wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2BTT
BMRB ID	:	6197
Title	:	NMR Structure of MYO3-SH3 domain from Myosin-typeI from S. cerevisiae
Authors	:	Musi, V.; Birdsall, B.; Pastore, A.
Deposited on	:	2005-06-06

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

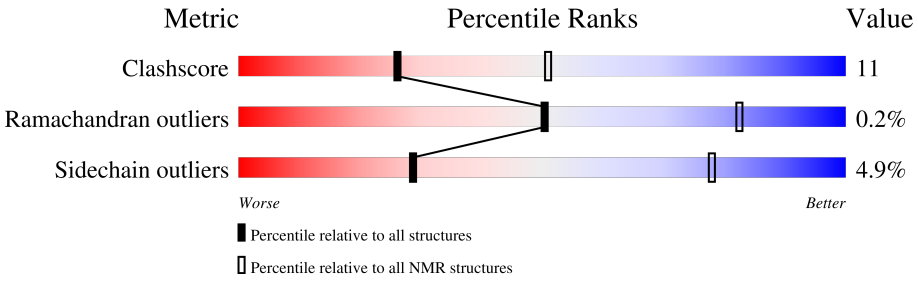
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	69	55% 20% 25%

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1123-A:1132, A:1140-A:1181 (52)	0.32	19

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 868 atoms, of which 332 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MYOSIN-3 ISOFORM.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	69	868	344	332	85	106	1	0

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: MYOSIN-3 ISOFORM

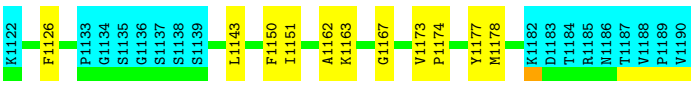
Chain A:

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 19. Colouring as in section 4.1 above.

• Molecule 1: MYOSIN-3 ISOFORM

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA 1.2*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
ARIA	refinement	1.2
XEASY	structure solution	
Sparky	structure solution	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	804
Number of shifts mapped to atoms	613
Number of unparsed shifts	0
Number of shifts with mapping errors	191
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	416	257	401	9±2
All	All	8320	5140	8020	183

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 11.

5 of 54 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1143:LEU:HD12	1:A:1173:VAL:HG21	0.79	1.54	10	14
1:A:1149:VAL:HG12	1:A:1164:LEU:HA	0.65	1.68	6	5
1:A:1130:TYR:HB2	1:A:1177:TYR:CD2	0.64	2.26	9	2
1:A:1174:PRO:HG2	1:A:1177:TYR:CE2	0.64	2.28	4	11
1:A:1132:PHE:CD2	1:A:1173:VAL:HG23	0.62	2.29	8	5

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	52/69 (75%)	49±1 (93±2%)	3±1 (6±2%)	0±0 (0±1%)	50 82
All	All	1040/1380 (75%)	972 (93%)	66 (6%)	2 (0%)	50 82

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	1145	LYS	1
1	A	1175	THR	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	44/59 (75%)	42±1 (95±2%)	2±1 (5±2%)	29 78
All	All	880/1180 (75%)	837 (95%)	43 (5%)	29 78

5 of 14 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	1178	MET	10
1	A	1141	LEU	9
1	A	1170	GLU	8
1	A	1140	GLU	3
1	A	1173	VAL	2

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 monosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	804
Number of shifts mapped to atoms	613
Number of unparsed shifts	0
Number of shifts with mapping errors	191
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. First 5 (of 191) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	GLY	C	174.933	0.05	1
1	A	1122	LYS	HB2	1.745	0.02	2
1	A	1122	LYS	HB3	1.835	0.02	2
1	A	1122	LYS	HD2	1.673	0.02	1
1	A	1122	LYS	HD3	1.673	0.02	1
1	A	1122	LYS	HE2	2.994	0.02	1
1	A	1122	LYS	HE3	2.994	0.02	1
1	A	1122	LYS	HG2	1.414	0.02	1
1	A	1122	LYS	HG3	1.414	0.02	1
1	A	1123	ASP	HB2	2.223	0.02	2
1	A	1123	ASP	HB3	2.748	0.02	2
1	A	1124	PRO	HB2	2.188	0.02	2
1	A	1124	PRO	HB3	2.381	0.02	2
1	A	1124	PRO	HD2	4.181	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1124	PRO	HD3	3.917	0.02	2
1	A	1124	PRO	HG2	2.243	0.02	2
1	A	1124	PRO	HG3	2.418	0.02	2
1	A	1125	LYS	HB2	1.769	0.02	2
1	A	1125	LYS	HB3	1.379	0.02	2
1	A	1125	LYS	HD2	1.474	0.02	2
1	A	1125	LYS	HD3	1.383	0.02	2
1	A	1125	LYS	HE2	2.667	0.02	2
1	A	1125	LYS	HE3	2.846	0.02	2
1	A	1125	LYS	HG2	1.606	0.02	2
1	A	1125	LYS	HG3	0.816	0.02	2
1	A	1126	PHE	HB2	2.578	0.02	2
1	A	1126	PHE	HB3	2.746	0.02	2
1	A	1127	GLU	HB2	1.913	0.02	2
1	A	1127	GLU	HB3	1.812	0.02	2
1	A	1127	GLU	HG2	1.968	0.02	2
1	A	1127	GLU	HG3	1.979	0.02	2
1	A	1130	TYR	HB2	1.771	0.02	1
1	A	1130	TYR	HB3	1.771	0.02	1
1	A	1131	ASP	HB2	2.652	0.02	2
1	A	1131	ASP	HB3	2.727	0.02	2
1	A	1132	PHE	HB2	3.124	0.02	2
1	A	1132	PHE	HB3	3.28	0.02	2
1	A	1133	PRO	HB2	2.283	0.02	2
1	A	1133	PRO	HB3	1.965	0.02	2
1	A	1133	PRO	HD2	3.997	0.02	2
1	A	1133	PRO	HD3	3.595	0.02	2
1	A	1133	PRO	HG2	2.123	0.02	1
1	A	1133	PRO	HG3	2.123	0.02	1
1	A	1135	SER	HB2	3.915	0.02	2
1	A	1135	SER	HB3	4.105	0.02	2
1	A	1137	SER	HB2	3.913	0.02	2
1	A	1137	SER	HB3	3.613	0.02	2
1	A	1138	SER	HB2	4.032	0.02	2
1	A	1138	SER	HB3	3.992	0.02	2
1	A	1139	SER	HB2	3.866	0.02	2
1	A	1139	SER	HB3	3.909	0.02	2
1	A	1140	GLU	HB2	2.253	0.02	2
1	A	1140	GLU	HB3	2.321	0.02	2
1	A	1140	GLU	HG2	2.463	0.02	2
1	A	1140	GLU	HG3	2.49	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1141	LEU	HB2	0.613	0.02	2
1	A	1141	LEU	HB3	1.903	0.02	2
1	A	1142	PRO	HB2	1.728	0.02	2
1	A	1142	PRO	HB3	2.183	0.02	2
1	A	1142	PRO	HD2	3.929	0.02	2
1	A	1142	PRO	HD3	3.575	0.02	2
1	A	1142	PRO	HG2	2.035	0.02	2
1	A	1142	PRO	HG3	2.178	0.02	2
1	A	1143	LEU	HB2	1.577	0.02	2
1	A	1143	LEU	HB3	1.799	0.02	2
1	A	1144	LYS	HB2	1.735	0.02	2
1	A	1144	LYS	HB3	1.754	0.02	2
1	A	1144	LYS	HD2	1.718	0.02	2
1	A	1144	LYS	HD3	1.705	0.02	2
1	A	1144	LYS	HE2	3.044	0.02	1
1	A	1144	LYS	HE3	3.044	0.02	1
1	A	1144	LYS	HG2	1.464	0.02	2
1	A	1144	LYS	HG3	1.469	0.02	2
1	A	1145	LYS	HB2	1.603	0.02	2
1	A	1145	LYS	HB3	1.486	0.02	2
1	A	1145	LYS	HD2	1.491	0.02	1
1	A	1145	LYS	HD3	1.491	0.02	1
1	A	1145	LYS	HE2	2.923	0.02	2
1	A	1145	LYS	HE3	2.91	0.02	2
1	A	1145	LYS	HG2	1.133	0.02	2
1	A	1145	LYS	HG3	1.071	0.02	2
1	A	1147	ASP	HB2	2.466	0.02	2
1	A	1147	ASP	HB3	2.9	0.02	2
1	A	1148	ILE	HG12	1.526	0.02	2
1	A	1148	ILE	HG13	0.682	0.02	2
1	A	1150	PHE	HB2	3.099	0.02	2
1	A	1150	PHE	HB3	2.842	0.02	2
1	A	1151	ILE	HG12	0.983	0.02	1
1	A	1151	ILE	HG13	0.896	0.02	1
1	A	1152	SER	HB2	3.737	0.02	2
1	A	1152	SER	HB3	3.719	0.02	2
1	A	1153	ARG	HB2	1.998	0.02	2
1	A	1153	ARG	HB3	1.853	0.02	2
1	A	1153	ARG	HD2	3.289	0.02	2
1	A	1153	ARG	HD3	3.22	0.02	2
1	A	1153	ARG	HG2	1.585	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1153	ARG	HG3	1.5	0.02	2
1	A	1154	ASP	HB2	2.756	0.02	2
1	A	1154	ASP	HB3	2.53	0.02	2
1	A	1155	GLU	HB2	2.348	0.02	2
1	A	1155	GLU	HB3	2.176	0.02	2
1	A	1155	GLU	HG2	2.464	0.02	2
1	A	1155	GLU	HG3	2.354	0.02	2
1	A	1156	PRO	HB2	2.41	0.02	2
1	A	1156	PRO	HB3	2.118	0.02	2
1	A	1156	PRO	HD2	3.904	0.02	2
1	A	1156	PRO	HD3	4.091	0.02	2
1	A	1156	PRO	HG2	1.931	0.02	2
1	A	1156	PRO	HG3	2.115	0.02	2
1	A	1157	SER	HB2	3.841	0.02	2
1	A	1157	SER	HB3	3.784	0.02	2
1	A	1159	TRP	HB2	3.452	0.02	2
1	A	1159	TRP	HB3	2.619	0.02	2
1	A	1160	SER	HB2	3.949	0.02	2
1	A	1160	SER	HB3	3.254	0.02	2
1	A	1161	LEU	HB2	1.397	0.02	2
1	A	1161	LEU	HB3	-0.368	0.02	2
1	A	1163	LYS	HB2	1.881	0.02	2
1	A	1163	LYS	HB3	1.795	0.02	2
1	A	1163	LYS	HD2	1.646	0.02	2
1	A	1163	LYS	HD3	1.648	0.02	2
1	A	1163	LYS	HE2	2.856	0.02	2
1	A	1163	LYS	HE3	2.849	0.02	2
1	A	1163	LYS	HG2	1.461	0.02	2
1	A	1163	LYS	HG3	1.819	0.02	2
1	A	1164	LEU	HB2	1.897	0.02	2
1	A	1164	LEU	HB3	1.772	0.02	2
1	A	1165	LEU	HB2	1.477	0.02	2
1	A	1165	LEU	HB3	1.607	0.02	2
1	A	1166	ASP	HB2	3.166	0.02	2
1	A	1166	ASP	HB3	2.649	0.02	2
1	A	1168	SER	HB2	3.883	0.02	2
1	A	1168	SER	HB3	3.799	0.02	2
1	A	1169	LYS	HB2	1.742	0.02	2
1	A	1169	LYS	HB3	1.666	0.02	2
1	A	1169	LYS	HD2	1.73	0.02	2
1	A	1169	LYS	HD3	1.724	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1169	LYS	HE2	3.046	0.02	1
1	A	1169	LYS	HE3	3.046	0.02	1
1	A	1169	LYS	HG2	1.497	0.02	2
1	A	1169	LYS	HG3	1.475	0.02	2
1	A	1170	GLU	HB2	1.92	0.02	2
1	A	1170	GLU	HB3	1.928	0.02	2
1	A	1170	GLU	HG2	2.022	0.02	2
1	A	1170	GLU	HG3	2.017	0.02	2
1	A	1172	TRP	HB2	3.346	0.02	2
1	A	1172	TRP	HB3	2.827	0.02	2
1	A	1174	PRO	HB2	1.017	0.02	1
1	A	1174	PRO	HB3	1.017	0.02	1
1	A	1174	PRO	HD2	1.983	0.02	2
1	A	1174	PRO	HD3	1.799	0.02	2
1	A	1174	PRO	HG2	0.444	0.02	2
1	A	1174	PRO	HG3	0.242	0.02	2
1	A	1177	TYR	HB2	3.161	0.02	2
1	A	1177	TYR	HB3	3.34	0.02	2
1	A	1178	MET	HB2	2.179	0.02	2
1	A	1178	MET	HB3	1.726	0.02	2
1	A	1178	MET	HG2	2.578	0.02	1
1	A	1178	MET	HG3	2.578	0.02	1
1	A	1180	PRO	HB2	2.097	0.02	2
1	A	1180	PRO	HB3	1.673	0.02	2
1	A	1180	PRO	HD2	4.101	0.02	2
1	A	1180	PRO	HD3	3.799	0.02	2
1	A	1180	PRO	HG2	1.932	0.02	2
1	A	1180	PRO	HG3	2.093	0.02	2
1	A	1181	TYR	HB2	2.515	0.02	2
1	A	1181	TYR	HB3	2.495	0.02	2
1	A	1182	LYS	HB2	1.494	0.02	2
1	A	1182	LYS	HB3	1.588	0.02	2
1	A	1182	LYS	HD2	1.566	0.02	2
1	A	1182	LYS	HD3	1.567	0.02	2
1	A	1182	LYS	HE2	2.884	0.02	1
1	A	1182	LYS	HE3	2.884	0.02	1
1	A	1182	LYS	HG2	1.156	0.02	2
1	A	1182	LYS	HG3	1.222	0.02	2
1	A	1183	ASP	HB2	2.739	0.02	2
1	A	1183	ASP	HB3	2.526	0.02	2
1	A	1185	ARG	HB2	1.858	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1185	ARG	HB3	1.81	0.02	2
1	A	1185	ARG	HD2	3.204	0.02	2
1	A	1185	ARG	HD3	3.196	0.02	2
1	A	1185	ARG	HG2	1.647	0.02	2
1	A	1185	ARG	HG3	1.625	0.02	2
1	A	1186	ASN	HB2	2.862	0.02	2
1	A	1186	ASN	HB3	2.762	0.02	2
1	A	1189	PRO	HB2	1.953	0.02	2
1	A	1189	PRO	HB3	2.276	0.02	2
1	A	1189	PRO	HD2	3.687	0.02	2
1	A	1189	PRO	HD3	3.884	0.02	2
1	A	1189	PRO	HG2	1.983	0.02	2
1	A	1189	PRO	HG3	2.053	0.02	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	69	0.07 ± 0.19	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	62	-0.11 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	55	-0.04 ± 0.11	None needed (< 0.5 ppm)
^{15}N	56	0.11 ± 0.35	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 91%, i.e. 631 atoms were assigned a chemical shift out of a possible 696. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	242/254 (95%)	101/103 (98%)	96/104 (92%)	45/47 (96%)
Sidechain	335/361 (93%)	230/235 (98%)	105/118 (89%)	0/8 (0%)
Aromatic	54/81 (67%)	28/39 (72%)	24/40 (60%)	2/2 (100%)
Overall	631/696 (91%)	359/377 (95%)	225/262 (86%)	47/57 (82%)

7.1.4 Statistically unusual chemical shifts (i)

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

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	1161	LEU	HB3	-0.37	-0.26 – 3.31	-5.3
1	A	1174	PRO	HG3	0.24	0.33 – 3.48	-5.3

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: