



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 06:34 PM BST

PDB ID : 2A9H
Title : NMR structural studies of a potassium channel / charybdotoxin complex
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Deposited on : 2005-07-11

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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

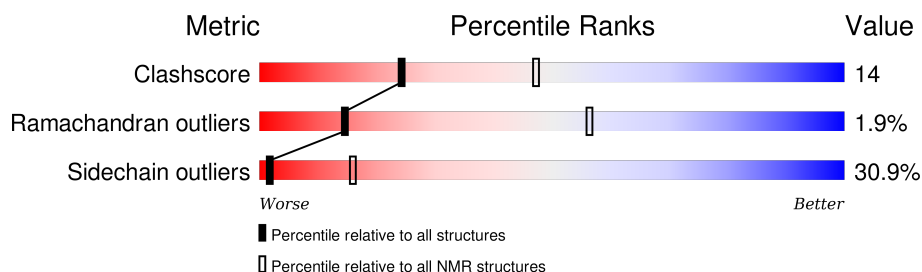
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	155	
1	B	155	
1	C	155	
1	D	155	
2	E	37	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6381 atoms, of which 3202 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Voltage-gated potassium channel.

Mol	Chain	Residues	Atoms						Trace
1	A	97	Total	C	H	N	O	S	0
			1451	478	730	117	124	2	
1	B	97	Total	C	H	N	O	S	0
			1451	478	730	117	124	2	
1	C	97	Total	C	H	N	O	S	0
			1451	478	730	117	124	2	
1	D	97	Total	C	H	N	O	S	0
			1451	478	730	117	124	2	

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	CLONING ARTIFACT	UNP P0A334
A	-21	SER	-	CLONING ARTIFACT	UNP P0A334
A	-20	GLY	-	CLONING ARTIFACT	UNP P0A334
A	-19	SER	-	CLONING ARTIFACT	UNP P0A334
A	-18	HIS	-	EXPRESSION TAG	UNP P0A334
A	-17	HIS	-	EXPRESSION TAG	UNP P0A334
A	-16	HIS	-	EXPRESSION TAG	UNP P0A334
A	-15	HIS	-	EXPRESSION TAG	UNP P0A334
A	-14	HIS	-	EXPRESSION TAG	UNP P0A334
A	-13	HIS	-	EXPRESSION TAG	UNP P0A334
A	-12	SER	-	CLONING ARTIFACT	UNP P0A334
A	-11	SER	-	CLONING ARTIFACT	UNP P0A334
A	-10	GLY	-	CLONING ARTIFACT	UNP P0A334
A	-9	ILE	-	CLONING ARTIFACT	UNP P0A334
A	-8	GLU	-	CLONING ARTIFACT	UNP P0A334
A	-7	GLY	-	CLONING ARTIFACT	UNP P0A334
A	-6	ARG	-	CLONING ARTIFACT	UNP P0A334
A	-5	GLY	-	CLONING ARTIFACT	UNP P0A334
A	-4	ARG	-	CLONING ARTIFACT	UNP P0A334
A	-3	LEU	-	CLONING ARTIFACT	UNP P0A334
A	-2	ILE	-	CLONING ARTIFACT	UNP P0A334
A	-1	LYS	-	CLONING ARTIFACT	UNP P0A334
A	0	HIS	-	CLONING ARTIFACT	UNP P0A334
A	58	ALA	GLN	ENGINEERED	UNP P0A334
A	61	SER	THR	ENGINEERED	UNP P0A334

