

Full wwPDB NMR Structure Validation Report (i)

Apr 16, 2023 – 08:04 AM EDT

PDB ID	:	8BM4
BMRB ID	:	34768
Title	:	Hairpin adopted by modified oligonucleotide A32_mod found in the promoter of AUTS2 gene.
Authors	:	Novotny, A.
Deposited on	:	2022-11-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

Clashscore

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment is 30%.

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.

Metri	: Р	Percentile Ranks		
Clashscore			0	
	Worse		Better	
	Percentile relative to all structure	es		
	Percentile relative to all NMR st	tructures		
ЪЛани	Whole arch	ive NMR archiv	/e	
Metr	$\mathbf{c} (\# \text{Entries})$	s) (#Entries)		

158937

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 <=5%

12864

Mol	Chain	Length	Quality of chain		
1	А	32	28%	69%	•



2 Ensemble composition and analysis (i)

This entry contains 10 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1018 atoms, of which 356 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called A32_mod.

Mol	Chain	Residues			Ator	ns			Trace
1	Λ	32	Total	С	Н	Ν	0	Р	0
1	A	52	1018	312	356	138	181	31	0



4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: A32_mod

Chain A:	28%	69%	•
61 42 63 63 63 63 63 64 61 61 612 612	614 614 A16 A16 A16 A16 C19 C19 C19 C21 C21 C21 C21 C21 C25 C26 C26 C26 C26 C26 C26 C26 C26 C26 C26		

4.2 Scores per residue for each member of the ensemble

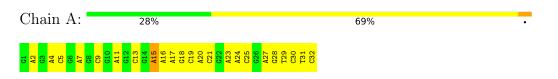
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1



4.2.2 Score per residue for model 2

• Molecule 1: A32_mod





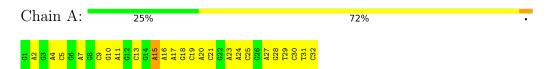
4.2.3 Score per residue for model 3

• Molecule 1: A32_mod



4.2.4 Score per residue for model 4

• Molecule 1: A32_mod



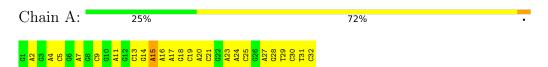
4.2.5 Score per residue for model 5

 \bullet Molecule 1: A32_mod

Chain A:	22%	75%	•
<mark>G1</mark> A2 G3 A4 C5 G6 G5 A7	G8 C9 C9 C9 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	019 021 021 022 022 022 022 022 023 023 023 023 023	

4.2.6 Score per residue for model 6

• Molecule 1: A32_mod



4.2.7 Score per residue for model 7

 \bullet Molecule 1: A32_mod





G1 A2

A4 C5 C5 A7 A7

4.2.8Score per residue for model 8

• Molecule 1: A32_mod

<mark>8</mark> ຄ

Chain A: 28% 69% •

Score per residue for model 9 4.2.9

• Molecule 1: A32_mod

Chain A:	28%	69% ·
G1 A2 A2 A4 A7 A7 G1 G1 C9 G1 C9 A11 C1 C9 C9 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	C13 A16 A16 A16 A16 C19 C19 C26 A23 A23 A23 A23 A23 C26 C26 C26 C26 C26 C26 C26 C26 C26 C26	

4.2.10Score per residue for model 10

• Molecule 1: A32_mod

Chain A:	22%	75%	•
G1 A2 G3 A4 C5 G6 G6	GB C9 610 610 612 613 613 8115 613 8116 613 618 618	C19 C21 C21 C21 C22 C25 C25 C25 C25 C25 C25 C25 C22 C22	



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Amber	structure calculation	2020

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	200
Number of shifts mapped to atoms	200
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	30%



6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles		
	Unam	RMSZ	$\#Z{>}5$	RMSZ	#Z > 5	
1	А	$1.63 {\pm} 0.00$	$0{\pm}0/747~(~0.0{\pm}~0.0\%)$	2.43 ± 0.01	$58{\pm}2/1152~(~5.1{\pm}~0.1\%)$	
All	All	1.63	0/7470~(~0.0%)	2.43	585/11520~(~5.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	А	$0.0{\pm}0.0$	$1.0{\pm}0.0$
All	All	0	10

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Trune	Atoma	Z	Observed(0)		Models	
	Chain	nes	Type	Atoms		$\mathbf{Observed}(^{o})$	$\mathrm{Ideal}(^{o})$	Worst	Total
1	А	15	DA	N1-C6-N6	-9.96	112.63	118.60	2	10
1	А	20	DA	N1-C6-N6	-9.74	112.76	118.60	7	10
1	А	27	DA	N1-C6-N6	-9.69	112.79	118.60	8	10
1	А	23	DA	N1-C6-N6	-9.54	112.88	118.60	6	10
1	А	16	DA	N1-C6-N6	-9.44	112.93	118.60	7	10
1	А	17	DA	N1-C6-N6	-9.10	113.14	118.60	1	10
1	А	7	DA	N1-C6-N6	-9.06	113.16	118.60	8	10
1	А	4	DA	N1-C6-N6	-8.89	113.26	118.60	8	10
1	А	27	DA	C5-C6-N1	8.73	122.06	117.70	1	10
1	А	7	DA	C5-C6-N1	8.36	121.88	117.70	5	10
1	А	2	DA	N1-C6-N6	-8.34	113.59	118.60	7	10
1	А	24	DA	N1-C6-N6	-8.32	113.61	118.60	9	10
1	А	15	DA	O4'-C1'-N9	8.26	113.78	108.00	6	10
1	А	11	DA	N1-C6-N6	-8.14	113.71	118.60	1	10
1	А	17	DA	C5-C6-N1	8.05	121.73	117.70	1	10

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Mol	nued from	Res			Z	Observed (0)	Ideal(0)	Mo	dels
IVIOI	Chain	Res	Type	Atoms		$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$	Worst	Total
1	А	11	DA	C5-C6-N1	7.93	121.67	117.70	9	10
1	А	13	DC	N3-C2-O2	-7.89	116.38	121.90	1	10
1	А	15	DA	C5-C6-N1	7.82	121.61	117.70	2	10
1	А	16	DA	C5-C6-N1	7.73	121.57	117.70	4	10
1	А	24	DA	C5-C6-N1	7.72	121.56	117.70	6	10
1	А	20	DA	C5-C6-N1	7.69	121.54	117.70	7	10
1	А	30	DC	N3-C2-O2	-7.65	116.54	121.90	4	10
1	А	32	DC	N3-C2-O2	-7.55	116.61	121.90	2	10
1	А	23	DA	C5-C6-N1	7.52	121.46	117.70	1	10
1	А	2	DA	C5-C6-N1	7.47	121.44	117.70	9	10
1	А	25	DC	N3-C2-O2	-7.41	116.71	121.90	6	10
1	А	4	DA	C5-C6-N1	7.40	121.40	117.70	3	10
1	А	20	DA	C4-C5-C6	-7.37	113.31	117.00	7	10
1	А	9	DC	N3-C2-O2	-7.37	116.74	121.90	2	10
1	А	27	DA	C4-C5-C6	-7.32	113.34	117.00	1	10
1	А	15	DA	C4-C5-C6	-7.24	113.38	117.00	8	10
1	А	5	DC	N3-C2-O2	-7.21	116.85	121.90	1	10
1	А	11	DA	C4-C5-C6	-7.05	113.47	117.00	9	10
1	А	7	DA	C4-C5-C6	-7.02	113.49	117.00	5	10
1	А	17	DA	C4-C5-C6	-6.91	113.55	117.00	1	10
1	А	4	DA	C4-C5-C6	-6.89	113.55	117.00	8	10
1	А	24	DA	C4-C5-C6	-6.87	113.56	117.00	4	10
1	А	23	DA	C4-C5-C6	-6.87	113.57	117.00	6	10
1	А	2	DA	C4-C5-C6	-6.80	113.60	117.00	3	10
1	А	13	DC	N1-C2-O2	6.78	122.97	118.90	1	10
1	А	11	DA	O4'-C1'-N9	6.76	112.73	108.00	1	10
1	А	19	DC	N3-C2-O2	-6.66	117.24	121.90	3	10
1	А	21	DC	N3-C2-O2	-6.64	117.25	121.90	6	10
1	А	16	DA	C4-C5-C6	-6.60	113.70	117.00	5	10
1	А	2	DA	O4'-C1'-N9	6.27	112.39	108.00	9	1
1	А	32	DC	N1-C2-O2	6.09	122.55	118.90	1	10
1	А	30	DC	N1-C2-O2	6.07	122.54	118.90	6	10
1	А	25	DC	N1-C2-O2	6.03	122.52	118.90	6	10
1	А	31	DT	C6-C5-C7	-6.02	119.29	122.90	6	10
1	А	5	DC	N1-C2-O2	5.99	122.49	118.90	1	10
1	А	15	DA	P-O3'-C3'	5.95	126.84	119.70	10	2
1	А	29	DT	C6-C5-C7	-5.74	119.45	122.90	9	10
1	А	21	DC	N1-C2-O2	5.71	122.33	118.90	5	10
1	А	18	DG	O4'-C1'-N9	5.69	111.99	108.00	1	1
1	А	32	DC	O4'-C1'-N1	5.66	111.97	108.00	9	1
1	А	9	DC	N1-C2-O2	5.51	122.20	118.90	2	10

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	Chain	hain Des Turne		A t a m a a	7	Oh a survey $\mathbf{d}(\theta)$		Models	
Mol	Chain	Res	Type	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$	Worst	Total
1	А	28	DG	O4'-C4'-C3'	5.49	109.29	106.00	7	10
1	А	18	DG	N1-C6-O6	-5.44	116.64	119.90	1	9
1	А	19	DC	N1-C2-O2	5.44	122.17	118.90	10	10
1	А	19	DC	N3-C4-C5	5.38	124.05	121.90	8	7
1	А	10	DG	O4'-C1'-N9	5.33	111.73	108.00	4	3
1	А	19	DC	O4'-C4'-C3'	5.28	109.17	106.00	8	3
1	А	31	DT	N3-C2-O2	-5.19	119.19	122.30	10	6
1	А	14	DG	O4'-C4'-C3'	5.14	109.09	106.00	1	3
1	А	29	DT	O4'-C4'-C3'	5.12	109.08	106.00	4	4
1	А	23	DA	O4'-C1'-N9	5.04	111.53	108.00	6	2
1	А	12	DG	O4'-C1'-N9	5.03	111.52	108.00	5	1
1	А	13	DC	O4'-C4'-C3'	5.02	109.01	106.00	8	1
1	А	12	DG	N1-C6-O6	-5.00	116.90	119.90	8	1

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There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	А	15	DA	Sidechain	10

6.2 Too-close contacts (i)

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
All	All	6620	3560	3560	-

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is -.

There are no clashes.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

There are no protein molecules in this entry.



6.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 30% for the well-defined parts and 30% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping (i)

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	200
Number of shifts mapped to atoms	200
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 30%, i.e. 194 atoms were assigned a chemical shift out of a possible 647. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N
Sugar	150/384~(39%)	150/224~(67%)	0/160~(0%)	0/0 (%)
Base	44/263~(17%)	44/167~(26%)	0/53~(0%)	0/43~(0%)
Overall	194/647~(30%)	194/391~(50%)	0/213~(0%)	0/43~(0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 194 atoms were assigned a chemical shift out of a possible 647. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Sugar	150/384~(39%)	150/224~(67%)	0/160~(0%)	0/0 (%)
Base	44/263~(17%)	44/167~(26%)	0/53~(0%)	0/43~(0%)
Overall	194/647~(30%)	194/391~(50%)	0/213~(0%)	0/43~(0%)

7.1.4 Statistically unusual chemical shifts (i)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	А	7	DA	H2'	1.01	1.39 - 3.84	-6.6
1	А	27	DA	H2'	1.12	1.39 - 3.84	-6.1

7.1.5 Random Coil Index (RCI) plots (i)

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

