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wwPDB NMR Structure Validation Summary Report (i)

Apr 27, 2016 – 03:39 AM BST

PDB ID	:	2MTP
Title	:	The structure of Filamin repeat 21 bound to integrin
Authors	:	Liu, J.; Qin, J.
Deposited on	:	2014-08-28

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

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

A user guide is available at

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

with specific help available everywhere you see the (i) symbol.

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

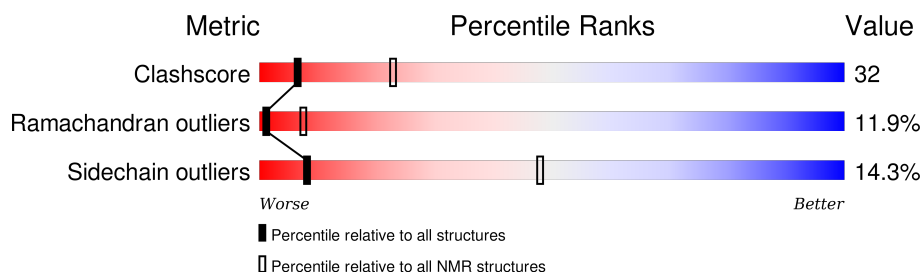|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
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 69%.

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		32
Ramachandran outliers		11.9%
Sidechain outliers		14.3%

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	95	53% 40% 6% ·
2	B	21	24% 19% 5% 52%
3	C	47	· 9% · 87%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 17 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:2237-A:2330, B:988-B:997, C:746-C:751 (110)	0.47	17

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 11, 17, 18, 20
2	8, 9, 10, 12, 14
3	1, 2, 4
4	3, 13, 15
Single-model clusters	16; 19

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2464 atoms, of which 1195 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Filamin-A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1332	431	643	118	139	1	0

- Molecule 2 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	21	347	115	164	31	37	0

- Molecule 3 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
3	C	47	785	250	388	72	75	0

There are 2 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
C	717	LYS	LEU	ENGINEERED MUTATION	UNP P05106
C	718	LYS	LEU	ENGINEERED MUTATION	UNP P05106

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Filamin-A

Chain A:
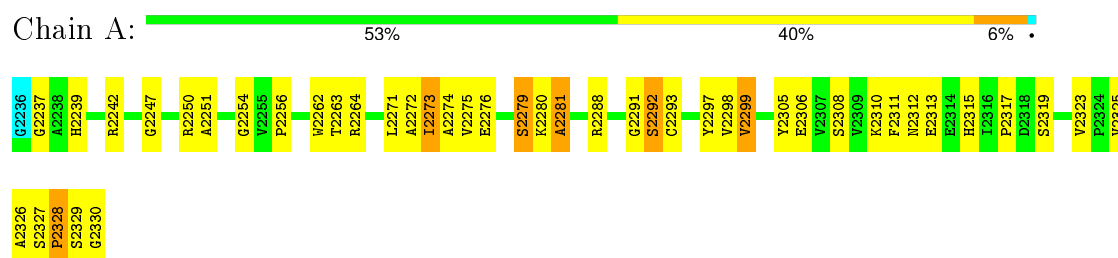
- Molecule 2: Integrin alpha-IIb
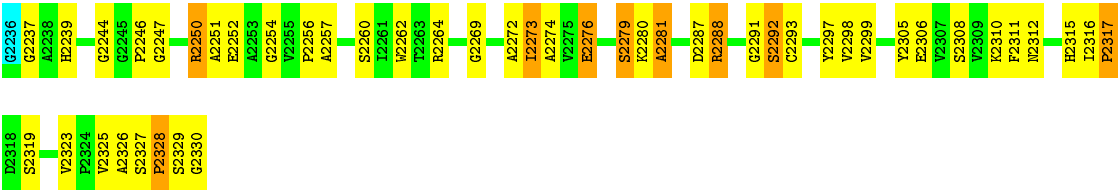
Chain B:

- Molecule 3: Integrin beta-3

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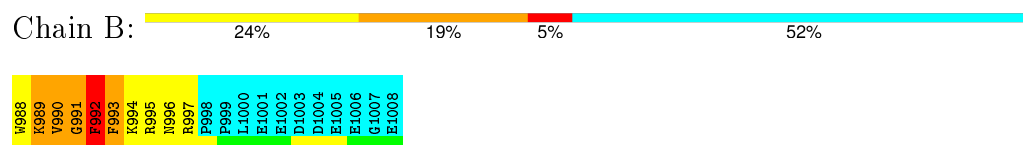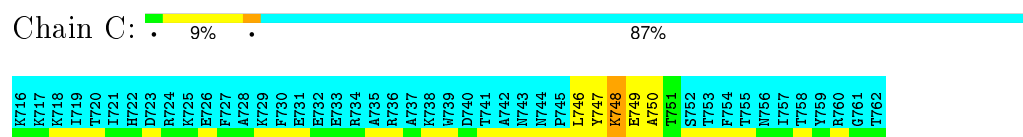
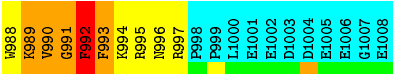## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: Filamin-A

Chain A:

G2236 G2237 A2238 H2239 G2244 G2245 P2246 G2247 R2250 A2251 E2252 A2253 G2254 V2255 P2256 A2257 S2260 I2261 W2262 T2263 R2264 G2269 A2272 I2273 A2274 V2275 E2276 S2279 K2280 A2281 D2287 R2288 G2291 S2292 C2293 Y2297 V2298 V2299 Y2305 E2306 V2307 S2308 V2309 K2310 F2311 N2312 H2315 I2316 P2317

D2318 S2319 V2323 P2324 V2325 A2326 S2327 P2328 S2329 G2330

• Molecule 2: Integrin alpha-IIb

Chain B:　　24%　　　　19%　　5%　　　　　52%

W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

• Molecule 3: Integrin beta-3

Chain C: ․ ․ ․ ․ 　　　　　　　　　　87%

K716 K717 K718 I719 T720 I721 H722 D723 R724 K725 E726 F727 A728 K729 F730 E731 E732 E733 R734 A735 R736 A737 K738 W739 D740 T741 A742 N743 N744 P745 L746 Y747 K748 E749 A750 T751 S752 T753 F754 T755 N756 I757 T758 Y759 R760 G761 T762

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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)	2mtp_cs.str
Number of chemical shift lists	1
Total number of shifts	1430
Number of shifts mapped to atoms	1430
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

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)

There are no covalent bond-length or bond-angle outliers.

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	3.2±0.7
All	All	0	65

There are no bond-length outliers.

There are no bond-angle outliers.

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)
1	A	2288	ARG	Sidechain	20
1	A	2264	ARG	Sidechain	18
1	A	2242	ARG	Sidechain	14
1	A	2250	ARG	Sidechain	13

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	685	640	650	34±4
2	B	95	98	97	19±2
3	C	50	50	51	4±1
All	All	16600	15760	15960	1054

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 32.

5 of 265 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
2:B:989:LYS:O	2:B:991:GLY:N	1.02	1.92	2	20
2:B:993:PHE:CD1	2:B:994:LYS:N	0.72	2.58	15	20
2:B:992:PHE:CD1	2:B:993:PHE:N	0.69	2.60	1	20
2:B:992:PHE:CE1	2:B:993:PHE:CD1	0.67	2.83	7	20
2:B:992:PHE:CG	2:B:993:PHE:N	0.66	2.63	7	20

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	93/95 (98%)	73±2 (79±2%)	13±2 (14±2%)	7±1 (7±1%)	3	18
2	B	9/21 (43%)	4±0 (40±5%)	1±1 (9±8%)	5±1 (51±9%)	0	0
3	C	6/47 (13%)	3±1 (47±15%)	1±1 (24±12%)	2±1 (29±12%)	0	1
All	All	2160/3260 (66%)	1596 (74%)	306 (14%)	258 (12%)	1	7

5 of 25 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	992	PHE	20
1	A	2329	SER	20
1	A	2281	ALA	20
2	B	991	GLY	20
2	B	990	VAL	20

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	69/69 (100%)	61±2 (89±3%)	8±2 (11±3%)	12	56
2	B	9/19 (47%)	6±1 (64±9%)	3±1 (36±9%)	1	9
3	C	5/41 (12%)	4±1 (80±11%)	1±1 (20±11%)	5	36
All	All	1660/2580 (64%)	1423 (86%)	237 (14%)	8	48

5 of 37 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	2279	SER	20
2	B	993	PHE	20
2	B	992	PHE	18
1	A	2273	ILE	18
3	C	748	LYS	17

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

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 69% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: 2mtp_cs.str

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	1430
Number of shifts mapped to atoms	1430
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	149

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	142	-0.18 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	127	-0.21 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	133	0.00 ± 0.00	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 69%, i.e. 884 atoms were assigned a chemical shift out of a possible 1278. 12 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	403/534 (75%)	211/212 (100%)	100/220 (45%)	92/102 (90%)
Sidechain	453/630 (72%)	274/372 (74%)	179/230 (78%)	0/28 (0%)

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	Total	**¹H**	**¹³C**	**¹⁵N**
Aromatic	28/114 (25%)	27/62 (44%)	1/50 (2%)	0/2 (0%)
Overall	884/1278 (69%)	512/646 (79%)	280/500 (56%)	92/132 (70%)

7.1.4   Statistically unusual chemical shifts ⓘ

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	2321	PHE	CE2	51.05	136.81 − 124.71	-65.9
1	A	2313	GLU	N	17.84	138.24 − 103.14	-29.3
1	A	2247	GLY	N	12.01	129.07 − 90.27	-25.2
1	A	2279	SER	N	26.47	134.24 − 98.34	-25.0
1	A	2319	SER	N	29.28	134.24 − 98.34	-24.2
3	C	761	GLY	N	17.20	129.07 − 90.27	-23.8
1	A	2301	GLU	N	37.06	138.24 − 103.14	-23.8
1	A	2267	GLY	N	17.46	129.07 − 90.27	-23.8
1	A	2270	GLY	N	17.79	129.07 − 90.27	-23.7
1	A	2265	GLU	N	37.59	138.24 − 103.14	-23.7
1	A	2244	GLY	N	18.65	129.07 − 90.27	-23.5
1	A	2303	GLY	N	19.32	129.07 − 90.27	-23.3
1	A	2250	ARG	N	35.91	139.40 − 102.20	-22.8
1	A	2260	SER	N	35.00	134.24 − 98.34	-22.6
1	A	2237	GLY	N	22.00	129.07 − 90.27	-22.6
1	A	2254	GLY	N	22.89	129.07 − 90.27	-22.4
1	A	2239	HIS	N	29.47	139.70 − 99.40	-22.4
1	A	2258	GLU	N	42.47	138.24 − 103.14	-22.3
1	A	2291	GLY	N	23.41	129.07 − 90.27	-22.2
1	A	2236	GLY	N	23.65	129.07 − 90.27	-22.2
1	A	2269	GLY	N	24.73	129.07 − 90.27	-21.9
1	A	2327	SER	N	37.84	134.24 − 98.34	-21.9
1	A	2318	ASP	N	35.40	140.24 − 101.14	-21.8
1	A	2249	GLU	N	44.26	138.24 − 103.14	-21.8
1	A	2300	GLN	N	41.20	138.01 − 101.71	-21.7
1	A	2314	GLU	N	45.32	138.24 − 103.14	-21.5
1	A	2329	SER	N	39.93	134.24 − 98.34	-21.3
1	A	2292	SER	N	40.26	134.24 − 98.34	-21.2
3	C	752	SER	N	40.29	134.24 − 98.34	-21.2
1	A	2248	LEU	N	37.83	141.70 − 102.00	-21.2
1	A	2306	GLU	N	46.48	138.24 − 103.14	-21.1
1	A	2266	ALA	N	47.76	141.07 − 105.37	-21.1

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	2251	ALA	N	47.79	141.07 − 105.37	-21.1
1	A	2240	LYS	N	41.60	140.01 − 102.11	-21.0
1	A	2252	GLU	N	47.30	138.24 − 103.14	-20.9
3	C	736	ARG	N	43.35	139.40 − 102.20	-20.8
3	C	743	ASN	N	35.10	139.12 − 98.82	-20.8
1	A	2290	ASP	N	39.77	140.24 − 101.14	-20.7
3	C	732	GLU	N	48.46	138.24 − 103.14	-20.6
3	C	726	GLU	N	48.65	138.24 − 103.14	-20.5
3	C	738	LYS	N	43.35	140.01 − 102.11	-20.5
1	A	2268	ALA	N	50.07	141.07 − 105.37	-20.5
1	A	2245	GLY	N	30.39	129.07 − 90.27	-20.4
1	A	2238	ALA	N	50.29	141.07 − 105.37	-20.4
3	C	731	GLU	N	49.24	138.24 − 103.14	-20.4
1	A	2277	GLY	N	30.98	129.07 − 90.27	-20.3
1	A	2259	PHE	N	36.48	141.27 − 99.77	-20.3
3	C	733	GLU	N	49.96	138.24 − 103.14	-20.2
3	C	729	LYS	N	45.31	140.01 − 102.11	-20.0
1	A	2282	GLU	N	50.59	138.24 − 103.14	-20.0
1	A	2294	GLY	N	32.30	129.07 − 90.27	-19.9
1	A	2289	LYS	N	45.71	140.01 − 102.11	-19.9
3	C	749	GLU	N	51.60	138.24 − 103.14	-19.7
3	C	734	ARG	N	47.85	139.40 − 102.20	-19.6
1	A	2280	LYS	N	46.78	140.01 − 102.11	-19.6
1	A	2286	GLU	N	52.23	138.24 − 103.14	-19.5
3	C	735	ALA	N	53.95	141.07 − 105.37	-19.4
1	A	2243	ALA	N	54.00	141.07 − 105.37	-19.4
1	A	2264	ARG	N	49.34	139.40 − 102.20	-19.2
3	C	746	LEU	N	45.76	141.70 − 102.00	-19.2
1	A	2304	ASP	N	46.08	140.24 − 101.14	-19.1
3	C	737	ALA	N	55.49	141.07 − 105.37	-19.0
3	C	724	ARG	N	50.63	139.40 − 102.20	-18.9
1	A	2272	ALA	N	56.20	141.07 − 105.37	-18.8
3	C	751	THR	N	26.10	139.35 − 91.55	-18.7
1	A	2297	TYR	N	41.14	141.99 − 99.29	-18.6
1	A	2316	ILE	N	41.20	143.11 − 99.91	-18.6
3	C	728	ALA	N	57.03	141.07 − 105.37	-18.5
1	A	2242	ARG	N	51.90	139.40 − 102.20	-18.5
1	A	2310	LYS	N	51.59	140.01 − 102.11	-18.3
3	C	725	LYS	N	51.71	140.01 − 102.11	-18.3
1	A	2308	SER	N	50.88	134.24 − 98.34	-18.2
3	C	723	ASP	N	49.65	140.24 − 101.14	-18.2
3	C	744	ASN	N	45.76	139.12 − 98.82	-18.2

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	2330	GLY	N	39.48	129.07 – 90.27	-18.1
1	A	2281	ALA	N	58.65	141.07 – 105.37	-18.1
3	C	742	ALA	N	58.82	141.07 – 105.37	-18.0
3	C	741	THR	N	29.61	139.35 – 91.55	-18.0
3	C	740	ASP	N	50.85	140.24 – 101.14	-17.9
1	A	2284	SER	N	52.20	134.24 – 98.34	-17.9
3	C	739	TRP	N	47.20	142.48 – 100.78	-17.8
1	A	2288	ARG	N	54.62	139.40 – 102.20	-17.8
3	C	716	LYS	N	53.66	140.01 – 102.11	-17.8
3	C	717	LYS	N	53.77	140.01 – 102.11	-17.8
1	A	2276	GLU	N	58.49	138.24 – 103.14	-17.7
3	C	727	PHE	N	47.07	141.27 – 99.77	-17.7
1	A	2253	ALA	N	60.10	141.07 – 105.37	-17.7
1	A	2296	ALA	N	60.10	141.07 – 105.37	-17.7
1	A	2261	ILE	N	45.26	143.11 – 99.91	-17.6
3	C	747	TYR	N	45.30	141.99 – 99.29	-17.6
3	C	750	ALA	N	60.48	141.07 – 105.37	-17.6
3	C	730	PHE	N	47.72	141.27 – 99.77	-17.5
3	C	748	LYS	N	54.75	140.01 – 102.11	-17.5
1	A	2298	VAL	N	41.09	144.09 – 98.19	-17.4
1	A	2321	PHE	N	48.97	141.27 – 99.77	-17.2
3	C	756	ASN	N	49.59	139.12 – 98.82	-17.2
1	A	2271	LEU	N	53.76	141.70 – 102.00	-17.2
1	A	2285	PHE	N	49.50	141.27 – 99.77	-17.1
3	C	718	LYS	N	56.29	140.01 – 102.11	-17.1
1	A	2311	PHE	N	49.73	141.27 – 99.77	-17.1
3	C	755	THR	N	33.93	139.35 – 91.55	-17.1
1	A	2293	CYS	N	41.57	143.21 – 97.11	-17.0
3	C	753	THR	N	34.07	139.35 – 91.55	-17.0
1	A	2274	ALA	N	62.57	141.07 – 105.37	-17.0
1	A	2263	THR	N	34.39	139.35 – 91.55	-17.0
1	A	2315	HIS	N	51.59	139.70 – 99.40	-16.9
3	C	760	ARG	N	58.14	139.40 – 102.20	-16.8
3	C	757	ILE	N	49.44	143.11 – 99.91	-16.7
3	C	754	PHE	N	51.97	141.27 – 99.77	-16.5
1	A	2305	TYR	N	50.29	141.99 – 99.29	-16.5
3	C	722	HIS	N	54.39	139.70 – 99.40	-16.2
1	A	2299	VAL	N	47.91	144.09 – 98.19	-16.0
1	A	2275	VAL	N	48.20	144.09 – 98.19	-15.9
1	A	2287	ASP	N	58.65	140.24 – 101.14	-15.9
1	A	2273	ILE	N	53.38	143.11 – 99.91	-15.8
1	A	2257	ALA	N	67.07	141.07 – 105.37	-15.7

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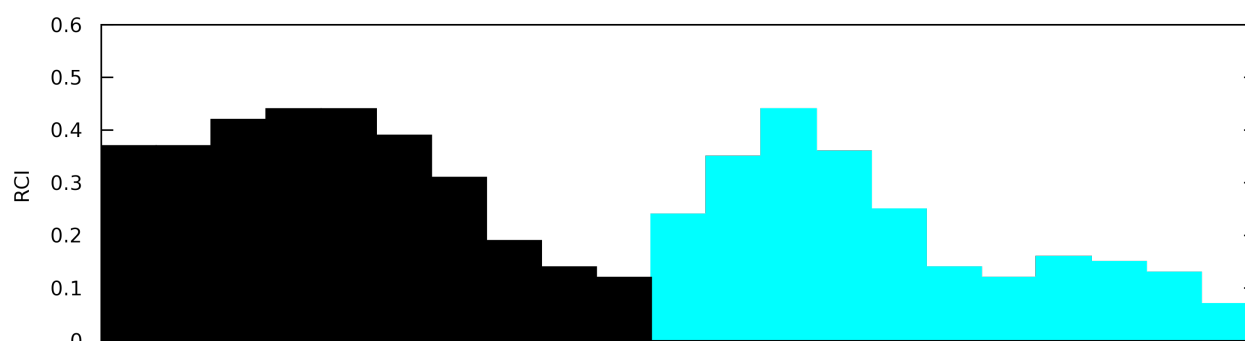| Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
3	C	762	THR	N	41.00	139.35 − 91.55	-15.6
3	C	758	THR	N	41.13	139.35 − 91.55	-15.5
1	A	2326	ALA	N	67.77	141.07 − 105.37	-15.5
3	C	721	ILE	N	54.59	143.11 − 99.91	-15.5
1	A	2255	VAL	N	51.02	144.09 − 98.19	-15.3
3	C	719	ILE	N	55.91	143.11 − 99.91	-15.2
3	C	759	TYR	N	56.19	141.99 − 99.29	-15.1
1	A	2241	VAL	N	51.95	144.09 − 98.19	-15.1
1	A	2283	ILE	N	57.63	143.11 − 99.91	-14.8
3	C	720	THR	N	45.51	139.35 − 91.55	-14.6
1	A	2295	VAL	N	54.21	144.09 − 98.19	-14.6
1	A	2262	TRP	N	61.30	142.48 − 100.78	-14.5
1	A	2309	VAL	N	54.87	144.09 − 98.19	-14.4
1	A	2312	ASN	N	60.81	139.12 − 98.82	-14.4
1	A	2322	VAL	N	55.13	144.09 − 98.19	-14.4
1	A	2325	VAL	N	57.87	144.09 − 98.19	-13.8
3	C	738	LYS	CD	43.08	34.86 − 23.06	12.0
3	C	729	LYS	CD	43.08	34.86 − 23.06	12.0
1	A	2307	VAL	N	66.60	144.09 − 98.19	-11.9
1	A	2323	VAL	N	68.80	144.09 − 98.19	-11.4
1	A	2273	ILE	CG2	29.60	24.63 − 10.43	8.5
1	A	2278	PRO	CD	43.01	55.31 − 45.41	-7.4
1	A	2264	ARG	CD	49.65	47.57 − 38.77	7.4
1	A	2283	ILE	CG2	27.81	24.63 − 10.43	7.2
1	A	2261	ILE	CG2	27.81	24.63 − 10.43	7.2
1	A	2273	ILE	CD1	25.14	21.91 − 5.01	6.9
1	A	2310	LYS	CG	32.61	30.67 − 19.17	6.7
3	C	757	ILE	CG2	26.99	24.63 − 10.43	6.7
3	C	721	ILE	CG2	26.99	24.63 − 10.43	6.7
3	C	719	ILE	CG2	26.99	24.63 − 10.43	6.7
3	C	738	LYS	HD2	3.02	2.76 − 0.46	6.1
3	C	729	LYS	HD2	3.02	2.76 − 0.46	6.1
3	C	739	TRP	HE1	7.12	12.85 − 7.35	-5.4

7.1.5   Random Coil Index (RCI) plots ⓘ

The images below report *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:
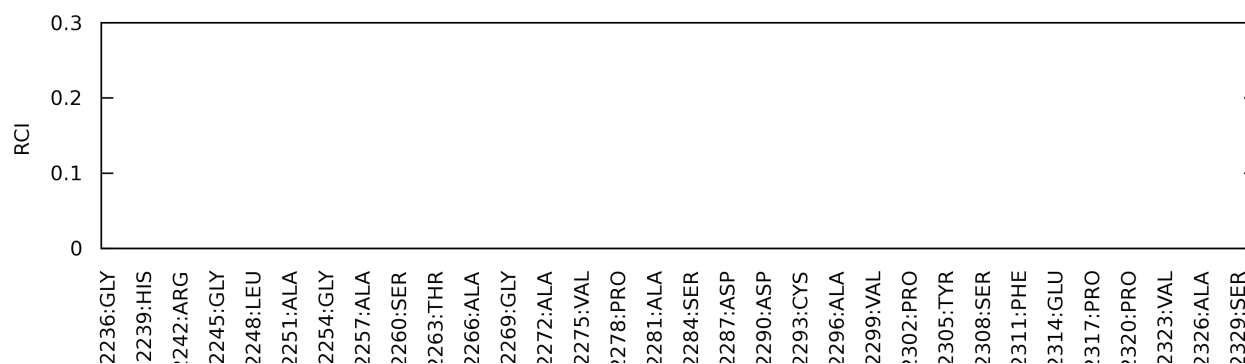
Random coil index (RCI) for chain B:

Random coil index (RCI) for chain C: