Chemical Shift Validation Report

November 28, 2022 – 2:50pm EST

Entry ID	:	51294
Title	:	Backbone assignment of Hepatitis B virus core protein Cp149 dimer by solution NMR at pH 7.5
Authors	:	Lauriane Lecoq; Mathilde Briday; Anja Bockmann
Deposited on	:	2022-01-27

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 an oligomer with 2 chains made by one Entity.

1.1 Entity information

1.1.1 Entity 1

Type	:	polymer
Polymer type	:	polypeptide(L)
Name	:	entity_1
Sequence length	:	149
Sequence	:	MDIDPYKEFGATVELLSFLP SDFFPSVRDLLDTASALYRE ALESPEHCSPHHTALRQAIL CWGELMTLATWVGVNLEDPA SRDLVVSYVNTNMGLKFRQL LWFHISCLTFGRETVIEYLV SFGVWIRTPPAYRPPNAPIL STLPETTVV

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_chemical_shifts_1
Saveframe ID	1
Ionic Strength	0 M
PH	7.5 pH
Pressure	1 atm
Temperature	295 K
Number of shifts	382
Number of shift outliers	0
Assignment completeness	18.5%

2 Completeness

Completeness information for Entity 1. It is a polypeptide(L) polymer. 0 out of 32 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	378/727 (52.0%)	98/292 (33.6%)	182/298 (61.1%)	98/137 (71.5%)

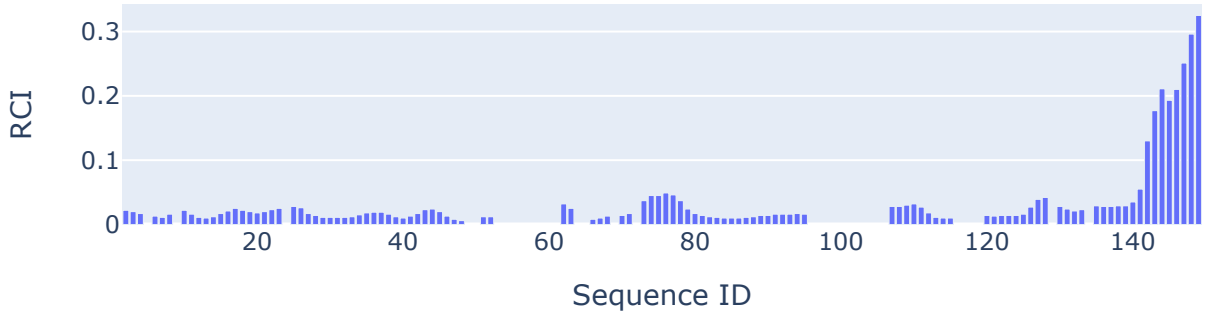
Sidechain	0/1129 (0.0%)	0/761 (0.0%)	0/352 (0.0%)	0/32 (0.0%)
Aromatic	4/210 (1.9%)	2/109 (1.8%)	0/93 (0.0%)	2/12 (16.7%)
Overall	382/2066 (18.5%)	100/1162 (8.6%)	182/743 (24.5%)	100/181 (55.2%)

3 Statistically unusual chemical shifts

There are no chemical shift outliers.

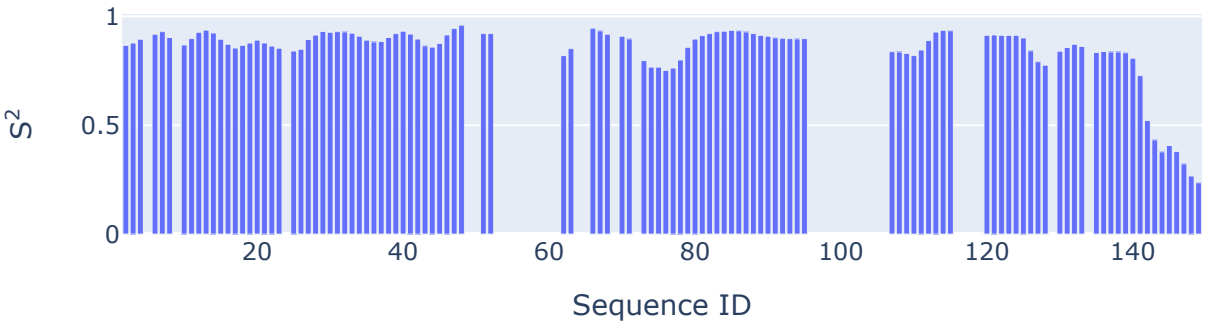
4 RCI

RCI plot for the chemical shifts from the save frame *assigned_chemical_shifts_1*

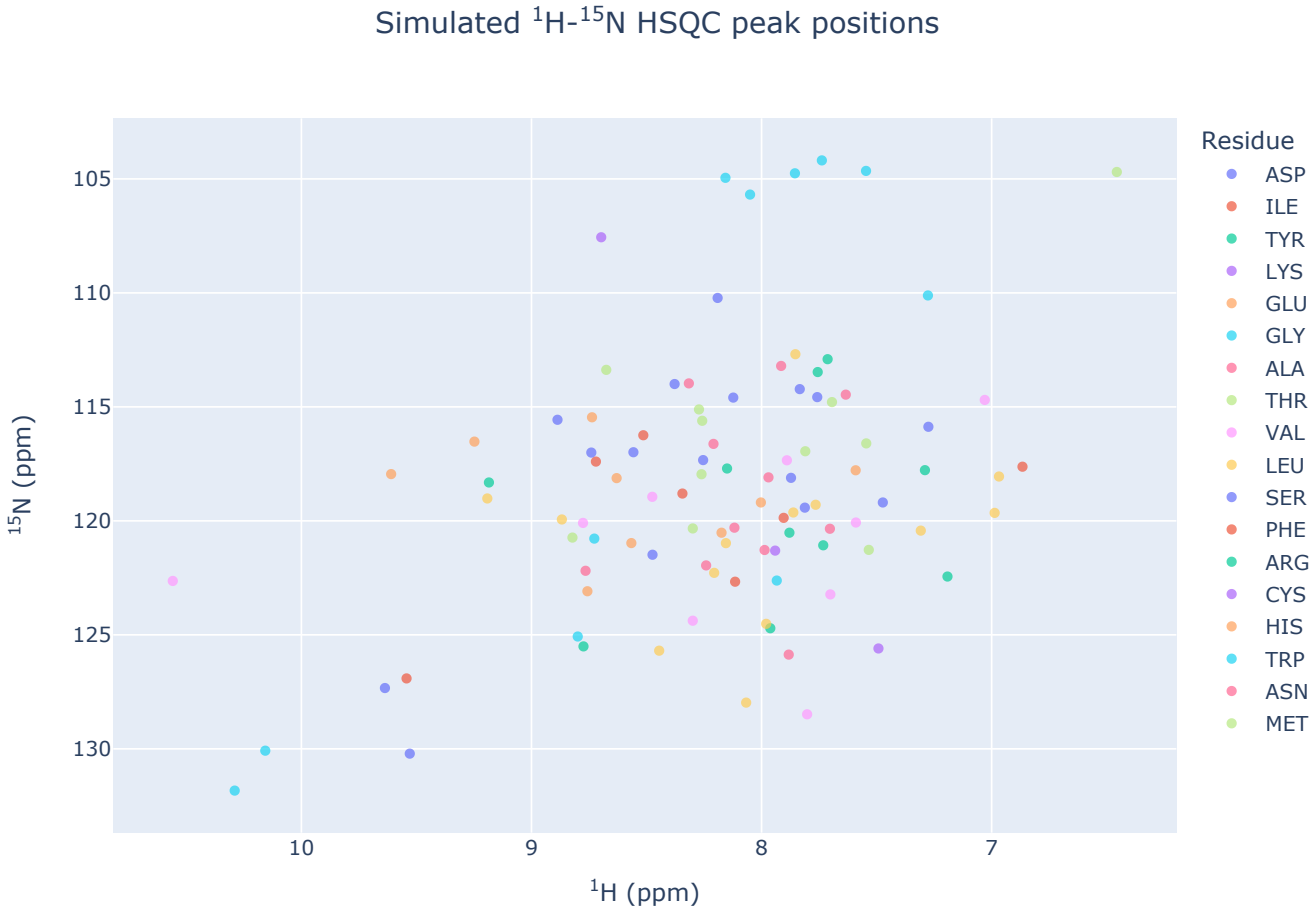


5 Order parameter

Order parameter plot for the chemical shifts from the save frame *assigned_chemical_shifts_1*



6 Simulated peak positions



7 LACS

Place holder for LACS results

8 Analysis data

place holder for the numerical values and tables.