



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 09:47 PM UTC

PDB ID : 2MLX / pdb_00002mlx
BMRB ID : 19835
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

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

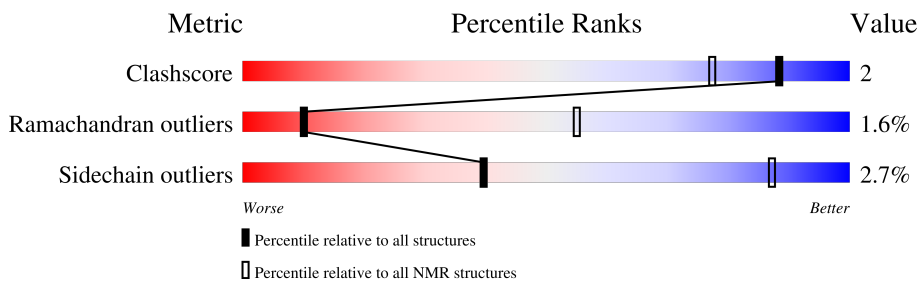
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 37%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	443	94%
2	B	93	33% 8% 57%

2 Ensemble composition and analysis i

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)	1.73	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

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:

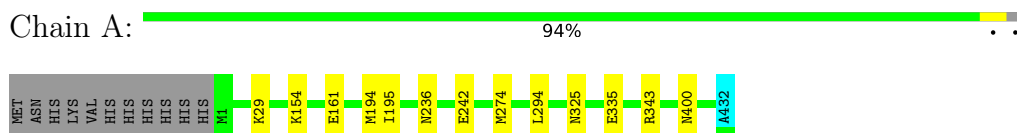
Chain	Residue	Modelled	Actual	Comment	Reference
B	218	HIS	-	expression tag	UNP U6N3P1
B	219	MET	-	expression tag	UNP U6N3P1

4 Residue-property plots [i](#)

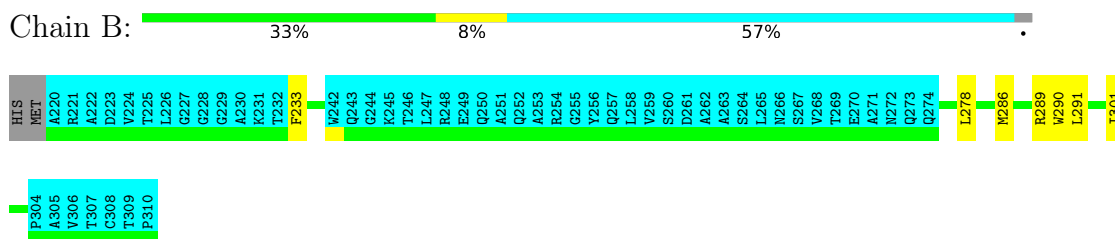
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Trigger factor



- Molecule 2: Alkaline phosphatase

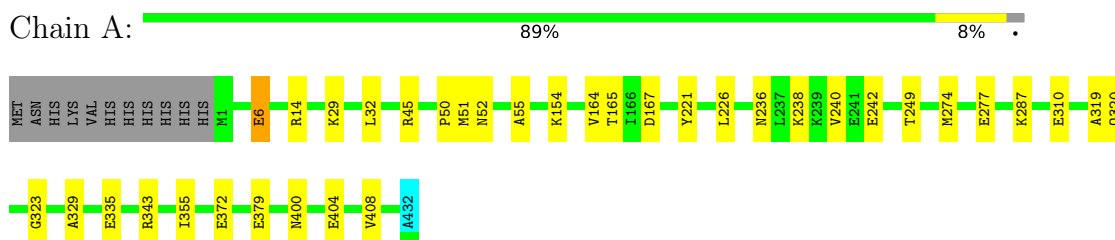


4.2 Scores per residue for each member of the ensemble

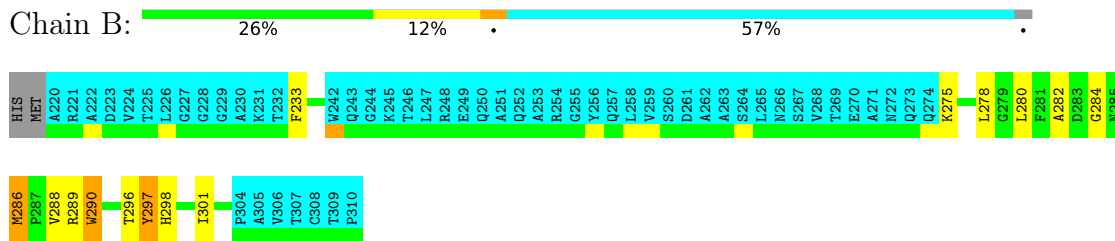
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Trigger factor

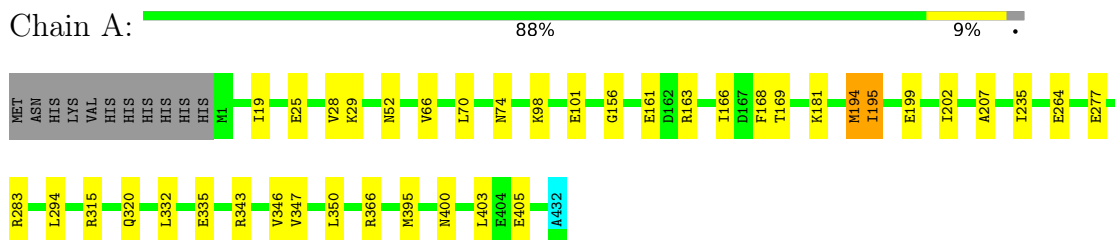


- Molecule 2: Alkaline phosphatase

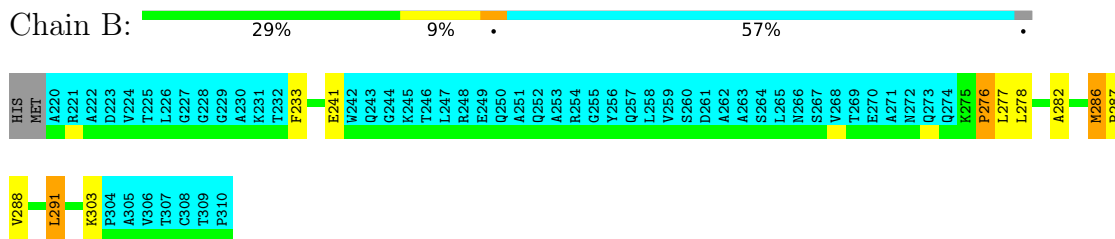


4.2.2 Score per residue for model 2

- Molecule 1: Trigger factor

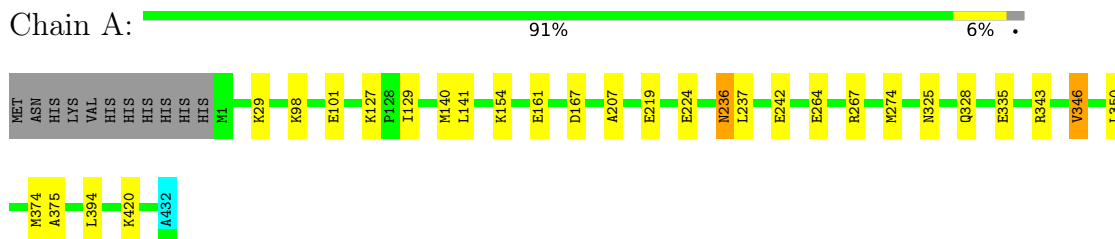


- Molecule 2: Alkaline phosphatase



4.2.3 Score per residue for model 3

- Molecule 1: Trigger factor



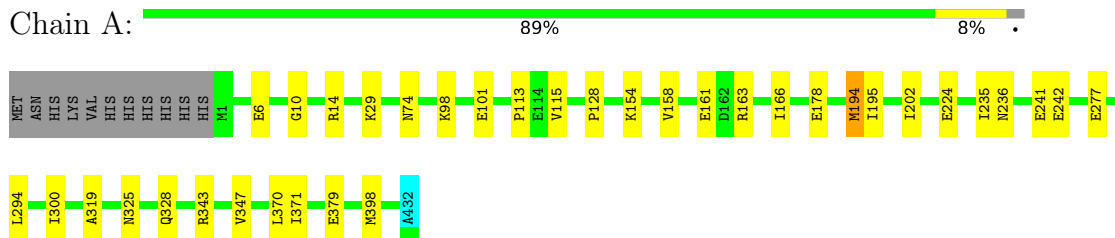
- Molecule 2: Alkaline phosphatase



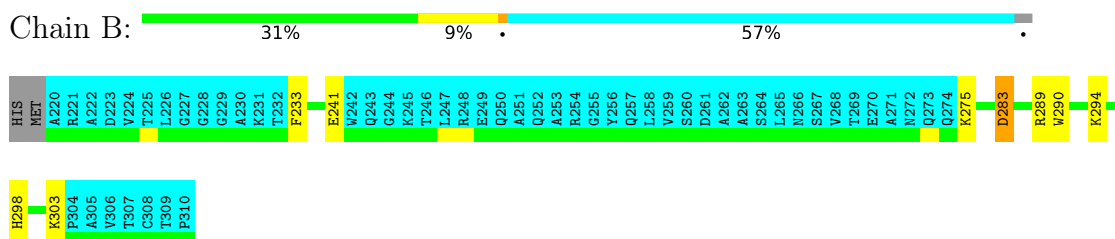


4.2.4 Score per residue for model 4

- Molecule 1: Trigger factor

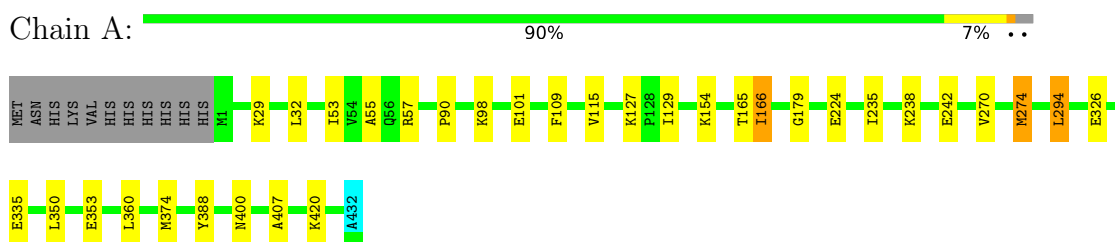


- Molecule 2: Alkaline phosphatase

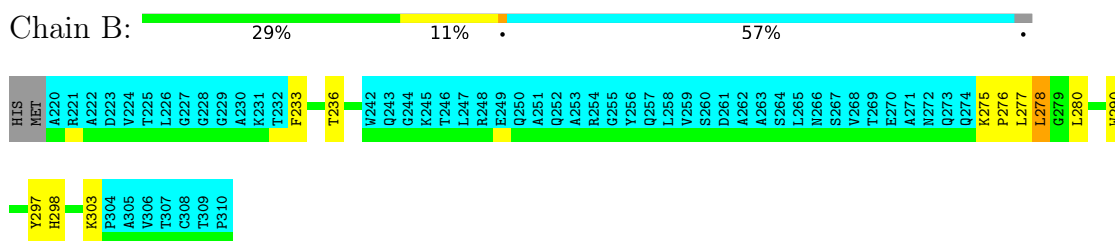


4.2.5 Score per residue for model 5

- Molecule 1: Trigger factor

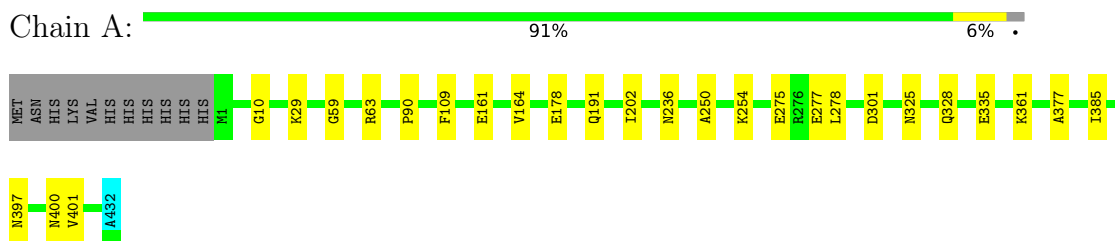


- Molecule 2: Alkaline phosphatase

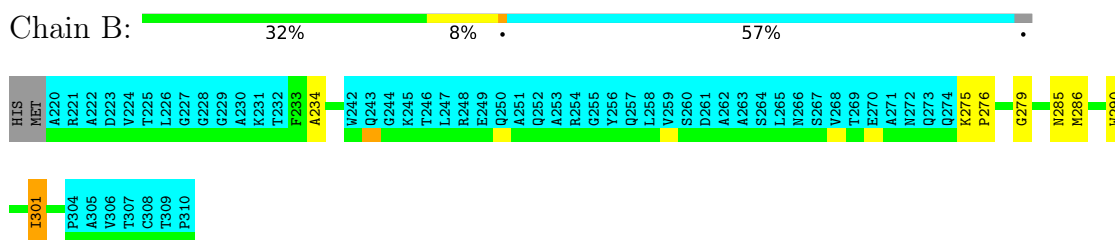


4.2.6 Score per residue for model 6

- Molecule 1: Trigger factor

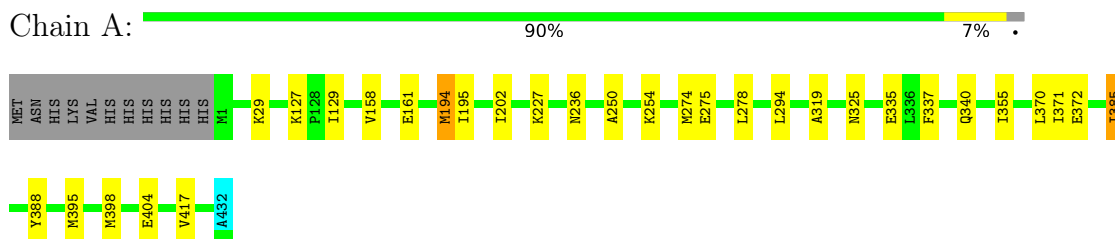


- Molecule 2: Alkaline phosphatase

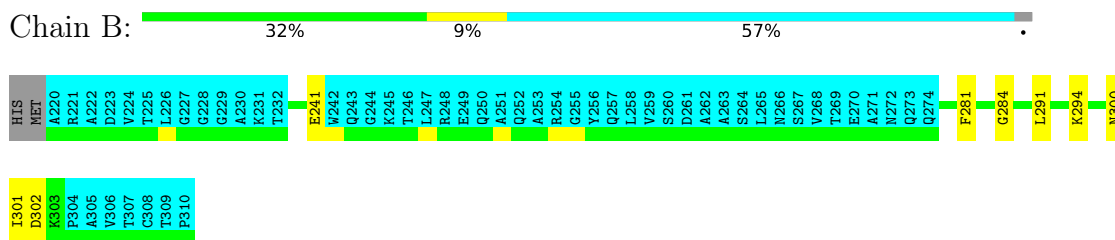


4.2.7 Score per residue for model 7

- Molecule 1: Trigger factor



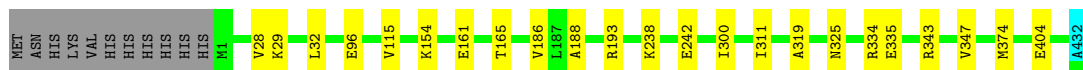
- Molecule 2: Alkaline phosphatase



4.2.8 Score per residue for model 8 (medoid)

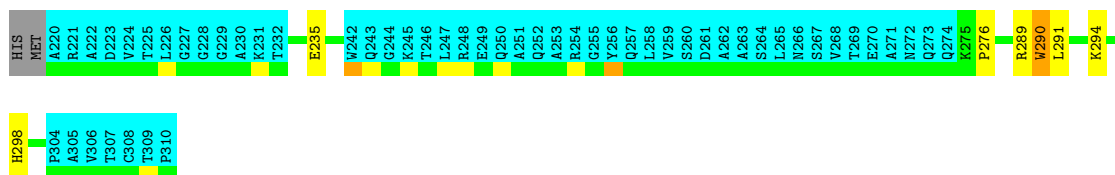
- Molecule 1: Trigger factor

Chain A:  92% 5%




- Molecule 2: Alkaline phosphatase

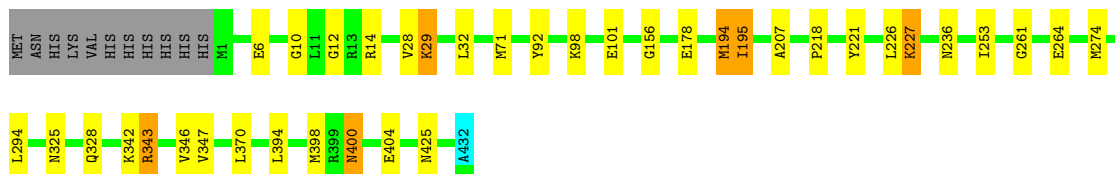
Chain B:  33% 6% 57%



4.2.9 Score per residue for model 9

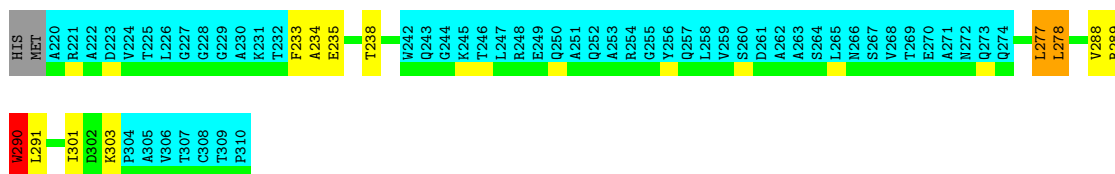
- Molecule 1: Trigger factor

Chain A:  89% 7%




- Molecule 2: Alkaline phosphatase

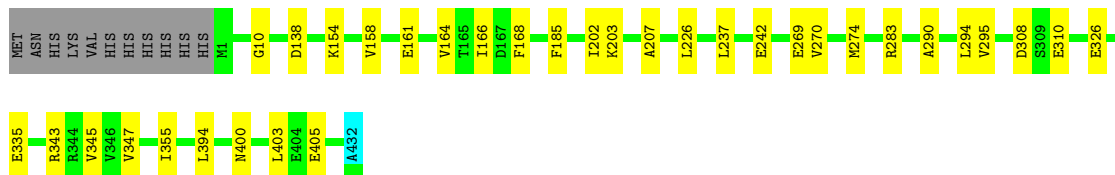
Chain B:  28% 10% 57%



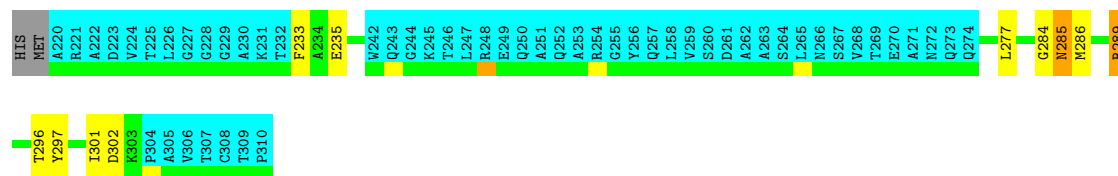
4.2.10 Score per residue for model 10

- Molecule 1: Trigger factor

Chain A:  90% 8%



● Molecule 2: Alkaline phosphatase

Chain B:  29% 10% 57%

5 Refinement protocol and experimental data overview

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)	working_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)	37%

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	1.21±0.01	1±1/3421 (0.0± 0.0%)	1.01±0.02	0±0/4601 (0.0± 0.0%)
2	B	1.40±0.05	0±0/297 (0.1± 0.2%)	1.07±0.06	0±1/405 (0.1± 0.2%)
All	All	1.22	10/37180 (0.0%)	1.01	6/50060 (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

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	371	ILE	CA-CB	5.96	1.60	1.54	7	2
2	B	286	MET	C-N	5.91	1.40	1.33	1	1
2	B	303	LYS	C-N	5.73	1.40	1.33	4	1
1	A	385	ILE	CA-CB	5.30	1.61	1.54	7	2
2	B	296	THR	CA-C	5.30	1.55	1.52	10	1
1	A	417	VAL	CA-CB	5.26	1.59	1.53	7	1
2	B	290	TRP	N-CA	5.18	1.52	1.46	9	1
1	A	346	VAL	CA-CB	5.01	1.60	1.54	3	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)	Models	
								Worst	Total
2	B	303	LYS	CA-C-N	5.26	126.42	119.84	3	1
2	B	303	LYS	C-N-CA	5.26	126.42	119.84	3	1
1	A	168	PHE	CA-CB-CG	5.16	118.96	113.80	2	2
2	B	275	LYS	CA-C-N	5.15	126.28	119.84	5	1
2	B	275	LYS	C-N-CA	5.15	126.28	119.84	5	1

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 \pm 3
2	B	288	284	283	3 \pm 2
All	All	36680	36820	36810	143

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.

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

Atom-1	Atom-2	Clash(\AA)	Distance(\AA)	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
1:A:319:ALA:HB1	1:A:325:ASN:HB2	0.54	1.79	8	2
1:A:403:LEU:HD11	2:B:301:ILE:HD11	0.54	1.78	10	1
1:A:141:LEU:HD11	1:A:267:ARG:HG2	0.54	1.79	3	1
1:A:194:MET:SD	1:A:195:ILE:HG22	0.53	2.43	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LYS:HB2	1:A:101:GLU:HB2	0.52	1.81	9	5
1:A:163:ARG:HG3	1:A:241:GLU:HB2	0.52	1.82	4	1
2:B:276:PRO:HB3	2:B:286:MET:HB3	0.52	1.81	6	1
1:A:113:PRO:HG2	1:A:300:ILE:HD11	0.52	1.82	4	1
1:A:115:VAL:HB	1:A:353:GLU:HB2	0.51	1.82	5	1
1:A:319:ALA:HB1	1:A:325:ASN:HB3	0.51	1.82	7	1
1:A:372:GLU:HG2	1:A:385:ILE:HD11	0.51	1.83	7	1
2:B:301:ILE:HG22	2:B:303:LYS:H	0.50	1.67	9	1
1:A:156:GLY:H	1:A:207:ALA:HB2	0.50	1.66	9	2
1:A:319:ALA:HB2	1:A:329:ALA:HB2	0.50	1.83	1	1
1:A:226:LEU:HD11	2:B:233:PHE:HA	0.49	1.84	1	2
1:A:374:MET:SD	2:B:290:TRP:CH2	0.49	3.06	8	1
2:B:296:THR:HG22	2:B:297:TYR:H	0.48	1.68	1	1
1:A:355:ILE:HG21	2:B:301:ILE:HD13	0.48	1.84	7	3
1:A:165:THR:HG22	1:A:238:LYS:HD3	0.48	1.85	1	3
1:A:127:LYS:HE2	1:A:129:ILE:HD11	0.48	1.84	3	3
1:A:167:ASP:HB2	1:A:236:ASN:HB2	0.48	1.85	3	1
1:A:6:GLU:HB2	1:A:14:ARG:HB3	0.48	1.84	1	3
1:A:90:PRO:HA	1:A:109:PHE:HB3	0.48	1.86	6	2
1:A:140:MET:HG2	1:A:274:MET:SD	0.48	2.49	3	1
1:A:158:VAL:HB	1:A:203:LYS:HA	0.47	1.86	10	1
1:A:294:LEU:HD22	1:A:350:LEU:HD13	0.47	1.85	5	1
1:A:394:LEU:HD22	2:B:289:ARG:H	0.47	1.69	3	1
1:A:32:LEU:HD11	1:A:55:ALA:HA	0.47	1.85	5	1
1:A:311:ILE:HD13	1:A:334:ARG:HG3	0.46	1.88	8	1
2:B:280:LEU:H	2:B:280:LEU:HD23	0.46	1.70	1	1
1:A:28:VAL:HA	1:A:66:VAL:HG21	0.46	1.87	2	1
2:B:286:MET:H	2:B:287:PRO:HD2	0.46	1.70	2	1
1:A:295:VAL:HG21	1:A:347:VAL:HG22	0.46	1.86	10	1
1:A:253:ILE:HG21	1:A:261:GLY:HA2	0.46	1.88	9	1
1:A:218:PRO:HD2	1:A:221:TYR:HB2	0.46	1.88	9	1
1:A:169:THR:HG22	1:A:181:LYS:HG3	0.46	1.88	2	1
1:A:270:VAL:HG13	1:A:274:MET:SD	0.45	2.52	10	1
1:A:45:ARG:HH22	1:A:51:MET:HA	0.45	1.71	1	1
2:B:291:LEU:HD23	2:B:291:LEU:H	0.45	1.71	2	1
1:A:366:ARG:NH2	1:A:405:GLU:HB2	0.45	2.26	2	1
1:A:269:GLU:HG3	2:B:277:LEU:HD22	0.45	1.89	10	1
1:A:374:MET:HE3	2:B:287:PRO:HB3	0.45	1.88	3	1
1:A:32:LEU:HD13	1:A:55:ALA:HA	0.45	1.87	1	1
1:A:361:LYS:HA	2:B:301:ILE:HD13	0.45	1.88	6	1
1:A:375:ALA:HA	2:B:287:PRO:HG3	0.44	1.90	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:346:VAL:O	1:A:350:LEU:HG	0.44	2.12	2	2
1:A:250:ALA:O	1:A:254:LYS:HG2	0.44	2.13	6	2
1:A:275:GLU:HA	1:A:278:LEU:HB3	0.44	1.89	7	2
2:B:278:LEU:HD13	2:B:278:LEU:H	0.44	1.73	5	1
1:A:370:LEU:HB3	1:A:398:MET:HE1	0.44	1.89	7	1
2:B:301:ILE:HG12	2:B:302:ASP:N	0.44	2.28	3	1
1:A:287:LYS:HA	1:A:408:VAL:HG11	0.44	1.90	1	1
1:A:394:LEU:HD22	2:B:289:ARG:NH2	0.44	2.28	10	1
1:A:207:ALA:O	1:A:237:LEU:HG	0.44	2.13	10	2
1:A:277:GLU:HG3	2:B:283:ASP:HB2	0.43	1.90	4	1
1:A:28:VAL:O	1:A:32:LEU:HG	0.43	2.13	9	2
1:A:388:TYR:HB3	1:A:395:MET:SD	0.43	2.54	7	1
1:A:188:ALA:HB3	1:A:193:ARG:HH21	0.43	1.73	8	1
1:A:290:ALA:O	1:A:294:LEU:HB2	0.43	2.13	10	1
1:A:163:ARG:NH2	2:B:241:GLU:HB3	0.43	2.29	4	2
1:A:343:ARG:O	1:A:347:VAL:HG23	0.43	2.14	2	4
1:A:59:GLY:O	1:A:63:ARG:HG3	0.43	2.14	6	1
1:A:370:LEU:HB3	1:A:398:MET:HE3	0.43	1.91	9	1
1:A:394:LEU:HD11	2:B:290:TRP:HZ3	0.43	1.74	9	1
1:A:179:GLY:HA3	2:B:236:THR:HG21	0.43	1.91	5	1
1:A:374:MET:SD	1:A:388:TYR:CD2	0.43	3.12	5	1
1:A:115:VAL:HA	1:A:300:ILE:HD13	0.43	1.90	8	2
1:A:370:LEU:HB2	1:A:398:MET:SD	0.43	2.54	4	1
1:A:315:ARG:HD2	1:A:332:LEU:HB2	0.42	1.91	2	1
1:A:226:LEU:HD21	2:B:233:PHE:CZ	0.42	2.49	9	1
1:A:53:ILE:HG23	1:A:57:ARG:HD2	0.42	1.91	5	1
2:B:277:LEU:HG	2:B:278:LEU:HD12	0.42	1.92	2	1
1:A:29:LYS:HE3	1:A:52:ASN:HA	0.42	1.92	2	1
1:A:342:LYS:O	1:A:346:VAL:HG23	0.42	2.14	9	1
1:A:277:GLU:HA	2:B:285:ASN:ND2	0.42	2.29	6	1
2:B:277:LEU:HG	2:B:278:LEU:H	0.42	1.75	9	1
1:A:164:VAL:HG21	1:A:202:ILE:HG21	0.41	1.92	6	1
1:A:164:VAL:HG11	1:A:202:ILE:HG21	0.41	1.90	10	1
1:A:287:LYS:HG3	1:A:408:VAL:HG21	0.41	1.91	1	1
1:A:166:ILE:HG21	1:A:235:ILE:HG23	0.41	1.92	5	3
1:A:400:ASN:HA	1:A:403:LEU:HB3	0.41	1.93	2	1
1:A:360:LEU:HD13	1:A:407:ALA:HA	0.41	1.92	5	1
1:A:397:ASN:O	1:A:401:VAL:HG23	0.41	2.16	6	1
1:A:25:GLU:HG3	1:A:29:LYS:NZ	0.41	2.30	2	1
1:A:166:ILE:HG22	1:A:237:LEU:HA	0.41	1.92	10	1
1:A:50:PRO:HB2	1:A:52:ASN:ND2	0.41	2.31	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:158:VAL:HG11	1:A:202:ILE:HG22	0.41	1.93	4	2
1:A:400:ASN:O	1:A:404:GLU:HB2	0.41	2.16	9	1
1:A:164:VAL:HG22	1:A:240:VAL:HG13	0.41	1.93	1	1
1:A:283:ARG:NH2	1:A:366:ARG:NH2	0.41	2.69	2	1
1:A:270:VAL:O	1:A:274:MET:HB2	0.41	2.16	5	1
1:A:310:GLU:HG3	1:A:345:VAL:HG22	0.41	1.92	10	1
1:A:337:PHE:HA	1:A:340:GLN:HE21	0.41	1.76	7	1
2:B:286:MET:SD	2:B:286:MET:C	0.40	3.04	10	1
1:A:199:GLU:HA	1:A:202:ILE:HD12	0.40	1.94	2	1
1:A:29:LYS:NZ	1:A:29:LYS:HB2	0.40	2.31	9	1
1:A:71:MET:SD	1:A:92:TYR:HB3	0.40	2.57	9	1
1:A:277:GLU:HG3	2:B:284:GLY:HA3	0.40	1.92	1	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%)	37	78
2	B	38/93 (41%)	20±3 (52±8%)	12±3 (32±8%)	6±1 (16±3%)	0	4
All	All	4680/5360 (87%)	4156 (89%)	451 (10%)	73 (2%)	10	55

All 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
2	B	288	VAL	4
2	B	289	ARG	4
2	B	298	HIS	4
2	B	291	LEU	4
1	A	10	GLY	4
2	B	297	TYR	3
2	B	233	PHE	3
2	B	276	PRO	3

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Mol	Chain	Res	Type	Models (Total)
2	B	234	ALA	3
2	B	235	GLU	3
2	B	282	ALA	2
2	B	286	MET	2
2	B	278	LEU	2
1	A	326	GLU	2
2	B	284	GLY	2
2	B	302	ASP	2
1	A	6	GLU	1
1	A	323	GLY	1
2	B	293	PRO	1
1	A	128	PRO	1
2	B	283	ASP	1
2	B	277	LEU	1
2	B	303	LYS	1
1	A	301	ASP	1
2	B	279	GLY	1
2	B	301	ILE	1
2	B	241	GLU	1
2	B	281	PHE	1
2	B	300	ASN	1
1	A	96	GLU	1
1	A	12	GLY	1
1	A	227	LYS	1
2	B	238	THR	1
1	A	185	PHE	1
2	B	285	ASN	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	359/370 (97%)	350±3 (98±1%)	9±3 (2±1%)	43 89
2	B	28/69 (41%)	26±0 (94±1%)	2±0 (6±1%)	18 67
All	All	3870/4390 (88%)	3766 (97%)	104 (3%)	40 87

All 44 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	29	LYS	8
1	A	335	GLU	8
1	A	161	GLU	7
1	A	236	ASN	6
1	A	400	ASN	5
1	A	294	LEU	5
1	A	274	MET	4
1	A	343	ARG	4
1	A	194	MET	4
1	A	404	GLU	3
1	A	264	GLU	3
1	A	224	GLU	3
1	A	178	GLU	3
2	B	294	LYS	3
1	A	320	GLN	2
2	B	278	LEU	2
2	B	290	TRP	2
1	A	74	ASN	2
1	A	195	ILE	2
1	A	420	LYS	2
2	B	275	LYS	2
1	A	227	LYS	2
1	A	167	ASP	1
1	A	221	TYR	1
1	A	249	THR	1
1	A	310	GLU	1
1	A	372	GLU	1
1	A	277	GLU	1
1	A	395	MET	1
2	B	276	PRO	1
2	B	303	LYS	1
1	A	219	GLU	1
2	B	236	THR	1
2	B	301	ILE	1
1	A	379	GLU	1
2	B	280	LEU	1
1	A	191	GLN	1
2	B	291	LEU	1
1	A	425	ASN	1
2	B	277	LEU	1
1	A	138	ASP	1
1	A	308	ASP	1

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Mol	Chain	Res	Type	Models (Total)
2	B	285	ASN	1
2	B	289	ARG	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 oligosaccharides 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 37% for the well-defined parts and 35% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

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	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

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
¹³ C _α	0	—	None (insufficient data)
¹³ C _β	40	-0.05 \pm 0.32	None needed (< 0.5 ppm)
¹³ C'	0	—	None (insufficient data)
¹⁵ N	0	—	None (insufficient data)

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 12%, i.e. 765 atoms were assigned a chemical shift out of a possible 6403. 0 out of 78 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/2352 (0%)	0/960 (0%)	0/938 (0%)	0/454 (0%)
Sidechain	765/3732 (20%)	574/2408 (24%)	191/1171 (16%)	0/153 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/319 (0%)	0/155 (0%)	0/156 (0%)	0/8 (0%)
Overall	765/6403 (12%)	574/3523 (16%)	191/2265 (8%)	0/615 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 769 atoms were assigned a chemical shift out of a possible 7075. 0 out of 86 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/2623 (0%)	0/1071 (0%)	0/1046 (0%)	0/506 (0%)
Sidechain	769/4112 (19%)	577/2655 (22%)	192/1285 (15%)	0/172 (0%)
Aromatic	0/340 (0%)	0/165 (0%)	0/166 (0%)	0/9 (0%)
Overall	769/7075 (11%)	577/3891 (15%)	192/2497 (8%)	0/687 (0%)

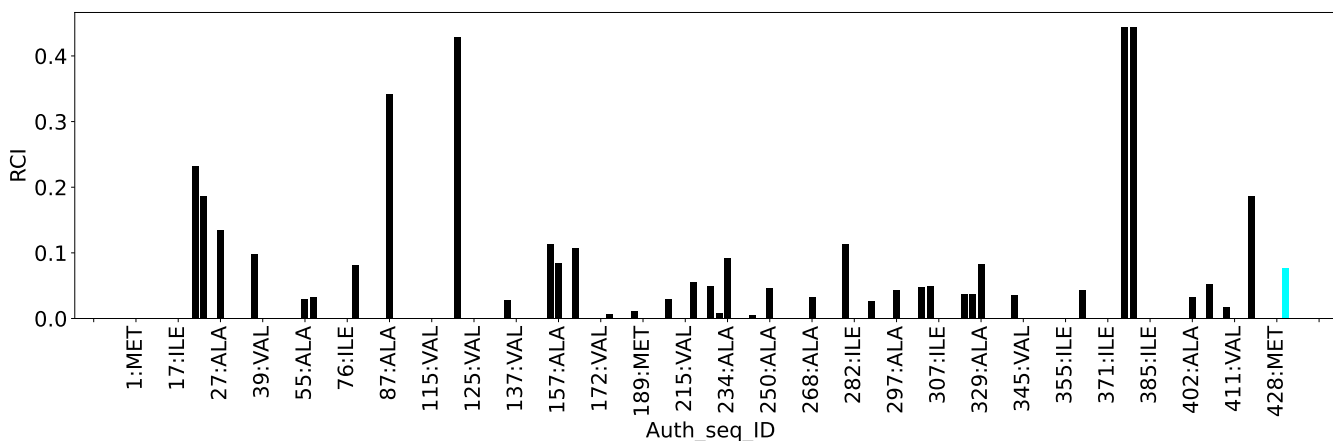
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	86	-0.02 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	100	0.01 ± 0.29	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	395	0.13 ± 0.32	None needed (< 0.5 ppm)

7.2.3 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 35%, i.e. 2234 atoms were assigned a chemical shift out of a possible 6403. 0 out of 78 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	972/2352 (41%)	492/960 (51%)	86/938 (9%)	394/454 (87%)
Sidechain	1172/3732 (31%)	846/2408 (35%)	326/1171 (28%)	0/153 (0%)
Aromatic	90/319 (28%)	45/155 (29%)	44/156 (28%)	1/8 (12%)
Overall	2234/6403 (35%)	1383/3523 (39%)	456/2265 (20%)	395/615 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 2240 atoms were assigned a chemical shift out of a possible 7075. 0 out of 86 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	974/2623 (37%)	493/1071 (46%)	86/1046 (8%)	395/506 (78%)
Sidechain	1176/4112 (29%)	849/2655 (32%)	327/1285 (25%)	0/172 (0%)
Aromatic	90/340 (26%)	45/165 (27%)	44/166 (27%)	1/9 (11%)
Overall	2240/7075 (32%)	1387/3891 (36%)	457/2497 (18%)	396/687 (58%)

7.2.4 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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	432	ALA	H	131.62	5.31 – 11.08	213.9
2	A	421	GLU	H	130.90	5.45 – 11.20	213.2
2	A	363	ASP	H	125.16	5.52 – 11.08	210.2
2	A	127	LYS	H	131.42	5.24 – 11.12	209.6
2	A	304	ALA	H	128.66	5.31 – 11.08	208.8
2	A	126	GLU	H	128.15	5.45 – 11.20	208.4
2	A	301	ASP	H	124.12	5.52 – 11.08	208.3
2	A	364	GLU	H	127.93	5.45 – 11.20	208.0
2	A	124	GLU	H	127.44	5.45 – 11.20	207.1
2	A	259	GLU	H	127.17	5.45 – 11.20	206.7
2	A	299	ASP	H	122.93	5.52 – 11.08	206.2
2	A	116	GLU	H	126.84	5.45 – 11.20	206.1
2	A	362	ALA	H	126.88	5.31 – 11.08	205.7
2	A	131	GLU	H	125.77	5.45 – 11.20	204.2
2	A	136	ASP	H	121.66	5.52 – 11.08	203.9
2	A	407	ALA	H	125.63	5.31 – 11.08	203.5
2	A	281	ALA	H	125.43	5.31 – 11.08	203.2
2	A	134	ASP	H	121.11	5.52 – 11.08	202.9
2	A	396	ASP	H	120.99	5.52 – 11.08	202.7
2	A	140	MET	H	123.97	5.39 – 11.10	202.7
2	A	118	GLN	H	122.90	5.39 – 11.05	202.6
2	A	392	LYS	H	127.16	5.24 – 11.12	202.4
2	A	138	ASP	H	120.66	5.52 – 11.08	202.1
2	A	419	GLU	H	124.47	5.45 – 11.20	202.0
2	A	308	ASP	H	120.45	5.52 – 11.08	201.7
2	A	290	ALA	H	124.39	5.31 – 11.08	201.4
2	A	310	GLU	H	124.08	5.45 – 11.20	201.3
2	A	353	GLU	H	123.88	5.45 – 11.20	201.0
2	A	149	ALA	H	123.98	5.31 – 11.08	200.7
2	A	250	ALA	H	123.77	5.31 – 11.08	200.3
2	A	431	GLN	H	121.47	5.39 – 11.05	200.1

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	142	ASP	H	119.40	5.52 – 11.08	199.8
2	A	312	ASP	H	119.38	5.52 – 11.08	199.8
2	A	410	ALA	H	123.45	5.31 – 11.08	199.8
2	A	340	GLN	H	121.11	5.39 – 11.05	199.4
2	A	402	ALA	H	123.15	5.31 – 11.08	199.2
2	A	318	ALA	H	123.12	5.31 – 11.08	199.2
2	A	329	ALA	H	122.97	5.31 – 11.08	198.9
2	A	377	ALA	H	122.87	5.31 – 11.08	198.7
2	A	374	MET	H	121.54	5.39 – 11.10	198.4
2	A	420	LYS	H	124.59	5.24 – 11.12	198.0
2	A	341	ALA	H	122.22	5.31 – 11.08	197.6
2	A	326	GLU	H	121.83	5.45 – 11.20	197.4
2	A	430	GLN	H	119.81	5.39 – 11.05	197.2
2	A	406	GLN	H	119.75	5.39 – 11.05	197.1
2	A	415	ALA	H	121.75	5.31 – 11.08	196.8
2	A	289	GLN	H	119.50	5.39 – 11.05	196.6
2	A	264	GLU	H	121.38	5.45 – 11.20	196.6
2	A	135	ALA	H	121.61	5.31 – 11.08	196.6
2	A	269	GLU	H	121.10	5.45 – 11.20	196.1
2	A	380	ASP	H	117.25	5.52 – 11.08	196.0
2	A	386	GLU	H	120.82	5.45 – 11.20	195.6
2	A	375	ALA	H	120.99	5.31 – 11.08	195.5
2	A	260	ASP	H	116.94	5.52 – 11.08	195.4
2	A	147	GLN	H	118.69	5.39 – 11.05	195.2
2	A	148	GLN	H	118.63	5.39 – 11.05	195.1
2	A	277	GLU	H	120.43	5.45 – 11.20	194.9
2	A	372	GLU	H	120.41	5.45 – 11.20	194.9
2	A	328	GLN	H	118.35	5.39 – 11.05	194.6
2	A	395	MET	H	119.32	5.39 – 11.10	194.5
2	A	339	GLU	H	120.15	5.45 – 11.20	194.5
2	A	398	MET	H	119.25	5.39 – 11.10	194.4
2	A	122	ALA	H	120.33	5.31 – 11.08	194.3
2	A	404	GLU	H	120.03	5.45 – 11.20	194.3
2	A	338	GLU	H	120.02	5.45 – 11.20	194.2
2	A	319	ALA	H	120.07	5.31 – 11.08	193.9
2	A	373	GLU	H	119.68	5.45 – 11.20	193.7
2	A	268	ALA	H	119.86	5.31 – 11.08	193.5
2	A	292	GLU	H	119.56	5.45 – 11.20	193.4
2	A	383	GLU	H	119.55	5.45 – 11.20	193.4
2	A	320	GLN	H	117.53	5.39 – 11.05	193.1
2	A	409	GLU	H	119.30	5.45 – 11.20	193.0
2	A	271	ARG	H	123.43	5.25 – 11.22	192.9

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	285	ARG	H	123.39	5.25 – 11.22	192.9
2	A	416	LYS	H	121.41	5.24 – 11.12	192.6
2	A	334	ARG	H	123.17	5.25 – 11.22	192.5
2	A	359	GLU	H	118.94	5.45 – 11.20	192.4
2	A	426	GLU	H	118.92	5.45 – 11.20	192.3
2	A	361	LYS	H	121.03	5.24 – 11.12	191.9
2	A	393	GLU	H	118.46	5.45 – 11.20	191.5
2	A	287	LYS	H	120.71	5.24 – 11.12	191.4
2	A	413	ALA	H	118.51	5.31 – 11.08	191.2
2	A	418	THR	H	124.18	5.19 – 11.27	190.7
2	A	315	ARG	H	122.04	5.25 – 11.22	190.6
2	A	335	GLU	H	117.94	5.45 – 11.20	190.6
2	A	262	SER	H	115.80	5.45 – 11.10	190.3
2	A	327	LYS	H	120.07	5.24 – 11.12	190.3
2	A	331	GLU	H	117.62	5.45 – 11.20	190.1
2	A	305	ALA	H	117.60	5.31 – 11.08	189.6
2	A	133	THR	H	123.41	5.19 – 11.27	189.4
2	A	251	GLU	H	117.06	5.45 – 11.20	189.1
2	A	146	LYS	H	119.32	5.24 – 11.12	189.0
2	A	399	ARG	H	120.99	5.25 – 11.22	188.9
2	A	297	ALA	H	117.05	5.31 – 11.08	188.7
2	A	279	LYS	H	119.06	5.24 – 11.12	188.6
2	A	296	LYS	H	119.01	5.24 – 11.12	188.5
2	A	309	SER	H	114.50	5.45 – 11.10	188.0
2	A	368	LYS	H	118.69	5.24 – 11.12	188.0
2	A	390	LYS	H	118.55	5.24 – 11.12	187.7
2	A	280	SER	H	114.32	5.45 – 11.10	187.7
2	A	117	LEU	H	125.36	5.09 – 11.34	187.4
2	A	314	LEU	H	125.15	5.09 – 11.34	187.1
2	A	428	MET	H	115.03	5.39 – 11.10	187.0
2	A	266	LEU	H	124.73	5.09 – 11.34	186.4
2	A	391	ASN	H	121.66	5.28 – 11.36	186.4
2	A	145	ARG	H	119.43	5.25 – 11.22	186.2
2	A	370	LEU	H	124.55	5.09 – 11.34	186.1
2	A	356	ARG	H	119.30	5.25 – 11.22	186.0
2	A	342	LYS	H	117.54	5.24 – 11.12	186.0
2	A	283	ARG	H	119.16	5.25 – 11.22	185.8
2	A	321	ARG	H	118.99	5.25 – 11.22	185.5
2	A	267	ARG	H	118.79	5.25 – 11.22	185.2
2	A	422	THR	H	120.71	5.19 – 11.27	185.0
2	A	288	SER	H	112.59	5.45 – 11.10	184.6
2	A	417	VAL	H	129.55	4.98 – 11.56	184.3

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	349	LEU	H	123.31	5.09 – 11.34	184.2
2	A	343	ARG	H	117.92	5.25 – 11.22	183.7
2	A	344	ARG	H	117.63	5.25 – 11.22	183.2
2	A	382	LYS	H	115.81	5.24 – 11.12	183.1
2	A	278	LEU	H	122.60	5.09 – 11.34	183.0
2	A	121	GLU	H	113.50	5.45 – 11.20	182.9
2	A	325	ASN	H	119.49	5.28 – 11.36	182.8
2	A	397	ASN	H	119.47	5.28 – 11.36	182.8
2	A	144	LEU	H	122.45	5.09 – 11.34	182.8
2	A	414	LYS	H	115.41	5.24 – 11.12	182.4
2	A	120	LEU	H	121.60	5.09 – 11.34	181.4
2	A	141	LEU	H	121.55	5.09 – 11.34	181.3
2	A	389	SER	H	110.69	5.45 – 11.10	181.3
2	A	298	ASN	H	118.41	5.28 – 11.36	181.1
2	A	143	THR	H	118.18	5.19 – 11.27	180.8
2	A	400	ASN	H	117.91	5.28 – 11.36	180.2
2	A	429	ASN	H	117.62	5.28 – 11.36	179.8
2	A	394	LEU	H	120.51	5.09 – 11.34	179.7
2	A	350	LEU	H	120.47	5.09 – 11.34	179.6
2	A	284	ASN	H	117.50	5.28 – 11.36	179.6
2	A	130	VAL	H	126.20	4.98 – 11.56	179.2
2	A	427	LEU	H	120.09	5.09 – 11.34	179.0
2	A	412	LEU	H	120.04	5.09 – 11.34	178.9
2	A	358	ASN	H	116.63	5.28 – 11.36	178.1
2	A	336	LEU	H	119.29	5.09 – 11.34	177.7
2	A	354	VAL	H	125.20	4.98 – 11.56	177.7
2	A	425	ASN	H	116.07	5.28 – 11.36	177.2
2	A	403	LEU	H	118.86	5.09 – 11.34	177.0
2	A	351	LEU	H	118.33	5.09 – 11.34	176.2
2	A	263	VAL	H	123.72	4.98 – 11.56	175.4
2	A	115	VAL	H	123.60	4.98 – 11.56	175.3
2	A	401	VAL	H	123.54	4.98 – 11.56	175.2
2	A	125	VAL	H	123.45	4.98 – 11.56	175.0
2	A	137	VAL	H	123.14	4.98 – 11.56	174.6
2	A	249	THR	H	114.27	5.19 – 11.27	174.4
2	A	129	ILE	H	125.13	4.90 – 11.63	173.7
2	A	330	LEU	H	116.66	5.09 – 11.34	173.5
2	A	302	VAL	H	122.08	4.98 – 11.56	173.0
2	A	132	VAL	H	122.04	4.98 – 11.56	172.9
2	A	360	LEU	H	116.26	5.09 – 11.34	172.9
2	A	423	THR	H	112.74	5.19 – 11.27	171.9
2	A	313	VAL	H	121.34	4.98 – 11.56	171.8

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	384	VAL	H	121.26	4.98 – 11.56	171.7
2	A	346	VAL	H	121.24	4.98 – 11.56	171.7
2	A	306	LEU	H	115.48	5.09 – 11.34	171.6
2	A	357	THR	H	112.44	5.19 – 11.27	171.4
2	A	367	VAL	H	120.67	4.98 – 11.56	170.8
2	A	411	VAL	H	120.58	4.98 – 11.56	170.7
2	A	258	VAL	H	120.48	4.98 – 11.56	170.5
2	A	123	ILE	H	122.86	4.90 – 11.63	170.3
2	A	286	VAL	H	120.17	4.98 – 11.56	170.1
2	A	347	VAL	H	120.05	4.98 – 11.56	169.9
2	A	345	VAL	H	119.99	4.98 – 11.56	169.8
2	A	270	VAL	H	119.89	4.98 – 11.56	169.6
2	A	295	VAL	H	119.42	4.98 – 11.56	168.9
2	A	355	ILE	H	121.73	4.90 – 11.63	168.6
2	A	408	VAL	H	119.19	4.98 – 11.56	168.6
2	A	371	ILE	H	121.56	4.90 – 11.63	168.3
2	A	311	ILE	H	121.49	4.90 – 11.63	168.2
2	A	307	ILE	H	121.08	4.90 – 11.63	167.6
2	A	385	ILE	H	120.97	4.90 – 11.63	167.5
2	A	282	ILE	H	120.78	4.90 – 11.63	167.2
2	A	253	ILE	H	120.64	4.90 – 11.63	167.0
2	A	300	ILE	H	120.28	4.90 – 11.63	166.4
2	A	323	GLY	H	110.69	5.23 – 11.42	165.4
2	A	265	GLY	H	110.39	5.23 – 11.42	164.9
2	A	424	PHE	H	124.76	4.79 – 11.87	164.4
2	A	324	GLY	H	108.59	5.23 – 11.42	162.0
2	A	261	GLY	H	108.32	5.23 – 11.42	161.5
2	A	291	ILE	H	116.53	4.90 – 11.63	160.9
2	A	139	GLY	H	107.80	5.23 – 11.42	160.7
2	A	252	PHE	H	121.87	4.79 – 11.87	160.4
2	A	352	GLY	H	107.01	5.23 – 11.42	159.4
2	A	387	PHE	H	121.13	4.79 – 11.87	159.3
2	A	369	GLY	H	106.89	5.23 – 11.42	159.2
2	A	257	GLY	H	105.52	5.23 – 11.42	157.0
2	A	119	GLY	H	105.40	5.23 – 11.42	156.8
2	A	348	GLY	H	105.22	5.23 – 11.42	156.5
2	A	293	GLY	H	105.17	5.23 – 11.42	156.4
2	A	388	TYR	H	119.60	4.70 – 11.88	155.0
2	A	378	TYR	H	118.45	4.70 – 11.88	153.4
2	A	322	PHE	H	116.85	4.79 – 11.87	153.3
2	A	337	PHE	H	114.26	4.79 – 11.87	149.6
2	A	347	VAL	HG11	25.98	-0.48 – 2.12	96.7

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	347	VAL	HG12	25.98	-0.48 – 2.12	96.7
2	A	347	VAL	HG13	25.98	-0.48 – 2.12	96.7
2	A	411	VAL	HG11	25.82	-0.48 – 2.12	96.1
2	A	411	VAL	HG12	25.82	-0.48 – 2.12	96.1
2	A	411	VAL	HG13	25.82	-0.48 – 2.12	96.1
2	A	278	LEU	HD11	26.67	-0.61 – 2.12	94.9
2	A	278	LEU	HD12	26.67	-0.61 – 2.12	94.9
2	A	278	LEU	HD13	26.67	-0.61 – 2.12	94.9
2	A	332	LEU	HD11	26.46	-0.61 – 2.12	94.2
2	A	332	LEU	HD12	26.46	-0.61 – 2.12	94.2
2	A	332	LEU	HD13	26.46	-0.61 – 2.12	94.2
2	A	144	LEU	HD11	26.44	-0.61 – 2.12	94.1
2	A	144	LEU	HD12	26.44	-0.61 – 2.12	94.1
2	A	144	LEU	HD13	26.44	-0.61 – 2.12	94.1
2	A	349	LEU	HD11	26.44	-0.61 – 2.12	94.1
2	A	349	LEU	HD12	26.44	-0.61 – 2.12	94.1
2	A	349	LEU	HD13	26.44	-0.61 – 2.12	94.1
2	A	427	LEU	HD11	26.44	-0.61 – 2.12	94.1
2	A	427	LEU	HD12	26.44	-0.61 – 2.12	94.1
2	A	427	LEU	HD13	26.44	-0.61 – 2.12	94.1
2	A	314	LEU	HD21	26.57	-0.65 – 2.13	92.9
2	A	314	LEU	HD22	26.57	-0.65 – 2.13	92.9
2	A	314	LEU	HD23	26.57	-0.65 – 2.13	92.9
2	A	370	LEU	HD11	26.05	-0.61 – 2.12	92.7
2	A	370	LEU	HD12	26.05	-0.61 – 2.12	92.7
2	A	370	LEU	HD13	26.05	-0.61 – 2.12	92.7
2	A	132	VAL	HG11	24.88	-0.48 – 2.12	92.5
2	A	132	VAL	HG12	24.88	-0.48 – 2.12	92.5
2	A	132	VAL	HG13	24.88	-0.48 – 2.12	92.5
2	A	117	LEU	HD11	25.99	-0.61 – 2.12	92.4
2	A	117	LEU	HD12	25.99	-0.61 – 2.12	92.4
2	A	117	LEU	HD13	25.99	-0.61 – 2.12	92.4
2	A	266	LEU	HD21	26.14	-0.65 – 2.13	91.4
2	A	266	LEU	HD22	26.14	-0.65 – 2.13	91.4
2	A	266	LEU	HD23	26.14	-0.65 – 2.13	91.4
2	A	412	LEU	HD11	25.67	-0.61 – 2.12	91.2
2	A	412	LEU	HD12	25.67	-0.61 – 2.12	91.2
2	A	412	LEU	HD13	25.67	-0.61 – 2.12	91.2
2	A	248	LEU	HD11	25.41	-0.61 – 2.12	90.3
2	A	248	LEU	HD12	25.41	-0.61 – 2.12	90.3
2	A	248	LEU	HD13	25.41	-0.61 – 2.12	90.3
2	A	141	LEU	HD11	25.40	-0.61 – 2.12	90.3

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	141	LEU	HD12	25.40	-0.61 – 2.12	90.3
2	A	141	LEU	HD13	25.40	-0.61 – 2.12	90.3
2	A	120	LEU	HD11	25.30	-0.61 – 2.12	89.9
2	A	120	LEU	HD12	25.30	-0.61 – 2.12	89.9
2	A	120	LEU	HD13	25.30	-0.61 – 2.12	89.9
2	A	360	LEU	HD11	25.21	-0.61 – 2.12	89.6
2	A	360	LEU	HD12	25.21	-0.61 – 2.12	89.6
2	A	360	LEU	HD13	25.21	-0.61 – 2.12	89.6
2	A	367	VAL	HG11	23.97	-0.48 – 2.12	89.0
2	A	367	VAL	HG12	23.97	-0.48 – 2.12	89.0
2	A	367	VAL	HG13	23.97	-0.48 – 2.12	89.0
2	A	306	LEU	HD11	25.02	-0.61 – 2.12	88.9
2	A	306	LEU	HD12	25.02	-0.61 – 2.12	88.9
2	A	306	LEU	HD13	25.02	-0.61 – 2.12	88.9
2	A	302	VAL	HG11	23.93	-0.48 – 2.12	88.9
2	A	302	VAL	HG12	23.93	-0.48 – 2.12	88.9
2	A	302	VAL	HG13	23.93	-0.48 – 2.12	88.9
2	A	394	LEU	HD11	24.98	-0.61 – 2.12	88.7
2	A	394	LEU	HD12	24.98	-0.61 – 2.12	88.7
2	A	394	LEU	HD13	24.98	-0.61 – 2.12	88.7
2	A	330	LEU	HD11	24.88	-0.61 – 2.12	88.3
2	A	330	LEU	HD12	24.88	-0.61 – 2.12	88.3
2	A	330	LEU	HD13	24.88	-0.61 – 2.12	88.3
2	A	336	LEU	HD21	25.05	-0.65 – 2.13	87.5
2	A	336	LEU	HD22	25.05	-0.65 – 2.13	87.5
2	A	336	LEU	HD23	25.05	-0.65 – 2.13	87.5
2	A	403	LEU	HD11	24.37	-0.61 – 2.12	86.5
2	A	403	LEU	HD12	24.37	-0.61 – 2.12	86.5
2	A	403	LEU	HD13	24.37	-0.61 – 2.12	86.5
2	A	408	VAL	HG11	23.18	-0.48 – 2.12	86.0
2	A	408	VAL	HG12	23.18	-0.48 – 2.12	86.0
2	A	408	VAL	HG13	23.18	-0.48 – 2.12	86.0
2	A	403	LEU	HD21	24.51	-0.65 – 2.13	85.5
2	A	403	LEU	HD22	24.51	-0.65 – 2.13	85.5
2	A	403	LEU	HD23	24.51	-0.65 – 2.13	85.5
2	A	345	VAL	HG11	22.91	-0.48 – 2.12	85.0
2	A	345	VAL	HG12	22.91	-0.48 – 2.12	85.0
2	A	345	VAL	HG13	22.91	-0.48 – 2.12	85.0
2	A	427	LEU	HD21	24.25	-0.65 – 2.13	84.6
2	A	427	LEU	HD22	24.25	-0.65 – 2.13	84.6
2	A	427	LEU	HD23	24.25	-0.65 – 2.13	84.6
2	A	294	LEU	HD11	23.84	-0.61 – 2.12	84.5

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	294	LEU	HD12	23.84	-0.61 – 2.12	84.5
2	A	294	LEU	HD13	23.84	-0.61 – 2.12	84.5
2	A	351	LEU	HD11	23.78	-0.61 – 2.12	84.3
2	A	351	LEU	HD12	23.78	-0.61 – 2.12	84.3
2	A	351	LEU	HD13	23.78	-0.61 – 2.12	84.3
2	A	294	LEU	HD21	24.15	-0.65 – 2.13	84.2
2	A	294	LEU	HD22	24.15	-0.65 – 2.13	84.2
2	A	294	LEU	HD23	24.15	-0.65 – 2.13	84.2
2	A	270	VAL	HG11	22.69	-0.48 – 2.12	84.1
2	A	270	VAL	HG12	22.69	-0.48 – 2.12	84.1
2	A	270	VAL	HG13	22.69	-0.48 – 2.12	84.1
2	A	412	LEU	HD21	24.06	-0.65 – 2.13	83.9
2	A	412	LEU	HD22	24.06	-0.65 – 2.13	83.9
2	A	412	LEU	HD23	24.06	-0.65 – 2.13	83.9
2	A	141	LEU	HD21	24.05	-0.65 – 2.13	83.8
2	A	141	LEU	HD22	24.05	-0.65 – 2.13	83.8
2	A	141	LEU	HD23	24.05	-0.65 – 2.13	83.8
2	A	278	LEU	HD21	24.05	-0.65 – 2.13	83.8
2	A	278	LEU	HD22	24.05	-0.65 – 2.13	83.8
2	A	278	LEU	HD23	24.05	-0.65 – 2.13	83.8
2	A	120	LEU	HD21	23.95	-0.65 – 2.13	83.5
2	A	120	LEU	HD22	23.95	-0.65 – 2.13	83.5
2	A	120	LEU	HD23	23.95	-0.65 – 2.13	83.5
2	A	117	LEU	HD21	23.84	-0.65 – 2.13	83.1
2	A	117	LEU	HD22	23.84	-0.65 – 2.13	83.1
2	A	117	LEU	HD23	23.84	-0.65 – 2.13	83.1
2	A	401	VAL	HG11	22.29	-0.48 – 2.12	82.5
2	A	401	VAL	HG12	22.29	-0.48 – 2.12	82.5
2	A	401	VAL	HG13	22.29	-0.48 – 2.12	82.5
2	A	354	VAL	HG11	22.28	-0.48 – 2.12	82.5
2	A	354	VAL	HG12	22.28	-0.48 – 2.12	82.5
2	A	354	VAL	HG13	22.28	-0.48 – 2.12	82.5
2	A	286	VAL	HG11	22.17	-0.48 – 2.12	82.1
2	A	286	VAL	HG12	22.17	-0.48 – 2.12	82.1
2	A	286	VAL	HG13	22.17	-0.48 – 2.12	82.1
2	A	411	VAL	HG21	23.29	-0.58 – 2.19	81.2
2	A	411	VAL	HG22	23.29	-0.58 – 2.19	81.2
2	A	411	VAL	HG23	23.29	-0.58 – 2.19	81.2
2	A	132	VAL	HG21	23.25	-0.58 – 2.19	81.0
2	A	132	VAL	HG22	23.25	-0.58 – 2.19	81.0
2	A	132	VAL	HG23	23.25	-0.58 – 2.19	81.0
2	A	345	VAL	HG21	23.02	-0.58 – 2.19	80.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	345	VAL	HG22	23.02	-0.58 – 2.19	80.2
2	A	345	VAL	HG23	23.02	-0.58 – 2.19	80.2
2	A	336	LEU	HD11	22.60	-0.61 – 2.12	80.0
2	A	336	LEU	HD12	22.60	-0.61 – 2.12	80.0
2	A	336	LEU	HD13	22.60	-0.61 – 2.12	80.0
2	A	248	LEU	HD21	22.91	-0.65 – 2.13	79.8
2	A	248	LEU	HD22	22.91	-0.65 – 2.13	79.8
2	A	248	LEU	HD23	22.91	-0.65 – 2.13	79.8
2	A	370	LEU	HD21	22.87	-0.65 – 2.13	79.6
2	A	370	LEU	HD22	22.87	-0.65 – 2.13	79.6
2	A	370	LEU	HD23	22.87	-0.65 – 2.13	79.6
2	A	349	LEU	HD21	22.82	-0.65 – 2.13	79.5
2	A	349	LEU	HD22	22.82	-0.65 – 2.13	79.5
2	A	349	LEU	HD23	22.82	-0.65 – 2.13	79.5
2	A	332	LEU	HD21	22.65	-0.65 – 2.13	78.8
2	A	332	LEU	HD22	22.65	-0.65 – 2.13	78.8
2	A	332	LEU	HD23	22.65	-0.65 – 2.13	78.8
2	A	330	LEU	HD21	22.63	-0.65 – 2.13	78.8
2	A	330	LEU	HD22	22.63	-0.65 – 2.13	78.8
2	A	330	LEU	HD23	22.63	-0.65 – 2.13	78.8
2	A	137	VAL	HG21	22.60	-0.58 – 2.19	78.7
2	A	137	VAL	HG22	22.60	-0.58 – 2.19	78.7
2	A	137	VAL	HG23	22.60	-0.58 – 2.19	78.7
2	A	394	LEU	HD21	22.60	-0.65 – 2.13	78.6
2	A	394	LEU	HD22	22.60	-0.65 – 2.13	78.6
2	A	394	LEU	HD23	22.60	-0.65 – 2.13	78.6
2	A	306	LEU	HD21	22.55	-0.65 – 2.13	78.5
2	A	306	LEU	HD22	22.55	-0.65 – 2.13	78.5
2	A	306	LEU	HD23	22.55	-0.65 – 2.13	78.5
2	A	144	LEU	HD21	22.46	-0.65 – 2.13	78.1
2	A	144	LEU	HD22	22.46	-0.65 – 2.13	78.1
2	A	144	LEU	HD23	22.46	-0.65 – 2.13	78.1
2	A	258	VAL	HG11	21.14	-0.48 – 2.12	78.1
2	A	258	VAL	HG12	21.14	-0.48 – 2.12	78.1
2	A	258	VAL	HG13	21.14	-0.48 – 2.12	78.1
2	A	263	VAL	HG11	21.13	-0.48 – 2.12	78.1
2	A	263	VAL	HG12	21.13	-0.48 – 2.12	78.1
2	A	263	VAL	HG13	21.13	-0.48 – 2.12	78.1
2	A	341	ALA	HB1	20.40	0.14 – 2.58	78.0
2	A	341	ALA	HB2	20.40	0.14 – 2.58	78.0
2	A	341	ALA	HB3	20.40	0.14 – 2.58	78.0
2	A	297	ALA	HB1	20.37	0.14 – 2.58	77.9

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	297	ALA	HB2	20.37	0.14 – 2.58	77.9
2	A	297	ALA	HB3	20.37	0.14 – 2.58	77.9
2	A	125	VAL	HG11	21.07	-0.48 – 2.12	77.9
2	A	125	VAL	HG12	21.07	-0.48 – 2.12	77.9
2	A	125	VAL	HG13	21.07	-0.48 – 2.12	77.9
2	A	360	LEU	HD21	22.34	-0.65 – 2.13	77.7
2	A	360	LEU	HD22	22.34	-0.65 – 2.13	77.7
2	A	360	LEU	HD23	22.34	-0.65 – 2.13	77.7
2	A	115	VAL	HG11	21.02	-0.48 – 2.12	77.7
2	A	115	VAL	HG12	21.02	-0.48 – 2.12	77.7
2	A	115	VAL	HG13	21.02	-0.48 – 2.12	77.7
2	A	384	VAL	HG11	21.02	-0.48 – 2.12	77.7
2	A	384	VAL	HG12	21.02	-0.48 – 2.12	77.7
2	A	384	VAL	HG13	21.02	-0.48 – 2.12	77.7
2	A	417	VAL	HG11	21.02	-0.48 – 2.12	77.7
2	A	417	VAL	HG12	21.02	-0.48 – 2.12	77.7
2	A	417	VAL	HG13	21.02	-0.48 – 2.12	77.7
2	A	270	VAL	HG21	22.22	-0.58 – 2.19	77.3
2	A	270	VAL	HG22	22.22	-0.58 – 2.19	77.3
2	A	270	VAL	HG23	22.22	-0.58 – 2.19	77.3
2	A	263	VAL	HG21	22.18	-0.58 – 2.19	77.2
2	A	263	VAL	HG22	22.18	-0.58 – 2.19	77.2
2	A	263	VAL	HG23	22.18	-0.58 – 2.19	77.2
2	A	314	LEU	HD11	21.79	-0.61 – 2.12	77.0
2	A	314	LEU	HD12	21.79	-0.61 – 2.12	77.0
2	A	314	LEU	HD13	21.79	-0.61 – 2.12	77.0
2	A	432	ALA	HB1	19.95	0.14 – 2.58	76.2
2	A	432	ALA	HB2	19.95	0.14 – 2.58	76.2
2	A	432	ALA	HB3	19.95	0.14 – 2.58	76.2
2	A	401	VAL	HG21	21.78	-0.58 – 2.19	75.7
2	A	401	VAL	HG22	21.78	-0.58 – 2.19	75.7
2	A	401	VAL	HG23	21.78	-0.58 – 2.19	75.7
2	A	417	VAL	HG21	21.76	-0.58 – 2.19	75.6
2	A	417	VAL	HG22	21.76	-0.58 – 2.19	75.6
2	A	417	VAL	HG23	21.76	-0.58 – 2.19	75.6
2	A	130	VAL	HG11	20.39	-0.48 – 2.12	75.2
2	A	130	VAL	HG12	20.39	-0.48 – 2.12	75.2
2	A	130	VAL	HG13	20.39	-0.48 – 2.12	75.2
2	A	384	VAL	HG21	21.65	-0.58 – 2.19	75.2
2	A	384	VAL	HG22	21.65	-0.58 – 2.19	75.2
2	A	384	VAL	HG23	21.65	-0.58 – 2.19	75.2
2	A	415	ALA	HB1	19.71	0.14 – 2.58	75.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	415	ALA	HB2	19.71	0.14 – 2.58	75.2
2	A	415	ALA	HB3	19.71	0.14 – 2.58	75.2
2	A	367	VAL	HG21	21.64	-0.58 – 2.19	75.2
2	A	367	VAL	HG22	21.64	-0.58 – 2.19	75.2
2	A	367	VAL	HG23	21.64	-0.58 – 2.19	75.2
2	A	347	VAL	HG21	21.59	-0.58 – 2.19	75.0
2	A	347	VAL	HG22	21.59	-0.58 – 2.19	75.0
2	A	347	VAL	HG23	21.59	-0.58 – 2.19	75.0
2	A	130	VAL	HG21	21.58	-0.58 – 2.19	75.0
2	A	130	VAL	HG22	21.58	-0.58 – 2.19	75.0
2	A	130	VAL	HG23	21.58	-0.58 – 2.19	75.0
2	A	351	LEU	HD21	21.35	-0.65 – 2.13	74.1
2	A	351	LEU	HD22	21.35	-0.65 – 2.13	74.1
2	A	351	LEU	HD23	21.35	-0.65 – 2.13	74.1
2	A	408	VAL	HG21	21.28	-0.58 – 2.19	73.9
2	A	408	VAL	HG22	21.28	-0.58 – 2.19	73.9
2	A	408	VAL	HG23	21.28	-0.58 – 2.19	73.9
2	A	302	VAL	HG21	21.21	-0.58 – 2.19	73.7
2	A	302	VAL	HG22	21.21	-0.58 – 2.19	73.7
2	A	302	VAL	HG23	21.21	-0.58 – 2.19	73.7
2	A	375	ALA	HB1	19.18	0.14 – 2.58	73.0
2	A	375	ALA	HB2	19.18	0.14 – 2.58	73.0
2	A	375	ALA	HB3	19.18	0.14 – 2.58	73.0
2	A	377	ALA	HB1	19.08	0.14 – 2.58	72.6
2	A	377	ALA	HB2	19.08	0.14 – 2.58	72.6
2	A	377	ALA	HB3	19.08	0.14 – 2.58	72.6
2	A	122	ALA	HB1	19.07	0.14 – 2.58	72.6
2	A	122	ALA	HB2	19.07	0.14 – 2.58	72.6
2	A	122	ALA	HB3	19.07	0.14 – 2.58	72.6
2	A	115	VAL	HG21	20.87	-0.58 – 2.19	72.4
2	A	115	VAL	HG22	20.87	-0.58 – 2.19	72.4
2	A	115	VAL	HG23	20.87	-0.58 – 2.19	72.4
2	A	281	ALA	HB1	18.77	0.14 – 2.58	71.3
2	A	281	ALA	HB2	18.77	0.14 – 2.58	71.3
2	A	281	ALA	HB3	18.77	0.14 – 2.58	71.3
2	A	149	ALA	HB1	18.74	0.14 – 2.58	71.3
2	A	149	ALA	HB2	18.74	0.14 – 2.58	71.3
2	A	149	ALA	HB3	18.74	0.14 – 2.58	71.3
2	A	125	VAL	HG21	20.33	-0.58 – 2.19	70.5
2	A	125	VAL	HG22	20.33	-0.58 – 2.19	70.5
2	A	125	VAL	HG23	20.33	-0.58 – 2.19	70.5
2	A	258	VAL	HG21	20.27	-0.58 – 2.19	70.3

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	258	VAL	HG22	20.27	-0.58 – 2.19	70.3
2	A	258	VAL	HG23	20.27	-0.58 – 2.19	70.3
2	A	407	ALA	HB1	18.47	0.14 – 2.58	70.2
2	A	407	ALA	HB2	18.47	0.14 – 2.58	70.2
2	A	407	ALA	HB3	18.47	0.14 – 2.58	70.2
2	A	329	ALA	HB1	18.45	0.14 – 2.58	70.1
2	A	329	ALA	HB2	18.45	0.14 – 2.58	70.1
2	A	329	ALA	HB3	18.45	0.14 – 2.58	70.1
2	A	305	ALA	HB1	18.40	0.14 – 2.58	69.9
2	A	305	ALA	HB2	18.40	0.14 – 2.58	69.9
2	A	305	ALA	HB3	18.40	0.14 – 2.58	69.9
2	A	413	ALA	HB1	18.34	0.14 – 2.58	69.6
2	A	413	ALA	HB2	18.34	0.14 – 2.58	69.6
2	A	413	ALA	HB3	18.34	0.14 – 2.58	69.6
2	A	362	ALA	HB1	18.31	0.14 – 2.58	69.5
2	A	362	ALA	HB2	18.31	0.14 – 2.58	69.5
2	A	362	ALA	HB3	18.31	0.14 – 2.58	69.5
2	A	250	ALA	HB1	18.30	0.14 – 2.58	69.4
2	A	250	ALA	HB2	18.30	0.14 – 2.58	69.4
2	A	250	ALA	HB3	18.30	0.14 – 2.58	69.4
2	A	304	ALA	HB1	18.29	0.14 – 2.58	69.4
2	A	304	ALA	HB2	18.29	0.14 – 2.58	69.4
2	A	304	ALA	HB3	18.29	0.14 – 2.58	69.4
2	A	402	ALA	HB1	18.11	0.14 – 2.58	68.7
2	A	402	ALA	HB2	18.11	0.14 – 2.58	68.7
2	A	402	ALA	HB3	18.11	0.14 – 2.58	68.7
2	A	318	ALA	HB1	18.07	0.14 – 2.58	68.5
2	A	318	ALA	HB2	18.07	0.14 – 2.58	68.5
2	A	318	ALA	HB3	18.07	0.14 – 2.58	68.5
2	A	268	ALA	HB1	18.02	0.14 – 2.58	68.3
2	A	268	ALA	HB2	18.02	0.14 – 2.58	68.3
2	A	268	ALA	HB3	18.02	0.14 – 2.58	68.3
2	A	319	ALA	HB1	17.96	0.14 – 2.58	68.0
2	A	319	ALA	HB2	17.96	0.14 – 2.58	68.0
2	A	319	ALA	HB3	17.96	0.14 – 2.58	68.0
2	A	135	ALA	HB1	17.81	0.14 – 2.58	67.4
2	A	135	ALA	HB2	17.81	0.14 – 2.58	67.4
2	A	135	ALA	HB3	17.81	0.14 – 2.58	67.4
2	A	290	ALA	HB1	17.65	0.14 – 2.58	66.8
2	A	290	ALA	HB2	17.65	0.14 – 2.58	66.8
2	A	290	ALA	HB3	17.65	0.14 – 2.58	66.8
2	A	410	ALA	HB1	17.21	0.14 – 2.58	65.0

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	410	ALA	HB2	17.21	0.14 – 2.58	65.0
2	A	410	ALA	HB3	17.21	0.14 – 2.58	65.0
2	A	300	ILE	HD11	14.22	-0.72 – 2.09	48.2
2	A	300	ILE	HD12	14.22	-0.72 – 2.09	48.2
2	A	300	ILE	HD13	14.22	-0.72 – 2.09	48.2
2	A	371	ILE	HD11	14.18	-0.72 – 2.09	48.0
2	A	371	ILE	HD12	14.18	-0.72 – 2.09	48.0
2	A	371	ILE	HD13	14.18	-0.72 – 2.09	48.0
2	A	311	ILE	HD11	14.14	-0.72 – 2.09	47.9
2	A	311	ILE	HD12	14.14	-0.72 – 2.09	47.9
2	A	311	ILE	HD13	14.14	-0.72 – 2.09	47.9
2	A	282	ILE	HD11	14.10	-0.72 – 2.09	47.7
2	A	282	ILE	HD12	14.10	-0.72 – 2.09	47.7
2	A	282	ILE	HD13	14.10	-0.72 – 2.09	47.7
2	A	123	ILE	HD11	13.84	-0.72 – 2.09	46.8
2	A	123	ILE	HD12	13.84	-0.72 – 2.09	46.8
2	A	123	ILE	HD13	13.84	-0.72 – 2.09	46.8
2	A	355	ILE	HD11	13.83	-0.72 – 2.09	46.8
2	A	355	ILE	HD12	13.83	-0.72 – 2.09	46.8
2	A	355	ILE	HD13	13.83	-0.72 – 2.09	46.8
2	A	385	ILE	HD11	13.55	-0.72 – 2.09	45.8
2	A	385	ILE	HD12	13.55	-0.72 – 2.09	45.8
2	A	385	ILE	HD13	13.55	-0.72 – 2.09	45.8
2	A	253	ILE	HD11	13.06	-0.72 – 2.09	44.0
2	A	253	ILE	HD12	13.06	-0.72 – 2.09	44.0
2	A	253	ILE	HD13	13.06	-0.72 – 2.09	44.0
2	A	307	ILE	HD11	12.89	-0.72 – 2.09	43.5
2	A	307	ILE	HD12	12.89	-0.72 – 2.09	43.5
2	A	307	ILE	HD13	12.89	-0.72 – 2.09	43.5
2	A	291	ILE	HD11	12.09	-0.72 – 2.09	40.6
2	A	291	ILE	HD12	12.09	-0.72 – 2.09	40.6
2	A	291	ILE	HD13	12.09	-0.72 – 2.09	40.6
2	A	398	MET	HE1	17.44	-0.03 – 3.80	40.6
2	A	398	MET	HE2	17.44	-0.03 – 3.80	40.6
2	A	398	MET	HE3	17.44	-0.03 – 3.80	40.6
2	A	274	MET	HE1	17.34	-0.03 – 3.80	40.3
2	A	274	MET	HE2	17.34	-0.03 – 3.80	40.3
2	A	274	MET	HE3	17.34	-0.03 – 3.80	40.3
2	A	140	MET	HE1	17.09	-0.03 – 3.80	39.7
2	A	140	MET	HE2	17.09	-0.03 – 3.80	39.7
2	A	140	MET	HE3	17.09	-0.03 – 3.80	39.7
2	A	428	MET	HE1	16.71	-0.03 – 3.80	38.7

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	428	MET	HE2	16.71	-0.03 – 3.80	38.7
2	A	428	MET	HE3	16.71	-0.03 – 3.80	38.7
2	A	374	MET	HE1	16.53	-0.03 – 3.80	38.2
2	A	374	MET	HE2	16.53	-0.03 – 3.80	38.2
2	A	374	MET	HE3	16.53	-0.03 – 3.80	38.2
2	A	395	MET	HE1	15.86	-0.03 – 3.80	36.5
2	A	395	MET	HE2	15.86	-0.03 – 3.80	36.5
2	A	395	MET	HE3	15.86	-0.03 – 3.80	36.5
2	A	129	ILE	HD11	10.84	-0.72 – 2.09	36.1
2	A	129	ILE	HD12	10.84	-0.72 – 2.09	36.1
2	A	129	ILE	HD13	10.84	-0.72 – 2.09	36.1
2	A	415	ALA	N	7.11	106.13 – 140.55	-33.8
2	A	297	ALA	N	7.16	106.13 – 140.55	-33.8
2	A	122	ALA	N	7.26	106.13 – 140.55	-33.7
2	A	377	ALA	N	7.36	106.13 – 140.55	-33.7
2	A	413	ALA	N	7.57	106.13 – 140.55	-33.6
2	A	268	ALA	N	7.67	106.13 – 140.55	-33.6
2	A	410	ALA	N	7.83	106.13 – 140.55	-33.6
2	A	432	ALA	N	7.87	106.13 – 140.55	-33.5
2	A	318	ALA	N	7.98	106.13 – 140.55	-33.5
2	A	329	ALA	N	7.96	106.13 – 140.55	-33.5
2	A	149	ALA	N	7.99	106.13 – 140.55	-33.5
2	A	319	ALA	N	8.01	106.13 – 140.55	-33.5
2	A	135	ALA	N	8.03	106.13 – 140.55	-33.5
2	A	281	ALA	N	8.10	106.13 – 140.55	-33.5
2	A	402	ALA	N	8.14	106.13 – 140.55	-33.5
2	A	290	ALA	N	8.18	106.13 – 140.55	-33.5
2	A	375	ALA	N	8.39	106.13 – 140.55	-33.4
2	A	250	ALA	N	8.58	106.13 – 140.55	-33.3
2	A	304	ALA	N	8.66	106.13 – 140.55	-33.3
2	A	338	GLU	N	7.33	103.74 – 137.78	-33.3
2	A	341	ALA	N	8.64	106.13 – 140.55	-33.3
2	A	305	ALA	N	8.74	106.13 – 140.55	-33.3
2	A	310	GLU	N	7.49	103.74 – 137.78	-33.3
2	A	383	GLU	N	7.46	103.74 – 137.78	-33.3
2	A	407	ALA	N	8.79	106.13 – 140.55	-33.3
2	A	331	GLU	N	7.52	103.74 – 137.78	-33.3
2	A	362	ALA	N	8.90	106.13 – 140.55	-33.2
2	A	426	GLU	N	7.62	103.74 – 137.78	-33.2
2	A	353	GLU	N	7.67	103.74 – 137.78	-33.2
2	A	359	GLU	N	7.67	103.74 – 137.78	-33.2
2	A	269	GLU	N	7.87	103.74 – 137.78	-33.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	386	GLU	N	7.91	103.74 – 137.78	-33.1
2	A	404	GLU	N	7.96	103.74 – 137.78	-33.1
2	A	409	GLU	N	8.03	103.74 – 137.78	-33.1
2	A	373	GLU	N	8.04	103.74 – 137.78	-33.1
2	A	277	GLU	N	8.16	103.74 – 137.78	-33.1
2	A	292	GLU	N	8.23	103.74 – 137.78	-33.1
2	A	372	GLU	N	8.22	103.74 – 137.78	-33.1
2	A	124	GLU	N	8.27	103.74 – 137.78	-33.0
2	A	393	GLU	N	8.25	103.74 – 137.78	-33.0
2	A	251	GLU	N	8.29	103.74 – 137.78	-33.0
2	A	116	GLU	N	8.32	103.74 – 137.78	-33.0
2	A	131	GLU	N	8.53	103.74 – 137.78	-33.0
2	A	259	GLU	N	8.54	103.74 – 137.78	-33.0
2	A	326	GLU	N	8.53	103.74 – 137.78	-33.0
2	A	121	GLU	N	8.64	103.74 – 137.78	-32.9
2	A	339	GLU	N	8.63	103.74 – 137.78	-32.9
2	A	264	GLU	N	8.75	103.74 – 137.78	-32.9
2	A	419	GLU	N	8.72	103.74 – 137.78	-32.9
2	A	140	MET	N	7.69	102.99 – 137.21	-32.9
2	A	364	GLU	N	8.98	103.74 – 137.78	-32.8
2	A	374	MET	N	7.84	102.99 – 137.21	-32.8
2	A	126	GLU	N	9.11	103.74 – 137.78	-32.8
2	A	421	GLU	N	9.11	103.74 – 137.78	-32.8
2	A	428	MET	N	7.93	102.99 – 137.21	-32.8
2	A	395	MET	N	8.06	102.99 – 137.21	-32.7
2	A	398	MET	N	8.13	102.99 – 137.21	-32.7
2	A	335	GLU	N	9.49	103.74 – 137.78	-32.7
2	A	289	GLN	N	7.37	102.61 – 137.42	-32.4
2	A	320	GLN	N	7.67	102.61 – 137.42	-32.3
2	A	148	GLN	N	7.74	102.61 – 137.42	-32.2
2	A	430	GLN	N	7.75	102.61 – 137.42	-32.2
2	A	147	GLN	N	7.84	102.61 – 137.42	-32.2
2	A	328	GLN	N	7.88	102.61 – 137.42	-32.2
2	A	431	GLN	N	8.08	102.61 – 137.42	-32.1
2	A	340	GLN	N	8.57	102.61 – 137.42	-32.0
2	A	406	GLN	N	8.55	102.61 – 137.42	-32.0
2	A	118	GLN	N	9.38	102.61 – 137.42	-31.8
2	A	280	SER	N	7.55	99.14 – 133.45	-31.7
2	A	309	SER	N	7.62	99.14 – 133.45	-31.7
2	A	389	SER	N	7.88	99.14 – 133.45	-31.6
2	A	321	ARG	N	7.52	102.91 – 138.82	-31.6
2	A	271	ARG	N	7.61	102.91 – 138.82	-31.5

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	283	ARG	N	7.62	102.91 – 138.82	-31.5
2	A	343	ARG	N	7.63	102.91 – 138.82	-31.5
2	A	262	SER	N	8.14	99.14 – 133.45	-31.5
2	A	288	SER	N	8.30	99.14 – 133.45	-31.5
2	A	344	ARG	N	7.91	102.91 – 138.82	-31.5
2	A	356	ARG	N	8.03	102.91 – 138.82	-31.4
2	A	145	ARG	N	8.21	102.91 – 138.82	-31.4
2	A	285	ARG	N	8.20	102.91 – 138.82	-31.4
2	A	267	ARG	N	8.48	102.91 – 138.82	-31.3
2	A	399	ARG	N	8.56	102.91 – 138.82	-31.3
2	A	315	ARG	N	8.64	102.91 – 138.82	-31.2
2	A	334	ARG	N	8.69	102.91 – 138.82	-31.2
2	A	414	LYS	N	7.09	102.74 – 139.42	-31.1
2	A	390	LYS	N	7.16	102.74 – 139.42	-31.1
2	A	368	LYS	N	7.70	102.74 – 139.42	-30.9
2	A	146	LYS	N	7.85	102.74 – 139.42	-30.9
2	A	382	LYS	N	7.85	102.74 – 139.42	-30.9
2	A	279	LYS	N	7.96	102.74 – 139.42	-30.8
2	A	327	LYS	N	8.01	102.74 – 139.42	-30.8
2	A	296	LYS	N	8.18	102.74 – 139.42	-30.8
2	A	342	LYS	N	8.23	102.74 – 139.42	-30.8
2	A	420	LYS	N	8.23	102.74 – 139.42	-30.8
2	A	287	LYS	N	8.27	102.74 – 139.42	-30.8
2	A	361	LYS	N	8.28	102.74 – 139.42	-30.8
2	A	392	LYS	N	8.48	102.74 – 139.42	-30.7
2	A	416	LYS	N	8.64	102.74 – 139.42	-30.6
2	A	127	LYS	N	9.22	102.74 – 139.42	-30.5
2	A	312	ASP	N	7.32	102.08 – 139.36	-30.4
2	A	136	ASP	N	7.84	102.08 – 139.36	-30.3
2	A	142	ASP	N	7.93	102.08 – 139.36	-30.2
2	A	380	ASP	N	8.11	102.08 – 139.36	-30.2
2	A	260	ASP	N	8.20	102.08 – 139.36	-30.2
2	A	299	ASP	N	8.30	102.08 – 139.36	-30.2
2	A	301	ASP	N	8.39	102.08 – 139.36	-30.1
2	A	308	ASP	N	8.47	102.08 – 139.36	-30.1
2	A	306	LEU	N	7.18	102.77 – 140.89	-30.1
2	A	138	ASP	N	8.63	102.08 – 139.36	-30.1
2	A	396	ASP	N	8.69	102.08 – 139.36	-30.1
2	A	134	ASP	N	8.79	102.08 – 139.36	-30.0
2	A	336	LEU	N	7.43	102.77 – 140.89	-30.0
2	A	363	ASP	N	8.90	102.08 – 139.36	-30.0
2	A	394	LEU	N	7.57	102.77 – 140.89	-30.0

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	330	LEU	N	7.70	102.77 – 140.89	-29.9
2	A	427	LEU	N	7.87	102.77 – 140.89	-29.9
2	A	360	LEU	N	7.95	102.77 – 140.89	-29.9
2	A	266	LEU	N	8.02	102.77 – 140.89	-29.9
2	A	314	LEU	N	8.03	102.77 – 140.89	-29.9
2	A	120	LEU	N	8.12	102.77 – 140.89	-29.8
2	A	349	LEU	N	8.16	102.77 – 140.89	-29.8
2	A	370	LEU	N	8.21	102.77 – 140.89	-29.8
2	A	144	LEU	N	8.28	102.77 – 140.89	-29.8
2	A	403	LEU	N	8.31	102.77 – 140.89	-29.8
2	A	412	LEU	N	8.43	102.77 – 140.89	-29.8
2	A	141	LEU	N	8.51	102.77 – 140.89	-29.7
2	A	117	LEU	N	8.60	102.77 – 140.89	-29.7
2	A	350	LEU	N	8.61	102.77 – 140.89	-29.7
2	A	278	LEU	N	8.86	102.77 – 140.89	-29.6
2	A	351	LEU	N	9.03	102.77 – 140.89	-29.6
2	A	298	ASN	N	7.28	99.66 – 138.23	-28.9
2	A	358	ASN	N	7.37	99.66 – 138.23	-28.9
2	A	391	ASN	N	7.45	99.66 – 138.23	-28.9
2	A	429	ASN	N	7.52	99.66 – 138.23	-28.9
2	A	400	ASN	N	7.66	99.66 – 138.23	-28.9
2	A	397	ASN	N	7.88	99.66 – 138.23	-28.8
2	A	325	ASN	N	8.13	99.66 – 138.23	-28.7
2	A	284	ASN	N	8.33	99.66 – 138.23	-28.7
2	A	425	ASN	N	9.34	99.66 – 138.23	-28.4
2	A	257	GLY	N	7.69	91.59 – 127.52	-28.4
2	A	348	GLY	N	7.76	91.59 – 127.52	-28.3
2	A	369	GLY	N	7.83	91.59 – 127.52	-28.3
2	A	323	GLY	N	7.88	91.59 – 127.52	-28.3
2	A	293	GLY	N	8.03	91.59 – 127.52	-28.3
2	A	352	GLY	N	8.04	91.59 – 127.52	-28.2
2	A	261	GLY	N	8.09	91.59 – 127.52	-28.2
2	A	324	GLY	N	8.08	91.59 – 127.52	-28.2
2	A	139	GLY	N	8.12	91.59 – 127.52	-28.2
2	A	265	GLY	N	8.32	91.59 – 127.52	-28.2
2	A	119	GLY	N	8.46	91.59 – 127.52	-28.1
2	A	378	TYR	N	7.78	100.12 – 140.79	-27.7
2	A	322	PHE	N	7.57	99.93 – 140.82	-27.6
2	A	337	PHE	N	7.63	99.93 – 140.82	-27.6
2	A	252	PHE	N	7.90	99.93 – 140.82	-27.5
2	A	388	TYR	N	8.58	100.12 – 140.79	-27.5
2	A	387	PHE	N	7.97	99.93 – 140.82	-27.5

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	123	ILE	N	7.08	100.55 – 142.30	-27.4
2	A	307	ILE	N	7.13	100.55 – 142.30	-27.4
2	A	300	ILE	N	7.69	100.55 – 142.30	-27.2
2	A	371	ILE	N	7.96	100.55 – 142.30	-27.2
2	A	129	ILE	N	8.07	100.55 – 142.30	-27.1
2	A	385	ILE	N	8.14	100.55 – 142.30	-27.1
2	A	253	ILE	N	8.20	100.55 – 142.30	-27.1
2	A	291	ILE	N	8.35	100.55 – 142.30	-27.1
2	A	355	ILE	N	8.44	100.55 – 142.30	-27.1
2	A	424	PHE	N	9.79	99.93 – 140.82	-27.0
2	A	311	ILE	N	8.66	100.55 – 142.30	-27.0
2	A	282	ILE	N	8.74	100.55 – 142.30	-27.0
2	A	384	VAL	N	7.20	99.23 – 142.92	-26.1
2	A	313	VAL	N	7.33	99.23 – 142.92	-26.0
2	A	258	VAL	N	7.43	99.23 – 142.92	-26.0
2	A	137	VAL	N	7.60	99.23 – 142.92	-26.0
2	A	411	VAL	N	7.70	99.23 – 142.92	-25.9
2	A	401	VAL	N	7.88	99.23 – 142.92	-25.9
2	A	367	VAL	N	7.96	99.23 – 142.92	-25.9
2	A	130	VAL	N	8.04	99.23 – 142.92	-25.9
2	A	354	VAL	N	8.06	99.23 – 142.92	-25.9
2	A	302	VAL	N	8.10	99.23 – 142.92	-25.9
2	A	345	VAL	N	8.13	99.23 – 142.92	-25.9
2	A	408	VAL	N	8.12	99.23 – 142.92	-25.9
2	A	115	VAL	N	8.29	99.23 – 142.92	-25.8
2	A	270	VAL	N	8.31	99.23 – 142.92	-25.8
2	A	286	VAL	N	8.32	99.23 – 142.92	-25.8
2	A	295	VAL	N	8.35	99.23 – 142.92	-25.8
2	A	417	VAL	N	8.38	99.23 – 142.92	-25.8
2	A	125	VAL	N	8.41	99.23 – 142.92	-25.8
2	A	347	VAL	N	8.43	99.23 – 142.92	-25.8
2	A	346	VAL	N	8.55	99.23 – 142.92	-25.8
2	A	263	VAL	N	8.57	99.23 – 142.92	-25.8
2	A	132	VAL	N	8.64	99.23 – 142.92	-25.7
2	A	249	THR	N	7.89	91.89 – 138.78	-22.9
2	A	143	THR	N	7.97	91.89 – 138.78	-22.9
2	A	422	THR	N	8.37	91.89 – 138.78	-22.8
2	A	423	THR	N	8.45	91.89 – 138.78	-22.8
2	A	357	THR	N	8.64	91.89 – 138.78	-22.8
2	A	418	THR	N	8.89	91.89 – 138.78	-22.7
2	A	133	THR	N	9.65	91.89 – 138.78	-22.5
2	A	384	VAL	CG1	0.69	14.71 – 28.29	-15.3

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	394	LEU	CD1	0.38	16.71 – 32.55	-15.3
2	A	411	VAL	CG1	0.76	14.71 – 28.29	-15.3
2	A	115	VAL	CG1	0.78	14.71 – 28.29	-15.3
2	A	417	VAL	CG1	0.78	14.71 – 28.29	-15.3
2	A	130	VAL	CG1	0.81	14.71 – 28.29	-15.2
2	A	347	VAL	CG1	0.81	14.71 – 28.29	-15.2
2	A	270	VAL	CG1	0.88	14.71 – 28.29	-15.2
2	A	132	VAL	CG1	0.90	14.71 – 28.29	-15.2
2	A	125	VAL	CG1	0.91	14.71 – 28.29	-15.2
2	A	367	VAL	CG1	0.92	14.71 – 28.29	-15.2
2	A	258	VAL	CG1	0.94	14.71 – 28.29	-15.1
2	A	263	VAL	CG1	0.93	14.71 – 28.29	-15.1
2	A	354	VAL	CG1	0.94	14.71 – 28.29	-15.1
2	A	408	VAL	CG1	0.95	14.71 – 28.29	-15.1
2	A	360	LEU	CD1	0.69	16.71 – 32.55	-15.1
2	A	278	LEU	CD1	0.71	16.71 – 32.55	-15.1
2	A	336	LEU	CD1	0.71	16.71 – 32.55	-15.1
2	A	345	VAL	CG1	0.98	14.71 – 28.29	-15.1
2	A	412	LEU	CD1	0.76	16.71 – 32.55	-15.1
2	A	294	LEU	CD1	0.78	16.71 – 32.55	-15.1
2	A	248	LEU	CD1	0.79	16.71 – 32.55	-15.1
2	A	403	LEU	CD1	0.80	16.71 – 32.55	-15.1
2	A	314	LEU	CD1	0.83	16.71 – 32.55	-15.0
2	A	349	LEU	CD1	0.82	16.71 – 32.55	-15.0
2	A	120	LEU	CD1	0.84	16.71 – 32.55	-15.0
2	A	141	LEU	CD1	0.84	16.71 – 32.55	-15.0
2	A	370	LEU	CD1	0.83	16.71 – 32.55	-15.0
2	A	117	LEU	CD1	0.85	16.71 – 32.55	-15.0
2	A	330	LEU	CD1	0.85	16.71 – 32.55	-15.0
2	A	286	VAL	CG1	1.11	14.71 – 28.29	-15.0
2	A	302	VAL	CG1	1.11	14.71 – 28.29	-15.0
2	A	401	VAL	CG1	1.10	14.71 – 28.29	-15.0
2	A	306	LEU	CD1	0.95	16.71 – 32.55	-15.0
2	A	144	LEU	CD1	1.00	16.71 – 32.55	-14.9
2	A	427	LEU	CD1	1.00	16.71 – 32.55	-14.9
2	A	351	LEU	CD1	1.08	16.71 – 32.55	-14.9
2	A	332	LEU	CD1	1.14	16.71 – 32.55	-14.8
2	A	248	LEU	CD2	0.50	15.73 – 32.47	-14.1
2	A	351	LEU	CD2	0.63	15.73 – 32.47	-14.0
2	A	394	LEU	CD2	0.63	15.73 – 32.47	-14.0
2	A	412	LEU	CD2	0.72	15.73 – 32.47	-14.0
2	A	403	LEU	CD2	0.75	15.73 – 32.47	-13.9

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	144	LEU	CD2	0.76	15.73 – 32.47	-13.9
2	A	117	LEU	CD2	0.78	15.73 – 32.47	-13.9
2	A	141	LEU	CD2	0.77	15.73 – 32.47	-13.9
2	A	266	LEU	CD2	0.78	15.73 – 32.47	-13.9
2	A	278	LEU	CD2	0.77	15.73 – 32.47	-13.9
2	A	294	LEU	CD2	0.78	15.73 – 32.47	-13.9
2	A	330	LEU	CD2	0.77	15.73 – 32.47	-13.9
2	A	120	LEU	CD2	0.79	15.73 – 32.47	-13.9
2	A	360	LEU	CD2	0.81	15.73 – 32.47	-13.9
2	A	336	LEU	CD2	0.83	15.73 – 32.47	-13.9
2	A	349	LEU	CD2	0.87	15.73 – 32.47	-13.9
2	A	370	LEU	CD2	0.87	15.73 – 32.47	-13.9
2	A	306	LEU	CD2	0.89	15.73 – 32.47	-13.9
2	A	427	LEU	CD2	0.90	15.73 – 32.47	-13.9
2	A	314	LEU	CD2	0.97	15.73 – 32.47	-13.8
2	A	332	LEU	CD2	0.98	15.73 – 32.47	-13.8
2	A	384	VAL	CG2	0.59	13.71 – 28.88	-13.7
2	A	137	VAL	CG2	0.77	13.71 – 28.88	-13.5
2	A	130	VAL	CG2	0.80	13.71 – 28.88	-13.5
2	A	258	VAL	CG2	0.80	13.71 – 28.88	-13.5
2	A	417	VAL	CG2	0.81	13.71 – 28.88	-13.5
2	A	132	VAL	CG2	0.84	13.71 – 28.88	-13.5
2	A	367	VAL	CG2	0.84	13.71 – 28.88	-13.5
2	A	115	VAL	CG2	0.84	13.71 – 28.88	-13.5
2	A	302	VAL	CG2	0.86	13.71 – 28.88	-13.5
2	A	408	VAL	CG2	0.89	13.71 – 28.88	-13.5
2	A	345	VAL	CG2	0.90	13.71 – 28.88	-13.4
2	A	125	VAL	CG2	0.91	13.71 – 28.88	-13.4
2	A	347	VAL	CG2	0.90	13.71 – 28.88	-13.4
2	A	401	VAL	CG2	0.96	13.71 – 28.88	-13.4
2	A	263	VAL	CG2	1.02	13.71 – 28.88	-13.4
2	A	411	VAL	CG2	1.02	13.71 – 28.88	-13.4
2	A	270	VAL	CG2	1.03	13.71 – 28.88	-13.4
2	A	377	ALA	CB	1.21	10.19 – 27.75	-10.1
2	A	415	ALA	CB	1.25	10.19 – 27.75	-10.1
2	A	362	ALA	CB	1.27	10.19 – 27.75	-10.1
2	A	319	ALA	CB	1.28	10.19 – 27.75	-10.1
2	A	432	ALA	CB	1.31	10.19 – 27.75	-10.1
2	A	122	ALA	CB	1.34	10.19 – 27.75	-10.0
2	A	329	ALA	CB	1.34	10.19 – 27.75	-10.0
2	A	135	ALA	CB	1.39	10.19 – 27.75	-10.0
2	A	149	ALA	CB	1.41	10.19 – 27.75	-10.0

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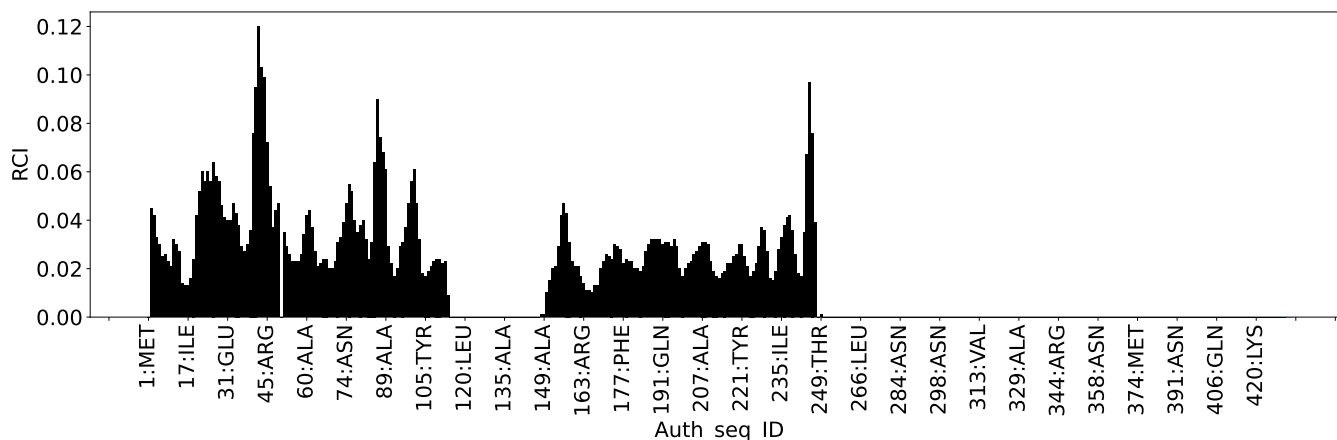
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	290	ALA	CB	1.40	10.19 – 27.75	-10.0
2	A	305	ALA	CB	1.40	10.19 – 27.75	-10.0
2	A	410	ALA	CB	1.40	10.19 – 27.75	-10.0
2	A	297	ALA	CB	1.44	10.19 – 27.75	-10.0
2	A	402	ALA	CB	1.45	10.19 – 27.75	-10.0
2	A	281	ALA	CB	1.46	10.19 – 27.75	-10.0
2	A	304	ALA	CB	1.46	10.19 – 27.75	-10.0
2	A	250	ALA	CB	1.48	10.19 – 27.75	-10.0
2	A	341	ALA	CB	1.49	10.19 – 27.75	-9.9
2	A	407	ALA	CB	1.49	10.19 – 27.75	-9.9
2	A	413	ALA	CB	1.49	10.19 – 27.75	-9.9
2	A	268	ALA	CB	1.51	10.19 – 27.75	-9.9
2	A	375	ALA	CB	1.52	10.19 – 27.75	-9.9
2	A	318	ALA	CB	1.66	10.19 – 27.75	-9.9
2	A	374	MET	CE	1.74	8.39 – 25.85	-8.8
2	A	428	MET	CE	1.74	8.39 – 25.85	-8.8
2	A	395	MET	CE	1.92	8.39 – 25.85	-8.7
2	A	398	MET	CE	1.96	8.39 – 25.85	-8.7
2	A	140	MET	CE	2.05	8.39 – 25.85	-8.6
2	A	274	MET	CE	2.09	8.39 – 25.85	-8.6
2	A	129	ILE	CD1	0.66	5.18 – 21.60	-7.8
2	A	253	ILE	CD1	0.68	5.18 – 21.60	-7.7
2	A	355	ILE	CD1	0.78	5.18 – 21.60	-7.7
2	A	291	ILE	CD1	0.80	5.18 – 21.60	-7.7
2	A	371	ILE	CD1	0.80	5.18 – 21.60	-7.7
2	A	385	ILE	CD1	0.80	5.18 – 21.60	-7.7
2	A	123	ILE	CD1	0.81	5.18 – 21.60	-7.7
2	A	300	ILE	CD1	0.82	5.18 – 21.60	-7.7
2	A	307	ILE	CD1	0.83	5.18 – 21.60	-7.7
2	A	282	ILE	CD1	0.84	5.18 – 21.60	-7.6
2	A	311	ILE	CD1	0.89	5.18 – 21.60	-7.6
2	A	163	ARG	HB3	0.14	0.43 – 3.11	-6.1

7.2.5 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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_dup*

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	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

7.3.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	2	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	49	-1.02 ± 0.30	Should be applied

7.3.3 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 2%, i.e. 132 atoms were assigned a chemical shift out of a possible 6403. 0 out of 78 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	23/2352 (1%)	15/960 (2%)	0/938 (0%)	8/454 (2%)
Sidechain	84/3732 (2%)	69/2408 (3%)	15/1171 (1%)	0/153 (0%)
Aromatic	25/319 (8%)	15/155 (10%)	10/156 (6%)	0/8 (0%)
Overall	132/6403 (2%)	99/3523 (3%)	25/2265 (1%)	8/615 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 228 atoms were assigned a chemical shift out of a possible 7075. 0 out of 86 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	107/2623 (4%)	58/1071 (5%)	0/1046 (0%)	49/506 (10%)
Sidechain	90/4112 (2%)	75/2655 (3%)	15/1285 (1%)	0/172 (0%)
Aromatic	31/340 (9%)	21/165 (13%)	10/166 (6%)	0/9 (0%)
Overall	228/7075 (3%)	154/3891 (4%)	25/2497 (1%)	49/687 (7%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:

