Chemical Shift Validation Report

November 28, 2022 – 2:50pm EST

Entry ID	:	18857
Title	:	Backbone 1H, 13C,and 15N chemical shift assignments for alpha-synuclein at different pH and temperature
Authors	:	Gergana A. Vandova; Kamil Tamiola; Nur A. Oktaviani; Frans A.A. Mulder
Deposited on	:	2012-11-25

The following versions of software and data were used in the production of this report:

PyNMRSTAR	:	3.3.0
RCI	:	1.1
ShiftChecker	:	1.2
LACS	:	VARLACSVER
AVS	:	VARAVSVER

1 Summary

The biological assembly is a monomer with one Entity.

1.1 Entity information

1.1.1 Entity 1

Type	:	polymer
Polymer type	:	polypeptide(L)
Name	:	alpha_synuclein
Sequence length	:	140
Sequence	:	MDVFMKGLSKAKEGVVAAAE KTKQGVAEAAGKTKEGVLYV GSKTKEGVVHGVATVAEKTK EQVTNVGGAVVTGVTAVAQK TVEGAGSIAAATGFVKKDQL GKNEEGAPQEGILEDMPVDP DNEAYEMPSEEGYQDYEPEA

1.2 Chemical shift list information

There are 33 chemical shift lists reproted. The summary of the chemical shift data is given below

Saveframe name	assigned_chem_shift_list_1
Saveframe ID	1
PH	2.16 pH
Temperature	283 K
Number of shifts	682
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_2
Saveframe ID	2
PH	2.36 pH
Temperature	283 K
Number of shifts	682
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_3
Saveframe ID	3
PH	2.61 pH

Temperature	283 K
Number of shifts	682
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_4
Saveframe ID	4
PH	2.82 pH
Temperature	283 K
Number of shifts	682
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_5
Saveframe ID	5
PH	3.11 pH
Temperature	283 K
Number of shifts	682
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_6
Saveframe ID	6
PH	3.19 pH
Temperature	283 K
Number of shifts	683
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_7
Saveframe ID	7
PH	3.38 pH
Temperature	283 K
Number of shifts	679
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_8
Saveframe ID	8
PH	3.58 pH
Temperature	283 K

Number of shifts	680
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_9
Saveframe ID	9
PH	3.78 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_10
Saveframe ID	10
PH	4.00 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_11
Saveframe ID	11
PH	4.21 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_12
Saveframe ID	12
PH	4.42 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_13
Saveframe ID	13
PH	4.67 pH
Temperature	283 K
Number of shifts	681

Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shif_list_14
Saveframe ID	14
PH	4.87 pH
Temperature	283 K
Number of shifts	547
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_15
Saveframe ID	15
PH	5.02 pH
Temperature	283 K
Number of shifts	682
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_16
Saveframe ID	16
PH	5.21 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_17
Saveframe ID	17
PH	5.42 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_18
Saveframe ID	18
PH	5.57 pH
Temperature	283 K
Number of shifts	682
Number of shift outliers	0

Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_19
Saveframe ID	19
PH	5.71 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_20
Saveframe ID	20
PH	5.85 pH
Temperature	283 K
Number of shifts	682
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_21
Saveframe ID	21
PH	6.09 pH
Temperature	283 K
Number of shifts	681
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_22
Saveframe ID	22
PH	6.34 pH
Temperature	283 K
Number of shifts	592
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_23
Saveframe ID	23
PH	6.55 pH
Temperature	283 K
Number of shifts	592
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_24
Saveframe ID	24
PH	6.74 pH
Temperature	283 K
Number of shifts	680
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_25
Saveframe ID	25
PH	6.94 pH
Temperature	283 K
Number of shifts	680
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_26
Saveframe ID	26
PH	7.10 pH
Temperature	283 K
Number of shifts	679
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_27
Saveframe ID	27
PH	7.34 pH
Temperature	283 K
Number of shifts	677
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_28
Saveframe ID	28
PH	7.51 pH
Temperature	283 K
Number of shifts	677
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_29

Saveframe ID	29
PH	5.87 pH
Temperature	278 K
Number of shifts	561
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_30
Saveframe ID	30
PH	5.87 pH
Temperature	288 K
Number of shifts	560
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_31
Saveframe ID	31
PH	5.87 pH
Temperature	293 K
Number of shifts	550
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_32
Saveframe ID	32
PH	5.87 pH
Temperature	298 K
Number of shifts	546
Number of shift outliers	0
Assignment completeness	37.8%

Saveframe name	assigned_chem_shift_list_33
Saveframe ID	33
PH	5.87 pH
Temperature	303 K
Number of shifts	546
Number of shift outliers	0
Assignment completeness	37.8%

2 Completeness

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	682/708 (96.3%)	279/293 (95.2%)	269/280 (96.1%)	134/135 (99.3%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	682/1724 (39.6%)	279/943 (29.6%)	269/620 (43.4%)	134/161 (83.2%)

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Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
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	Total	^1H	^{13}C	^{15}N
Backbone	681/708 (96.2%)	277/293 (94.5%)	270/280 (96.4%)	134/135 (99.3%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	681/1724 (39.5%)	277/943 (29.4%)	270/620 (43.5%)	134/161 (83.2%)

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	Total	^1H	^{13}C	^{15}N
Backbone	681/708 (96.2%)	277/293 (94.5%)	270/280 (96.4%)	134/135 (99.3%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	681/1724 (39.5%)	277/943 (29.4%)	270/620 (43.5%)	134/161 (83.2%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	681/708 (96.2%)	277/293 (94.5%)	270/280 (96.4%)	134/135 (99.3%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	681/1724 (39.5%)	277/943 (29.4%)	270/620 (43.5%)	134/161 (83.2%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	547/708 (77.3%)	277/293 (94.5%)	270/280 (96.4%)	0/135 (0.0%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	547/1724 (31.7%)	277/943 (29.4%)	270/620 (43.5%)	0/161 (0.0%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	682/708 (96.3%)	278/293 (94.9%)	270/280 (96.4%)	134/135 (99.3%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	682/1724 (39.6%)	278/943 (29.5%)	270/620 (43.5%)	134/161 (83.2%)

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Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	681/1724 (39.5%)	277/943 (29.4%)	270/620 (43.5%)	134/161 (83.2%)

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Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	681/1724 (39.5%)	278/943 (29.5%)	270/620 (43.5%)	133/161 (82.6%)

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	Total	^{1}H	^{13}C	^{15}N
Backbone	592/708 (83.6%)	277/293 (94.5%)	182/280 (65.0%)	133/135 (98.5%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
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Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	679/1724 (39.4%)	277/943 (29.4%)	270/620 (43.5%)	132/161 (82.0%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	677/708 (95.6%)	277/293 (94.5%)	269/280 (96.1%)	131/135 (97.0%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	677/1724 (39.3%)	277/943 (29.4%)	269/620 (43.4%)	131/161 (81.4%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	677/708 (95.6%)	276/293 (94.2%)	270/280 (96.4%)	131/135 (97.0%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	677/1724 (39.3%)	276/943 (29.3%)	270/620 (43.5%)	131/161 (81.4%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	561/708 (79.2%)	217/293 (74.1%)	219/280 (78.2%)	125/135 (92.6%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	561/1724 (32.5%)	217/943 (23.0%)	219/620 (35.3%)	125/161 (77.6%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	560/708 (79.1%)	219/293 (74.7%)	216/280 (77.1%)	125/135 (92.6%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	560/1724 (32.5%)	219/943 (23.2%)	216/620 (34.8%)	125/161 (77.6%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	550/708 (77.7%)	216/293 (73.7%)	211/280 (75.4%)	123/135 (91.1%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	550/1724 (31.9%)	216/943 (22.9%)	211/620 (34.0%)	123/161 (76.4%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	546/708 (77.1%)	213/293 (72.7%)	210/280 (75.0%)	123/135 (91.1%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	546/1724 (31.7%)	213/943 (22.6%)	210/620 (33.9%)	123/161 (76.4%)

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 23 methyl groups (LEU and VAL) were assigned stereospecifically.

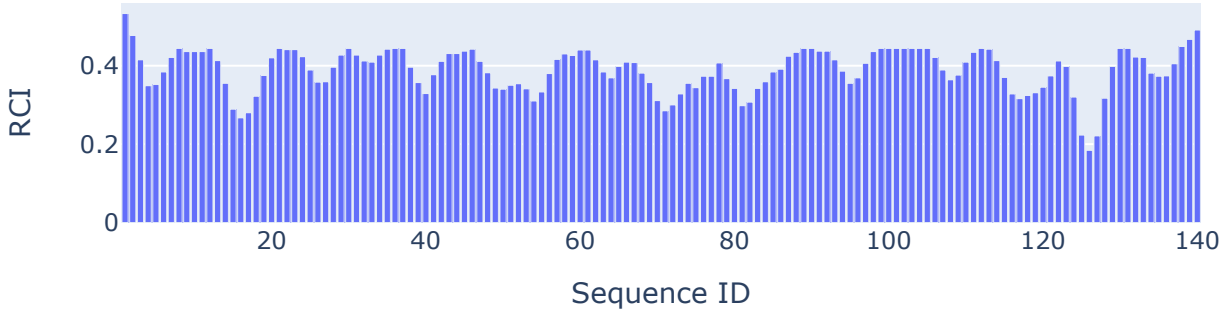
	Total	^{1}H	^{13}C	^{15}N
Backbone	546/708 (77.1%)	213/293 (72.7%)	210/280 (75.0%)	123/135 (91.1%)
Sidechain	0/948 (0.0%)	0/616 (0.0%)	0/308 (0.0%)	0/24 (0.0%)
Aromatic	0/68 (0.0%)	0/34 (0.0%)	0/32 (0.0%)	0/2 (0.0%)
Overall	546/1724 (31.7%)	213/943 (22.6%)	210/620 (33.9%)	123/161 (76.4%)

3 Statistically unusual chemical shifts

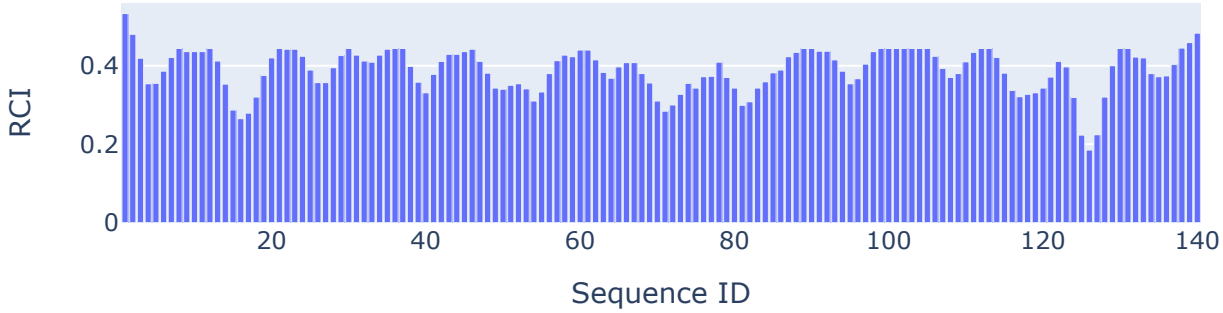
There are no chemical shift outliers.

4 RCI

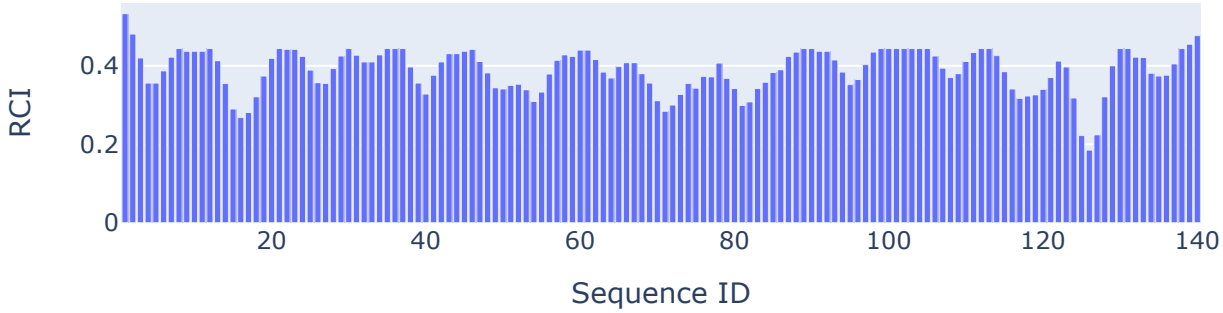
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_1*



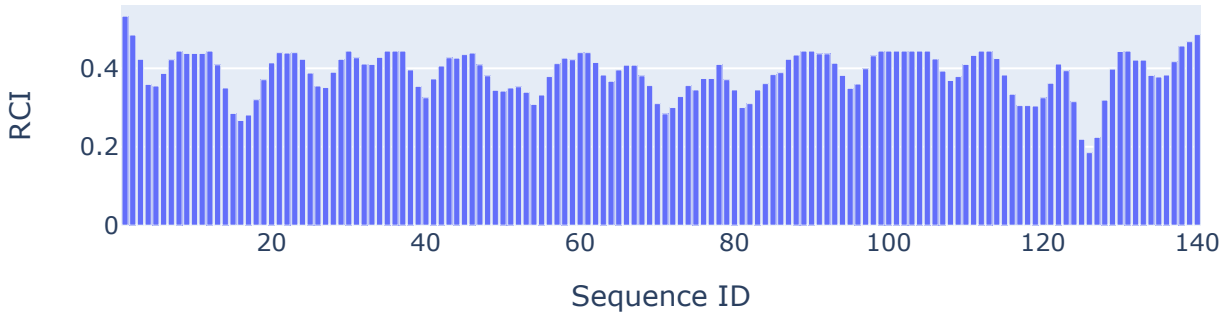
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_2*



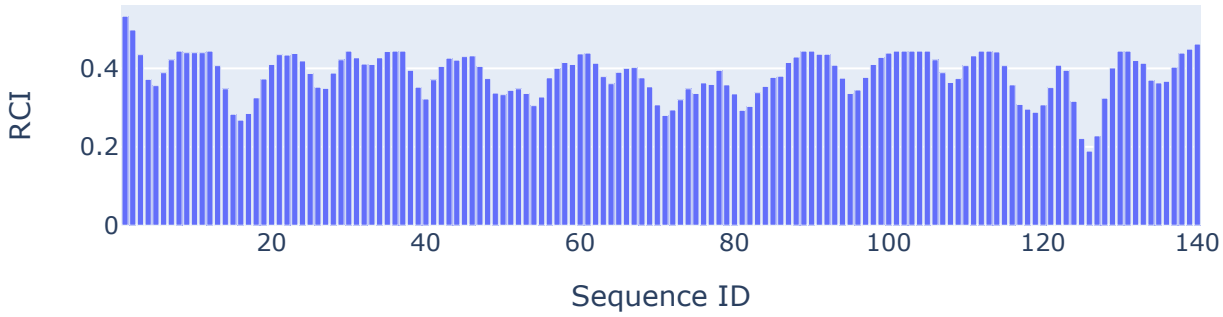
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_3*



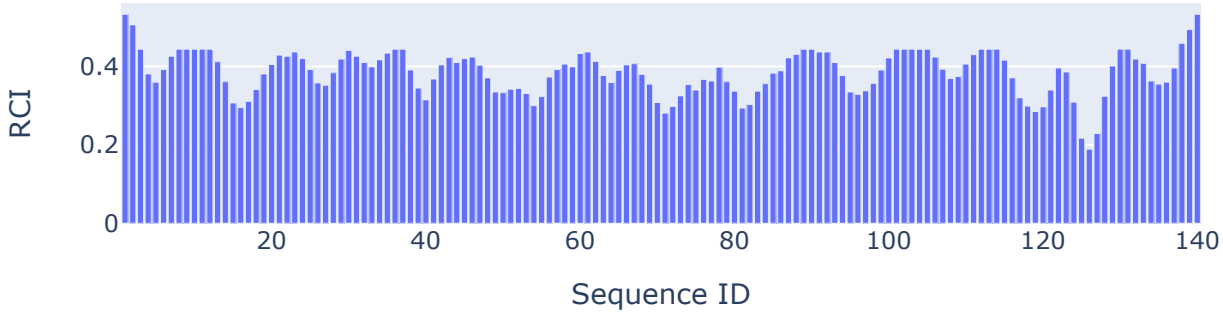
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_4*



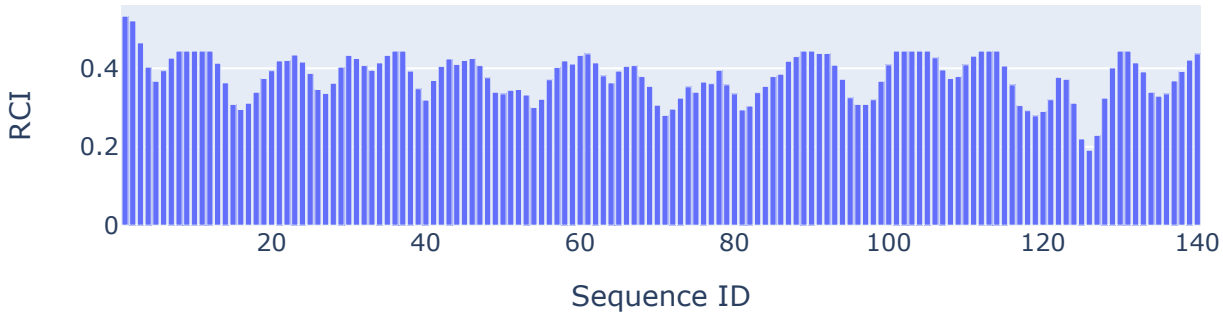
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_5*



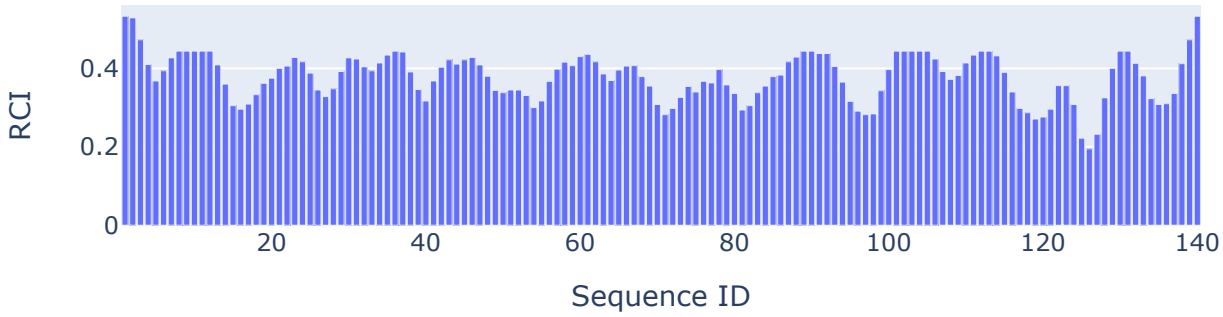
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_6*



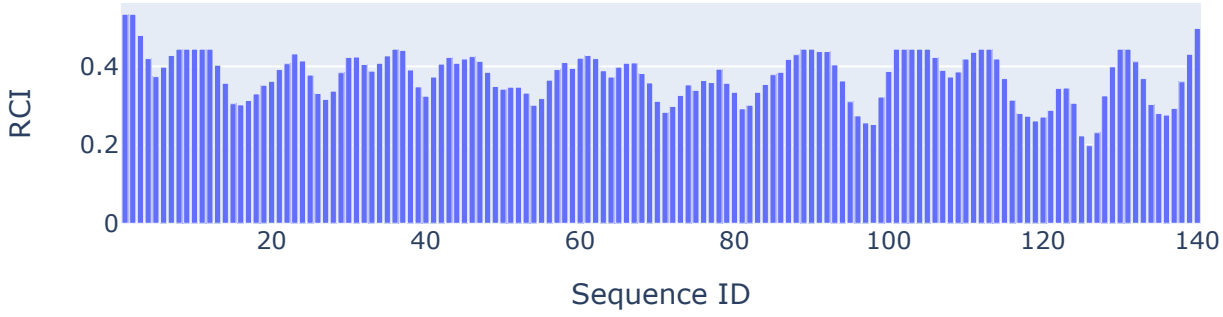
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_7*



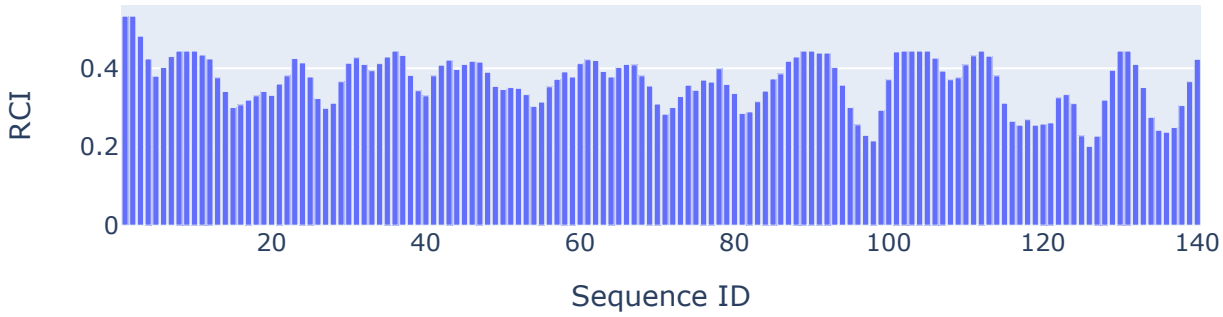
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_8*



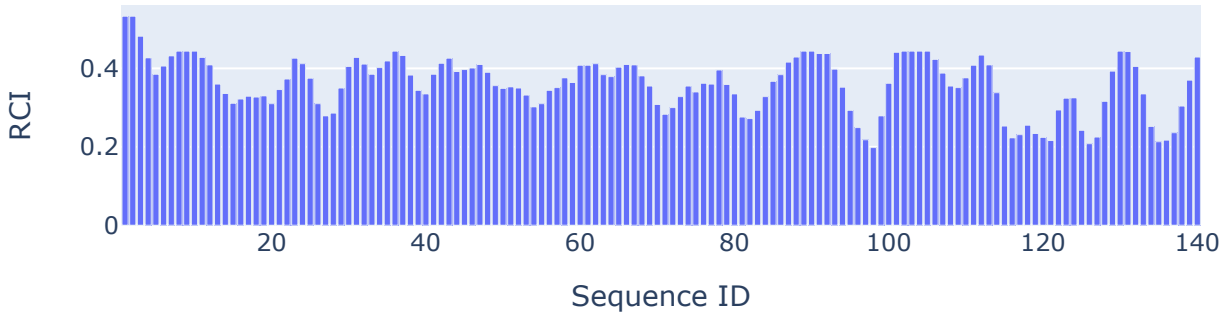
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_9*



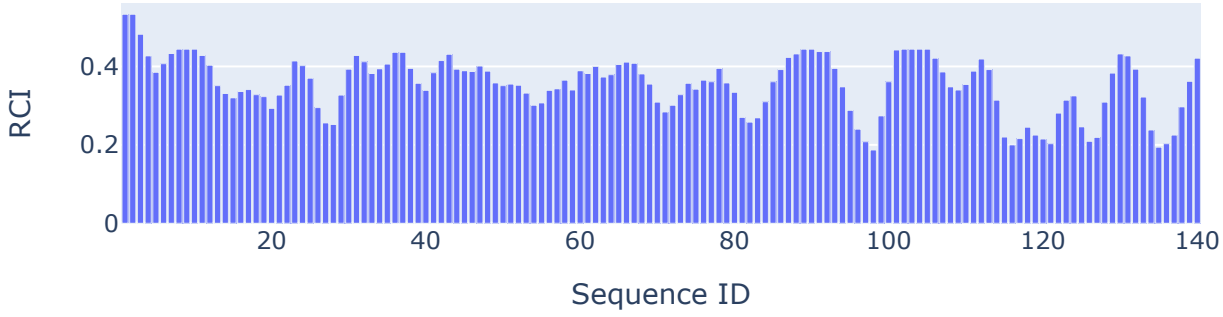
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_10*



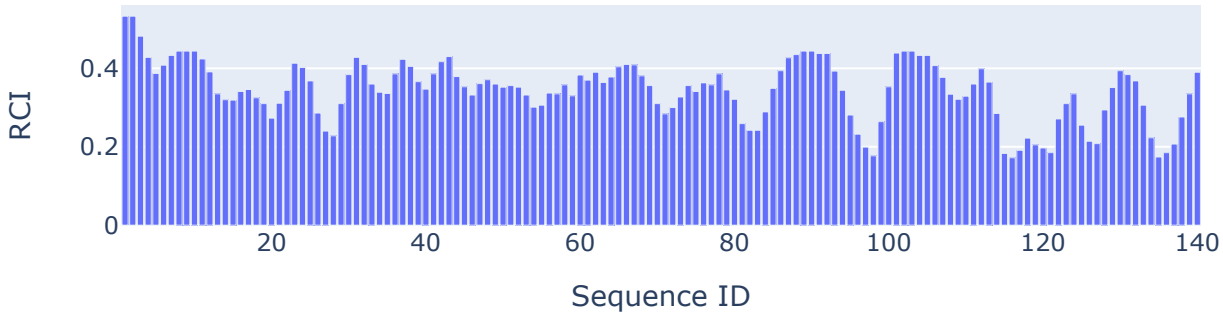
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_11*



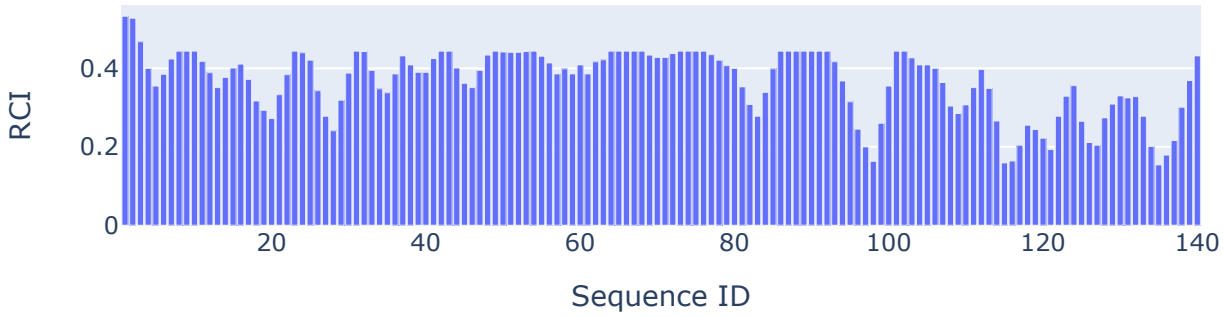
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_12*



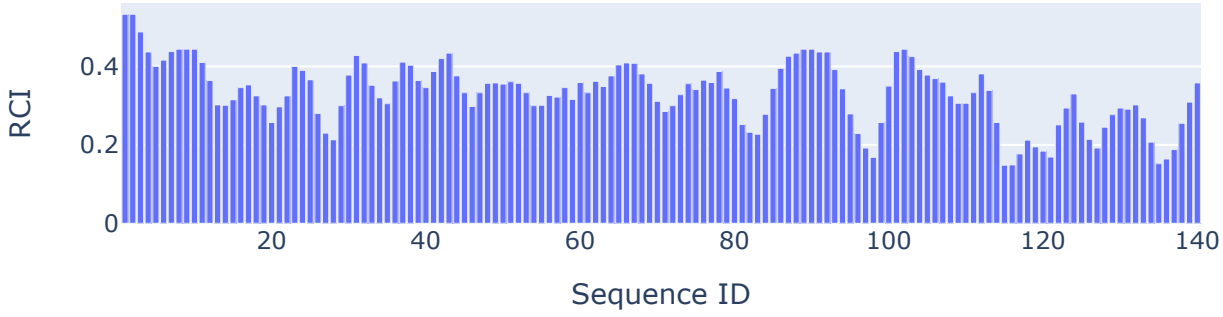
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_13*



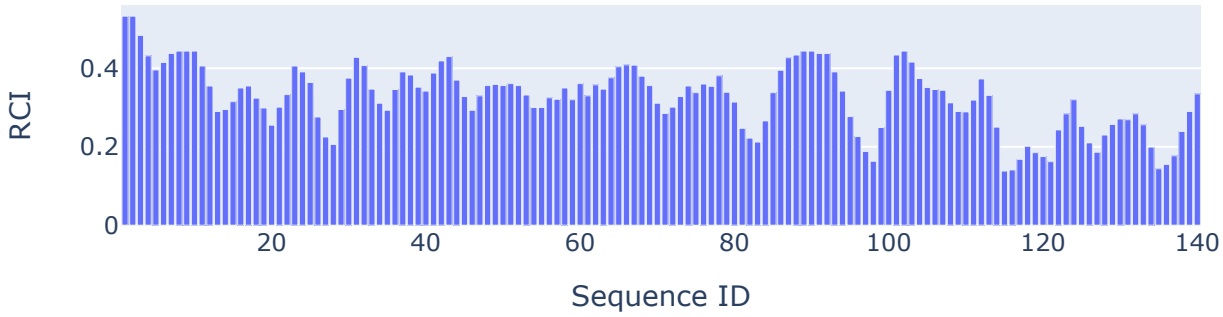
RCI plot for the chemical shifts from the save frame *assigned_chem_shif_list_14*



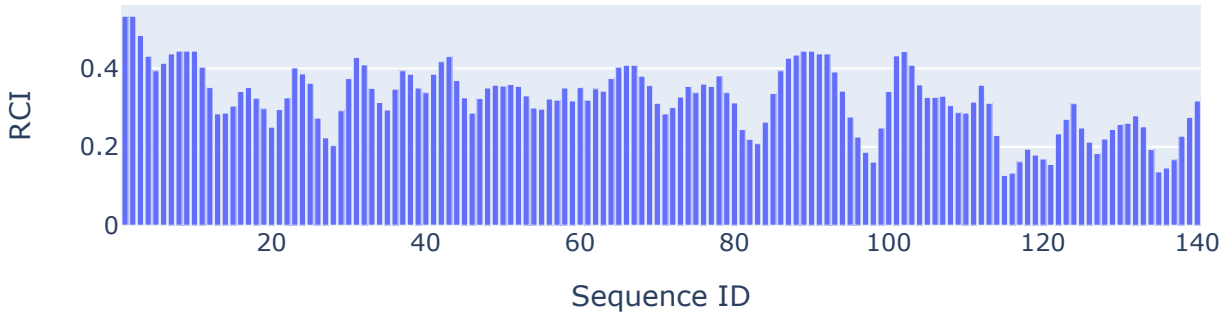
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_15*



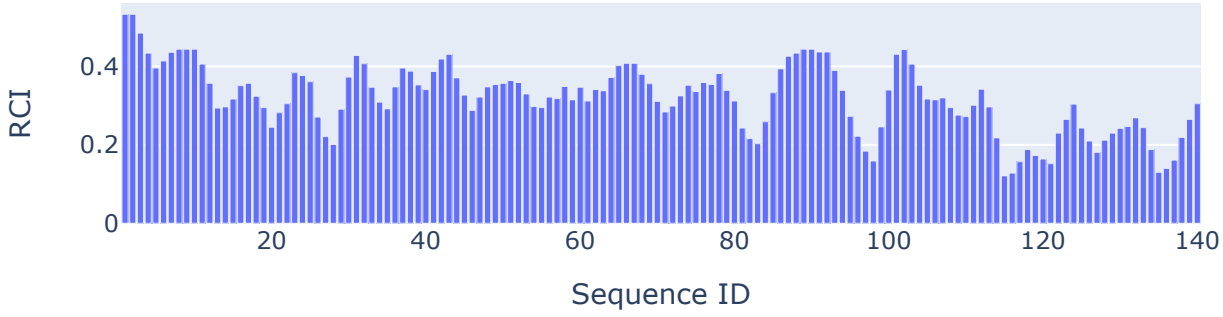
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_16*



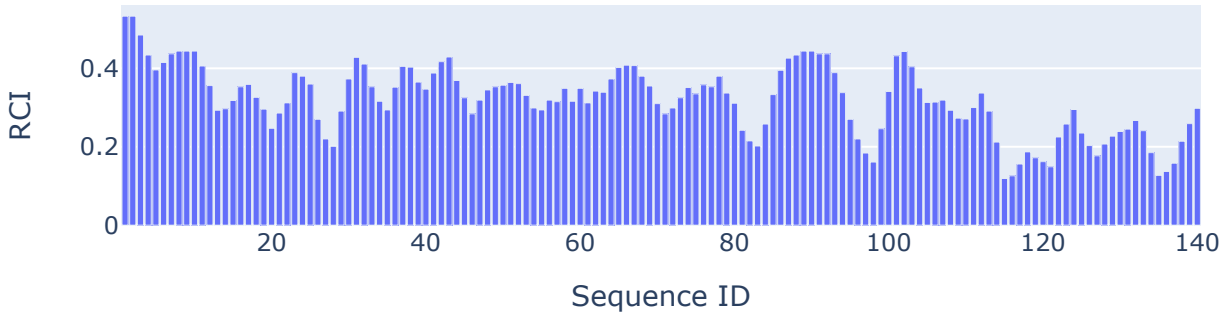
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_*17



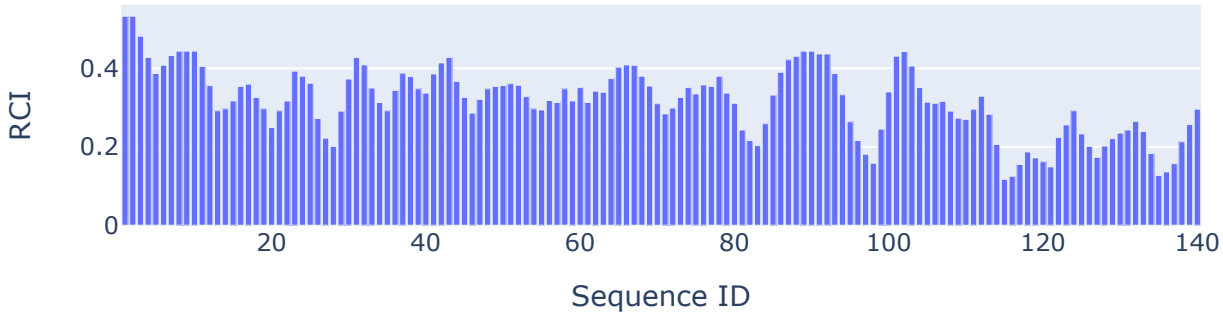
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_*18



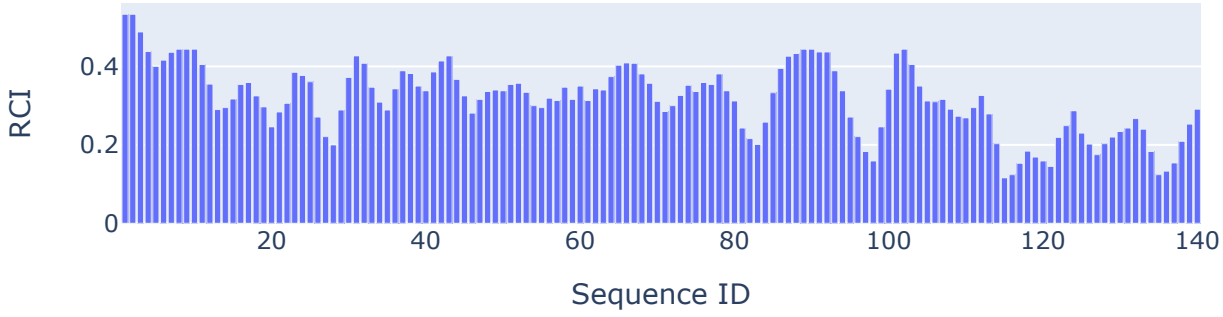
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_*19



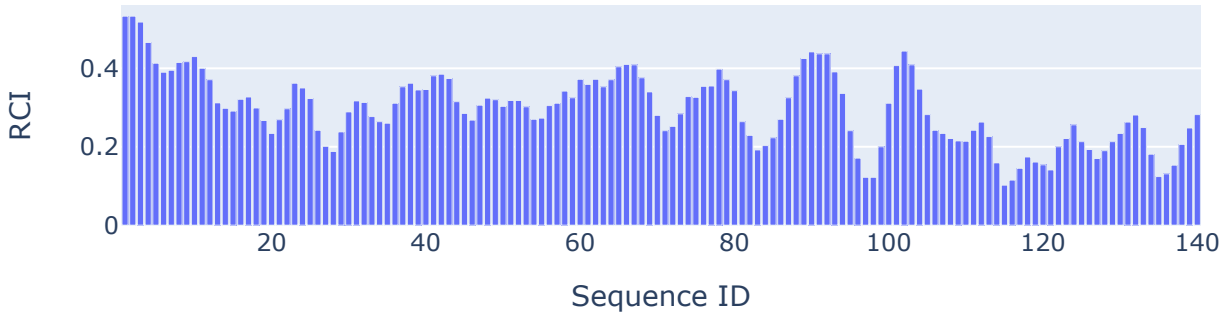
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_20*



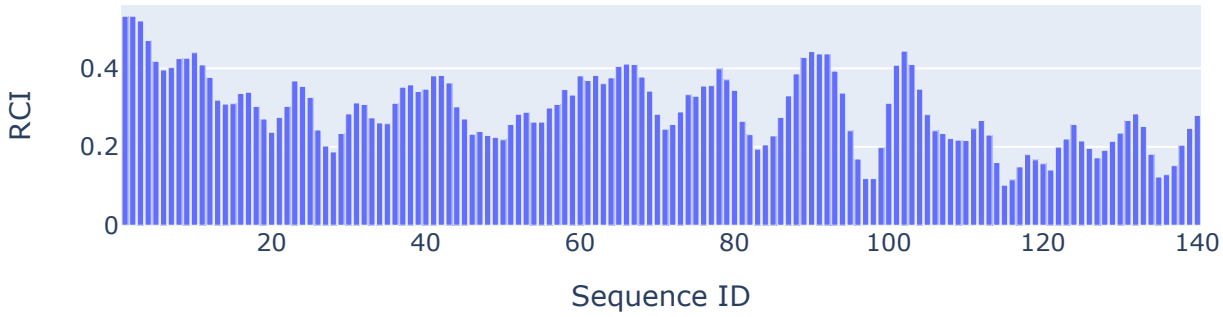
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_21*



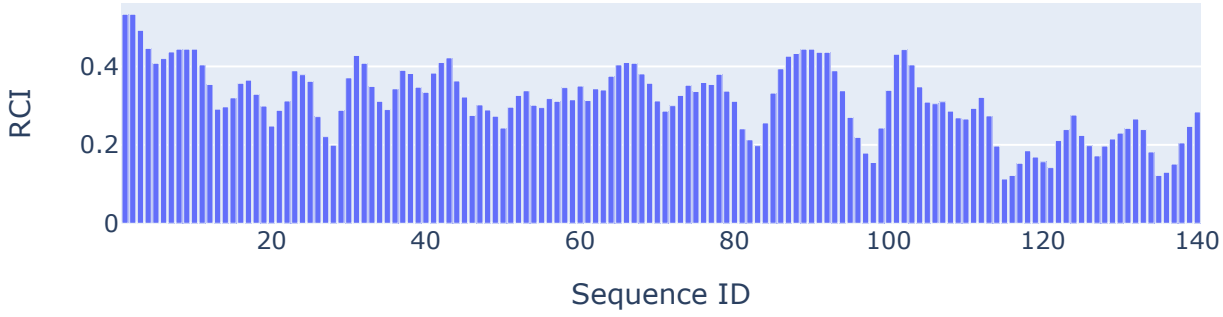
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_22*



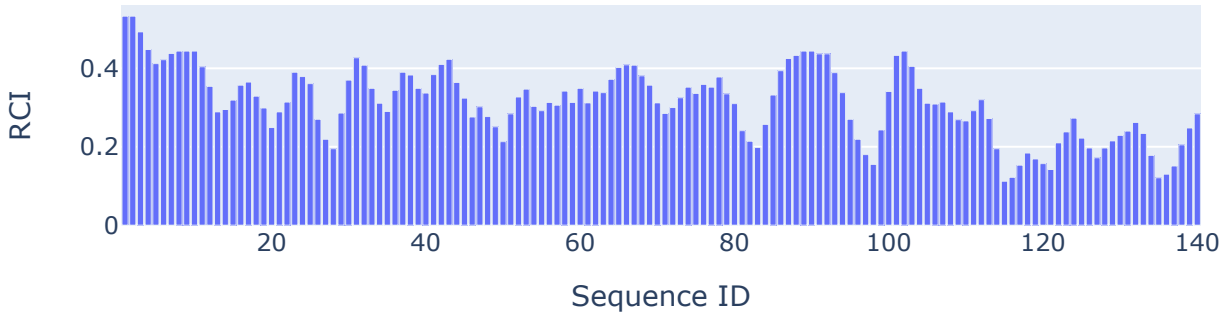
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_23*



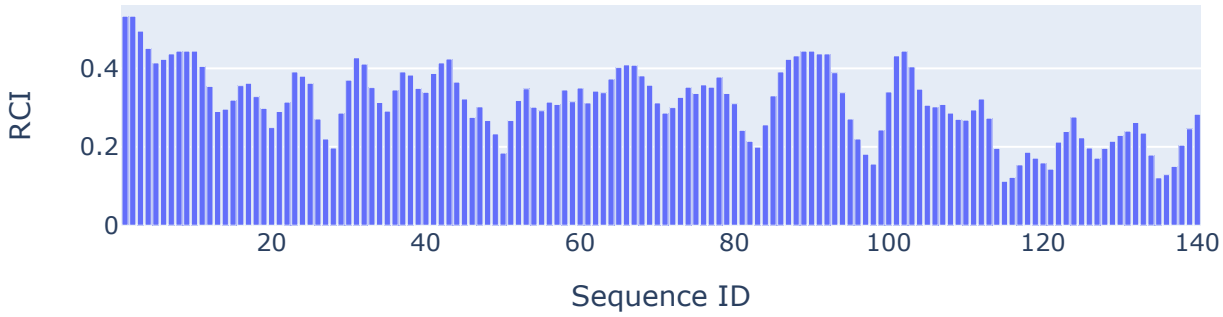
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_24*



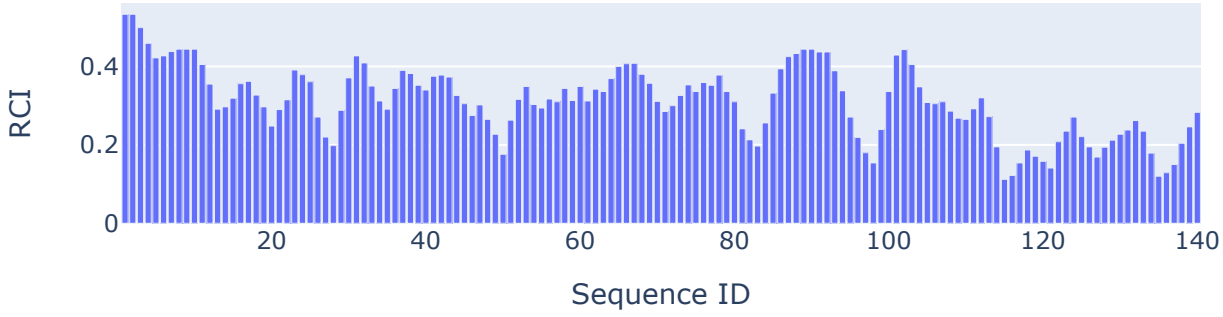
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_25*



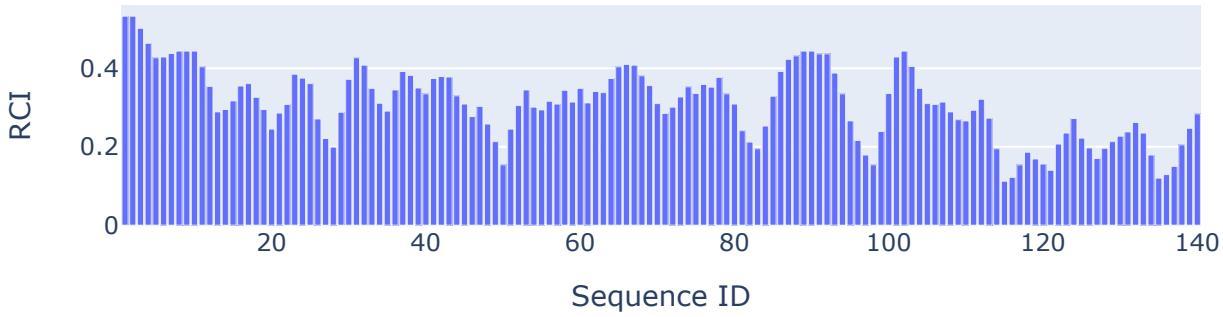
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_26*



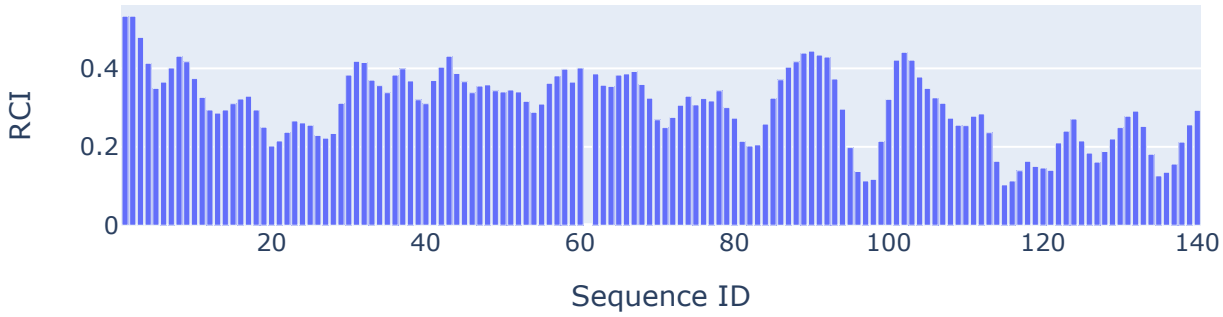
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_27*



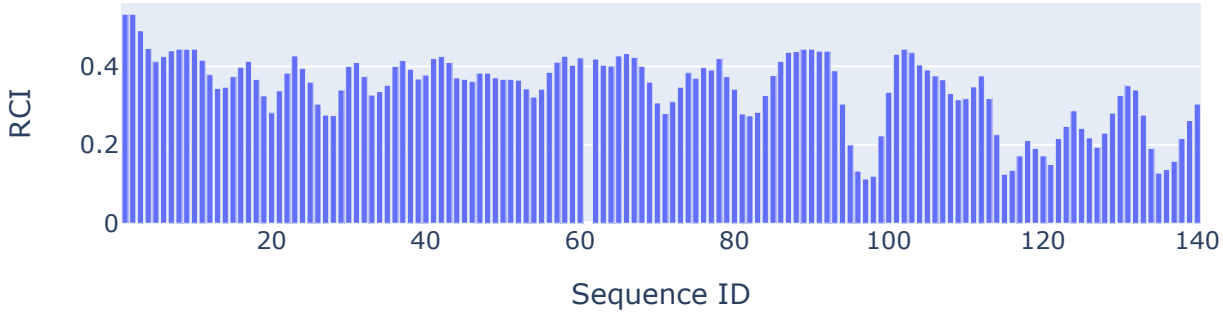
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_28*



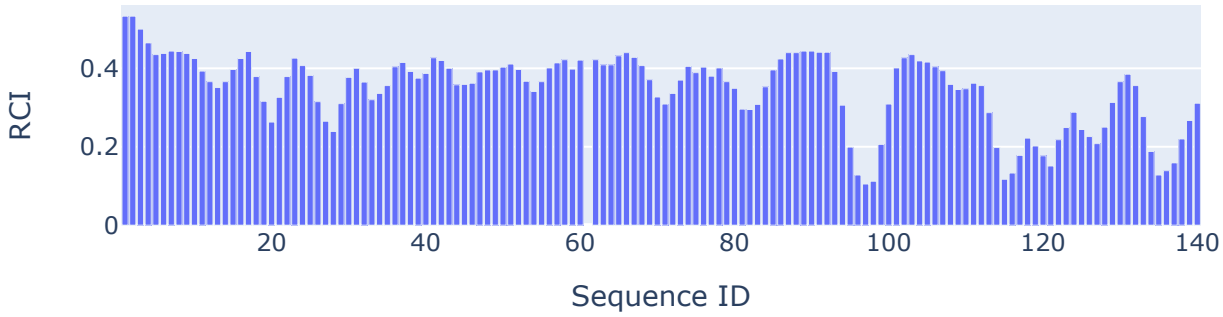
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_29*



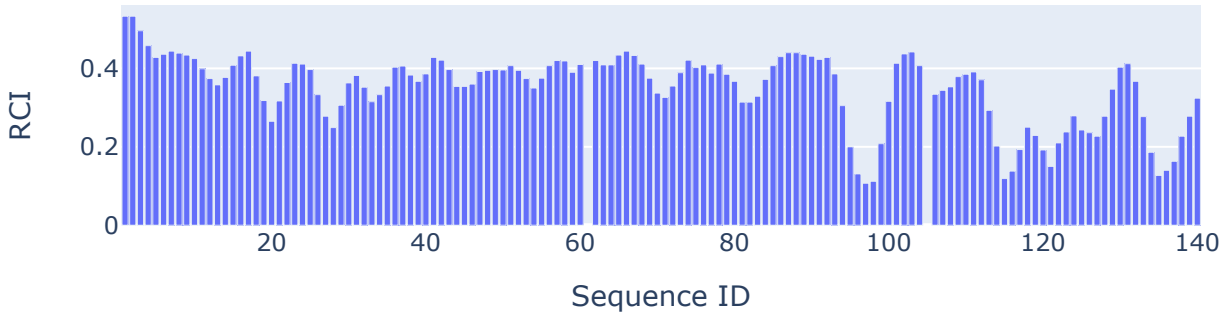
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_30*



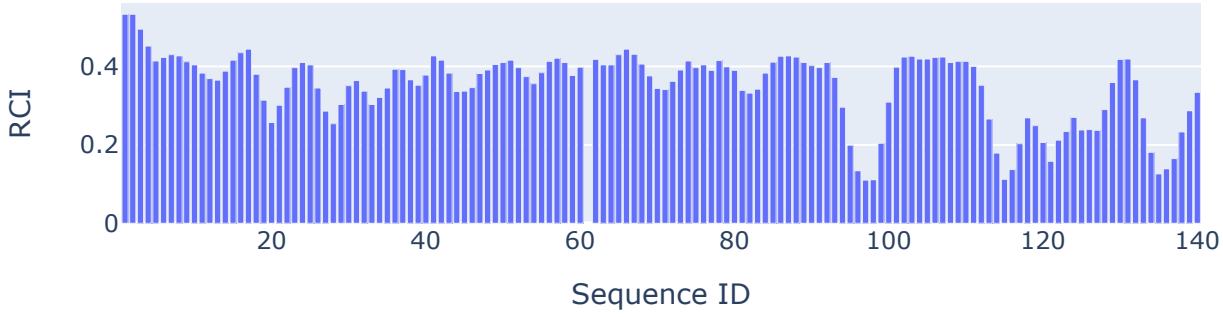
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_31*



RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_32*

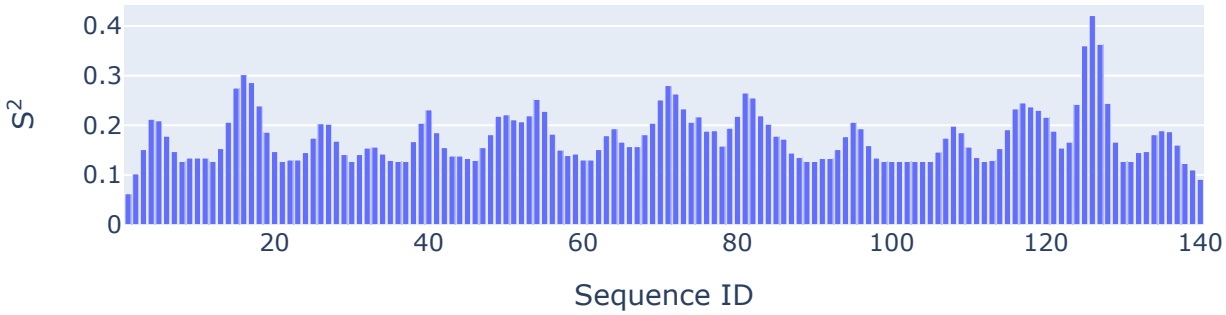


RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_33*

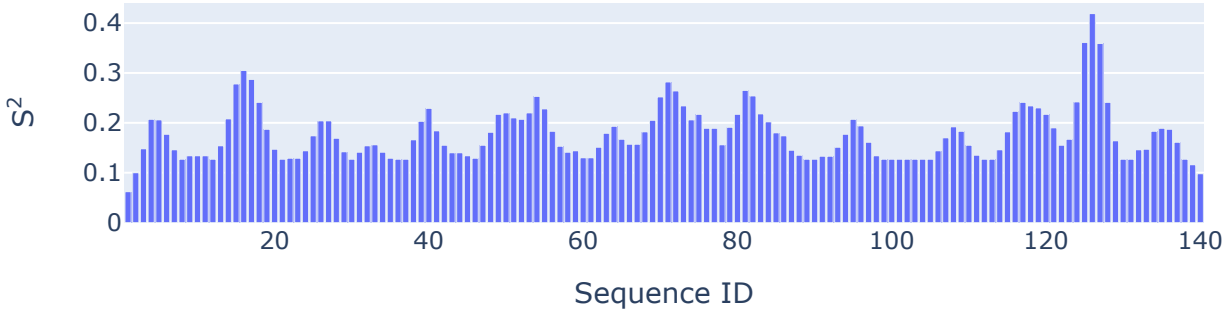


5 Order parameter

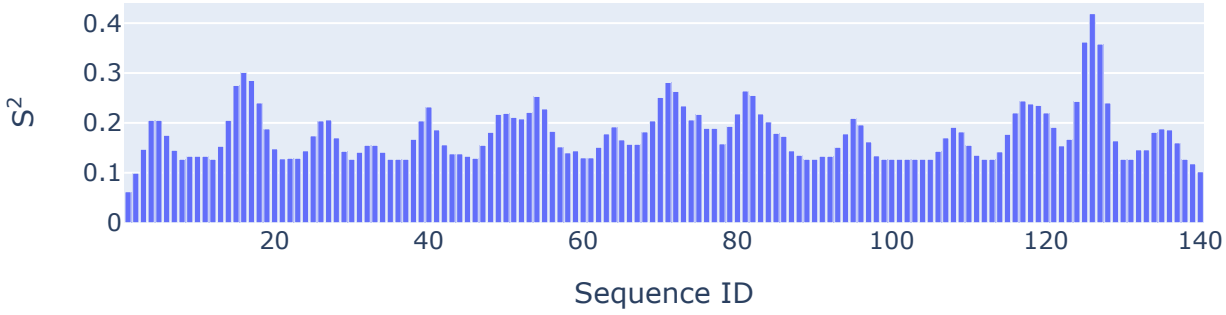
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_1*



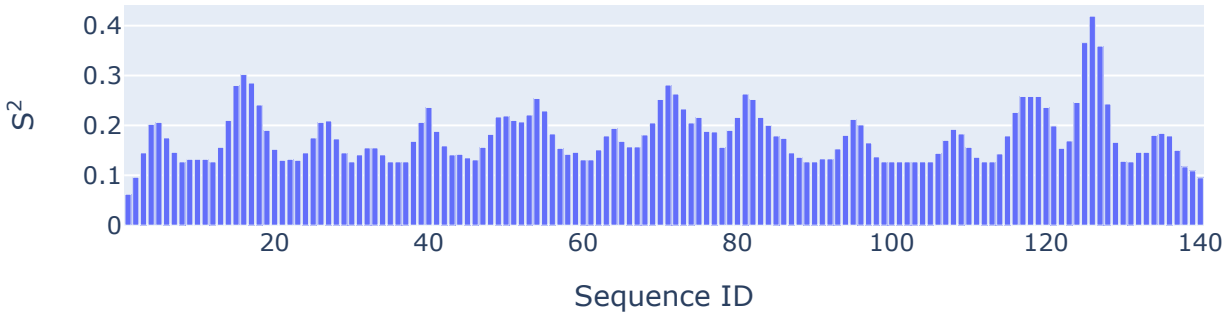
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_2*



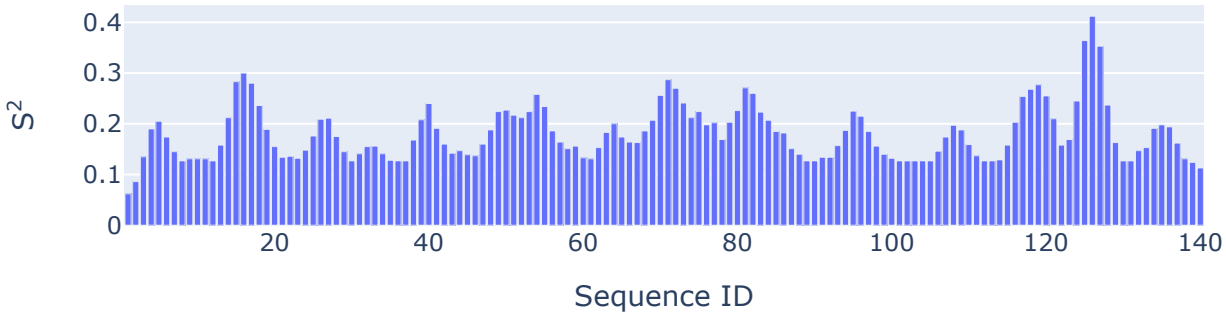
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_3*



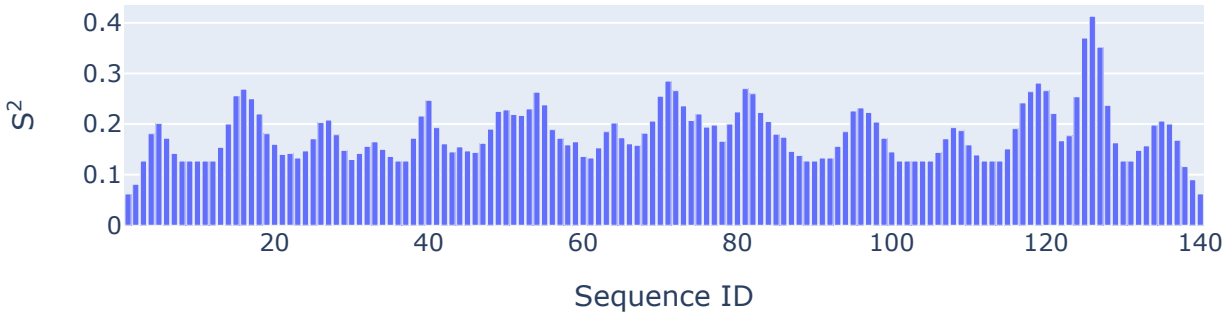
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_4*



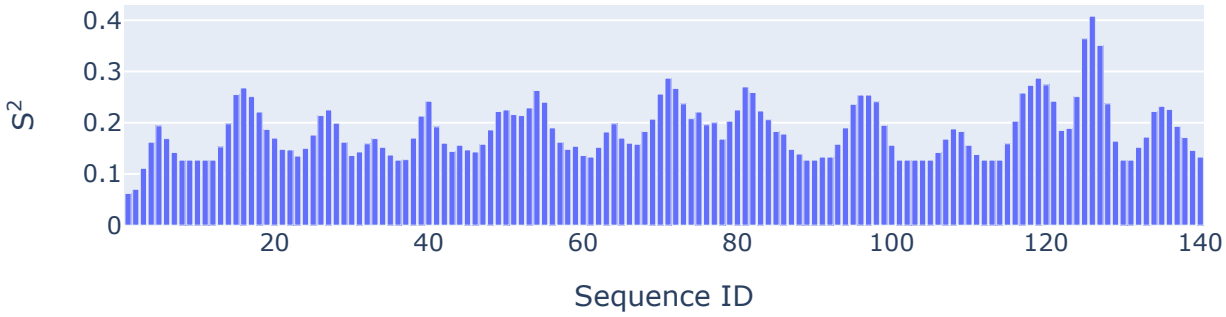
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_5*



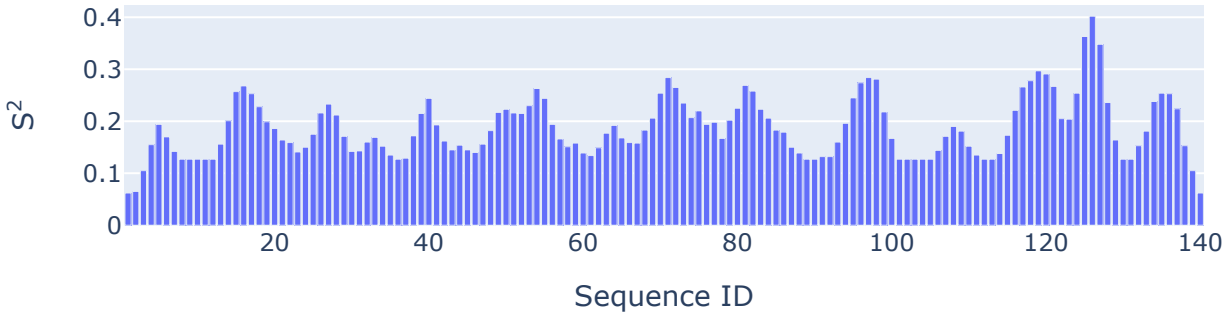
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_6*



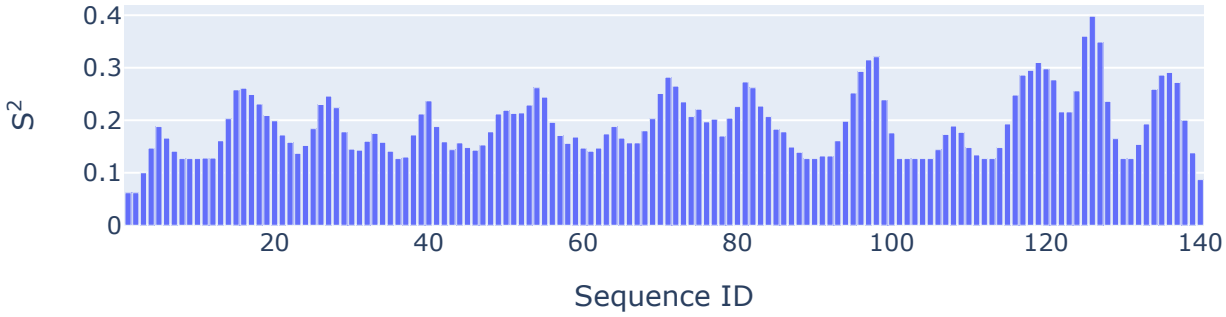
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_7*



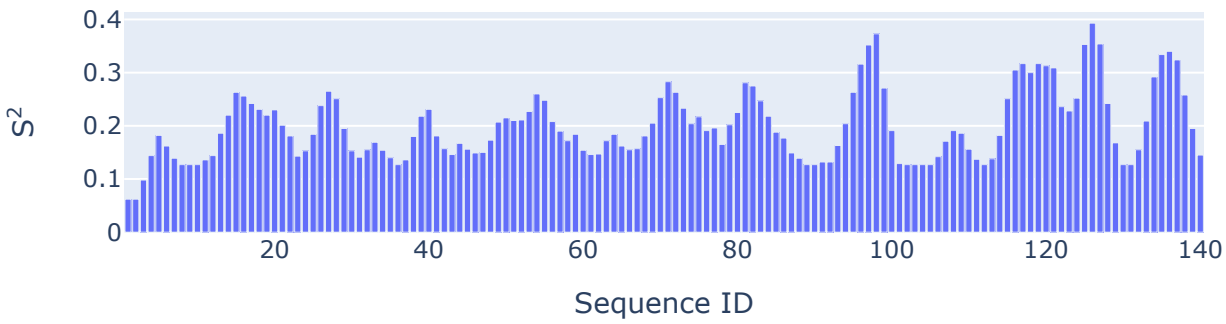
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_8*



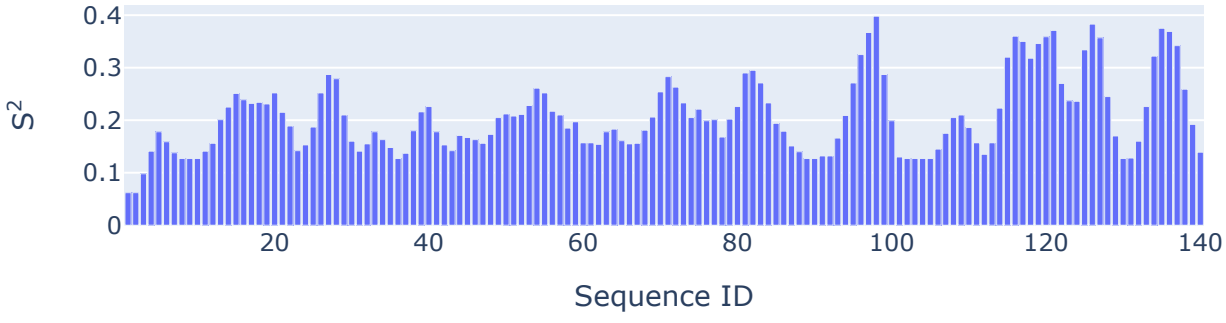
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_9*



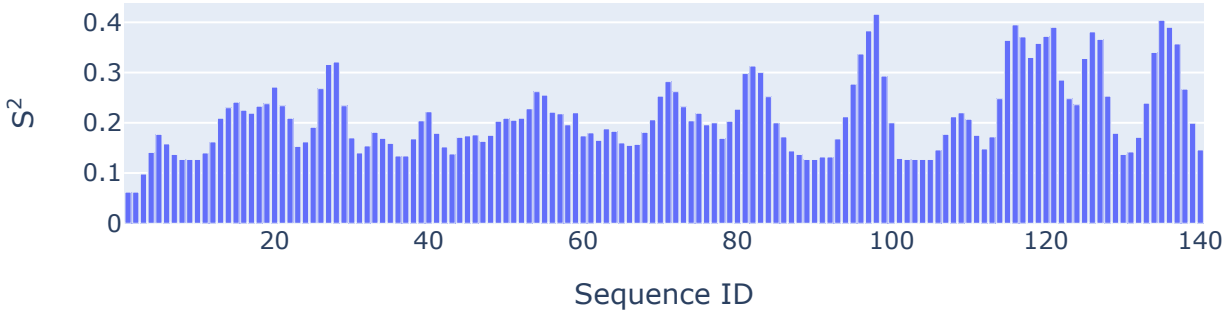
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_10*



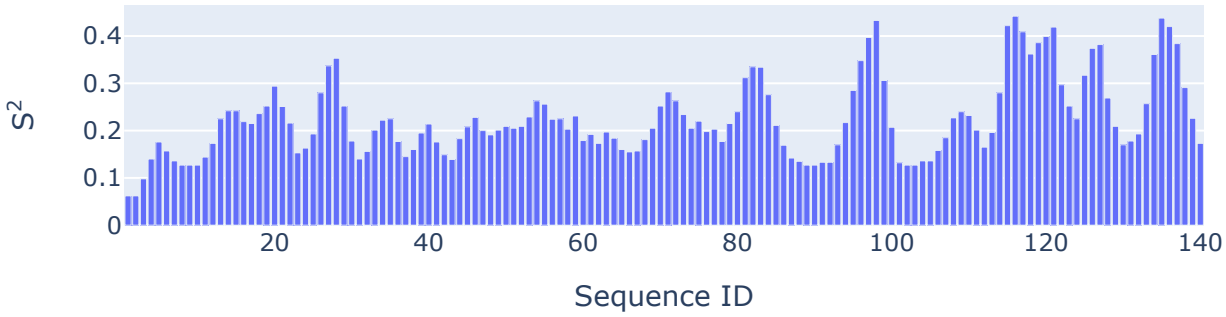
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_11*



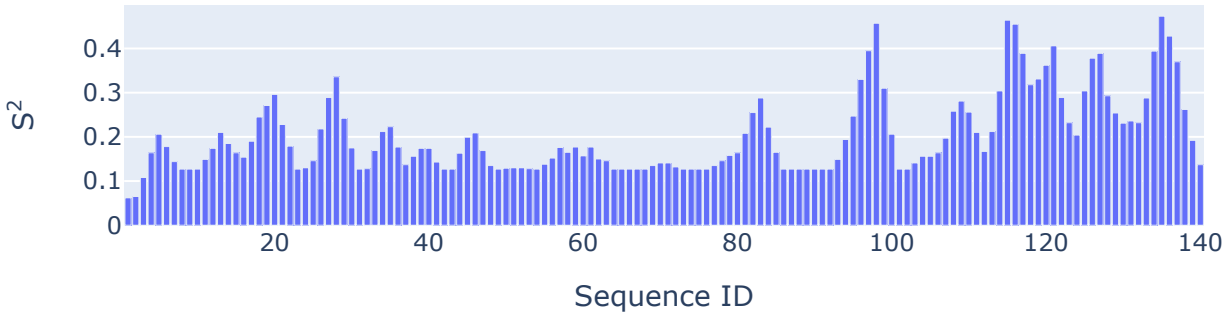
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_12*



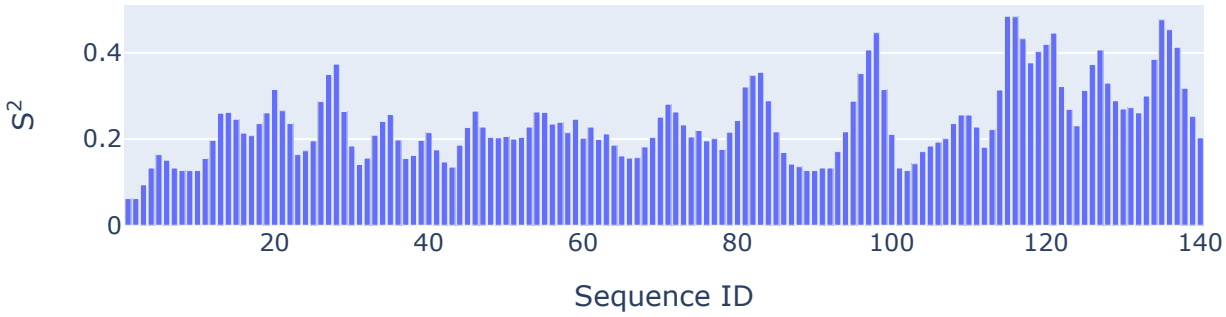
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_13*



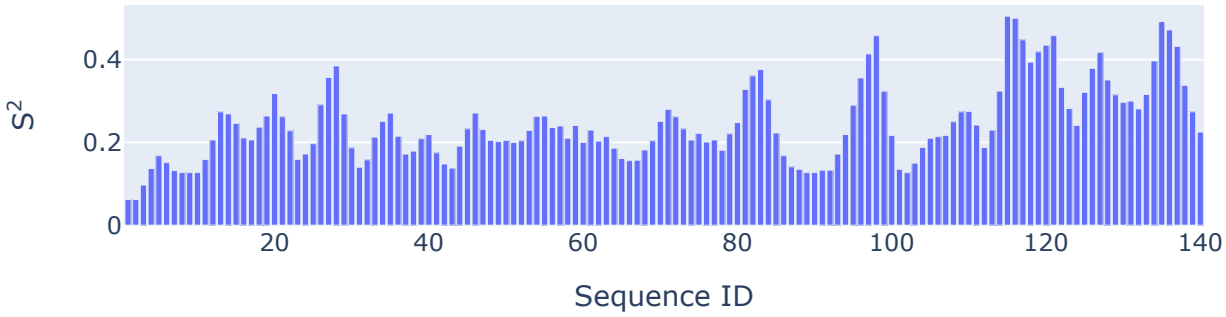
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shif_list_14*



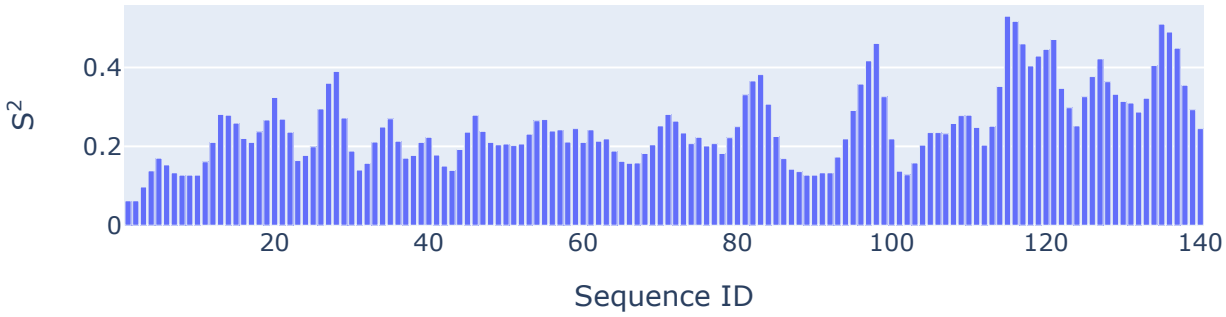
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_15*



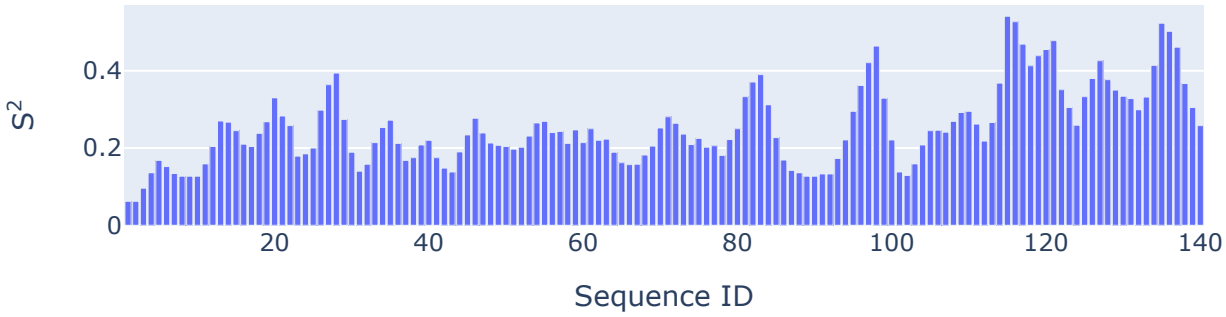
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_16*



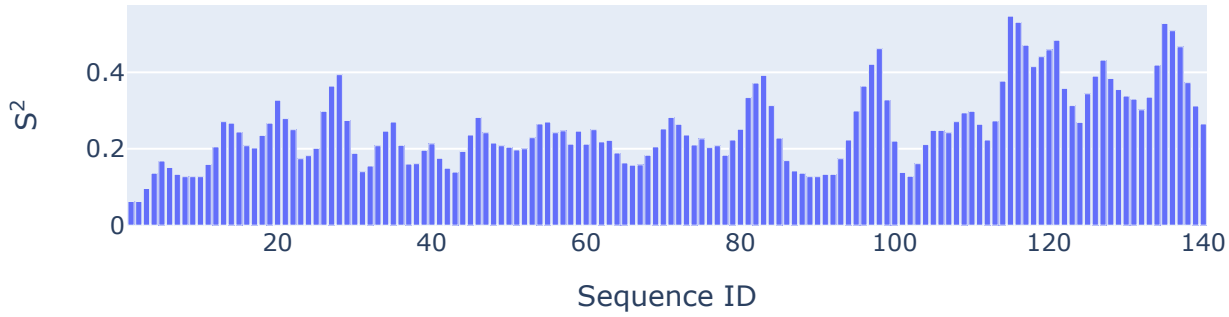
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_17*



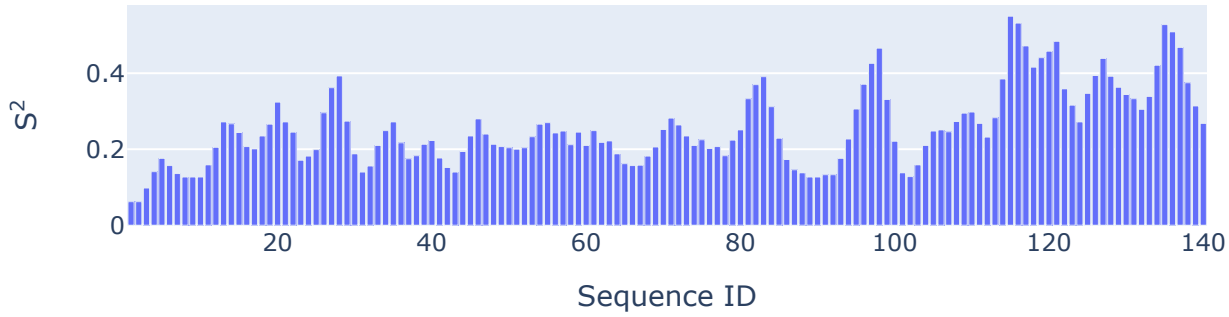
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_18*



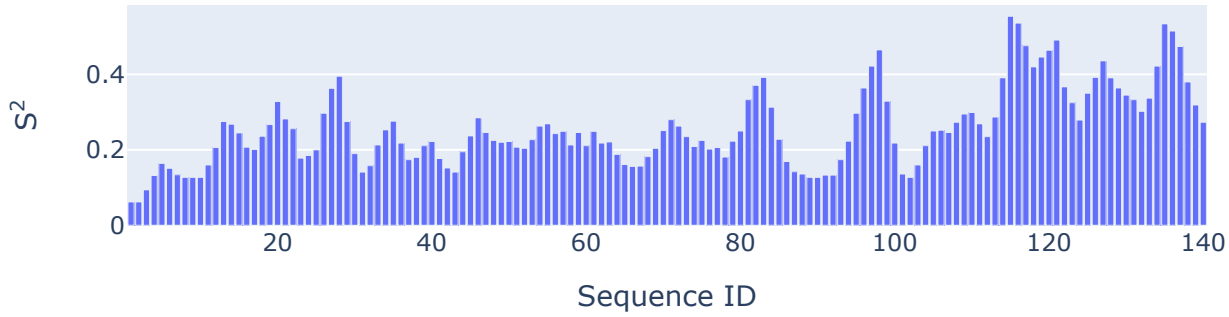
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_19*



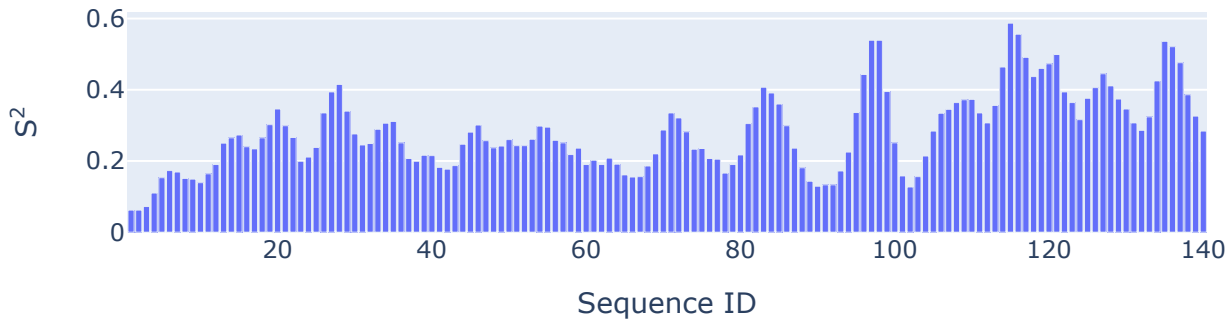
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_20*



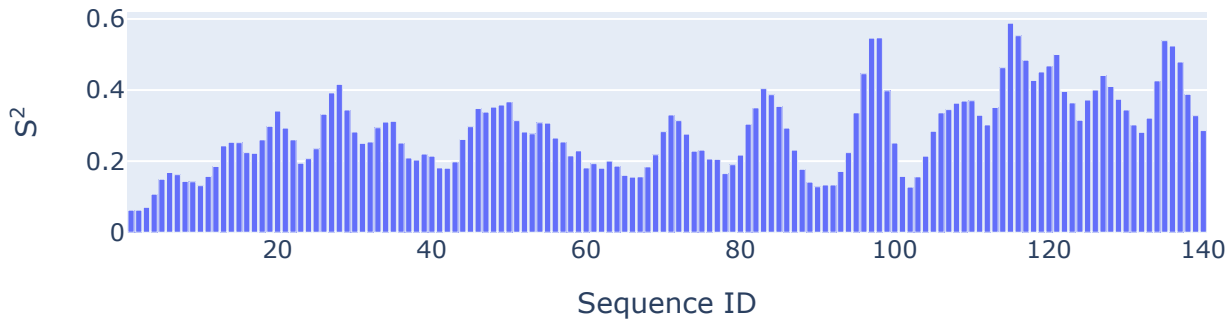
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_21*



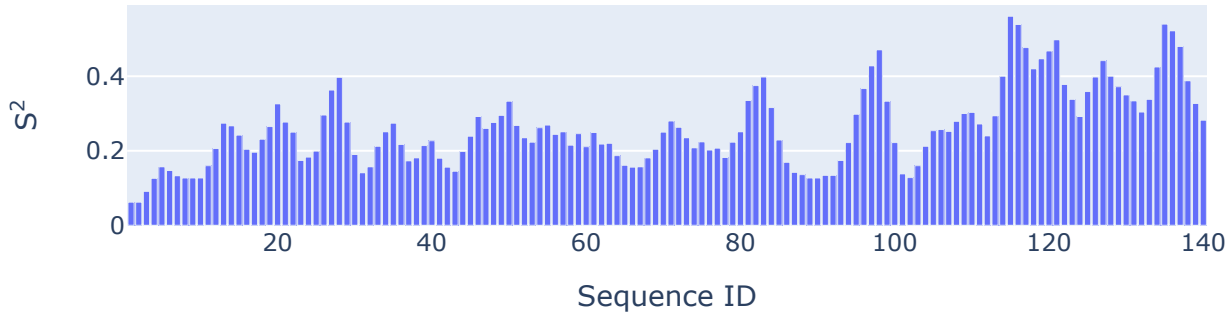
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_22*



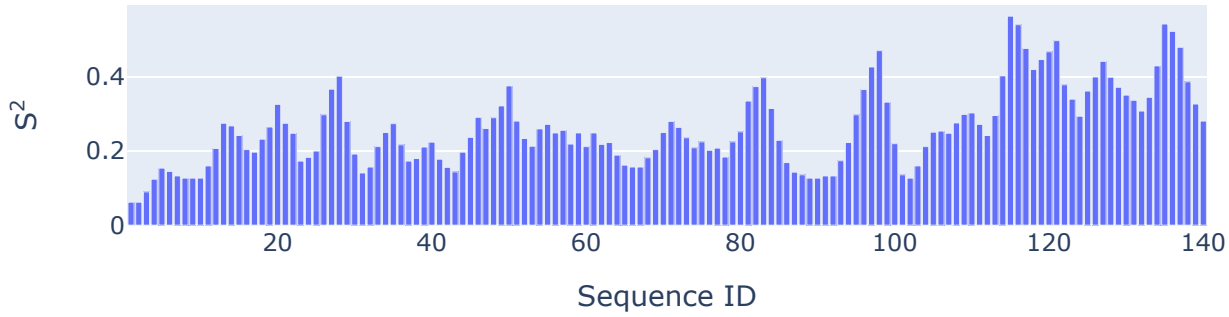
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_23*



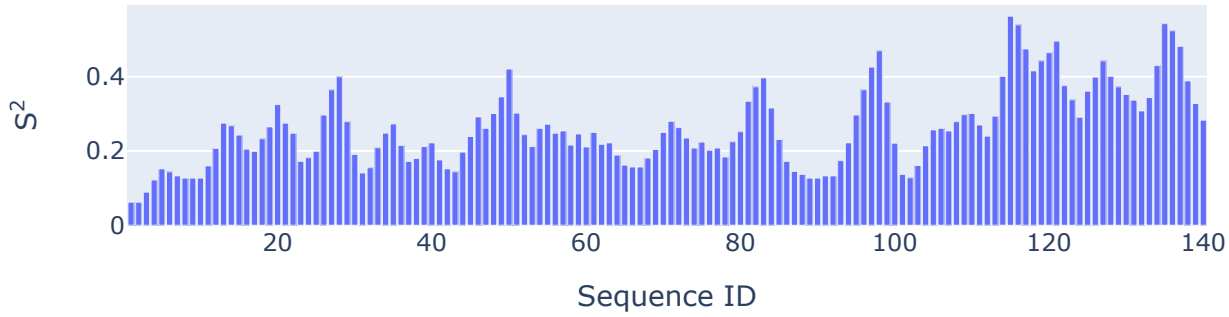
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_24*



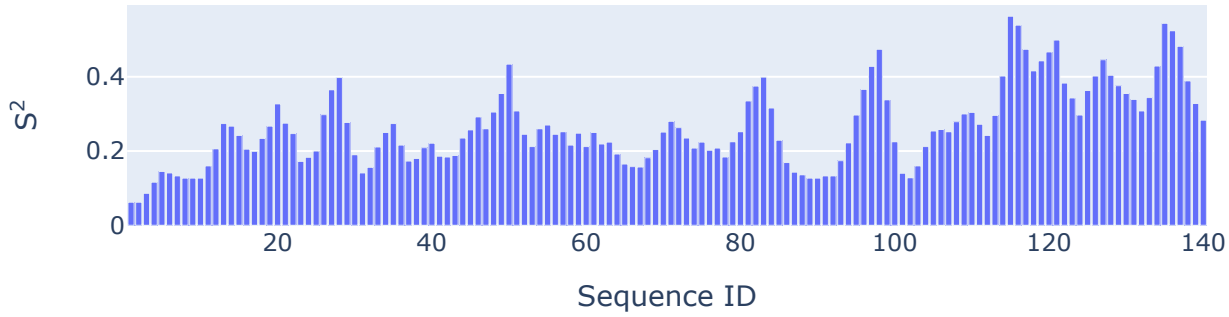
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_25*



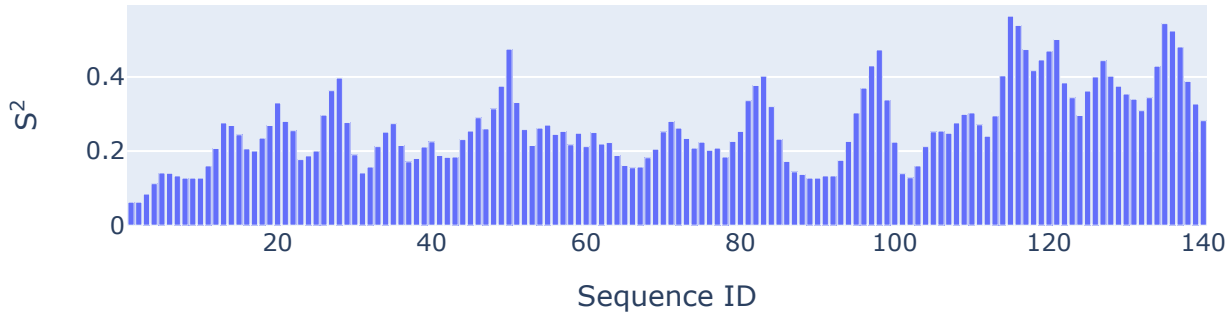
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_26*



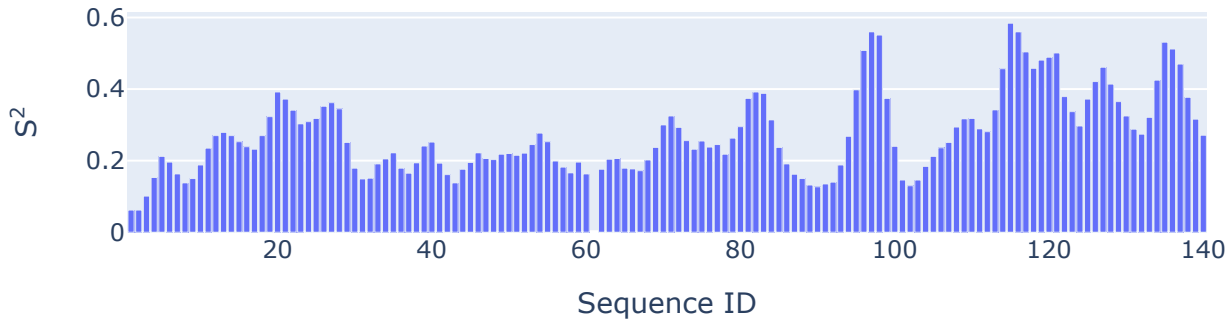
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_27*



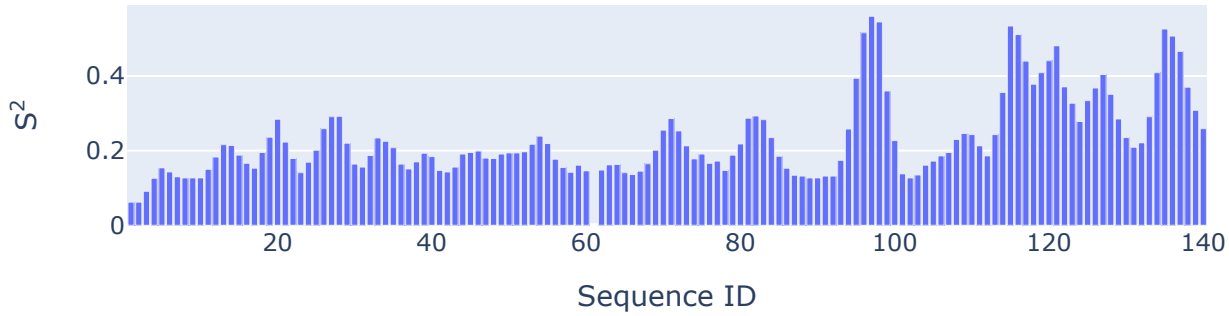
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_28*



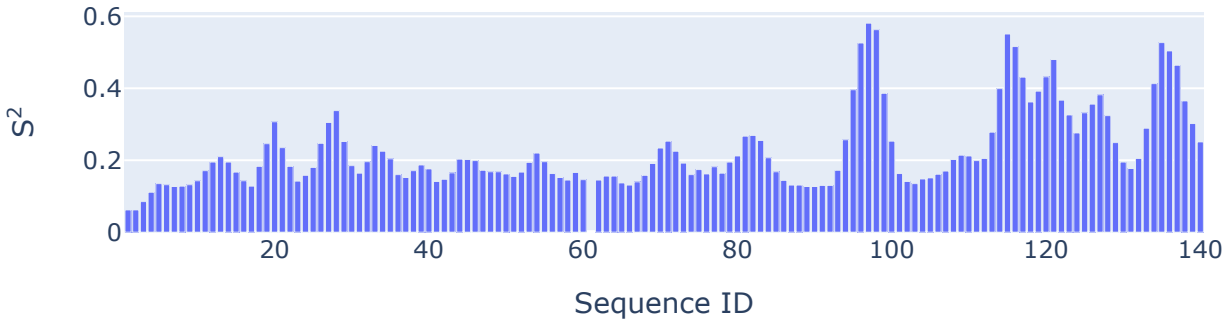
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_29*



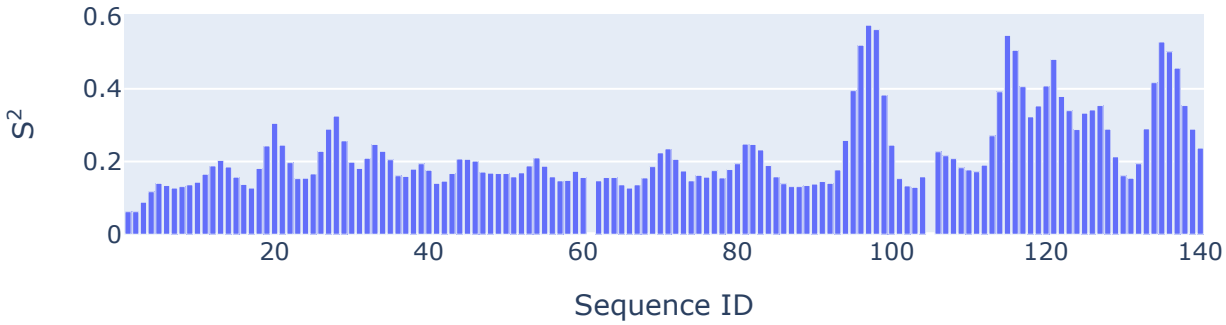
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_30*



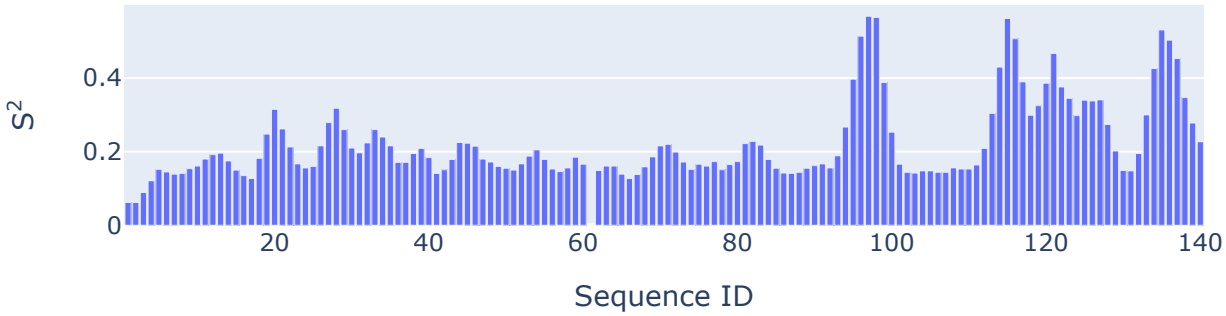
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_31*



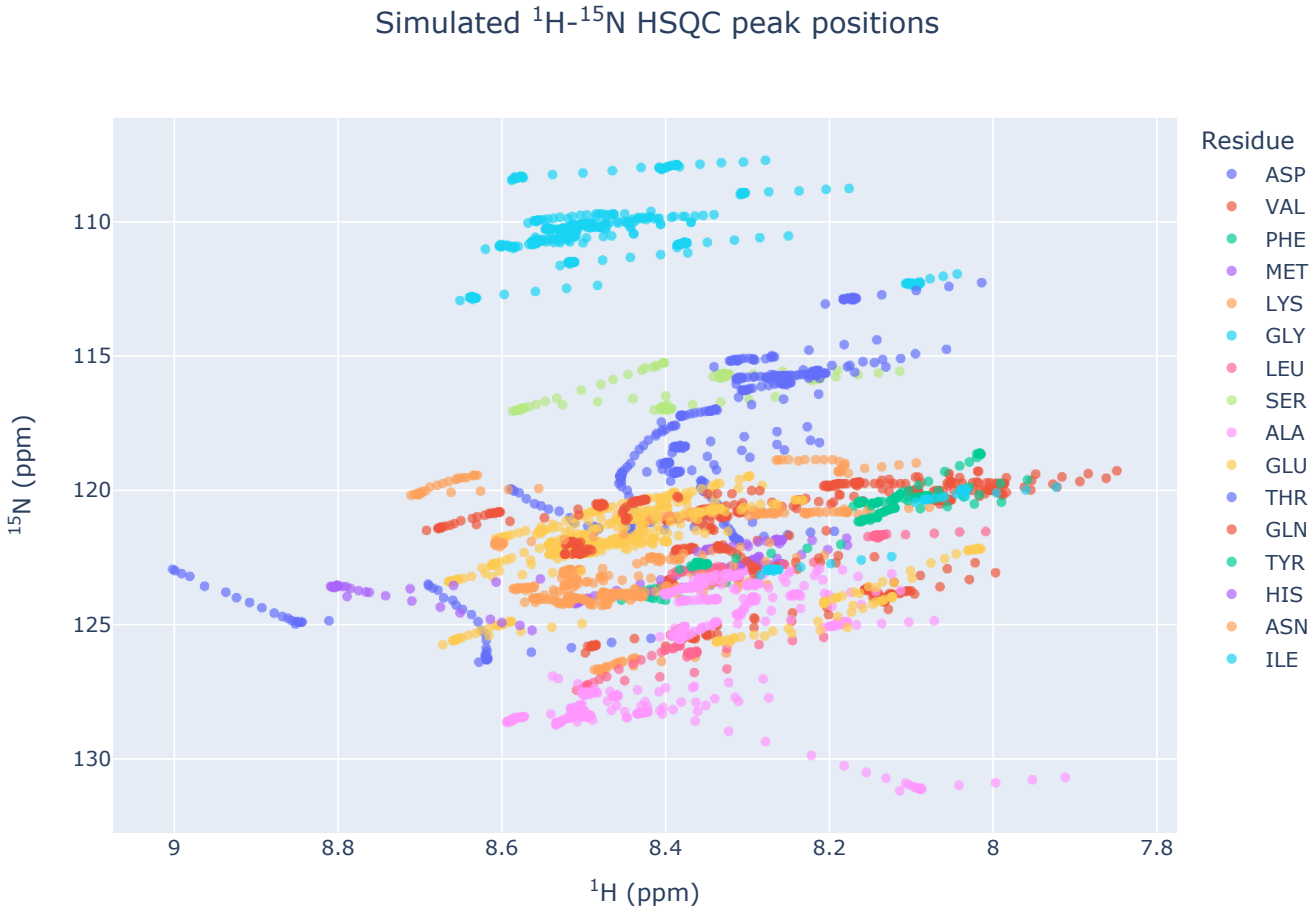
Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_32*



Order parameter plot for the chemical shifts from the save frame *assigned_chem_shift_list_33*



6 Simulated peak positions



7 LACS

Place holder for LACS results

8 Analysis data

place holder for the numerical values and tables.