Full wwPDB NMR Structure Validation Report (i)

Aug 20, 2022 – 09:21 AM EDT

PDB ID	:	1X26
Title	:	Solution structure of the AA-mismatch DNA complexed with naphthyridine-azaquinolone
Authors	:	Nakatani, K.; Hagihara, S.; Goto, Y.; Kobori, A.; Hagihara, M.; Hayashi, G.; Kyo, M.; Nomura, M.; Mishima, M.; Kojima, C.
Deposited on	:	2005-04-20

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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	FAILED
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 was not calculated.

There are no overall percentile quality scores available for this entry.

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	9% 91%
2	B	11	100%

2 Ensemble composition and analysis (i)

This entry contains 30 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. 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

There are 3 unique types of molecules in this entry. The entry contains 816 atoms, of which 302 are hydrogens and 0 are deuteriums.

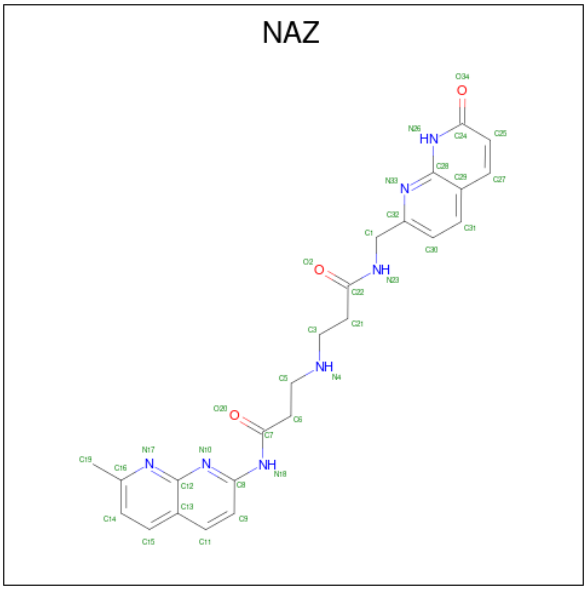
- Molecule 1 is a DNA chain called 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'.

Mol	Chain	Residues	Atoms						Trace
1	A	11	Total	C	H	N	O	P	0
			349	108	125	45	61	10	

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

Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	P	0
			349	108	127	39	65	10	

- Molecule 3 is N 3 -{3-[(7-METHYL-1,8-NAPHTHYRIDIN-2-YL)AMINO]-3-OXOPROPYL}-N 1 -[(7-OXO-7,8-DIHYDRO-1,8-NAPHTHYRIDIN-2-YL)METHYL]-BETA-ALANINAMIDE (three-letter code: NAZ) (formula: $C_{24}H_{25}N_7O_3$).



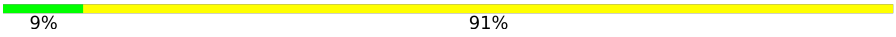
Mol	Chain	Residues	Atoms				
3	A	1	Total	C	H	N	O
			59	24	25	7	3
3	B	1	Total	C	H	N	O
			59	24	25	7	3

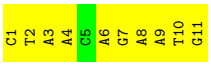
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

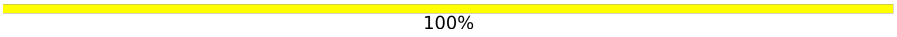
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

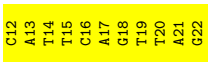
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 



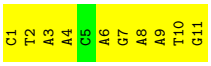
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



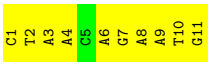
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

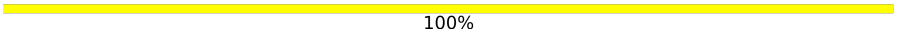
4.2.2 Score per residue for model 2

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

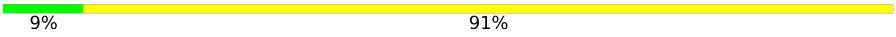


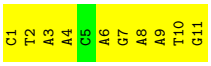
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

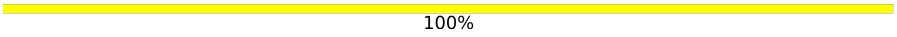
4.2.3 Score per residue for model 3

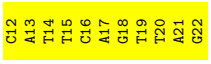
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

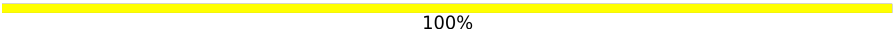


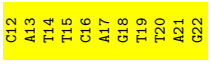
4.2.4 Score per residue for model 4

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

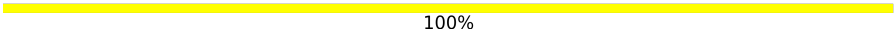
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

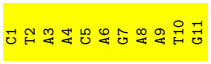
Chain B: 



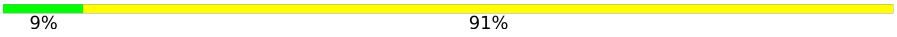
4.2.5 Score per residue for model 5

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

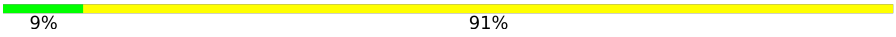


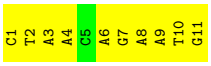
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

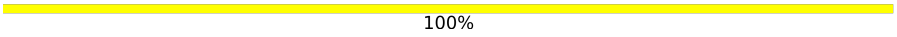
4.2.6 Score per residue for model 6

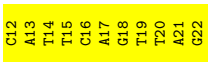
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

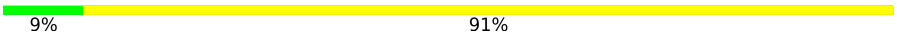


4.2.7 Score per residue for model 7

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

4.2.8 Score per residue for model 8

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 100%

C1 T2 A3 A4 C5 A6 G7 A8 A9 T10 G11

• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 100%

C12 A13 T14 T15 C16 A17 G18 T19 T20 A21 G22

4.2.9 Score per residue for model 9

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 9% 91%

C1 T2 A3 A4 C5 A6 G7 A8 A9 T10 G11

• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 9% 91%

C12 A13 T14 T15 C16 A17 G18 T19 T20 A21 G22

4.2.10 Score per residue for model 10

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 9% 91%

C1 T2 A3 A4 C5 A6 G7 A8 A9 T10 G11

• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

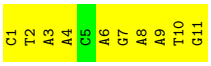
Chain B: 100%

C12 A13 T14 T15 C16 A17 G18 T19 T20 A21 G22

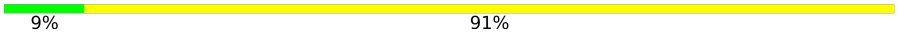
4.2.11 Score per residue for model 11

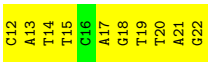
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



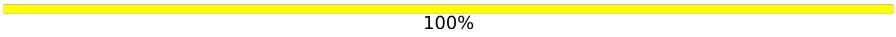
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

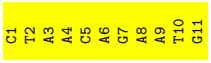
Chain B: 



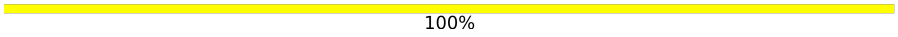
4.2.12 Score per residue for model 12

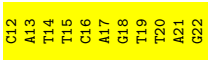
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

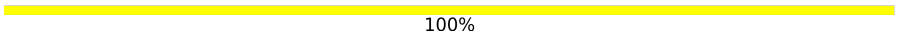


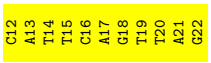
4.2.13 Score per residue for model 13

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

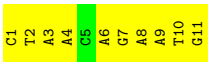
Chain B: 



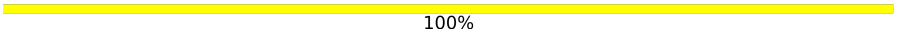
4.2.14 Score per residue for model 14

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

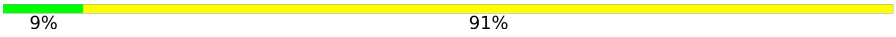


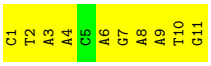
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

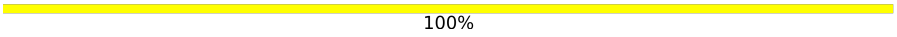
4.2.15 Score per residue for model 15

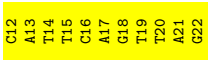
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



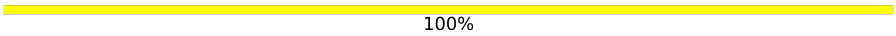
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

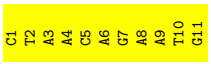
Chain B: 



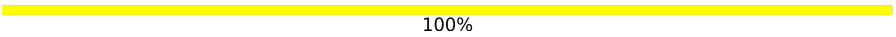
4.2.16 Score per residue for model 16

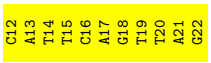
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



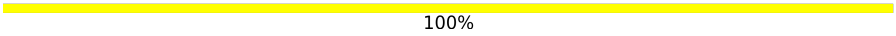
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

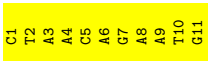
Chain B: 



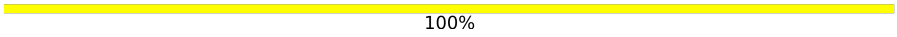
4.2.17 Score per residue for model 17

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

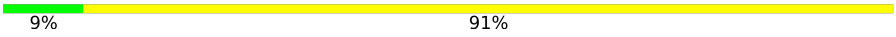


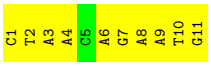
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

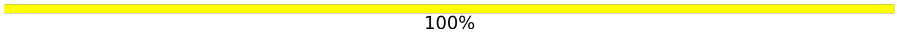
4.2.18 Score per residue for model 18

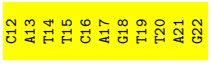
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

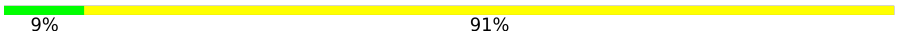


4.2.19 Score per residue for model 19

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

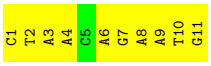
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

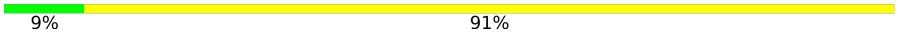
4.2.20 Score per residue for model 20

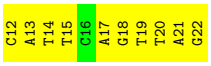
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



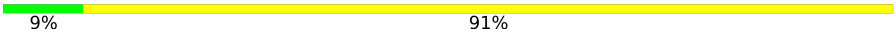
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

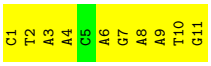
Chain B: 



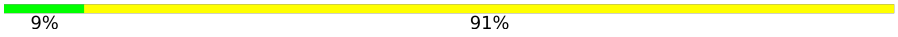
4.2.21 Score per residue for model 21

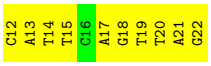
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

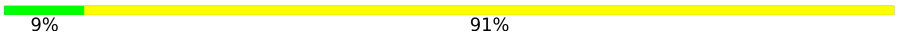


4.2.22 Score per residue for model 22

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

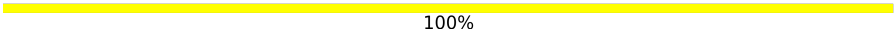
Chain A: 

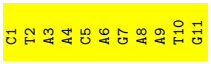
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

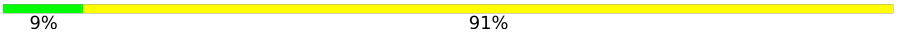
4.2.23 Score per residue for model 23

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

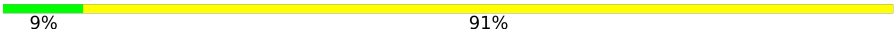


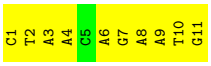
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

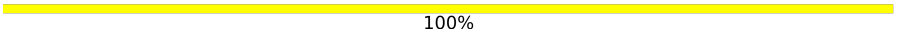
4.2.24 Score per residue for model 24

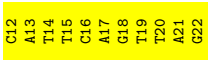
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

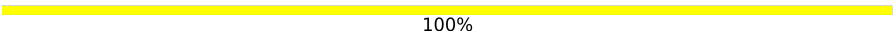


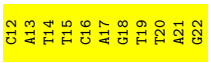
4.2.25 Score per residue for model 25

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

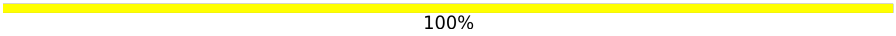
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

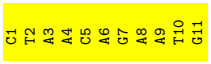
Chain B: 



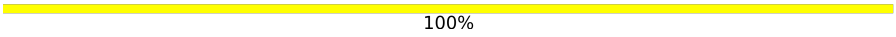
4.2.26 Score per residue for model 26

• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 

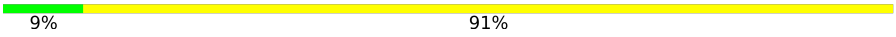


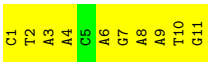
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 

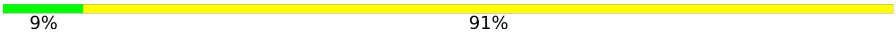
4.2.27 Score per residue for model 27

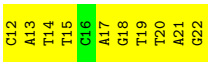
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



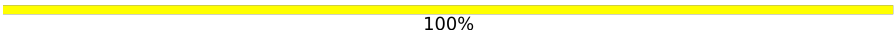
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

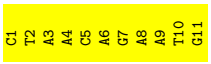
Chain B: 



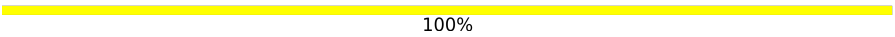
4.2.28 Score per residue for model 28

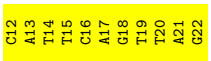
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

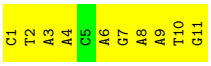
Chain B: 



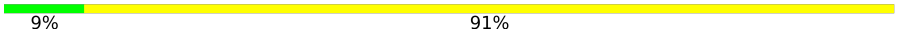
4.2.29 Score per residue for model 29

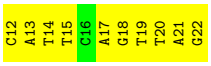
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



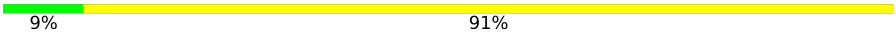
• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

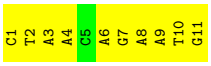
Chain B: 



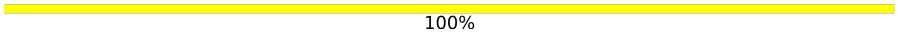
4.2.30 Score per residue for model 30

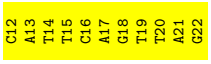
• Molecule 1: 5'-D(*CP*TP*AP*AP*CP*AP*GP*AP*AP*TP*G)-3'

Chain A: 



• Molecule 2: 5'-D(*CP*AP*TP*TP*CP*AP*GP*TP*TP*AP*G)-3'

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 30 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
MARDIGRAS	refinement	3.0
CNS	structure solution	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAZ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

6.2 Torsion angles

6.2.1 Protein backbone

There are no protein molecules in this entry.

6.2.2 Protein sidechains

There are no protein molecules in this entry.

6.2.3 RNA

There are no RNA molecules in this entry.

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

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

6.4 Carbohydrates

There are no monosaccharides in this entry.

6.5 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	NAZ	B	24	-	36,37,37	1.61±0.02	6±0 (16±0%)
3	NAZ	A	25	-	36,37,37	1.55±0.29	7±1 (19±3%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	NAZ	B	24	-	47,50,50	2.18±0.01	16±2 (34±3%)
3	NAZ	A	25	-	47,50,50	2.16±0.40	19±4 (40±7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAZ	B	24	-	-	0±0,17,17,17	0±0,4,4,4
3	NAZ	A	25	-	-	0±0,17,17,17	0±0,4,4,4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	24	NAZ	C32-N33	3.98	1.39	1.32	23	30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	24	NAZ	C28-N26	3.93	1.42	1.35	21	30
3	B	24	NAZ	C24-N26	3.77	1.39	1.33	2	30
3	A	25	NAZ	C32-N33	3.76	1.39	1.32	24	29
3	A	25	NAZ	C24-N26	3.73	1.39	1.33	30	29
3	A	25	NAZ	C28-N26	3.67	1.42	1.35	13	29
3	A	25	NAZ	C16-N17	3.09	1.39	1.33	28	29
3	B	24	NAZ	C16-N17	2.68	1.38	1.33	11	30
3	A	25	NAZ	C22-N23	2.61	1.39	1.33	21	29
3	B	24	NAZ	C22-N23	2.58	1.39	1.33	16	30
3	B	24	NAZ	C27-C29	2.57	1.48	1.41	6	30
3	A	25	NAZ	C27-C29	2.49	1.48	1.41	17	29
3	A	25	NAZ	C8-N10	2.28	1.39	1.33	1	29
3	A	25	NAZ	C7-N18	2.14	1.40	1.35	20	11

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	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	25	NAZ	C32-N33-C28	8.18	121.39	117.51	17	29
3	B	24	NAZ	C32-N33-C28	7.65	121.14	117.51	12	30
3	B	24	NAZ	C1-C32-N33	3.89	123.56	116.66	7	30
3	B	24	NAZ	C8-N18-C7	3.87	121.32	128.25	5	30
3	A	25	NAZ	C8-N18-C7	3.75	121.54	128.25	1	29
3	B	24	NAZ	C29-C28-N33	3.42	119.20	122.42	21	30
3	B	24	NAZ	C13-C12-N10	3.38	119.24	122.42	15	30
3	A	25	NAZ	C29-C28-N33	3.36	119.26	122.42	24	29
3	B	24	NAZ	C27-C29-C28	3.32	120.29	117.75	30	30
3	A	25	NAZ	C32-C1-N23	3.29	119.83	112.71	29	29
3	A	25	NAZ	C13-C12-N10	3.28	119.33	122.42	27	29
3	A	25	NAZ	C27-C29-C28	3.15	120.16	117.75	24	29
3	A	25	NAZ	C13-C12-N17	3.15	119.46	122.42	27	29
3	A	25	NAZ	C16-N17-C12	3.11	120.86	117.71	5	29
3	A	25	NAZ	C1-C32-N33	3.08	122.13	116.66	12	29
3	B	24	NAZ	C30-C32-N33	3.07	118.89	123.12	25	30
3	B	24	NAZ	C16-N17-C12	3.05	120.80	117.71	29	30
3	B	24	NAZ	N33-C28-N26	2.99	121.32	116.24	27	30
3	B	24	NAZ	C31-C29-C28	2.96	120.01	117.75	16	30
3	B	24	NAZ	C28-N26-C24	2.93	120.97	116.85	4	30
3	A	25	NAZ	C31-C29-C28	2.90	119.97	117.75	29	29
3	A	25	NAZ	C30-C32-N33	2.81	119.26	123.12	28	29
3	A	25	NAZ	C28-N26-C24	2.79	120.77	116.85	10	29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	25	NAZ	N33-C28-N26	2.75	120.90	116.24	24	29
3	B	24	NAZ	C13-C12-N17	2.72	119.86	122.42	5	30
3	A	25	NAZ	C11-C13-C12	2.65	119.77	117.75	2	29
3	B	24	NAZ	C11-C13-C12	2.61	119.75	117.75	15	30
3	A	25	NAZ	C6-C7-N18	2.52	119.03	114.59	24	29
3	B	24	NAZ	C3-C21-C22	2.39	108.39	112.36	11	10
3	A	25	NAZ	C15-C13-C12	2.38	119.57	117.75	27	29
3	B	24	NAZ	C15-C13-C12	2.28	119.49	117.75	3	19
3	B	24	NAZ	O20-C7-N18	2.24	119.54	123.63	7	10
3	B	24	NAZ	O2-C22-N23	2.23	118.81	123.01	21	3
3	A	25	NAZ	O20-C7-N18	2.21	119.59	123.63	19	17
3	A	25	NAZ	N17-C12-N10	2.21	121.21	115.97	27	29
3	A	25	NAZ	C9-C8-N10	2.19	118.84	123.30	11	29
3	A	25	NAZ	C19-C16-N17	2.18	120.80	117.23	18	24
3	B	24	NAZ	C19-C16-N17	2.17	120.78	117.23	11	29
3	B	24	NAZ	C1-C32-C30	2.14	117.01	121.48	7	5
3	A	25	NAZ	O20-C7-C6	2.12	118.14	122.02	16	10
3	B	24	NAZ	C32-C1-N23	2.10	117.26	112.71	26	2
3	A	25	NAZ	C1-N23-C22	2.10	119.07	122.34	14	5
3	B	24	NAZ	N17-C12-N10	2.04	120.81	115.97	15	11
3	B	24	NAZ	C9-C8-N10	2.04	119.15	123.30	4	4
3	B	24	NAZ	C1-N23-C22	2.04	119.17	122.34	12	2
3	B	24	NAZ	C21-C22-N23	2.01	119.81	116.42	16	1

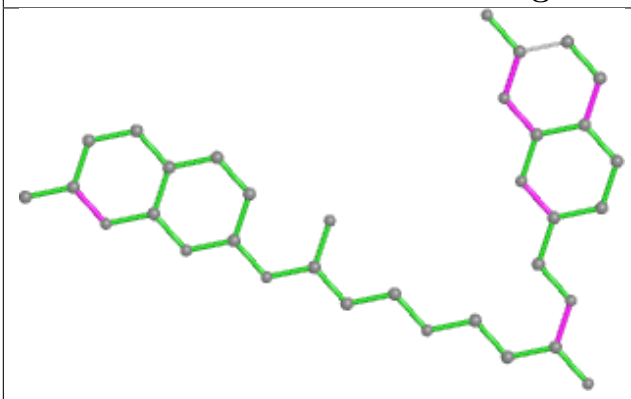
There are no chirality outliers.

There are no torsion outliers.

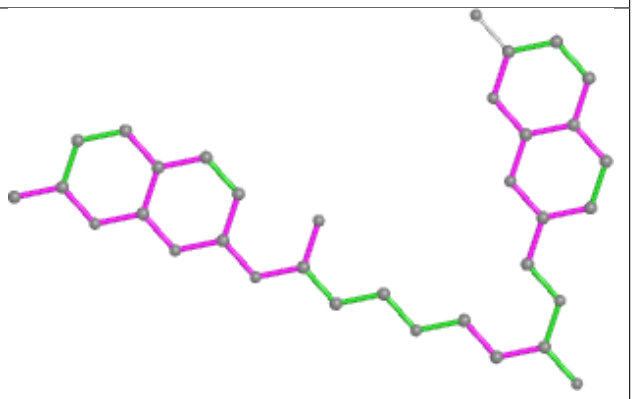
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

