.1
1	A	312	ASP	N	7.32	140.24 − 101.14	-29.0
1	A	306	LEU	N	7.18	141.70 − 102.00	-28.9
1	A	136	ASP	N	7.84	140.24 − 101.14	-28.9
1	A	142	ASP	N	7.93	140.24 − 101.14	-28.8
1	A	336	LEU	N	7.43	141.70 − 102.00	-28.8
1	A	380	ASP	N	8.11	140.24 − 101.14	-28.8
1	A	394	LEU	N	7.57	141.70 − 102.00	-28.8
1	A	260	ASP	N	8.20	140.24 − 101.14	-28.8
1	A	330	LEU	N	7.70	141.70 − 102.00	-28.8
1	A	299	ASP	N	8.30	140.24 − 101.14	-28.7
1	A	301	ASP	N	8.39	140.24 − 101.14	-28.7
1	A	427	LEU	N	7.87	141.70 − 102.00	-28.7
1	A	308	ASP	N	8.47	140.24 − 101.14	-28.7
1	A	360	LEU	N	7.95	141.70 − 102.00	-28.7
1	A	266	LEU	N	8.02	141.70 − 102.00	-28.7
1	A	314	LEU	N	8.03	141.70 − 102.00	-28.7

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	138	ASP	N	8.63	140.24 – 101.14	-28.7
1	A	120	LEU	N	8.12	141.70 – 102.00	-28.6
1	A	396	ASP	N	8.69	140.24 – 101.14	-28.6
1	A	349	LEU	N	8.16	141.70 – 102.00	-28.6
1	A	370	LEU	N	8.21	141.70 – 102.00	-28.6
1	A	134	ASP	N	8.79	140.24 – 101.14	-28.6
1	A	144	LEU	N	8.28	141.70 – 102.00	-28.6
1	A	403	LEU	N	8.31	141.70 – 102.00	-28.6
1	A	363	ASP	N	8.90	140.24 – 101.14	-28.6
1	A	412	LEU	N	8.43	141.70 – 102.00	-28.6
1	A	141	LEU	N	8.51	141.70 – 102.00	-28.5
1	A	117	LEU	N	8.60	141.70 – 102.00	-28.5
1	A	350	LEU	N	8.61	141.70 – 102.00	-28.5
1	A	278	LEU	N	8.86	141.70 – 102.00	-28.5
1	A	351	LEU	N	9.03	141.70 – 102.00	-28.4
1	A	298	ASN	N	7.28	139.12 – 98.82	-27.7
1	A	358	ASN	N	7.37	139.12 – 98.82	-27.7
1	A	391	ASN	N	7.45	139.12 – 98.82	-27.7
1	A	429	ASN	N	7.52	139.12 – 98.82	-27.7
1	A	400	ASN	N	7.66	139.12 – 98.82	-27.6
1	A	397	ASN	N	7.88	139.12 – 98.82	-27.6
1	A	325	ASN	N	8.13	139.12 – 98.82	-27.5
1	A	284	ASN	N	8.33	139.12 – 98.82	-27.5
1	A	322	PHE	N	7.57	141.27 – 99.77	-27.2
1	A	425	ASN	N	9.34	139.12 – 98.82	-27.2
1	A	337	PHE	N	7.63	141.27 – 99.77	-27.2
1	A	252	PHE	N	7.90	141.27 – 99.77	-27.1
1	A	387	PHE	N	7.97	141.27 – 99.77	-27.1
1	A	424	PHE	N	9.79	141.27 – 99.77	-26.7
1	A	123	ILE	N	7.08	143.11 – 99.91	-26.5
1	A	307	ILE	N	7.13	143.11 – 99.91	-26.5
1	A	378	TYR	N	7.78	141.99 – 99.29	-26.4
1	A	300	ILE	N	7.69	143.11 – 99.91	-26.3
1	A	371	ILE	N	7.96	143.11 – 99.91	-26.3
1	A	257	GLY	N	7.69	129.07 – 90.27	-26.3
1	A	348	GLY	N	7.76	129.07 – 90.27	-26.3
1	A	129	ILE	N	8.07	143.11 – 99.91	-26.3
1	A	369	GLY	N	7.83	129.07 – 90.27	-26.2
1	A	388	TYR	N	8.58	141.99 – 99.29	-26.2
1	A	385	ILE	N	8.14	143.11 – 99.91	-26.2
1	A	323	GLY	N	7.88	129.07 – 90.27	-26.2
1	A	253	ILE	N	8.20	143.11 – 99.91	-26.2