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Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ASP	ARG	ENGINEERED	UNP P0A334
A	90	CYS	LEU	ENGINEERED	UNP P0A334
A	103	TYR	PHE	ENGINEERED	UNP P0A334
A	107	PHE	THR	ENGINEERED	UNP P0A334
A	110	VAL	LEU	ENGINEERED	UNP P0A334
B	-22	MET	-	CLONING ARTIFACT	UNP P0A334
B	-21	SER	-	CLONING ARTIFACT	UNP P0A334
B	-20	GLY	-	CLONING ARTIFACT	UNP P0A334
B	-19	SER	-	CLONING ARTIFACT	UNP P0A334
B	-18	HIS	-	EXPRESSION TAG	UNP P0A334
B	-17	HIS	-	EXPRESSION TAG	UNP P0A334
B	-16	HIS	-	EXPRESSION TAG	UNP P0A334
B	-15	HIS	-	EXPRESSION TAG	UNP P0A334
B	-14	HIS	-	EXPRESSION TAG	UNP P0A334
B	-13	HIS	-	EXPRESSION TAG	UNP P0A334
B	-12	SER	-	CLONING ARTIFACT	UNP P0A334
B	-11	SER	-	CLONING ARTIFACT	UNP P0A334
B	-10	GLY	-	CLONING ARTIFACT	UNP P0A334
B	-9	ILE	-	CLONING ARTIFACT	UNP P0A334
B	-8	GLU	-	CLONING ARTIFACT	UNP P0A334
B	-7	GLY	-	CLONING ARTIFACT	UNP P0A334
B	-6	ARG	-	CLONING ARTIFACT	UNP P0A334
B	-5	GLY	-	CLONING ARTIFACT	UNP P0A334
B	-4	ARG	-	CLONING ARTIFACT	UNP P0A334
B	-3	LEU	-	CLONING ARTIFACT	UNP P0A334
B	-2	ILE	-	CLONING ARTIFACT	UNP P0A334
B	-1	LYS	-	CLONING ARTIFACT	UNP P0A334
B	0	HIS	-	CLONING ARTIFACT	UNP P0A334
B	58	ALA	GLN	ENGINEERED	UNP P0A334
B	61	SER	THR	ENGINEERED	UNP P0A334
B	64	ASP	ARG	ENGINEERED	UNP P0A334
B	90	CYS	LEU	ENGINEERED	UNP P0A334
B	103	TYR	PHE	ENGINEERED	UNP P0A334
B	107	PHE	THR	ENGINEERED	UNP P0A334
B	110	VAL	LEU	ENGINEERED	UNP P0A334
C	-22	MET	-	CLONING ARTIFACT	UNP P0A334
C	-21	SER	-	CLONING ARTIFACT	UNP P0A334
C	-20	GLY	-	CLONING ARTIFACT	UNP P0A334
C	-19	SER	-	CLONING ARTIFACT	UNP P0A334
C	-18	HIS	-	EXPRESSION TAG	UNP P0A334
C	-17	HIS	-	EXPRESSION TAG	UNP P0A334
C	-16	HIS	-	EXPRESSION TAG	UNP P0A334

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	HIS	-	EXPRESSION TAG	UNP P0A334
C	-14	HIS	-	EXPRESSION TAG	UNP P0A334
C	-13	HIS	-	EXPRESSION TAG	UNP P0A334
C	-12	SER	-	CLONING ARTIFACT	UNP P0A334
C	-11	SER	-	CLONING ARTIFACT	UNP P0A334
C	-10	GLY	-	CLONING ARTIFACT	UNP P0A334
C	-9	ILE	-	CLONING ARTIFACT	UNP P0A334
C	-8	GLU	-	CLONING ARTIFACT	UNP P0A334
C	-7	GLY	-	CLONING ARTIFACT	UNP P0A334
C	-6	ARG	-	CLONING ARTIFACT	UNP P0A334
C	-5	GLY	-	CLONING ARTIFACT	UNP P0A334
C	-4	ARG	-	CLONING ARTIFACT	UNP P0A334
C	-3	LEU	-	CLONING ARTIFACT	UNP P0A334
C	-2	ILE	-	CLONING ARTIFACT	UNP P0A334
C	-1	LYS	-	CLONING ARTIFACT	UNP P0A334
C	0	HIS	-	CLONING ARTIFACT	UNP P0A334
C	58	ALA	GLN	ENGINEERED	UNP P0A334
C	61	SER	THR	ENGINEERED	UNP P0A334
C	64	ASP	ARG	ENGINEERED	UNP P0A334
C	90	CYS	LEU	ENGINEERED	UNP P0A334
C	103	TYR	PHE	ENGINEERED	UNP P0A334
C	107	PHE	THR	ENGINEERED	UNP P0A334
C	110	VAL	LEU	ENGINEERED	UNP P0A334
D	-22	MET	-	CLONING ARTIFACT	UNP P0A334
D	-21	SER	-	CLONING ARTIFACT	UNP P0A334
D	-20	GLY	-	CLONING ARTIFACT	UNP P0A334
D	-19	SER	-	CLONING ARTIFACT	UNP P0A334
D	-18	HIS	-	EXPRESSION TAG	UNP P0A334
D	-17	HIS	-	EXPRESSION TAG	UNP P0A334
D	-16	HIS	-	EXPRESSION TAG	UNP P0A334
D	-15	HIS	-	EXPRESSION TAG	UNP P0A334
D	-14	HIS	-	EXPRESSION TAG	UNP P0A334
D	-13	HIS	-	EXPRESSION TAG	UNP P0A334
D	-12	SER	-	CLONING ARTIFACT	UNP P0A334
D	-11	SER	-	CLONING ARTIFACT	UNP P0A334
D	-10	GLY	-	CLONING ARTIFACT	UNP P0A334
D	-9	ILE	-	CLONING ARTIFACT	UNP P0A334
D	-8	GLU	-	CLONING ARTIFACT	UNP P0A334
D	-7	GLY	-	CLONING ARTIFACT	UNP P0A334
D	-6	ARG	-	CLONING ARTIFACT	UNP P0A334
D	-5	GLY	-	CLONING ARTIFACT	UNP P0A334
D	-4	ARG	-	CLONING ARTIFACT	UNP P0A334

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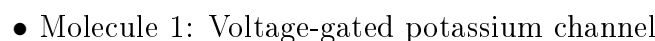
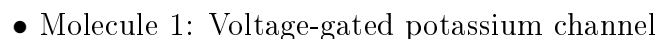
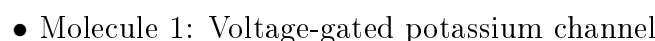
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	LEU	-	CLONING ARTIFACT	UNP P0A334
D	-2	ILE	-	CLONING ARTIFACT	UNP P0A334
D	-1	LYS	-	CLONING ARTIFACT	UNP P0A334
D	0	HIS	-	CLONING ARTIFACT	UNP P0A334
D	58	ALA	GLN	ENGINEERED	UNP P0A334
D	61	SER	THR	ENGINEERED	UNP P0A334
D	64	ASP	ARG	ENGINEERED	UNP P0A334
D	90	CYS	LEU	ENGINEERED	UNP P0A334
D	103	TYR	PHE	ENGINEERED	UNP P0A334
D	107	PHE	THR	ENGINEERED	UNP P0A334
D	110	VAL	LEU	ENGINEERED	UNP P0A334


- Molecule 2 is a protein called charybdotoxin.

Mol	Chain	Residues	Atoms						Trace
2	E	37	Total	C	H	N	O	S	0
			577	176	282	57	55	7	

- Molecule 1: Voltage-gated potassium channel



- Molecule 2: charybdotoxin

Chain E:  46% 54%

Chain	Color	Count
E801	Green	1
F802	Green	1
T803	Green	1
N804	Green	1
V805	Green	1
S806	Green	1
C807	Green	1
T808	Green	1
E812	Green	1
V816	Green	1
R819	Green	1
L820	Green	1
H821	Green	1
N822	Green	1
T823	Green	1
S824	Green	1
R825	Green	1
G826	Green	1
K827	Green	1
C828	Green	1
M829	Green	1
N830	Green	1
K831	Green	1
K832	Green	1
Y836	Green	1
S837	Green	1
E801	Yellow	0
F802	Yellow	0
T803	Yellow	0
N804	Yellow	0
V805	Yellow	0
S806	Yellow	0
C807	Yellow	0
T808	Yellow	0
E812	Yellow	0
V816	Yellow	0
R819	Yellow	0
L820	Yellow	0
H821	Yellow	0
N822	Yellow	0
T823	Yellow	0
S824	Yellow	0
R825	Yellow	0
G826	Yellow	0
K827	Yellow	0
C828	Yellow	0
M829	Yellow	0
N830	Yellow	0
K831	Yellow	0
K832	Yellow	0
Y836	Yellow	0
S837	Yellow	0

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *molecular SIMULATED ANNEALING / dynamics / docking*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
CNS	structure solution	2002
CNS	refinement	2002

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)	BMRB entry 6728
Number of chemical shift lists	1
Total number of shifts	188
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	188
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality

6.1 Standard geometry

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

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	721	730	729	21
1	B	721	730	729	25
1	C	721	730	729	28
1	D	721	730	729	28
2	E	295	282	281	2
All	All	3179	3202	3197	90

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 14.

5 of 90 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:D:57:ALA:HB2	1:D:82:TYR:O	0.77	1.79
1:A:24:LEU:HD22	1:D:117:ARG:HD2	0.69	1.63
1:D:80:ASP:O	1:D:81:LEU:HD23	0.68	1.89
1:A:24:LEU:HD22	1:D:117:ARG:CD	0.67	2.19
1:B:32:ALA:HB1	1:B:102:SER:HA	0.66	1.66

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	95/155 (61%)	78 (82%)	16 (17%)	1 (1%)	23	69
1	B	95/155 (61%)	78 (82%)	15 (16%)	2 (2%)	13	53
1	C	95/155 (61%)	77 (81%)	17 (18%)	1 (1%)	23	69
1	D	95/155 (61%)	76 (80%)	17 (18%)	2 (2%)	13	53
2	E	35/37 (95%)	27 (77%)	6 (17%)	2 (6%)	4	23
All	All	415/657 (63%)	336 (81%)	71 (17%)	8 (2%)	14	56

5 of 8 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	E	825	ARG
1	D	55	PRO
1	B	55	PRO
2	E	822	ASN
1	A	24	LEU

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	69/117 (59%)	49 (71%)	20 (29%)	2	19
1	B	69/117 (59%)	50 (72%)	19 (28%)	2	21
1	C	69/117 (59%)	48 (70%)	21 (30%)	2	17
1	D	69/117 (59%)	49 (71%)	20 (29%)	2	19
2	E	35/35 (100%)	19 (54%)	16 (46%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	311/503 (62%)	215 (69%)	96 (31%)	2 16

5 of 96 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	95	VAL
1	A	49	LEU
1	D	46	LEU
1	A	33	THR
2	E	820	LEU

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PCA	E	801	2	7,8,9	1.12	0 (0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PCA	E	801	2	9,10,12	1.13	0 (0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	E	801	2	-	0,0,11,13	0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

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

7.1 Chemical shift list 1

File name: BMRB entry 6728

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	188
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	188
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. First 5 (of 188) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	95	VAL	HG11	1.07	0.02	2
UNMAPPED	76	VAL	HG11	0.079	0.02	2
UNMAPPED	70	VAL	HG12	1.22	0.02	2
UNMAPPED	73	ALA	CB	18.28	0.2	1
UNMAPPED	105	LEU	CD1	24.299	0.2	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	—
$^{13}\text{C}_\beta$	11	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
¹⁵ N	0	—	—

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 4822. 0 out of 111 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/2096 (0%)	0/836 (0%)	0/848 (0%)	0/412 (0%)
Sidechain	0/2190 (0%)	0/1249 (0%)	0/872 (0%)	0/69 (0%)
Aromatic	0/536 (0%)	0/275 (0%)	0/235 (0%)	0/26 (0%)
Overall	0/4822 (0%)	0/2360 (0%)	0/1955 (0%)	0/507 (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](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.