



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:27 AM UTC

PDB ID : 1NK2 / pdb_00001nk2
Title : VND/NK-2 HOMEODOMAIN/DNA COMPLEX, NMR, 20 STRUCTURES
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Deposited on : 1998-05-06

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

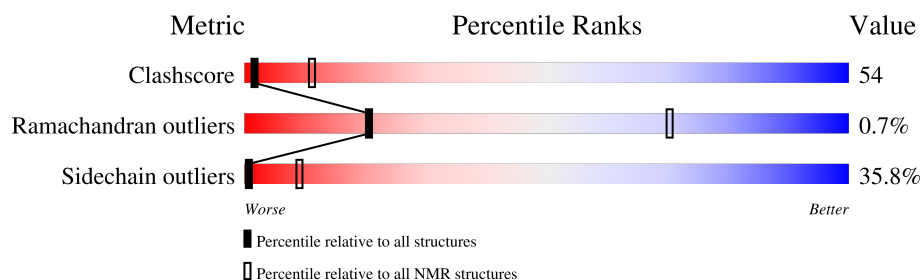
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	16	
2	B	16	
3	P	77	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	P:116-P:161 (46)	0.18	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 10, 12, 13, 14, 15, 18, 19, 20
2	11, 16
Single-model clusters	9; 17

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2358 atoms, of which 1045 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms						Trace
1	A	16	Total	C	H	N	O	P	0
			513	158	184	58	98	15	

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

Mol	Chain	Residues	Atoms						Trace
2	B	16	Total	C	H	N	O	P	0
			501	154	180	62	90	15	

- Molecule 3 is a protein called HOMEBOX PROTEIN VND.

Mol	Chain	Residues	Atoms					Trace
3	P	77	Total	C	H	N	O	0
			1344	416	681	134	113	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	101	ALA	GLY	conflict	UNP P22808

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: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A: 



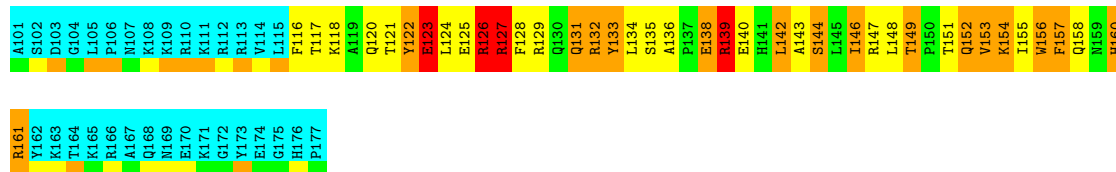
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B: 



- Molecule 3: HOMEBOX PROTEIN VND

Chain P: 

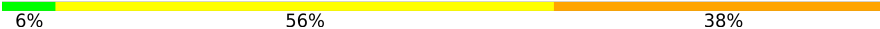


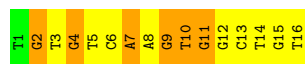
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

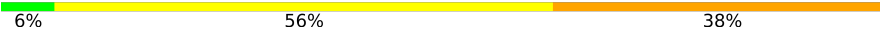
4.2.1 Score per residue for model 1

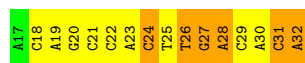
- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A: 

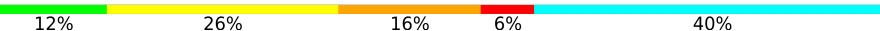


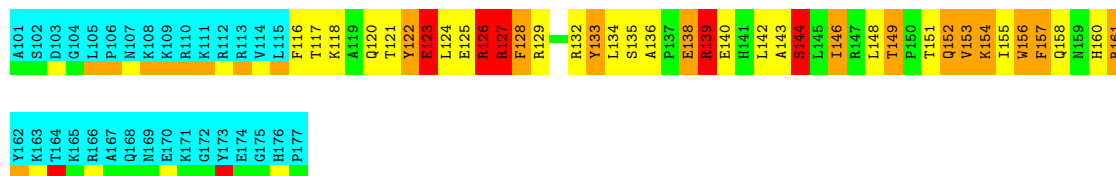
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B: 



- Molecule 3: HOMEBOX PROTEIN VND

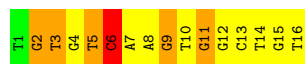
Chain P: 



4.2.2 Score per residue for model 2

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A: 



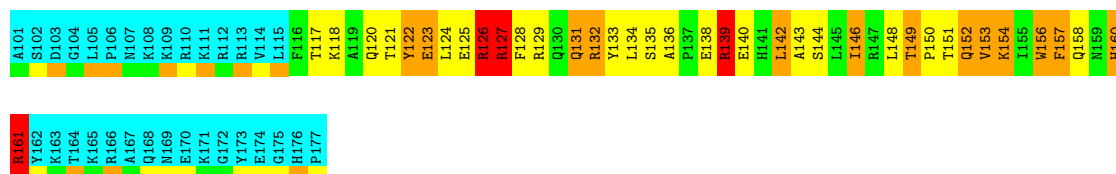
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B: 



- Molecule 3: HOMEBOX PROTEIN VND

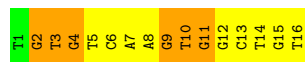
Chain P: 



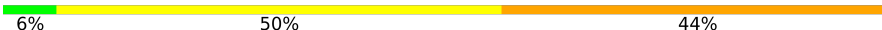
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A: 



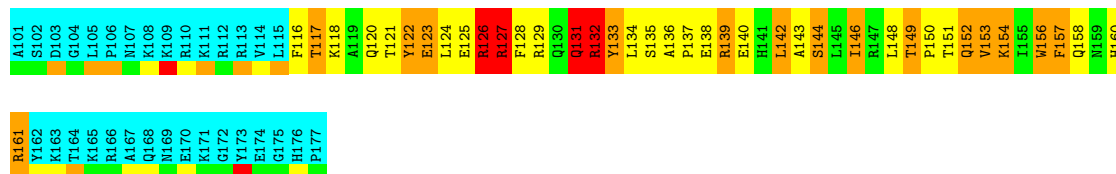
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B: 



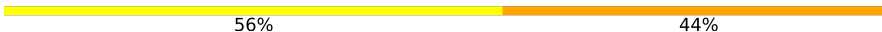
- Molecule 3: HOMEBOX PROTEIN VND

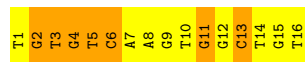
Chain P: 



4.2.4 Score per residue for model 4

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A: 



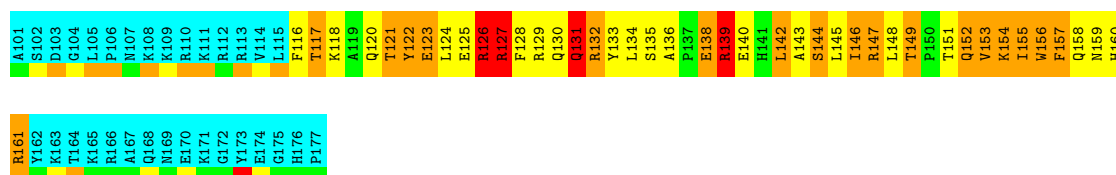
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B: 



- Molecule 3: HOMEBOX PROTEIN VND

Chain P: 

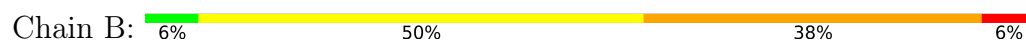


4.2.5 Score per residue for model 5

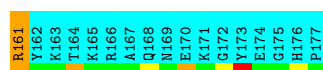
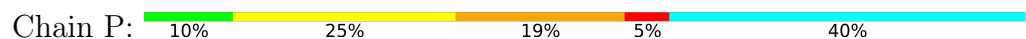
- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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

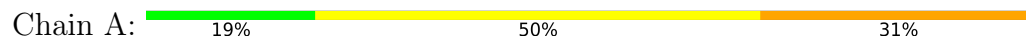


- Molecule 3: HOMEBOX PROTEIN VND

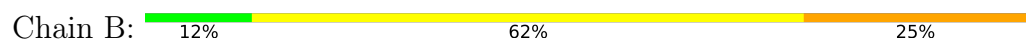


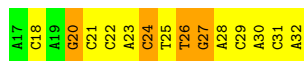
4.2.6 Score per residue for model 6

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

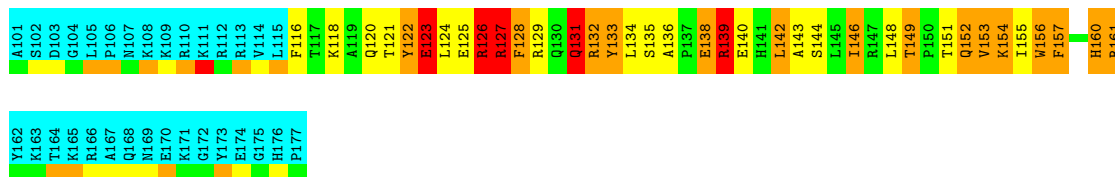
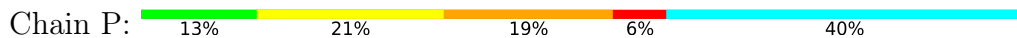


- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')





• Molecule 3: HOMEBOX PROTEIN VND



4.2.7 Score per residue for model 7

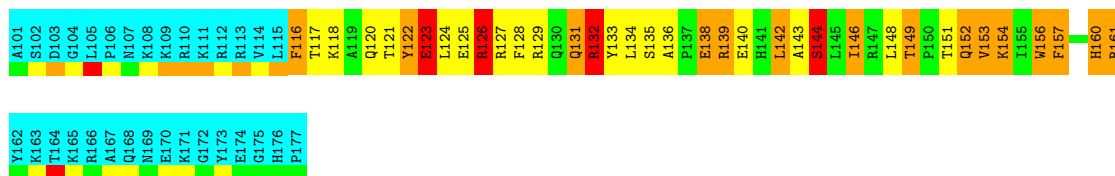
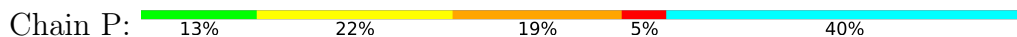
• Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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



• Molecule 3: HOMEBOX PROTEIN VND



4.2.8 Score per residue for model 8

• Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

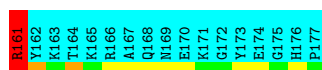
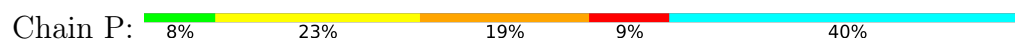




- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

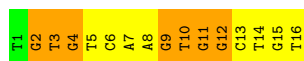


- Molecule 3: HOMEBOX PROTEIN VND

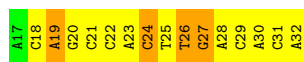
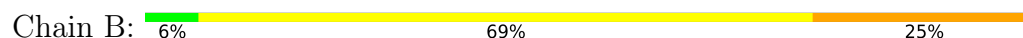


4.2.9 Score per residue for model 9

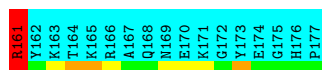
- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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



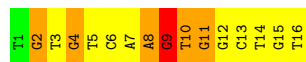
- Molecule 3: HOMEBOX PROTEIN VND



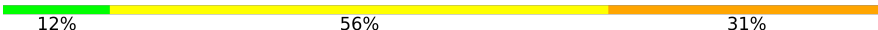
4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A: 



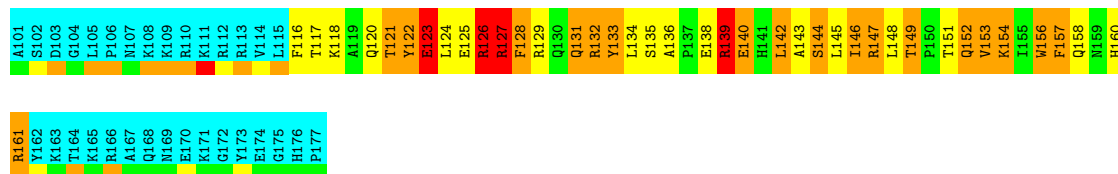
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B: 



- Molecule 3: HOMEBOX PROTEIN VND

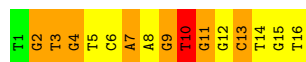
Chain P: 



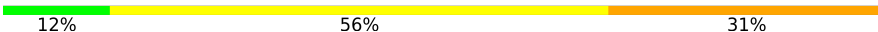
4.2.11 Score per residue for model 11

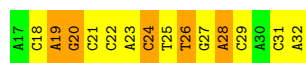
- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A: 



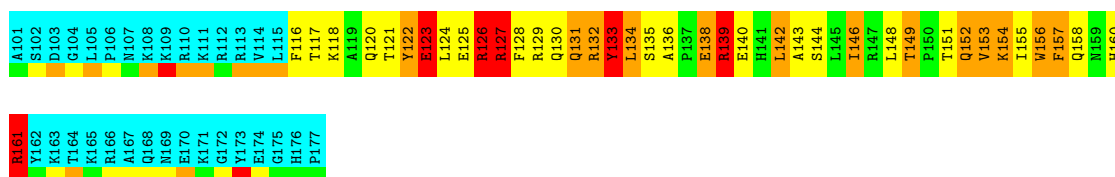
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B: 



- Molecule 3: HOMEBOX PROTEIN VND

Chain P: 

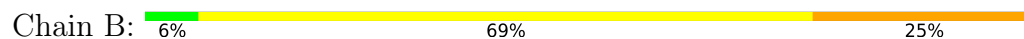


4.2.12 Score per residue for model 12

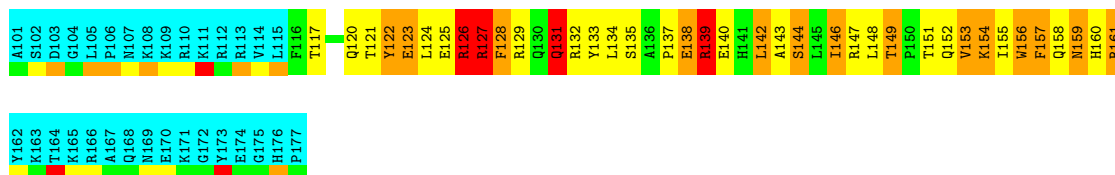
- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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

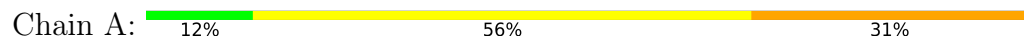


- Molecule 3: HOMEBOX PROTEIN VND



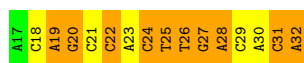
4.2.13 Score per residue for model 13

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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



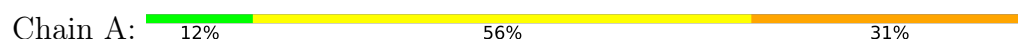


• Molecule 3: HOMEBOX PROTEIN VND



4.2.14 Score per residue for model 14

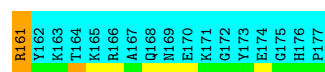
• Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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



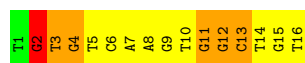
• Molecule 3: HOMEBOX PROTEIN VND



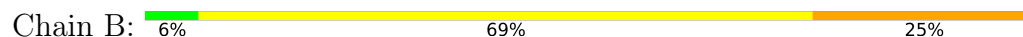
4.2.15 Score per residue for model 15

• Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

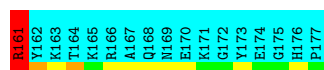
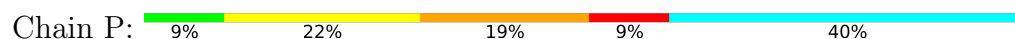




- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

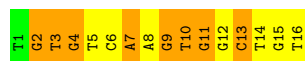


- Molecule 3: HOMEBOX PROTEIN VND

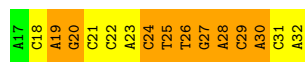


4.2.16 Score per residue for model 16

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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



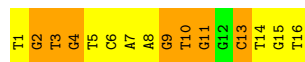
- Molecule 3: HOMEBOX PROTEIN VND



4.2.17 Score per residue for model 17

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A:  6% 50% 44%

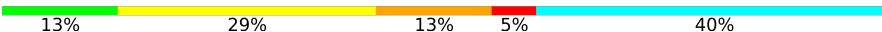


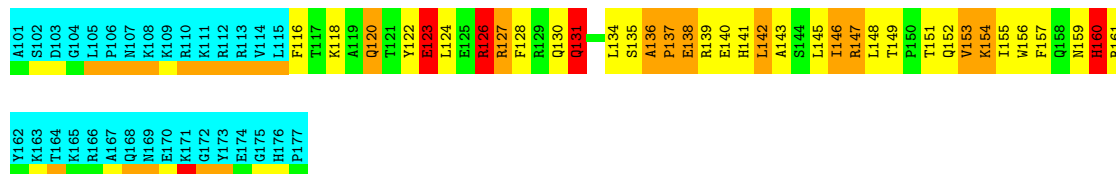
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B:  6% 44% 50%



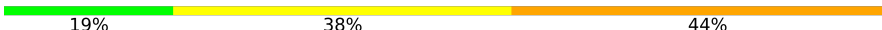
- Molecule 3: HOMEBOX PROTEIN VND

Chain P:  13% 29% 13% 5% 40%



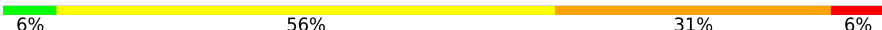
4.2.18 Score per residue for model 18

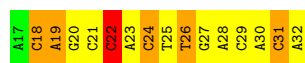
- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

Chain A:  19% 38% 44%



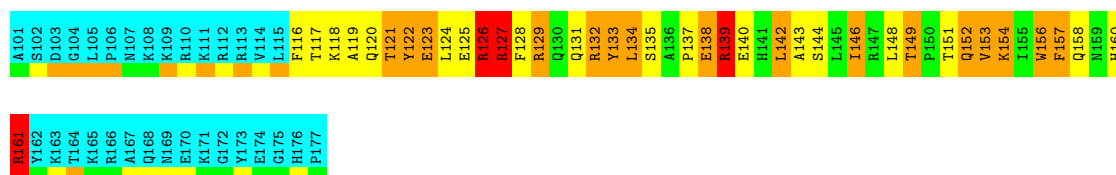
- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')

Chain B:  6% 56% 31% 6%



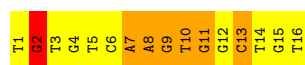
- Molecule 3: HOMEBOX PROTEIN VND

Chain P:  10% 23% 21% 5% 40%

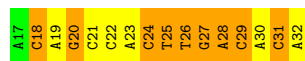


4.2.19 Score per residue for model 19

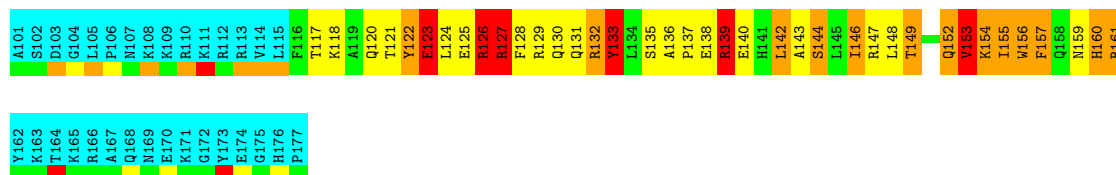
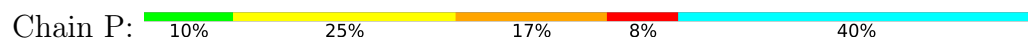
- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')



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

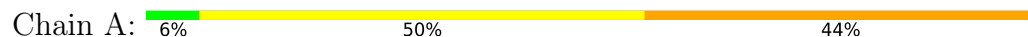


- Molecule 3: HOMEBOX PROTEIN VND

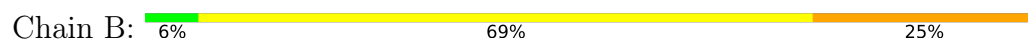


4.2.20 Score per residue for model 20

- Molecule 1: DNA (5'-D(*TP*GP*TP*GP*TP*CP*AP*AP*GP*TP*GP*GP*CP*TP*GP*T)-3')

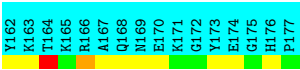
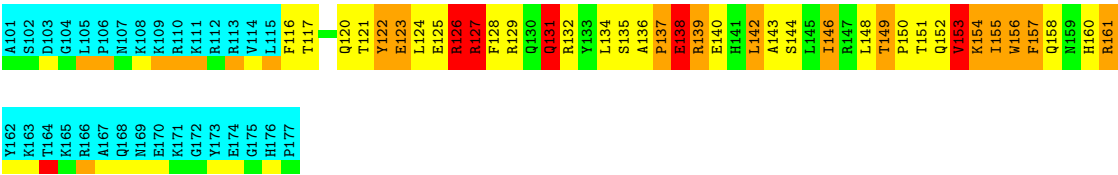
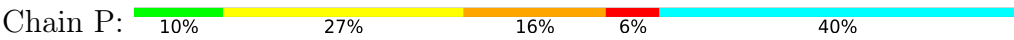


- Molecule 2: DNA (5'-D(*AP*CP*AP*GP*CP*CP*AP*CP*TP*TP*GP*AP*CP*AP*CP*A)-3')





● Molecule 3: HOMEBOX PROTEIN VND



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY/ SIMULATED ANNEALING*.

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
INSIGHT II 97 AUTHOR : MSI	refinement	MSI
NMR REFINER	structure solution	REFINE

No chemical shift data was provided.

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	1.02±0.02	0±0/368 (0.0± 0.0%)	1.29±0.03	1±1/568 (0.1± 0.2%)
2	B	1.01±0.01	0±0/360 (0.0± 0.0%)	1.25±0.03	0±1/552 (0.1± 0.1%)
3	P	1.94±0.10	7±1/418 (1.6± 0.4%)	1.91±0.06	8±4/564 (1.5± 0.7%)
All	All	1.43	131/22920 (0.6%)	1.52	187/33680 (0.6%)

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	A	0.0±0.0	7.0±1.2
2	B	0.0±0.0	8.0±1.2
3	P	0.0±0.0	2.6±1.1
All	All	0	353

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	P	133	TYR	C-N	6.45	1.42	1.33	18	7
3	P	149	THR	C-N	6.31	1.42	1.33	1	18
3	P	132	ARG	NE-CZ	5.70	1.39	1.33	15	18
3	P	127	ARG	NE-CZ	5.55	1.39	1.33	12	17
3	P	141	HIS	CG-CD2	5.49	1.41	1.35	17	1
3	P	161	ARG	NE-CZ	5.42	1.39	1.33	18	7
3	P	156	TRP	CG-CD2	5.40	1.53	1.43	3	19
3	P	136	ALA	CA-C	5.27	1.58	1.52	15	17
3	P	136	ALA	C-N	5.23	1.40	1.33	5	12
3	P	139	ARG	NE-CZ	5.20	1.38	1.33	18	8
3	P	160	HIS	CE1-NE2	5.18	1.37	1.32	17	1
3	P	141	HIS	CE1-NE2	5.14	1.37	1.32	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	P	130	GLN	C-N	5.12	1.39	1.33	11	2
3	P	137	PRO	N-CA	5.10	1.54	1.47	17	1
3	P	149	THR	CA-C	5.02	1.59	1.53	19	2

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(°)	Ideal(°)	Models	
								Worst	Total
3	P	159	ASN	CA-CB-CG	10.95	123.55	112.60	17	4
3	P	141	HIS	ND1-CE1-NE2	9.85	118.25	108.40	17	1
3	P	160	HIS	ND1-CE1-NE2	9.80	118.20	108.40	17	1
3	P	159	ASN	OD1-CG-ND2	-9.71	112.89	122.60	17	1
1	A	3	DT	P-O3'-C3'	9.49	134.43	120.20	15	1
3	P	135	SER	N-CA-CB	8.78	123.77	110.42	9	1
3	P	139	ARG	CA-CB-CG	8.59	131.28	114.10	12	19
3	P	160	HIS	CE1-NE2-CD2	-8.25	100.75	109.00	17	1
3	P	141	HIS	CE1-NE2-CD2	-8.22	100.78	109.00	17	1
3	P	131	GLN	CB-CG-CD	8.16	126.47	112.60	17	1
2	B	22	DC	P-O3'-C3'	8.08	132.32	120.20	18	3
1	A	4	DG	P-O3'-C3'	7.83	131.94	120.20	4	1
3	P	130	GLN	OE1-CD-NE2	-7.31	115.29	122.60	17	1
1	A	2	DG	P-O3'-C3'	7.28	131.12	120.20	19	2
3	P	130	GLN	CG-CD-NE2	7.15	127.12	116.40	17	1
1	A	6	DC	P-O3'-C3'	6.90	130.56	120.20	2	1
3	P	161	ARG	N-CA-CB	6.78	120.80	110.28	6	1
3	P	138	GLU	CA-CB-CG	6.77	127.64	114.10	15	5
3	P	141	HIS	CA-CB-CG	6.71	120.52	113.80	17	1
3	P	159	ASN	CB-CG-ND2	6.57	126.25	116.40	17	5
3	P	155	ILE	N-CA-CB	6.56	117.77	110.62	19	4
3	P	120	GLN	OE1-CD-NE2	-6.55	116.05	122.60	17	1
3	P	138	GLU	N-CA-CB	6.20	119.24	109.82	12	2
3	P	140	GLU	CA-CB-CG	6.19	126.49	114.10	15	1
1	A	11	DG	P-O3'-C3'	6.15	129.43	120.20	5	1
2	B	31	DC	P-O3'-C3'	6.15	129.42	120.20	18	1
3	P	126	ARG	CG-CD-NE	6.02	125.24	112.00	17	20
2	B	18	DC	P-O3'-C3'	5.98	129.17	120.20	5	1
1	A	10	DT	P-O3'-C3'	5.97	129.15	120.20	17	2
3	P	120	GLN	CG-CD-NE2	5.91	125.26	116.40	17	1
1	A	5	DT	P-O3'-C3'	5.88	129.01	120.20	2	1
3	P	130	GLN	CB-CG-CD	5.78	122.43	112.60	17	1
3	P	123	GLU	CB-CG-CD	5.77	122.41	112.60	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	DA	C2'-C3'-O3'	5.76	120.14	111.50	5	1
3	P	141	HIS	CB-CG-CD2	-5.75	123.73	131.20	17	1
3	P	131	GLN	CA-CB-CG	5.65	125.40	114.10	20	9
3	P	133	TYR	CB-CA-C	-5.62	104.33	111.70	11	1
3	P	123	GLU	CA-CB-CG	5.62	125.33	114.10	5	18
3	P	152	GLN	N-CA-CB	5.58	118.93	110.28	7	16
3	P	152	GLN	N-CA-C	-5.54	105.40	111.82	1	10
3	P	149	THR	CA-C-N	5.49	124.95	119.24	2	4
3	P	149	THR	C-N-CA	5.49	124.95	119.24	2	4
1	A	1	DT	P-O3'-C3'	5.47	128.41	120.20	4	1
3	P	152	GLN	CG-CD-NE2	5.46	124.59	116.40	17	1
3	P	149	THR	N-CA-CB	5.37	116.53	110.03	18	4
3	P	152	GLN	OE1-CD-NE2	-5.37	117.23	122.60	17	1
1	A	8	DA	P-O3'-C3'	5.31	128.17	120.20	10	1
3	P	119	ALA	CA-C-N	5.30	127.33	120.44	18	1
3	P	119	ALA	C-N-CA	5.30	127.33	120.44	18	1
3	P	132	ARG	CA-CB-CG	5.30	124.69	114.10	8	1
3	P	144	SER	N-CA-CB	5.20	117.85	110.16	5	9
3	P	134	LEU	N-CA-CB	5.18	119.06	110.52	11	2
1	A	9	DG	P-O3'-C3'	5.15	127.93	120.20	10	1
2	B	29	DC	P-O3'-C3'	5.08	127.82	120.20	16	1
3	P	138	GLU	CA-C-O	5.05	126.10	120.90	17	1
3	P	157	PHE	N-CA-CB	5.05	117.63	110.16	20	1
3	P	137	PRO	CB-CA-C	-5.05	104.29	112.62	20	1
3	P	136	ALA	CA-C-N	5.04	125.32	119.47	17	1
3	P	136	ALA	C-N-CA	5.04	125.32	119.47	17	1
3	P	121	THR	N-CA-CB	5.04	117.48	109.82	15	4
3	P	130	GLN	N-CA-C	-5.03	107.22	113.55	13	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	11	DG	Sidechain	20
2	B	24	DC	Sidechain	20
2	B	26	DT	Sidechain	20
2	B	32	DA	Sidechain	20
1	A	2	DG	Sidechain	19
2	B	20	DG	Sidechain	19
1	A	9	DG	Sidechain	18

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Mol	Chain	Res	Type	Group	Models (Total)
3	P	157	PHE	Sidechain	18
1	A	4	DG	Sidechain	17
3	P	122	TYR	Sidechain	17
2	B	25	DT	Sidechain	16
1	A	10	DT	Sidechain	15
2	B	27	DG	Sidechain	15
1	A	3	DT	Sidechain	15
1	A	12	DG	Sidechain	14
1	A	13	DC	Sidechain	13
2	B	28	DA	Sidechain	11
2	B	19	DA	Sidechain	10
2	B	31	DC	Sidechain	8
3	P	128	PHE	Sidechain	8
2	B	18	DC	Sidechain	8
3	P	133	TYR	Sidechain	7
2	B	29	DC	Sidechain	6
1	A	7	DA	Sidechain	5
2	B	22	DC	Sidechain	5
1	A	6	DC	Sidechain	2
2	B	30	DA	Sidechain	2
1	A	5	DT	Sidechain	1
3	P	116	PHE	Sidechain	1
1	A	1	DT	Sidechain	1
1	A	8	DA	Sidechain	1
3	P	127	ARG	Sidechain	1

6.2 Too-close contacts

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	329	184	184	31±5
2	B	321	180	180	23±4
3	P	407	411	409	49±6
All	All	21140	15500	15460	1978

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 54.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:146:ILE:HD11	3:P:148:LEU:HD12	1.12	1.18	18	20
3:P:139:ARG:CZ	3:P:154:LYS:HG2	0.93	1.92	12	15
3:P:123:GLU:CD	3:P:146:ILE:HG22	0.91	1.91	16	8
3:P:139:ARG:NH2	3:P:154:LYS:HG3	0.90	1.81	7	2
1:A:7:DA:H2''	1:A:8:DA:H5'	0.87	1.46	18	3
3:P:153:VAL:HG13	3:P:157:PHE:CE2	0.85	2.05	12	12
3:P:146:ILE:HD11	3:P:148:LEU:CD1	0.84	2.00	7	20
1:A:7:DA:H2''	1:A:8:DA:H5''	0.84	1.48	15	9
1:A:13:DC:C6	1:A:14:DT:H72	0.84	2.07	12	2
1:A:15:DG:C2'	1:A:16:DT:H71	0.84	2.03	1	13
1:A:15:DG:C4	1:A:16:DT:H71	0.83	2.07	5	6
3:P:146:ILE:CD1	3:P:148:LEU:HD12	0.83	2.03	15	20
3:P:139:ARG:CZ	3:P:154:LYS:HG3	0.82	2.03	9	4
1:A:15:DG:H2''	1:A:16:DT:H5'	0.80	1.52	5	2
3:P:153:VAL:HG13	3:P:157:PHE:CD2	0.77	2.13	12	14
3:P:127:ARG:CG	3:P:142:LEU:HD13	0.76	2.10	2	11
1:A:15:DG:H2''	1:A:16:DT:C5'	0.74	2.12	5	2
1:A:8:DA:H2''	1:A:9:DG:C5'	0.73	2.13	7	2
3:P:139:ARG:NE	3:P:154:LYS:HG2	0.72	1.98	12	11
3:P:136:ALA:HB3	3:P:137:PRO:HD3	0.72	1.61	17	2
1:A:14:DT:H2''	1:A:15:DG:H5''	0.72	1.61	9	8
3:P:128:PHE:N	3:P:157:PHE:HE1	0.72	1.81	12	17
1:A:15:DG:N9	1:A:16:DT:H71	0.71	1.99	2	14
1:A:8:DA:H2''	1:A:9:DG:H5''	0.71	1.63	3	8
3:P:123:GLU:OE2	3:P:146:ILE:HG22	0.71	1.84	2	2
2:B:21:DC:H2''	2:B:22:DC:H5''	0.71	1.60	15	1
3:P:127:ARG:HG2	3:P:142:LEU:HD13	0.70	1.63	20	6
1:A:2:DG:H2'	1:A:3:DT:H72	0.70	1.63	10	6
1:A:13:DC:H2'	1:A:14:DT:H71	0.68	1.64	16	1
3:P:124:LEU:HD22	3:P:156:TRP:HB3	0.68	1.65	1	19
3:P:156:TRP:CZ2	3:P:160:HIS:CE1	0.68	2.82	17	1
3:P:123:GLU:CG	3:P:146:ILE:HG22	0.67	2.18	9	18
1:A:2:DG:C2'	1:A:3:DT:H72	0.67	2.20	11	5
1:A:7:DA:C6	1:A:8:DA:C6	0.67	2.83	12	20
3:P:127:ARG:HG3	3:P:142:LEU:HD13	0.67	1.67	2	7
3:P:128:PHE:N	3:P:157:PHE:HE2	0.66	1.87	4	3
1:A:2:DG:C2'	1:A:3:DT:H71	0.66	2.20	7	5
3:P:149:THR:O	3:P:152:GLN:N	0.65	2.30	1	19
1:A:15:DG:H2'	1:A:16:DT:H71	0.65	1.67	15	6
3:P:140:GLU:O	3:P:144:SER:N	0.64	2.30	19	19
2:B:23:DA:C2	2:B:24:DC:C2	0.64	2.86	5	19
1:A:8:DA:H2''	1:A:9:DG:H5'	0.63	1.70	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:27:DG:C5	2:B:28:DA:C6	0.63	2.87	16	20
3:P:127:ARG:CD	3:P:134:LEU:HD11	0.63	2.23	15	6
2:B:25:DT:C2	2:B:26:DT:C4	0.63	2.85	12	9
2:B:28:DA:C2	2:B:29:DC:C2	0.63	2.86	14	15
1:A:8:DA:C5'	3:P:155:ILE:HG21	0.63	2.24	11	2
1:A:7:DA:C2'	1:A:8:DA:H5'	0.63	2.23	18	2
3:P:139:ARG:HB2	3:P:153:VAL:HG11	0.63	1.69	11	4
3:P:116:PHE:CD1	3:P:148:LEU:HD22	0.62	2.29	17	9
1:A:7:DA:C2'	1:A:8:DA:H5''	0.62	2.25	11	4
1:A:2:DG:H2'	1:A:3:DT:H71	0.62	1.71	7	3
1:A:7:DA:C2	1:A:8:DA:C2	0.61	2.88	5	20
1:A:9:DG:C5	1:A:10:DT:C4	0.61	2.88	18	19
1:A:8:DA:H5'	3:P:155:ILE:HG21	0.61	1.71	11	2
3:P:123:GLU:C	3:P:142:LEU:HD21	0.61	2.21	20	6
3:P:145:LEU:O	3:P:147:ARG:HD2	0.61	1.96	4	4
2:B:30:DA:C2	2:B:31:DC:C2	0.60	2.90	12	16
3:P:127:ARG:HD2	3:P:134:LEU:HD21	0.60	1.74	13	2
3:P:121:THR:HA	3:P:124:LEU:HD12	0.60	1.72	16	18
2:B:18:DC:C4	2:B:19:DA:C6	0.60	2.90	13	17
3:P:140:GLU:O	3:P:143:ALA:HB3	0.60	1.96	18	20
3:P:139:ARG:CZ	3:P:154:LYS:CG	0.60	2.80	10	18
1:A:9:DG:C2	1:A:10:DT:C2	0.60	2.90	17	4
1:A:6:DC:C5	1:A:7:DA:C6	0.60	2.90	14	18
1:A:1:DT:C4	2:B:32:DA:C2	0.60	2.90	7	1
2:B:27:DG:C2	2:B:28:DA:C2	0.59	2.90	12	13
3:P:132:ARG:O	3:P:133:TYR:HD1	0.59	1.80	6	3
3:P:133:TYR:HE1	3:P:161:ARG:CD	0.59	2.10	13	7
3:P:153:VAL:HG12	3:P:154:LYS:N	0.59	2.13	20	19
3:P:122:TYR:HE1	3:P:126:ARG:NH1	0.59	1.96	8	11
3:P:128:PHE:CA	3:P:157:PHE:HE1	0.59	2.11	9	15
3:P:132:ARG:C	3:P:133:TYR:HD1	0.59	2.05	6	1
3:P:123:GLU:HG3	3:P:146:ILE:HG22	0.58	1.75	13	11
3:P:116:PHE:CD1	3:P:148:LEU:CD2	0.58	2.87	17	13
3:P:129:ARG:HB3	3:P:129:ARG:NH1	0.58	2.14	11	3
3:P:122:TYR:CE1	3:P:126:ARG:CZ	0.58	2.87	8	12
3:P:125:GLU:O	3:P:129:ARG:N	0.58	2.34	10	19
3:P:133:TYR:CD1	3:P:161:ARG:CZ	0.58	2.87	15	6
1:A:2:DG:H2''	1:A:3:DT:H71	0.57	1.75	2	6
3:P:122:TYR:CZ	3:P:126:ARG:CZ	0.57	2.87	5	5
3:P:133:TYR:HE1	3:P:161:ARG:HD3	0.57	1.58	3	4
1:A:10:DT:C4	1:A:11:DG:C6	0.57	2.92	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:DG:C2	2:B:23:DA:C2	0.57	2.92	1	10
1:A:13:DC:H2'	1:A:14:DT:H72	0.57	1.74	20	3
1:A:8:DA:H2''	1:A:9:DG:C8	0.57	2.35	4	8
1:A:7:DA:C2	2:B:27:DG:C2	0.57	2.93	16	19
3:P:122:TYR:CE2	3:P:126:ARG:CZ	0.57	2.87	4	2
2:B:27:DG:C4	2:B:28:DA:C6	0.57	2.93	4	4
1:A:8:DA:H2''	1:A:9:DG:O5'	0.57	1.99	2	6
1:A:7:DA:C6	1:A:8:DA:N6	0.56	2.72	19	15
1:A:9:DG:C8	1:A:10:DT:C7	0.56	2.89	20	19
3:P:133:TYR:HD1	3:P:161:ARG:CZ	0.56	2.13	18	4
3:P:139:ARG:NE	3:P:154:LYS:HG3	0.56	2.16	17	5
2:B:21:DC:H2''	2:B:22:DC:C6	0.56	2.36	7	18
1:A:15:DG:C8	1:A:16:DT:H71	0.56	2.35	5	5
3:P:116:PHE:HD1	3:P:148:LEU:CD2	0.56	2.13	6	6
3:P:128:PHE:CE2	3:P:160:HIS:ND1	0.56	2.74	4	1
3:P:122:TYR:CE1	3:P:126:ARG:CG	0.56	2.88	7	9
2:B:28:DA:C2	2:B:29:DC:N3	0.56	2.74	5	17
1:A:6:DC:C2'	1:A:7:DA:C8	0.56	2.88	2	17
3:P:123:GLU:CG	3:P:146:ILE:CG2	0.56	2.83	7	12
1:A:4:DG:C5	1:A:5:DT:C4	0.56	2.93	13	20
1:A:5:DT:C2	1:A:6:DC:N3	0.55	2.75	20	20
1:A:6:DC:C5	1:A:7:DA:N6	0.55	2.74	17	18
1:A:1:DT:H73	1:A:2:DG:O6	0.55	2.00	19	1
1:A:13:DC:C5	1:A:14:DT:H72	0.55	2.35	12	2
1:A:9:DG:C8	1:A:10:DT:C5	0.55	2.94	17	7
3:P:133:TYR:CE1	3:P:161:ARG:CD	0.55	2.90	6	11
3:P:131:GLN:OE1	3:P:134:LEU:HD23	0.55	2.02	11	1
3:P:139:ARG:NE	3:P:154:LYS:CG	0.55	2.70	12	13
2:B:23:DA:N3	2:B:24:DC:C2	0.55	2.74	7	9
3:P:134:LEU:HD22	3:P:138:GLU:HG3	0.55	1.78	1	12
3:P:154:LYS:O	3:P:158:GLN:N	0.55	2.39	20	14
3:P:123:GLU:HB2	3:P:146:ILE:HG21	0.55	1.79	9	9
1:A:8:DA:C2'	1:A:9:DG:C8	0.55	2.90	5	9
1:A:5:DT:C2	1:A:6:DC:C2	0.55	2.95	9	19
3:P:156:TRP:CH2	3:P:160:HIS:CE1	0.54	2.95	17	1
3:P:128:PHE:N	3:P:157:PHE:CE1	0.54	2.74	19	17
2:B:26:DT:C2'	2:B:27:DG:C8	0.54	2.91	5	20
1:A:2:DG:N1	2:B:32:DA:C2	0.54	2.75	4	1
1:A:15:DG:C4	1:A:16:DT:C7	0.54	2.90	9	3
1:A:4:DG:C8	1:A:5:DT:H73	0.54	2.37	16	2
3:P:120:GLN:O	3:P:124:LEU:HD12	0.54	2.03	17	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:131:GLN:CD	3:P:134:LEU:HD23	0.54	2.27	11	1
1:A:15:DG:H2''	1:A:16:DT:H71	0.54	1.79	1	1
3:P:122:TYR:HE1	3:P:126:ARG:CZ	0.54	2.16	7	9
3:P:142:LEU:O	3:P:146:ILE:HG23	0.54	2.02	1	15
3:P:122:TYR:CE2	3:P:126:ARG:CG	0.54	2.90	18	2
2:B:24:DC:C5	2:B:25:DT:H73	0.54	2.38	8	8
3:P:128:PHE:N	3:P:157:PHE:CE2	0.54	2.76	17	3
2:B:26:DT:H2''	2:B:27:DG:C8	0.53	2.37	5	19
1:A:11:DG:N2	2:B:23:DA:C2	0.53	2.76	10	18
1:A:15:DG:C2'	1:A:16:DT:H73	0.53	2.33	3	1
3:P:134:LEU:HD22	3:P:138:GLU:CG	0.53	2.34	15	2
1:A:13:DC:N3	1:A:14:DT:C4	0.53	2.77	6	13
2:B:23:DA:C2	2:B:24:DC:N3	0.53	2.76	17	12
3:P:128:PHE:CZ	3:P:160:HIS:ND1	0.53	2.76	15	2
2:B:28:DA:C5	2:B:29:DC:C4	0.53	2.96	12	6
3:P:142:LEU:CD1	3:P:146:ILE:HD13	0.53	2.34	8	2
1:A:13:DC:C2'	1:A:14:DT:H72	0.53	2.33	4	2
1:A:7:DA:C2	2:B:27:DG:N2	0.52	2.77	16	19
1:A:6:DC:H2''	1:A:7:DA:C8	0.52	2.40	15	12
3:P:122:TYR:CZ	3:P:126:ARG:HG3	0.52	2.39	18	2
3:P:132:ARG:NH1	3:P:133:TYR:CE2	0.52	2.78	15	4
1:A:7:DA:C4	1:A:8:DA:C5	0.52	2.96	5	3
1:A:15:DG:C5	1:A:16:DT:H72	0.52	2.38	17	1
2:B:28:DA:C5	2:B:29:DC:N4	0.52	2.78	19	6
1:A:12:DG:H2''	1:A:13:DC:C6	0.52	2.40	5	1
3:P:128:PHE:CA	3:P:157:PHE:HE2	0.52	2.17	18	1
2:B:26:DT:C4	2:B:27:DG:C6	0.52	2.98	18	13
3:P:123:GLU:HB2	3:P:142:LEU:HD11	0.52	1.81	7	2
3:P:153:VAL:HG13	3:P:157:PHE:HE2	0.51	1.58	12	1
3:P:122:TYR:CD1	3:P:123:GLU:N	0.51	2.79	20	2
3:P:127:ARG:HB3	3:P:134:LEU:HD11	0.51	1.82	7	3
3:P:122:TYR:CE1	3:P:126:ARG:HG2	0.51	2.40	4	13
1:A:4:DG:C8	1:A:5:DT:C7	0.51	2.93	16	2
1:A:13:DC:C2	1:A:14:DT:C5	0.51	2.98	4	6
3:P:133:TYR:CE1	3:P:161:ARG:NH1	0.51	2.79	11	4
3:P:139:ARG:NH2	3:P:154:LYS:HG2	0.51	2.21	16	2
3:P:134:LEU:HD22	3:P:138:GLU:CB	0.51	2.36	15	2
2:B:30:DA:C2	2:B:31:DC:N3	0.51	2.79	16	12
3:P:155:ILE:HD13	3:P:158:GLN:OE1	0.51	2.06	12	2
3:P:147:ARG:O	3:P:147:ARG:HG3	0.51	2.05	13	1
3:P:122:TYR:CE2	3:P:126:ARG:NH1	0.51	2.79	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:128:PHE:CE1	3:P:160:HIS:ND1	0.51	2.79	15	1
1:A:4:DG:N2	2:B:29:DC:C2	0.51	2.79	17	1
3:P:155:ILE:HD13	3:P:158:GLN:CD	0.51	2.31	12	1
1:A:15:DG:H2''	1:A:16:DT:O5'	0.50	2.06	19	4
1:A:4:DG:C4	1:A:5:DT:C4	0.50	3.00	15	4
2:B:18:DC:C4	2:B:19:DA:N6	0.50	2.80	10	9
2:B:28:DA:C6	2:B:29:DC:N4	0.50	2.80	16	8
2:B:24:DC:H2''	2:B:25:DT:C5'	0.50	2.36	12	5
3:P:144:SER:O	3:P:147:ARG:HG3	0.50	2.06	4	3
3:P:150:PRO:O	3:P:154:LYS:N	0.50	2.40	13	1
2:B:18:DC:N3	2:B:19:DA:C6	0.50	2.80	10	6
2:B:26:DT:C2	2:B:27:DG:C5	0.50	3.00	5	11
3:P:123:GLU:OE1	3:P:146:ILE:HG22	0.50	2.06	16	3
2:B:22:DC:C5	2:B:23:DA:N6	0.50	2.79	19	2
3:P:132:ARG:NH1	3:P:133:TYR:CZ	0.50	2.80	3	1
1:A:15:DG:C6	2:B:18:DC:N3	0.50	2.80	9	2
3:P:121:THR:O	3:P:125:GLU:N	0.50	2.41	20	5
1:A:15:DG:C1'	1:A:16:DT:H71	0.49	2.36	1	2
1:A:10:DT:C2'	1:A:11:DG:C8	0.49	2.95	18	1
3:P:133:TYR:HE1	3:P:161:ARG:HD2	0.49	1.68	6	1
3:P:155:ILE:HD12	3:P:158:GLN:OE1	0.49	2.07	8	1
1:A:2:DG:C6	2:B:31:DC:N3	0.49	2.81	18	3
3:P:133:TYR:CD1	3:P:161:ARG:NH1	0.49	2.81	2	4
1:A:9:DG:H2''	1:A:10:DT:C5'	0.48	2.38	6	2
2:B:18:DC:C2'	2:B:19:DA:C8	0.48	2.96	10	1
1:A:2:DG:H2'	1:A:3:DT:C7	0.48	2.39	7	1
3:P:128:PHE:CD2	3:P:157:PHE:HD1	0.48	2.26	7	2
1:A:15:DG:C4	1:A:16:DT:C5	0.48	3.01	9	1
3:P:153:VAL:HG13	3:P:157:PHE:CD1	0.48	2.43	18	2
2:B:22:DC:H2''	2:B:23:DA:C8	0.48	2.44	20	6
3:P:132:ARG:C	3:P:133:TYR:CD1	0.48	2.91	6	1
3:P:128:PHE:CE1	3:P:160:HIS:CE1	0.48	3.02	15	1
2:B:28:DA:H2''	2:B:29:DC:C6	0.48	2.44	3	1
2:B:27:DG:C5	2:B:28:DA:N6	0.48	2.81	4	4
3:P:128:PHE:CA	3:P:157:PHE:CE2	0.48	2.96	18	1
3:P:120:GLN:C	3:P:124:LEU:HD12	0.48	2.34	17	3
3:P:120:GLN:CG	3:P:146:ILE:HG13	0.48	2.39	16	20
1:A:2:DG:H2''	1:A:3:DT:C5'	0.48	2.39	19	1
1:A:2:DG:N2	2:B:32:DA:C2	0.48	2.82	1	2
3:P:122:TYR:CD1	3:P:122:TYR:C	0.47	2.93	8	9
3:P:128:PHE:CE2	3:P:160:HIS:CE1	0.47	3.03	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:DA:H2''	1:A:9:DG:H8	0.47	1.70	4	6
1:A:3:DT:H2''	1:A:4:DG:C8	0.47	2.44	16	13
3:P:128:PHE:HD2	3:P:157:PHE:CD1	0.47	2.27	11	1
3:P:132:ARG:HG2	3:P:133:TYR:CD2	0.47	2.44	2	2
3:P:142:LEU:HD13	3:P:146:ILE:HG23	0.47	1.87	8	1
1:A:9:DG:C8	1:A:10:DT:H73	0.47	2.45	9	1
1:A:2:DG:C2'	1:A:3:DT:C7	0.47	2.92	2	7
2:B:20:DG:H2''	2:B:21:DC:C5	0.47	2.45	5	10
1:A:15:DG:H2''	1:A:16:DT:H73	0.47	1.85	3	1
1:A:13:DC:C2	1:A:14:DT:C4	0.47	3.03	4	4
3:P:133:TYR:CE1	3:P:161:ARG:HD3	0.47	2.45	13	2
3:P:153:VAL:HG13	3:P:157:PHE:CE1	0.47	2.44	18	1
1:A:6:DC:C4	1:A:7:DA:C6	0.46	3.03	17	7
3:P:123:GLU:HG2	3:P:146:ILE:CG2	0.46	2.41	15	12
3:P:122:TYR:CE1	3:P:126:ARG:NH1	0.46	2.83	8	5
3:P:156:TRP:O	3:P:156:TRP:CE3	0.46	2.68	12	20
3:P:127:ARG:C	3:P:157:PHE:HE2	0.46	2.18	17	1
3:P:128:PHE:CE2	3:P:160:HIS:HB3	0.46	2.46	1	15
3:P:139:ARG:NH2	3:P:154:LYS:CG	0.46	2.79	16	9
1:A:7:DA:N1	1:A:8:DA:N1	0.46	2.63	13	14
3:P:122:TYR:CE2	3:P:126:ARG:HG3	0.46	2.45	18	2
3:P:118:LYS:O	3:P:122:TYR:N	0.46	2.42	15	17
3:P:128:PHE:CA	3:P:157:PHE:CE1	0.46	2.98	10	7
3:P:124:LEU:HD22	3:P:156:TRP:CB	0.46	2.40	16	9
3:P:139:ARG:NH1	3:P:150:PRO:CB	0.46	2.79	20	3
3:P:131:GLN:HG3	3:P:134:LEU:CD2	0.46	2.40	7	13
1:A:5:DT:H2''	1:A:6:DC:C6	0.46	2.46	10	2
2:B:27:DG:H2''	2:B:28:DA:C8	0.46	2.46	6	18
1:A:13:DC:C2'	1:A:14:DT:C7	0.46	2.94	4	1
3:P:128:PHE:CD2	3:P:160:HIS:HB3	0.45	2.46	1	6
3:P:134:LEU:CD2	3:P:138:GLU:HG3	0.45	2.41	7	8
1:A:15:DG:C2'	1:A:16:DT:C7	0.45	2.90	11	3
1:A:15:DG:C5	1:A:16:DT:C7	0.45	3.00	5	1
1:A:10:DT:H2''	1:A:11:DG:C8	0.45	2.46	6	6
3:P:126:ARG:HG2	3:P:126:ARG:HH11	0.45	1.72	11	13
3:P:122:TYR:HE2	3:P:126:ARG:CZ	0.45	2.25	18	1
2:B:25:DT:H2'	2:B:26:DT:H71	0.45	1.88	11	1
1:A:9:DG:C5	1:A:10:DT:C5	0.45	3.05	5	1
1:A:13:DC:C6	1:A:14:DT:C7	0.45	3.00	16	1
3:P:120:GLN:OE1	3:P:148:LEU:HD21	0.45	2.12	17	4
1:A:9:DG:C8	1:A:10:DT:H71	0.45	2.46	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:134:LEU:HD22	3:P:138:GLU:HG2	0.45	1.89	15	1
3:P:139:ARG:HD3	3:P:153:VAL:HG12	0.44	1.88	11	1
3:P:129:ARG:CZ	3:P:129:ARG:HA	0.44	2.42	18	2
2:B:29:DC:H2''	2:B:30:DA:C8	0.44	2.48	17	3
2:B:24:DC:H2''	2:B:25:DT:H5'	0.44	1.90	8	4
3:P:128:PHE:HB2	3:P:157:PHE:CE1	0.44	2.48	19	5
3:P:128:PHE:CE1	3:P:160:HIS:HB3	0.44	2.48	14	2
1:A:7:DA:C5	1:A:8:DA:C6	0.44	3.06	19	2
3:P:122:TYR:CE2	3:P:126:ARG:NH2	0.43	2.85	4	1
1:A:8:DA:C4	1:A:9:DG:N7	0.43	2.86	7	1
3:P:144:SER:O	3:P:147:ARG:HD3	0.43	2.13	9	1
1:A:7:DA:H2''	1:A:8:DA:C5'	0.43	2.41	12	3
3:P:132:ARG:NH1	3:P:133:TYR:CD2	0.43	2.86	11	1
3:P:117:THR:O	3:P:121:THR:N	0.43	2.47	18	5
3:P:121:THR:CA	3:P:124:LEU:HD12	0.43	2.43	19	3
3:P:129:ARG:NE	3:P:129:ARG:HA	0.43	2.28	20	1
1:A:9:DG:C6	1:A:10:DT:C4	0.43	3.07	2	2
2:B:23:DA:H2''	2:B:24:DC:H5'	0.43	1.90	4	3
3:P:128:PHE:HD2	3:P:157:PHE:HD1	0.43	1.56	11	2
1:A:11:DG:H2''	1:A:12:DG:C8	0.43	2.49	7	4
2:B:24:DC:C5	2:B:25:DT:C7	0.43	3.02	3	2
2:B:23:DA:H2''	2:B:24:DC:C5'	0.43	2.44	4	1
3:P:132:ARG:HB3	3:P:133:TYR:CD1	0.43	2.48	6	1
3:P:142:LEU:HD13	3:P:146:ILE:CG2	0.43	2.43	8	1
3:P:127:ARG:HG2	3:P:127:ARG:NH1	0.43	2.28	20	1
1:A:13:DC:H2''	1:A:14:DT:C5'	0.43	2.43	3	1
3:P:128:PHE:CZ	3:P:161:ARG:HG3	0.43	2.49	6	1
1:A:9:DG:N2	2:B:25:DT:C2	0.43	2.87	8	1
3:P:157:PHE:HB3	3:P:161:ARG:NH2	0.43	2.29	13	5
3:P:132:ARG:HG2	3:P:133:TYR:CG	0.43	2.48	8	1
1:A:9:DG:H2'	1:A:10:DT:H71	0.43	1.91	15	1
3:P:123:GLU:CD	3:P:146:ILE:CG2	0.43	2.82	20	1
3:P:153:VAL:CG1	3:P:154:LYS:N	0.42	2.81	3	12
2:B:31:DC:C2	2:B:32:DA:C6	0.42	3.07	13	1
3:P:132:ARG:HD3	3:P:133:TYR:CD2	0.42	2.49	2	1
3:P:132:ARG:O	3:P:161:ARG:NE	0.42	2.52	15	6
3:P:127:ARG:HD3	3:P:134:LEU:HD11	0.42	1.90	17	2
3:P:123:GLU:O	3:P:142:LEU:HD21	0.42	2.13	17	1
3:P:134:LEU:HD22	3:P:138:GLU:HB3	0.42	1.91	17	1
1:A:5:DT:N3	1:A:6:DC:N3	0.42	2.67	16	2
1:A:15:DG:N3	1:A:16:DT:C6	0.42	2.88	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:142:LEU:O	3:P:142:LEU:HD13	0.42	2.13	7	2
1:A:15:DG:N1	2:B:18:DC:C2	0.42	2.87	9	1
1:A:7:DA:N3	2:B:27:DG:N2	0.42	2.68	14	5
3:P:129:ARG:HA	3:P:129:ARG:NE	0.42	2.29	14	2
1:A:7:DA:C2'	1:A:8:DA:C8	0.42	3.02	12	1
3:P:142:LEU:HD13	3:P:146:ILE:HD13	0.42	1.91	5	1
1:A:13:DC:N4	2:B:20:DG:C6	0.42	2.88	19	2
3:P:153:VAL:O	3:P:157:PHE:HD1	0.42	1.96	17	1
3:P:132:ARG:HG2	3:P:133:TYR:CD1	0.42	2.49	3	1
3:P:146:ILE:CD1	3:P:148:LEU:CD1	0.42	2.87	19	2
3:P:143:ALA:HB2	3:P:150:PRO:HA	0.42	1.92	15	1
2:B:27:DG:C6	2:B:28:DA:N1	0.42	2.88	11	4
1:A:9:DG:C4	1:A:10:DT:C6	0.42	3.08	5	1
3:P:143:ALA:HB1	3:P:148:LEU:O	0.42	2.15	17	4
1:A:7:DA:C3'	1:A:8:DA:H5''	0.42	2.44	11	1
3:P:131:GLN:OE1	3:P:134:LEU:CD2	0.42	2.67	11	1
2:B:26:DT:C6	2:B:27:DG:N7	0.42	2.88	17	1
3:P:123:GLU:HB3	3:P:142:LEU:HD11	0.42	1.90	20	1
2:B:24:DC:H2''	2:B:25:DT:H5''	0.42	1.90	13	1
2:B:21:DC:H2''	2:B:22:DC:C5'	0.42	2.41	15	1
3:P:153:VAL:HG13	3:P:157:PHE:HD2	0.42	1.71	16	1
3:P:126:ARG:HB3	3:P:130:GLN:NE2	0.41	2.30	4	1
3:P:139:ARG:HE	3:P:154:LYS:HG3	0.41	1.75	17	1
1:A:7:DA:N1	1:A:8:DA:C6	0.41	2.88	18	1
3:P:139:ARG:NH1	3:P:150:PRO:C	0.41	2.78	20	1
2:B:24:DC:C2'	2:B:25:DT:H5'	0.41	2.45	16	2
2:B:27:DG:N7	2:B:28:DA:N6	0.41	2.68	5	6
1:A:13:DC:C2'	1:A:14:DT:H71	0.41	2.43	16	1
2:B:23:DA:H2''	2:B:24:DC:C6	0.41	2.51	7	1
3:P:131:GLN:CD	3:P:133:TYR:O	0.41	2.62	8	1
3:P:128:PHE:CD2	3:P:157:PHE:CD1	0.41	3.08	11	1
1:A:4:DG:C2	1:A:5:DT:C2	0.41	3.08	6	1
1:A:9:DG:C4	1:A:10:DT:C4	0.41	3.08	19	1
3:P:132:ARG:CZ	3:P:133:TYR:CZ	0.41	3.04	3	2
1:A:4:DG:C8	1:A:5:DT:C5	0.41	3.09	13	1
1:A:13:DC:N4	2:B:20:DG:N1	0.41	2.68	16	1
3:P:122:TYR:CD1	3:P:126:ARG:HG2	0.41	2.50	4	1
2:B:18:DC:H2''	2:B:19:DA:C8	0.41	2.51	14	2
2:B:25:DT:H2'	2:B:26:DT:C7	0.41	2.45	11	1
2:B:18:DC:C2	2:B:19:DA:C5	0.41	3.09	16	1
3:P:122:TYR:CZ	3:P:126:ARG:CG	0.41	3.03	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:116:PHE:CE2	3:P:156:TRP:HB2	0.41	2.51	1	1
1:A:9:DG:H2''	1:A:10:DT:H5'	0.41	1.93	6	1
2:B:22:DC:C5	2:B:23:DA:C6	0.41	3.08	19	1
2:B:18:DC:N4	2:B:19:DA:N6	0.41	2.69	19	1
3:P:123:GLU:OE1	3:P:145:LEU:HD13	0.41	2.16	5	1
3:P:128:PHE:CE2	3:P:161:ARG:HG3	0.41	2.51	6	1
3:P:132:ARG:HB3	3:P:133:TYR:CD2	0.41	2.51	9	1
1:A:12:DG:H2''	1:A:13:DC:C5	0.41	2.50	14	1
3:P:116:PHE:HD1	3:P:148:LEU:HD21	0.41	1.74	15	1
3:P:122:TYR:CZ	3:P:126:ARG:CD	0.41	3.04	18	1
2:B:20:DG:H1'	2:B:21:DC:N3	0.41	2.31	19	1
1:A:13:DC:H2'	1:A:14:DT:C7	0.41	2.44	20	1
1:A:13:DC:H2''	1:A:14:DT:H5''	0.41	1.93	3	1
3:P:123:GLU:HG2	3:P:146:ILE:HG22	0.41	1.92	17	1
2:B:20:DG:N3	2:B:21:DC:N3	0.40	2.70	6	1
1:A:2:DG:H2''	1:A:3:DT:C7	0.40	2.46	9	1
1:A:13:DC:H2''	1:A:14:DT:H5'	0.40	1.93	15	1
1:A:7:DA:C2	1:A:8:DA:N1	0.40	2.90	17	1
3:P:117:THR:O	3:P:120:GLN:N	0.40	2.54	18	1
1:A:4:DG:H2''	1:A:5:DT:H5''	0.40	1.92	4	1
1:A:15:DG:C8	1:A:16:DT:C7	0.40	3.05	5	1
1:A:8:DA:C2'	1:A:9:DG:H5''	0.40	2.45	7	1
1:A:15:DG:N9	1:A:16:DT:C7	0.40	2.84	9	1
2:B:22:DC:C4	2:B:23:DA:C6	0.40	3.09	19	1
2:B:26:DT:C5	2:B:27:DG:O6	0.40	2.75	9	3
2:B:25:DT:H2''	2:B:26:DT:C6	0.40	2.51	11	1
2:B:18:DC:N4	2:B:19:DA:C6	0.40	2.90	15	1
1:A:7:DA:C2	1:A:8:DA:C6	0.40	3.10	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	46/77 (60%)	39±2 (84±3%)	7±2 (15±4%)	0±1 (1±1%)	20	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	920/1540 (60%)	774 (84%)	140 (15%)	6 (1%)	20 70

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	P	153	VAL	4
3	P	138	GLU	2

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	P	43/69 (62%)	28±1 (64±3%)	15±1 (36±3%)	1 9
All	All	860/1380 (62%)	552 (64%)	308 (36%)	1 9

All 28 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	P	126	ARG	20
3	P	146	ILE	20
3	P	153	VAL	20
3	P	154	LYS	20
3	P	127	ARG	19
3	P	135	SER	19
3	P	151	THR	19
3	P	161	ARG	19
3	P	142	LEU	18
3	P	131	GLN	17
3	P	139	ARG	16
3	P	117	THR	15
3	P	138	GLU	13
3	P	123	GLU	12
3	P	132	ARG	11
3	P	160	HIS	10
3	P	147	ARG	7

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Mol	Chain	Res	Type	Models (Total)
3	P	155	ILE	7
3	P	137	PRO	6
3	P	144	SER	4
3	P	150	PRO	3
3	P	116	PHE	3
3	P	140	GLU	2
3	P	133	TYR	2
3	P	129	ARG	2
3	P	122	TYR	2
3	P	159	ASN	1
3	P	118	LYS	1

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 oligosaccharides 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

No chemical shift data were provided