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	293	GLY	N	8.03	129.07 − 90.27	-26.2
1	A	352	GLY	N	8.04	129.07 − 90.27	-26.2
1	A	291	ILE	N	8.35	143.11 − 99.91	-26.2
1	A	324	GLY	N	8.08	129.07 − 90.27	-26.2
1	A	261	GLY	N	8.09	129.07 − 90.27	-26.2
1	A	355	ILE	N	8.44	143.11 − 99.91	-26.2
1	A	139	GLY	N	8.12	129.07 − 90.27	-26.2
1	A	311	ILE	N	8.66	143.11 − 99.91	-26.1
1	A	265	GLY	N	8.32	129.07 − 90.27	-26.1
1	A	282	ILE	N	8.74	143.11 − 99.91	-26.1
1	A	119	GLY	N	8.46	129.07 − 90.27	-26.1
1	A	384	VAL	N	7.20	144.09 − 98.19	-24.8
1	A	313	VAL	N	7.33	144.09 − 98.19	-24.8
1	A	258	VAL	N	7.43	144.09 − 98.19	-24.8
1	A	137	VAL	N	7.60	144.09 − 98.19	-24.7
1	A	411	VAL	N	7.70	144.09 − 98.19	-24.7
1	A	401	VAL	N	7.88	144.09 − 98.19	-24.7
1	A	367	VAL	N	7.96	144.09 − 98.19	-24.7
1	A	130	VAL	N	8.04	144.09 − 98.19	-24.6
1	A	354	VAL	N	8.06	144.09 − 98.19	-24.6
1	A	302	VAL	N	8.10	144.09 − 98.19	-24.6
1	A	408	VAL	N	8.12	144.09 − 98.19	-24.6
1	A	345	VAL	N	8.13	144.09 − 98.19	-24.6
1	A	115	VAL	N	8.29	144.09 − 98.19	-24.6
1	A	270	VAL	N	8.31	144.09 − 98.19	-24.6
1	A	286	VAL	N	8.32	144.09 − 98.19	-24.6
1	A	295	VAL	N	8.35	144.09 − 98.19	-24.6
1	A	417	VAL	N	8.38	144.09 − 98.19	-24.6
1	A	125	VAL	N	8.41	144.09 − 98.19	-24.6
1	A	347	VAL	N	8.43	144.09 − 98.19	-24.6
1	A	346	VAL	N	8.55	144.09 − 98.19	-24.5
1	A	263	VAL	N	8.57	144.09 − 98.19	-24.5
1	A	132	VAL	N	8.64	144.09 − 98.19	-24.5
1	A	249	THR	N	7.89	139.35 − 91.55	-22.5
1	A	143	THR	N	7.97	139.35 − 91.55	-22.5
1	A	422	THR	N	8.37	139.35 − 91.55	-22.4
1	A	423	THR	N	8.45	139.35 − 91.55	-22.4
1	A	357	THR	N	8.64	139.35 − 91.55	-22.3
1	A	418	THR	N	8.89	139.35 − 91.55	-22.3
1	A	133	THR	N	9.65	139.35 − 91.55	-22.1
1	A	384	VAL	CG1	0.69	28.40 − 14.60	-15.1
1	A	411	VAL	CG1	0.76	28.40 − 14.60	-15.0

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	115	VAL	CG1	0.78	28.40 − 14.60	-15.0
1	A	417	VAL	CG1	0.78	28.40 − 14.60	-15.0
1	A	394	LEU	CD1	0.38	32.77 − 16.57	-15.0
1	A	130	VAL	CG1	0.81	28.40 − 14.60	-15.0
1	A	347	VAL	CG1	0.81	28.40 − 14.60	-15.0
1	A	270	VAL	CG1	0.88	28.40 − 14.60	-14.9
1	A	132	VAL	CG1	0.90	28.40 − 14.60	-14.9
1	A	125	VAL	CG1	0.91	28.40 − 14.60	-14.9
1	A	367	VAL	CG1	0.92	28.40 − 14.60	-14.9
1	A	263	VAL	CG1	0.93	28.40 − 14.60	-14.9
1	A	258	VAL	CG1	0.94	28.40 − 14.60	-14.9
1	A	354	VAL	CG1	0.94	28.40 − 14.60	-14.9
1	A	408	VAL	CG1	0.95	28.40 − 14.60	-14.9
1	A	345	VAL	CG1	0.98	28.40 − 14.60	-14.9
1	A	360	LEU	CD1	0.69	32.77 − 16.57	-14.8
1	A	336	LEU	CD1	0.71	32.77 − 16.57	-14.8
1	A	278	LEU	CD1	0.71	32.77 − 16.57	-14.8
1	A	401	VAL	CG1	1.10	28.40 − 14.60	-14.8
1	A	302	VAL	CG1	1.11	28.40 − 14.60	-14.8
1	A	286	VAL	CG1	1.11	28.40 − 14.60	-14.8
1	A	412	LEU	CD1	0.76	32.77 − 16.57	-14.8
1	A	294	LEU	CD1	0.78	32.77 − 16.57	-14.7
1	A	248	LEU	CD1	0.79	32.77 − 16.57	-14.7
1	A	403	LEU	CD1	0.80	32.77 − 16.57	-14.7
1	A	349	LEU	CD1	0.82	32.77 − 16.57	-14.7
1	A	314	LEU	CD1	0.83	32.77 − 16.57	-14.7
1	A	370	LEU	CD1	0.83	32.77 − 16.57	-14.7
1	A	141	LEU	CD1	0.84	32.77 − 16.57	-14.7
1	A	120	LEU	CD1	0.84	32.77 − 16.57	-14.7
1	A	117	LEU	CD1	0.85	32.77 − 16.57	-14.7
1	A	330	LEU	CD1	0.85	32.77 − 16.57	-14.7
1	A	306	LEU	CD1	0.95	32.77 − 16.57	-14.6
1	A	427	LEU	CD1	1.00	32.77 − 16.57	-14.6
1	A	144	LEU	CD1	1.00	32.77 − 16.57	-14.6
1	A	351	LEU	CD1	1.08	32.77 − 16.57	-14.6
1	A	332	LEU	CD1	1.14	32.77 − 16.57	-14.5
1	A	248	LEU	CD2	0.50	32.60 − 15.60	-13.9
1	A	394	LEU	CD2	0.63	32.60 − 15.60	-13.8
1	A	351	LEU	CD2	0.63	32.60 − 15.60	-13.8
1	A	412	LEU	CD2	0.72	32.60 − 15.60	-13.8
1	A	403	LEU	CD2	0.75	32.60 − 15.60	-13.7
1	A	144	LEU	CD2	0.76	32.60 − 15.60	-13.7

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	141	LEU	CD2	0.77	32.60 − 15.60	-13.7
1	A	278	LEU	CD2	0.77	32.60 − 15.60	-13.7
1	A	330	LEU	CD2	0.77	32.60 − 15.60	-13.7
1	A	117	LEU	CD2	0.78	32.60 − 15.60	-13.7
1	A	266	LEU	CD2	0.78	32.60 − 15.60	-13.7
1	A	294	LEU	CD2	0.78	32.60 − 15.60	-13.7
1	A	120	LEU	CD2	0.79	32.60 − 15.60	-13.7
1	A	360	LEU	CD2	0.81	32.60 − 15.60	-13.7
1	A	336	LEU	CD2	0.83	32.60 − 15.60	-13.7
1	A	349	LEU	CD2	0.87	32.60 − 15.60	-13.7
1	A	370	LEU	CD2	0.87	32.60 − 15.60	-13.7
1	A	306	LEU	CD2	0.89	32.60 − 15.60	-13.7
1	A	427	LEU	CD2	0.90	32.60 − 15.60	-13.6
1	A	314	LEU	CD2	0.97	32.60 − 15.60	-13.6
1	A	332	LEU	CD2	0.98	32.60 − 15.60	-13.6
1	A	384	VAL	CG2	0.59	29.20 − 13.40	-13.1
1	A	137	VAL	CG2	0.77	29.20 − 13.40	-13.0
1	A	258	VAL	CG2	0.80	29.20 − 13.40	-13.0
1	A	130	VAL	CG2	0.80	29.20 − 13.40	-13.0
1	A	417	VAL	CG2	0.81	29.20 − 13.40	-13.0
1	A	132	VAL	CG2	0.84	29.20 − 13.40	-12.9
1	A	367	VAL	CG2	0.84	29.20 − 13.40	-12.9
1	A	115	VAL	CG2	0.84	29.20 − 13.40	-12.9
1	A	302	VAL	CG2	0.86	29.20 − 13.40	-12.9
1	A	408	VAL	CG2	0.89	29.20 − 13.40	-12.9
1	A	345	VAL	CG2	0.90	29.20 − 13.40	-12.9
1	A	347	VAL	CG2	0.90	29.20 − 13.40	-12.9
1	A	125	VAL	CG2	0.91	29.20 − 13.40	-12.9
1	A	401	VAL	CG2	0.96	29.20 − 13.40	-12.9
1	A	411	VAL	CG2	1.02	29.20 − 13.40	-12.8
1	A	263	VAL	CG2	1.02	29.20 − 13.40	-12.8
1	A	270	VAL	CG2	1.03	29.20 − 13.40	-12.8
1	A	377	ALA	CB	1.21	28.03 − 9.93	-9.8
1	A	415	ALA	CB	1.25	28.03 − 9.93	-9.8
1	A	362	ALA	CB	1.27	28.03 − 9.93	-9.8
1	A	319	ALA	CB	1.28	28.03 − 9.93	-9.8
1	A	432	ALA	CB	1.31	28.03 − 9.93	-9.8
1	A	329	ALA	CB	1.34	28.03 − 9.93	-9.7
1	A	122	ALA	CB	1.34	28.03 − 9.93	-9.7
1	A	135	ALA	CB	1.39	28.03 − 9.93	-9.7
1	A	290	ALA	CB	1.40	28.03 − 9.93	-9.7
1	A	410	ALA	CB	1.40	28.03 − 9.93	-9.7

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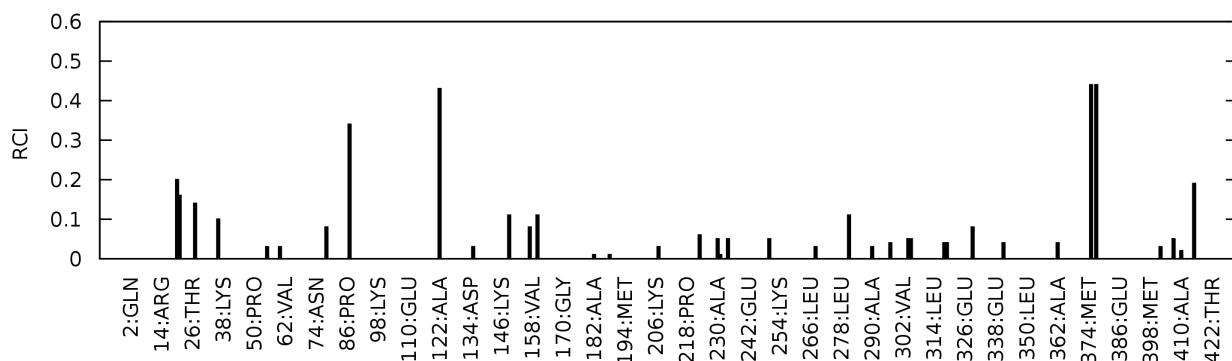
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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	305	ALA	CB	1.40	28.03 − 9.93	-9.7
1	A	149	ALA	CB	1.41	28.03 − 9.93	-9.7
1	A	297	ALA	CB	1.44	28.03 − 9.93	-9.7
1	A	402	ALA	CB	1.45	28.03 − 9.93	-9.7
1	A	281	ALA	CB	1.46	28.03 − 9.93	-9.7
1	A	304	ALA	CB	1.46	28.03 − 9.93	-9.7
1	A	250	ALA	CB	1.48	28.03 − 9.93	-9.7
1	A	407	ALA	CB	1.49	28.03 − 9.93	-9.7
1	A	341	ALA	CB	1.49	28.03 − 9.93	-9.7
1	A	413	ALA	CB	1.49	28.03 − 9.93	-9.7
1	A	268	ALA	CB	1.51	28.03 − 9.93	-9.6
1	A	375	ALA	CB	1.52	28.03 − 9.93	-9.6
1	A	318	ALA	CB	1.66	28.03 − 9.93	-9.6
1	A	428	MET	CE	1.74	26.97 − 7.37	-7.9
1	A	374	MET	CE	1.74	26.97 − 7.37	-7.9
1	A	395	MET	CE	1.92	26.97 − 7.37	-7.8
1	A	398	MET	CE	1.96	26.97 − 7.37	-7.8
1	A	140	MET	CE	2.05	26.97 − 7.37	-7.7
1	A	274	MET	CE	2.09	26.97 − 7.37	-7.7
1	A	129	ILE	CD1	0.66	21.91 − 5.01	-7.6
1	A	253	ILE	CD1	0.68	21.91 − 5.01	-7.6
1	A	355	ILE	CD1	0.78	21.91 − 5.01	-7.5
1	A	291	ILE	CD1	0.80	21.91 − 5.01	-7.5
1	A	371	ILE	CD1	0.80	21.91 − 5.01	-7.5
1	A	385	ILE	CD1	0.80	21.91 − 5.01	-7.5
1	A	123	ILE	CD1	0.81	21.91 − 5.01	-7.5
1	A	300	ILE	CD1	0.82	21.91 − 5.01	-7.5
1	A	307	ILE	CD1	0.83	21.91 − 5.01	-7.5
1	A	282	ILE	CD1	0.84	21.91 − 5.01	-7.5
1	A	311	ILE	CD1	0.89	21.91 − 5.01	-7.4
1	A	163	ARG	HB3	0.14	3.17 − 0.37	-5.8

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:

7.2 Chemical shift list 2

File name: 2mlx_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_dup*

7.2.1 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	228
Number of shifts mapped to atoms	228
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	0	—	—
$^{13}C_\beta$	2	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	49	-1.10 ± 0.81	None needed (imprecise)

7.2.3 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 2%, i.e. 92 atoms were assigned a chemical shift out of a possible 5764. 0 out of 78 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	23/2315 (1%)	15/923 (2%)	0/938 (0%)	8/454 (2%)
Sidechain	42/3158 (1%)	28/1834 (2%)	14/1171 (1%)	0/153 (0%)
Aromatic	27/291 (9%)	16/155 (10%)	11/128 (9%)	0/8 (0%)
Overall	92/5764 (2%)	59/2912 (2%)	25/2237 (1%)	8/615 (1%)
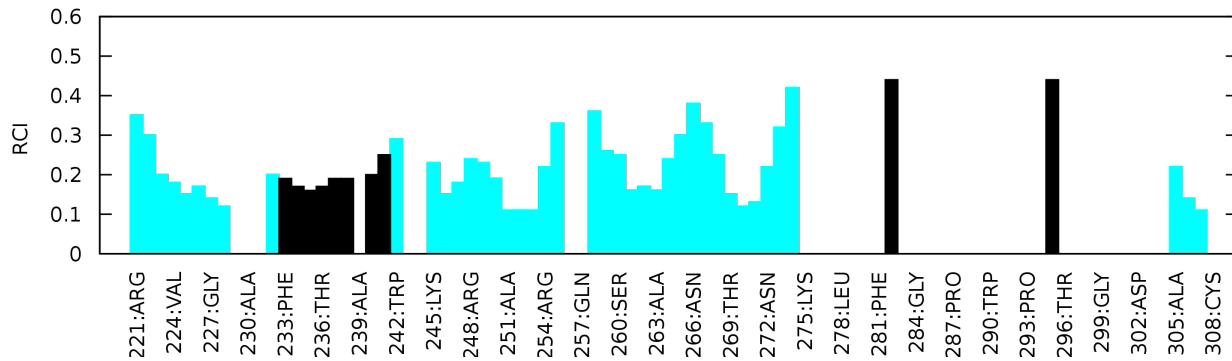
7.2.4   Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5   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 B:

7.3   Chemical shift list 3

File name: 2mlx_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.3.1   Bookkeeping (i)

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

Total number of shifts	769
Number of shifts mapped to atoms	769
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	40	-0.07 ± 0.35	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	0	—	—

7.3.3 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 7%, i.e. 383 atoms were assigned a chemical shift out of a possible 5764. 54 out of 78 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2315 (0%)	0/923 (0%)	0/938 (0%)	0/454 (0%)
Sidechain	383/3158 (12%)	192/1834 (10%)	191/1171 (16%)	0/153 (0%)
Aromatic	0/291 (0%)	0/155 (0%)	0/128 (0%)	0/8 (0%)
Overall	383/5764 (7%)	192/2912 (7%)	191/2237 (9%)	0/615 (0%)

7.3.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.3.5 Random Coil Index (RCI) plots ⓘ

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: