Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1AFZ
Title	:	SOLUTION NMR STRUCTURE OF AN 11 BASE-PAIR OLIGONUCLEOTIDE FROM THE HUMAN N-RAS PROTOONCOGENE ENCODING FOR AMINO ACIDS 11-13 OF P21, MINIMIZED AVERAGE STRUCTURE
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Deposited on	:	1997-03-18

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

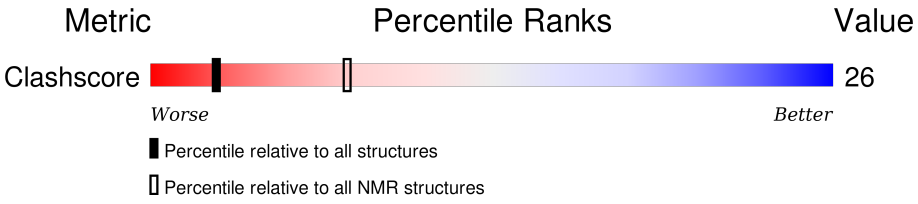
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment was not calculated.

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.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133

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%

Mol	Chain	Length	Quality of chain
1	A	11	45% 55%
2	B	11	100%

2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 694 atoms, of which 249 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*GP*GP*CP*AP*GP*GP*TP*GP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	11	356	109	125	47	65	10	0

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*CP*CP*AP*CP*CP*TP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	11	338	103	124	38	63	10	0

4 Residue-property plots (i)

These plots are provided for all protein, RNA and DNA 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: DNA (5'-D(*GP*GP*CP*AP*GP*GP*TP*GP*GP*TP*G)-3')

Chain A:

- Molecule 2: DNA (5'-D(*CP*AP*CP*CP*AP*CP*CP*TP*GP*CP*C)-3')

Chain B:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *NOE-RESTRAINED MOLECULAR DYNAMICS/SIMULATED ANNEALING*.

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *THIS STRUCTURE PROVIDED THE BEST-FIT FOR THE NOE DATA BASED ON THE RELAXATION MATRIX ANALYSIS USING CORMA.*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
FELIX	structure solution	
X-PLOR	structure solution	
MARDIGRAS	structure solution	
CORMA	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.24	2/260 (0.8%)	3.22	34/402 (8.5%)
2	B	1.49	0/238 (0.0%)	6.12	54/363 (14.9%)
All	All	1.36	2/498 (0.4%)	4.82	88/765 (11.5%)

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	DT	C5-C7	5.18	1.53	1.50
1	A	7	DT	C5-C7	5.02	1.53	1.50

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	13	DA	O5'-P-OP1	-30.18	74.48	110.70
1	A	4	DA	O5'-P-OP1	-25.48	80.13	110.70
2	B	21	DC	O5'-P-OP2	-23.46	82.55	110.70
2	B	19	DT	O5'-P-OP1	-22.84	83.30	110.70
2	B	18	DC	O5'-P-OP2	21.90	136.98	110.70
2	B	16	DA	O5'-P-OP2	-21.64	84.73	110.70
2	B	14	DC	O5'-P-OP1	-21.52	84.88	110.70
2	B	22	DC	O5'-P-OP2	-21.22	85.24	110.70
2	B	14	DC	O5'-P-OP2	20.34	135.11	110.70
2	B	16	DA	O5'-P-OP1	20.15	134.88	110.70
2	B	22	DC	O5'-P-OP1	20.12	134.84	110.70
2	B	17	DC	O3'-P-O5'	-19.32	67.30	104.00
2	B	15	DC	O3'-P-O5'	-19.21	67.50	104.00
2	B	19	DT	O5'-P-OP2	18.98	133.48	110.70
2	B	12	DC	O3'-P-O5'	-18.93	68.03	104.00
2	B	21	DC	O3'-P-O5'	-18.89	68.10	104.00
2	B	13	DA	O3'-P-O5'	-18.82	68.24	104.00
1	A	3	DC	O3'-P-O5'	-18.65	68.57	104.00
2	B	21	DC	O5'-P-OP1	18.65	133.07	110.70
2	B	20	DG	O3'-P-O5'	-18.52	68.80	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	18	DC	O3'-P-O5'	-18.44	68.96	104.00
2	B	18	DC	O5'-P-OP1	-18.23	88.82	110.70
1	A	4	DA	O5'-P-OP2	16.48	130.48	110.70
1	A	4	DA	OP1-P-OP2	-14.88	97.28	119.60
2	B	17	DC	OP2-P-O3'	-14.85	72.52	105.20
2	B	19	DT	OP1-P-OP2	-14.65	97.63	119.60
2	B	21	DC	OP1-P-OP2	-14.59	97.71	119.60
2	B	13	DA	OP2-P-O3'	-14.16	74.04	105.20
2	B	21	DC	OP1-P-O3'	-14.13	74.11	105.20
2	B	13	DA	O5'-P-OP2	14.02	127.53	110.70
2	B	15	DC	OP1-P-O3'	-13.88	74.66	105.20
2	B	13	DA	OP1-P-OP2	-13.64	99.14	119.60
2	B	18	DC	OP2-P-O3'	-13.61	75.25	105.20
2	B	12	DC	OP1-P-O3'	13.59	135.10	105.20
2	B	22	DC	OP1-P-OP2	-13.57	99.24	119.60
2	B	14	DC	OP1-P-OP2	-13.46	99.42	119.60
2	B	20	DG	OP1-P-O3'	-13.26	76.02	105.20
2	B	16	DA	OP1-P-OP2	-13.13	99.91	119.60
1	A	3	DC	OP1-P-O3'	12.33	132.33	105.20
1	A	3	DC	OP2-P-O3'	-12.07	78.65	105.20
2	B	18	DC	OP1-P-OP2	-11.68	102.08	119.60
2	B	20	DG	OP2-P-O3'	11.10	129.62	105.20
2	B	18	DC	OP1-P-O3'	10.82	129.00	105.20
2	B	21	DC	OP2-P-O3'	10.07	127.36	105.20
2	B	15	DC	OP2-P-O3'	9.98	127.16	105.20
2	B	13	DA	OP1-P-O3'	9.82	126.80	105.20
1	A	8	DG	N7-C8-N9	9.17	117.69	113.10
1	A	11	DG	N7-C8-N9	9.10	117.65	113.10
1	A	2	DG	N7-C8-N9	9.05	117.62	113.10
2	B	12	DC	OP2-P-O3'	-9.04	85.32	105.20
1	A	5	DG	N7-C8-N9	8.94	117.57	113.10
1	A	9	DG	N7-C8-N9	8.93	117.57	113.10
1	A	1	DG	N7-C8-N9	8.91	117.55	113.10
1	A	6	DG	N7-C8-N9	8.90	117.55	113.10
2	B	17	DC	OP1-P-O3'	8.89	124.75	105.20
2	B	20	DG	N7-C8-N9	8.78	117.49	113.10
1	A	4	DA	N7-C8-N9	7.83	117.72	113.80
1	A	8	DG	C8-N9-C4	-7.56	103.38	106.40
2	B	16	DA	N7-C8-N9	7.46	117.53	113.80
2	B	13	DA	N7-C8-N9	7.33	117.47	113.80
1	A	2	DG	C8-N9-C4	-7.23	103.51	106.40
1	A	11	DG	C8-N9-C4	-7.00	103.60	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	DG	C8-N9-C4	-6.72	103.71	106.40
1	A	6	DG	C8-N9-C4	-6.61	103.76	106.40
1	A	9	DG	C8-N9-C4	-6.60	103.76	106.40
1	A	5	DG	C8-N9-C4	-6.57	103.77	106.40
1	A	4	DA	C8-N9-C4	-6.10	103.36	105.80
2	B	20	DG	C8-N9-C4	-6.03	103.99	106.40
1	A	7	DT	C6-C5-C7	-5.93	119.34	122.90
2	B	17	DC	O4'-C1'-N1	5.83	112.08	108.00
2	B	19	DT	C6-C5-C7	-5.81	119.41	122.90
2	B	20	DG	O4'-C1'-N9	5.78	112.04	108.00
2	B	20	DG	C5-N7-C8	-5.50	101.55	104.30
1	A	3	DC	O4'-C1'-N1	5.41	111.79	108.00
1	A	4	DA	P-O3'-C3'	5.35	126.12	119.70
2	B	13	DA	O4'-C1'-N9	5.27	111.69	108.00
1	A	11	DG	C5-N7-C8	-5.21	101.69	104.30
2	B	15	DC	O4'-C1'-N1	5.20	111.64	108.00
2	B	21	DC	O4'-C1'-N1	5.18	111.63	108.00
1	A	9	DG	C5-N7-C8	-5.16	101.72	104.30
1	A	10	DT	C6-C5-C7	-5.16	119.80	122.90
1	A	10	DT	O4'-C1'-N1	5.13	111.59	108.00
1	A	5	DG	C5-N7-C8	-5.12	101.74	104.30
1	A	6	DG	C5-N7-C8	-5.12	101.74	104.30
1	A	1	DG	C5-N7-C8	-5.08	101.76	104.30
1	A	7	DT	C4-C5-C6	5.07	121.04	118.00
2	B	16	DA	C8-N9-C4	-5.05	103.78	105.80
1	A	10	DT	C4-C5-C6	5.02	121.01	118.00

There are no chirality outliers.

There are no planarity outliers.

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
1	A	231	125	125	5
2	B	214	124	124	13
All	All	445	249	249	18

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:8:DG:H2"	1:A:9:DG:O5'	0.83	1.71
1:A:4:DA:H2"	1:A:5:DG:O5'	0.78	1.79
2:B:21:DC:H2"	2:B:22:DC:O5'	0.58	1.98
2:B:17:DC:H2"	2:B:18:DC:C6	0.57	2.34
2:B:15:DC:H2"	2:B:16:DA:C8	0.56	2.35
1:A:2:DG:H2"	1:A:3:DC:O5'	0.54	2.03
2:B:13:DA:H2"	2:B:14:DC:O5'	0.53	2.03
2:B:15:DC:H2"	2:B:16:DA:O5'	0.52	2.05
2:B:20:DG:H2"	2:B:21:DC:O5'	0.51	2.05
2:B:17:DC:H2"	2:B:18:DC:O5'	0.51	2.06
2:B:20:DG:H2"	2:B:21:DC:C6	0.49	2.43
1:A:3:DC:H2"	1:A:4:DA:O5'	0.46	2.10
1:A:3:DC:H2"	1:A:4:DA:C8	0.44	2.47
2:B:16:DA:H2"	2:B:17:DC:O5'	0.44	2.11
2:B:12:DC:H2"	2:B:13:DA:O5'	0.43	2.14
2:B:21:DC:H2"	2:B:22:DC:C6	0.42	2.49
2:B:18:DC:H2"	2:B:19:DT:O5'	0.42	2.14
2:B:21:DC:C2'	2:B:22:DC:O5'	0.40	2.66

6.3 Torsion angles

6.3.1 Protein backbone

There are no protein molecules in this entry.

6.3.2 Protein sidechains

There are no protein molecules in this entry.

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided