Chemical Shift Validation Report

March 13, 2025 – 12:38pm EST

Entry ID	:	21103
Title	:	Solution structure of 12-meric d-form peptide
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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

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(D)
Name	:	Pap12-6-10
Sequence length	:	12
Sequence	:	(DAR)(DTR)(DLY)(DAL)(DPN)(DLY)(DLY)(DLE)(DLE)(DLY)(DLY)(DTR)(NH2)

1.2 Chemical shift list information

There is 1 chemical shift list reproted. The summary of the chemical shift data is given below

Saveframe name	assigned_chem_shift_list_1
Saveframe ID	1
Temperature	303 K
PH	5.9 pH
Number of shifts	116
Number of shift outliers	0
Assignment completeness	55.1%

2 Completeness

Completeness information for Entity 1. It is a polypeptide(D) polymer

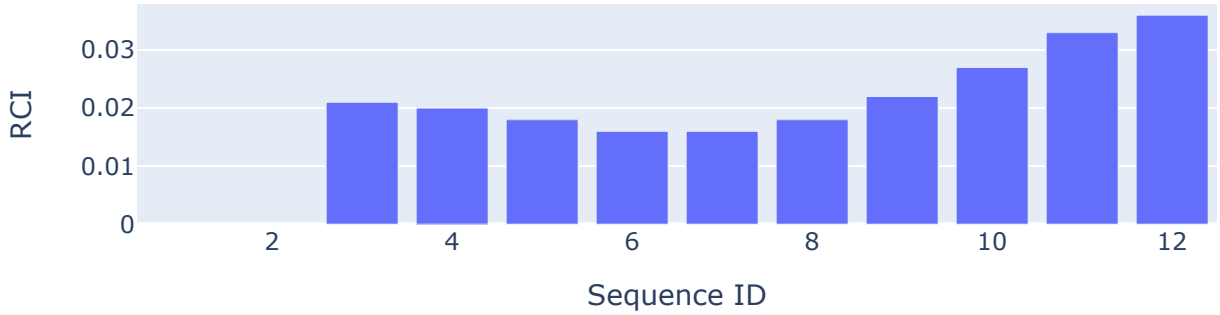
	Total	^{1}H	^{13}C	^{15}N
Backbone	30/60 (50.0%)	20/24 (83.3%)	10/24 (41.7%)	0/12 (0.0%)
Sidechain	72/122 (59.0%)	72/80 (90.0%)	0/36 (0.0%)	0/8 (0.0%)
Aromatic	14/34 (41.2%)	14/19 (73.7%)	0/15 (0.0%)	0/2 (0.0%)
Overall	119/216 (55.1%)	106/123 (86.2%)	10/75 (13.3%)	0/22 (0.0%)

3 Statistically unusual chemical shifts

There are no chemical shift outliers.
Note: Statistically unusual chemical shifts are determined using the BMRB chemical shift statistics. These chemical shifts are those that deviate from the mean value of the BMRB chemical shift distribution by more than five standard deviations, falling on either side of the mean. L- amino acid distributions are used to calcualte D- amino acid outliers

4 RCI

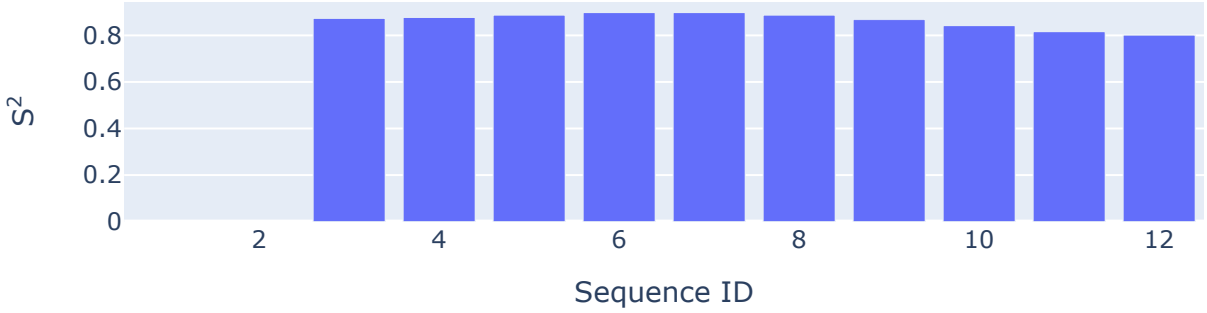
RCI plot for the chemical shifts from the save frame *assigned_chem_shift_list_1*



Note: D-amino acids are treated as L-amino acids to calcualte the RCI values.

5 Order parameter

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



Note: D-amino acids are treated as L-amino acids to calcualte the order parameter.