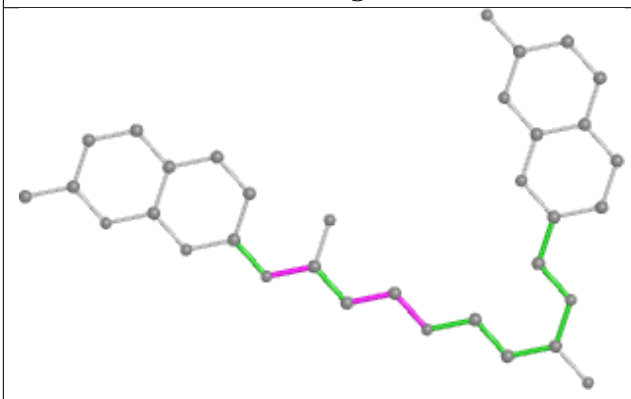
Ligand NAZ B 24



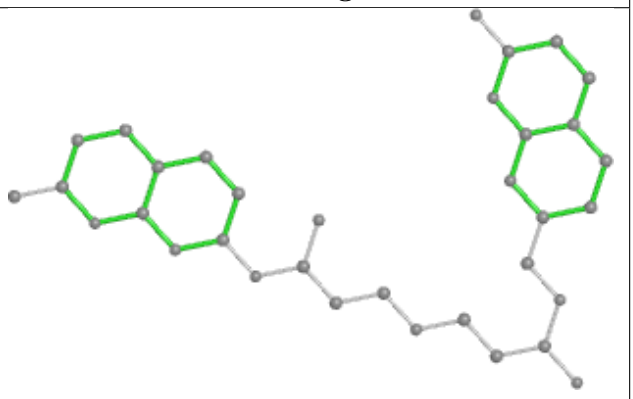
Bond lengths



Bond angles

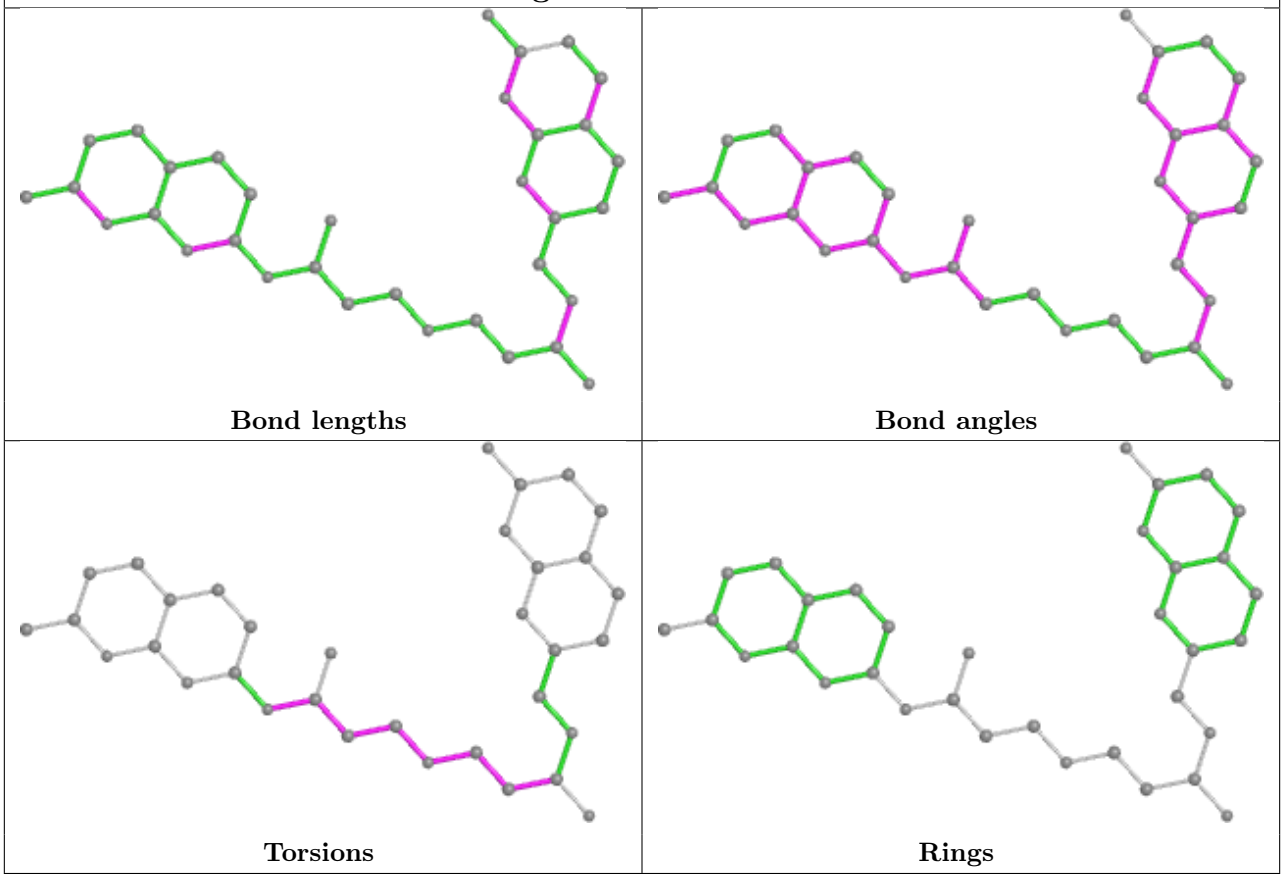


Torsions



Rings

Ligand NAZ A 25



6.6 Other polymers (i)

There are no such molecules in this entry.

6.7 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided