BMRB
Biological Magnetic Resonance Data Bank

Chemical Shift Validation Report

November 28, 2022 – 2:50pm EST

Entry ID	:	7354
Title	:	NMR STRUCTURE OF A PROTEIN-DNA COMPLEX OF AN ALTERED SPECIFICITY MUTANT OF THE LAC REPRESSOR THAT MIMICS THE GAL REPRESSOR
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Deposited on	:	2006-12-01

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 4 chains made by 2 Entities.

1.1 Entity information

1.1.1 Entity 1

Type	:	polymer
Polymer type	:	polydeoxyribonucleotide
Name	:	LAC-GAL_OPERATOR
Sequence length	:	22
Sequence	:	GAATTGTAAGCGCTTACAAT TC

1.1.2 Entity 2

Type	:	polymer
Polymer type	:	polypeptide(L)
Name	:	LAC_HEADPIECE_1-62
Sequence length	:	62
Sequence	:	MKPVTLYDVAEYAGVSVATV SRVVNQASHVSAKTREKVEA AMAELNYIPNRCAQQLAGKQ SL

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
Ionic Strength	20 mM
PH	6.0 pH
Pressure	1.0 atm
Temperature	315.0 K
Number of shifts	876
Number of shift outliers	3
Assignment completeness	67.2%

2 Completeness

Completeness information for Entity 1. It is a polydeoxyribonucleotide polymer

	Total	^{1}H	^{13}C	^{15}N
Sugar	91/264 (34.5%)	91/154 (59.1%)	0/110 (0.0%)	0/0 (0.0%)
Base	57/213 (26.8%)	57/121 (47.1%)	0/47 (0.0%)	0/45 (0.0%)
Overall	148/477 (31.0%)	148/275 (53.8%)	0/157 (0.0%)	0/45 (0.0%)

Completeness information for Entity 2. It is a polypeptide(L) polymer. 13 out of 13 methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	296/308 (96.1%)	120/124 (96.8%)	117/124 (94.4%)	59/60 (98.3%)
Sidechain	414/480 (86.2%)	282/321 (87.9%)	122/145 (84.1%)	11/20 (55.0%)
Aromatic	18/38 (47.4%)	9/19 (47.4%)	9/17 (52.9%)	0/2 (0.0%)
Overall	728/826 (88.1%)	411/464 (88.6%)	248/286 (86.7%)	70/82 (85.4%)

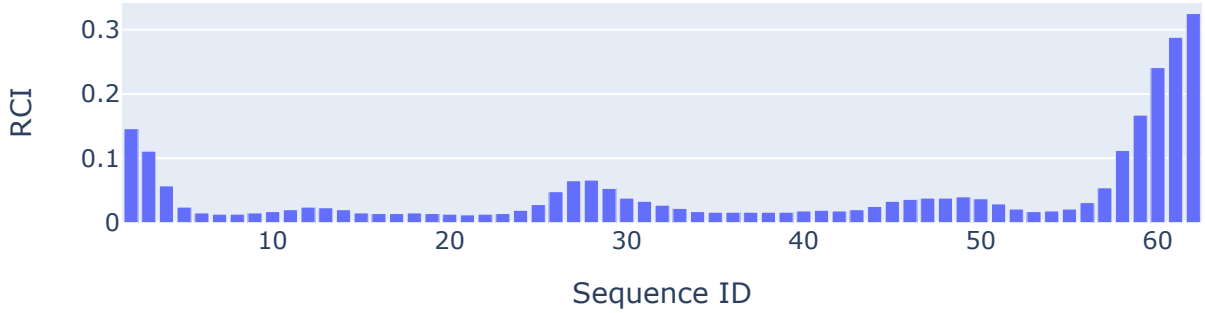
3 Statistically unusual chemical shifts

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

Entity	Seq	Res	Atom	Shift (ppm)	Expected range (ppm)	Z-score
2	12	TYR	CG	175.115	112.42 – 146.96	13.15
2	22	ARG	CB	40.076	21.74 – 39.52	5.31
2	35	ARG	NH1	113.702	49.05 – 99.42	7.84

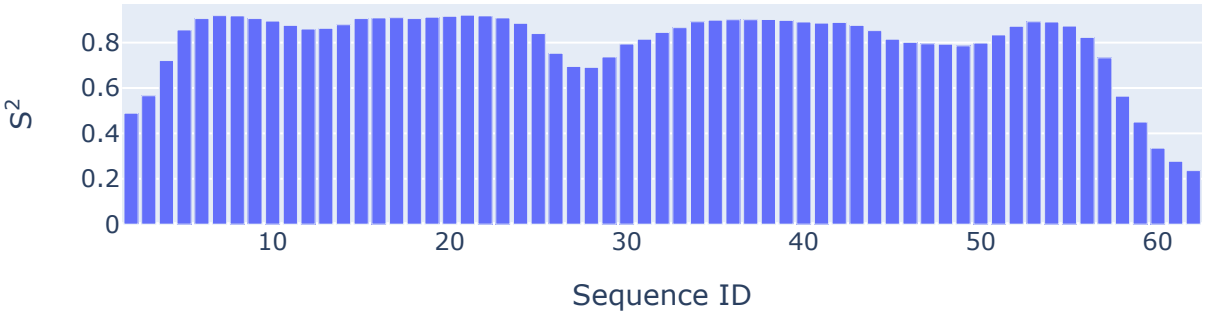
4 RCI

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

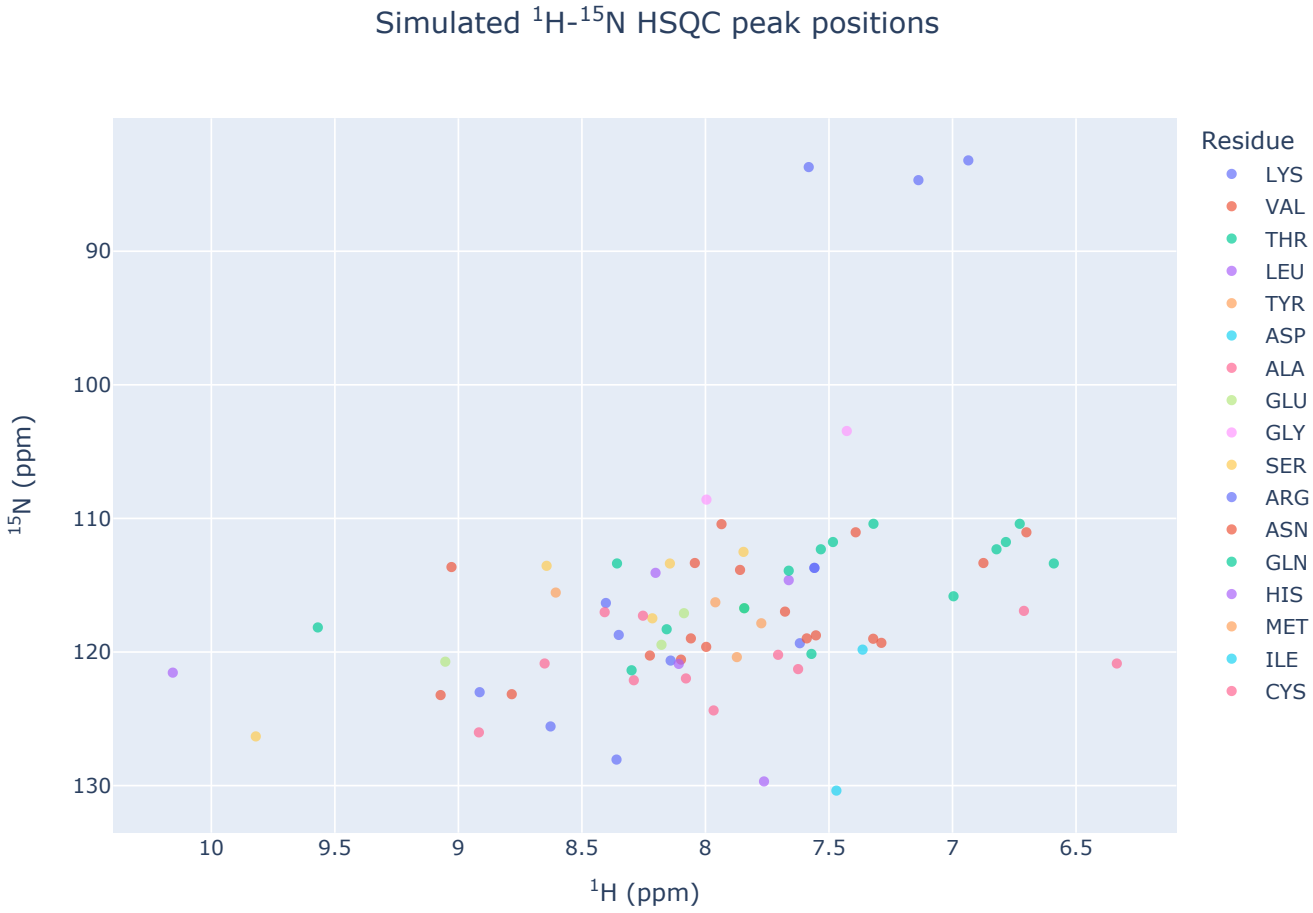


5 Order parameter

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



6 Simulated peak positions



7 LACS

Place holder for LACS results

8 Analysis data

place holder for the numerical values and tables.