



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:54 PM BST

PDB ID : 2JPA
Title : Structure of the Wilms Tumor Suppressor Protein Zinc Finger Domain Bound to DNA
Authors : Stoll, R.; Lee, B.M.; Debler, E.W.; Laity, J.H.; Wilson, I.A.; Dyson, H.J.; Wright, P.E.
Deposited on : 2007-05-01

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

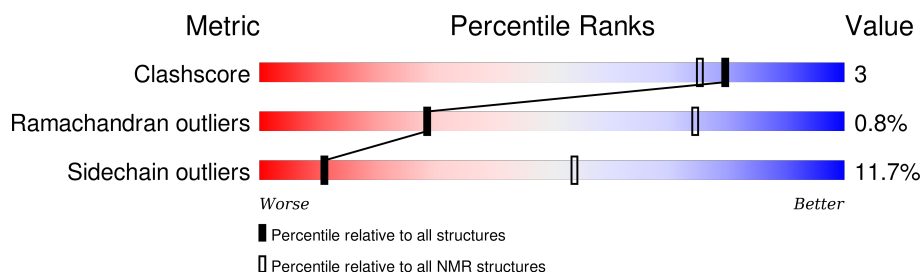
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 11%.

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
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	B	14	
2	C	14	
3	A	119	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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	A:7-A:119 (113)	0.70	11

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 1 single-model cluster was found.

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

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2880 atoms, of which 1291 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3').

Mol	Chain	Residues	Atoms						Trace
1	B	14	Total	C	H	N	O	P	0
			448	136	156	56	86	14	

- Molecule 2 is a DNA chain called DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DCP*DCP*DCP*DCP*DCP*DCP*DCP*DG)-3').

Mol	Chain	Residues	Atoms						Trace
2	C	14	Total	C	H	N	O	P	0
			436	132	154	54	82	14	

- Molecule 3 is a protein called Wilms tumor 1.

Mol	Chain	Residues	Atoms						Trace
3	A	119	Total	C	H	N	O	S	0
			1992	622	981	210	168	11	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP Q4VXV4

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	4	Total	Zn
			4	4

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

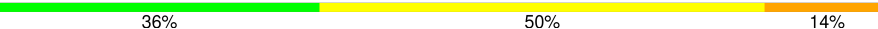
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain 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(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



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(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

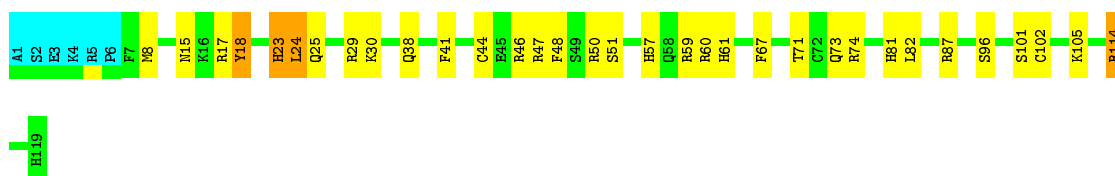
Chain B: 



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1



4.2.2 Score per residue for model 2

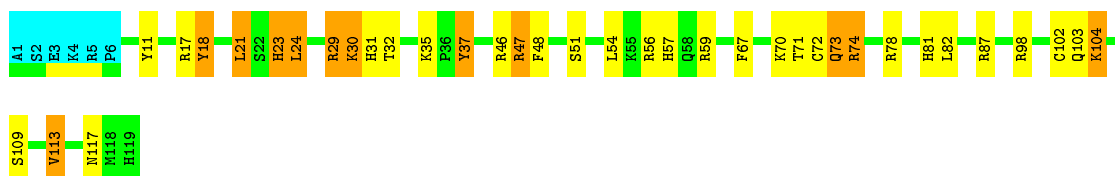
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



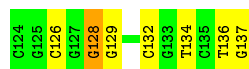
- Molecule 3: Wilms tumor 1



4.2.3 Score per residue for model 3

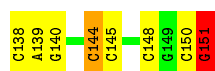
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



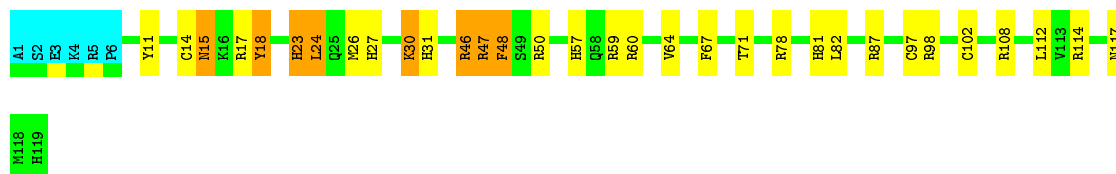
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



4.2.4 Score per residue for model 4

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



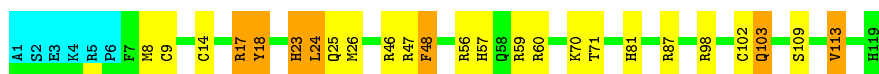
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



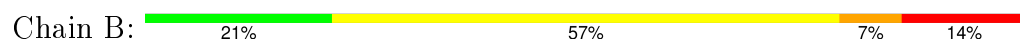
- Molecule 3: Wilms tumor 1

Chain A: 

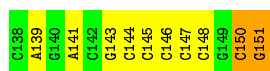


4.2.5 Score per residue for model 5

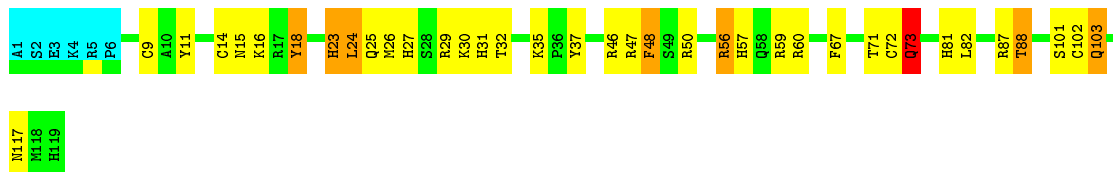
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

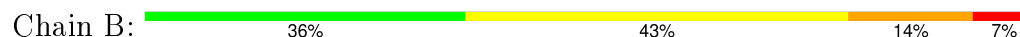


- Molecule 3: Wilms tumor 1

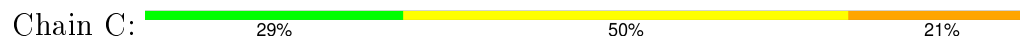


4.2.6 Score per residue for model 6

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1

Chain A: 



4.2.7 Score per residue for model 7

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



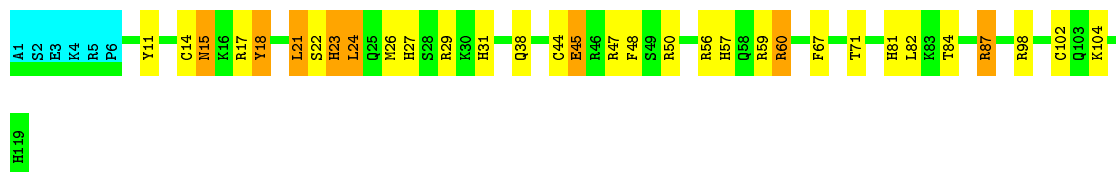
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



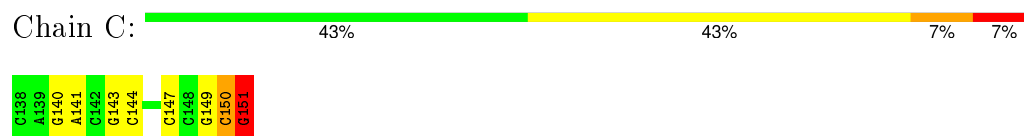
4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

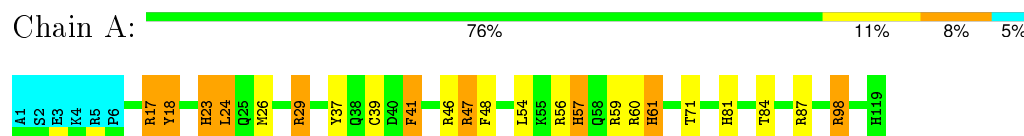
Chain B: 



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1



4.2.9 Score per residue for model 9

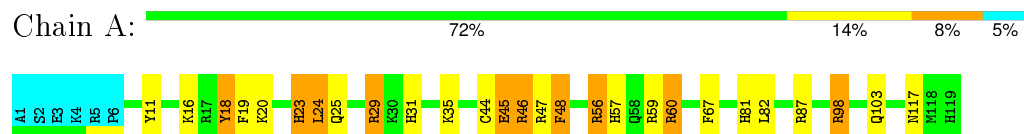
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

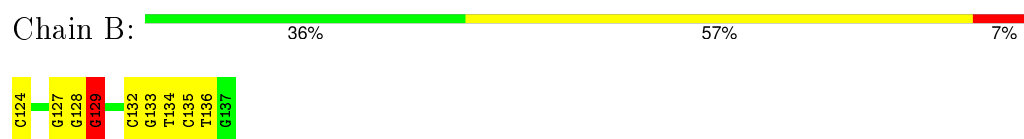


- Molecule 3: Wilms tumor 1



4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



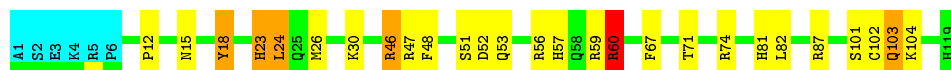
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



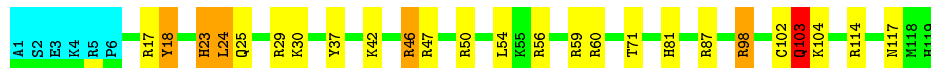
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



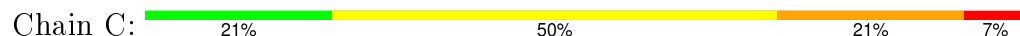
4.2.12 Score per residue for model 12

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1

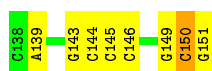


4.2.13 Score per residue for model 13

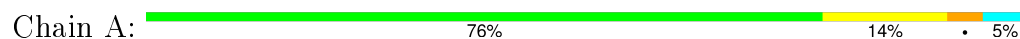
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1



4.2.14 Score per residue for model 14

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B:  36% 50% 14%



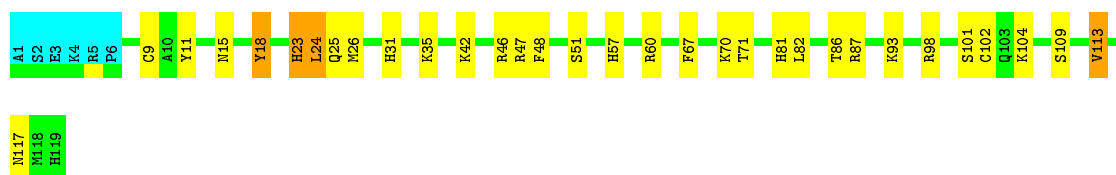
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:  29% 43% 29%



- Molecule 3: Wilms tumor 1

Chain A:  68% 24% 5%



4.2.15 Score per residue for model 15

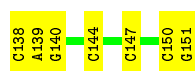
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B:  50% 29% 21%



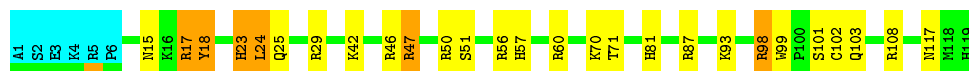
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:  50% 50%



- Molecule 3: Wilms tumor 1

Chain A:  72% 18% 5% 5%



4.2.16 Score per residue for model 16

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



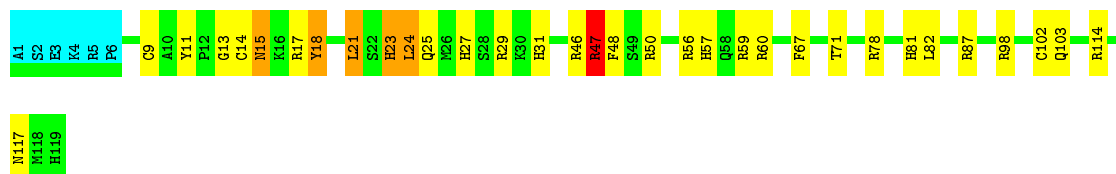
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



4.2.17 Score per residue for model 17

- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 

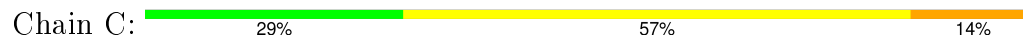


4.2.18 Score per residue for model 18

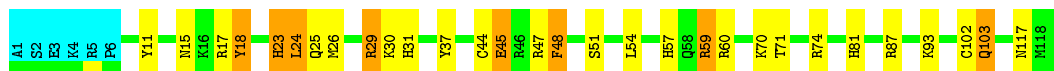
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1



4.2.19 Score per residue for model 19

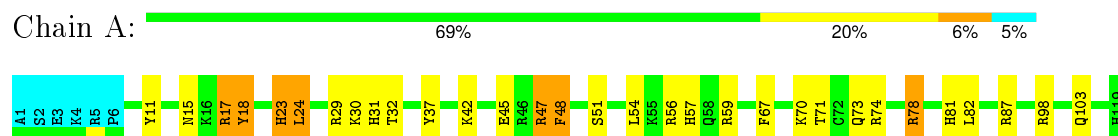
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1



4.2.20 Score per residue for model 20

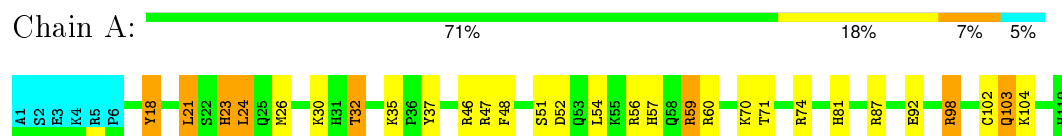
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')



- Molecule 3: Wilms tumor 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
AMBER	structure solution	
AMBER	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 15533
Number of chemical shift lists	1
Total number of shifts	236
Number of shifts mapped to atoms	236
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	11%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

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

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	B	1.83±0.15	5±3/327 (1.5±1.0%)	1.75±0.14	9±4/504 (1.8±0.8%)
2	C	1.64±0.12	2±2/315 (0.6±0.7%)	1.61±0.11	8±3/482 (1.6±0.5%)
3	A	0.72±0.01	0±0/992 (0.0±0.0%)	1.04±0.03	10±2/1320 (0.8±0.1%)
All	All	1.23	138/32680 (0.4%)	1.36	540/46120 (1.2%)

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	B	0.0±0.0	2.0±1.3
2	C	0.0±0.0	1.4±1.2
3	A	0.0±0.0	2.5±1.2
All	All	0	120

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
1	B	136	DT	C5-C7	14.44	1.58	1.50	4	8
1	B	136	DT	C4'-O4'	-9.22	1.35	1.45	9	4
1	B	134	DT	C5'-C4'	8.72	1.60	1.51	19	3
1	B	137	DG	N9-C4	8.12	1.44	1.38	9	1
1	B	134	DT	N1-C2	8.10	1.44	1.38	15	6
1	B	136	DT	C2'-C1'	7.82	1.60	1.52	13	2
1	B	127	DG	P-O5'	7.65	1.67	1.59	6	1
1	B	134	DT	C4'-O4'	-7.58	1.37	1.45	4	1
1	B	133	DG	C5'-C4'	7.49	1.59	1.51	9	2
1	B	134	DT	C5-C7	7.16	1.54	1.50	19	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	134	DT	C5-C6	7.06	1.39	1.34	13	3
1	B	128	DG	C4'-O4'	-6.77	1.38	1.45	6	1
1	B	134	DT	O4'-C1'	-6.75	1.34	1.42	4	1
1	B	129	DG	P-O5'	6.71	1.66	1.59	12	2
1	B	135	DC	C4-N4	-6.65	1.27	1.33	11	2
1	B	134	DT	P-O5'	6.62	1.66	1.59	3	1
1	B	136	DT	O4'-C1'	-6.47	1.34	1.42	4	1
1	B	129	DG	N1-C2	-6.47	1.32	1.37	6	1
2	C	143	DG	C4'-C3'	6.35	1.59	1.53	7	1
2	C	138	DC	C4-N4	-6.30	1.28	1.33	20	5
2	C	148	DC	C5'-C4'	6.26	1.58	1.51	18	1
2	C	144	DC	P-O5'	-6.11	1.53	1.59	7	1
2	C	140	DG	P-O5'	6.09	1.65	1.59	4	2
1	B	136	DT	C5'-C4'	6.02	1.57	1.51	9	1
1	B	129	DG	C5-C4	-5.94	1.34	1.38	18	1
1	B	133	DG	N9-C4	5.93	1.42	1.38	4	1
2	C	140	DG	C4'-O4'	-5.89	1.39	1.45	3	2
2	C	143	DG	C5-C6	5.88	1.48	1.42	19	1
1	B	132	DC	C4-N4	-5.86	1.28	1.33	3	2
1	B	137	DG	P-O5'	5.86	1.65	1.59	14	2
1	B	135	DC	P-O5'	-5.85	1.53	1.59	14	2
1	B	135	DC	C5'-C4'	5.85	1.57	1.51	8	1
1	B	130	DG	C4'-O4'	-5.84	1.39	1.45	19	1
2	C	145	DC	C4-N4	-5.83	1.28	1.33	16	2
2	C	146	DC	C5'-C4'	5.81	1.57	1.51	19	1
1	B	134	DT	N3-C4	5.79	1.43	1.38	9	3
2	C	149	DG	C6-N1	-5.78	1.35	1.39	18	1
2	C	143	DG	N7-C5	5.76	1.42	1.39	7	1
1	B	136	DT	C4'-C3'	5.74	1.59	1.53	9	1
2	C	139	DA	C6-N6	-5.74	1.29	1.33	9	1
1	B	131	DG	P-O5'	5.72	1.65	1.59	19	1
1	B	128	DG	C2-N2	-5.72	1.28	1.34	6	1
2	C	143	DG	C2-N2	-5.70	1.28	1.34	7	2
1	B	137	DG	N9-C8	-5.69	1.33	1.37	9	1
1	B	137	DG	C6-N1	-5.67	1.35	1.39	4	1
2	C	143	DG	P-O5'	5.60	1.65	1.59	7	2
1	B	137	DG	C5'-C4'	5.58	1.57	1.51	1	1
1	B	128	DG	C5'-C4'	5.57	1.57	1.51	5	1
1	B	130	DG	N3-C4	5.57	1.39	1.35	19	1
1	B	134	DT	C4'-C3'	5.54	1.58	1.53	3	1
1	B	134	DT	C3'-O3'	-5.51	1.36	1.44	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	138	DC	C4'-O4'	-5.50	1.39	1.45	4	1
2	C	149	DG	C2'-C1'	-5.47	1.46	1.52	18	1
1	B	136	DT	C5-C6	5.47	1.38	1.34	6	1
2	C	141	DA	O3'-P	5.46	1.67	1.61	16	1
1	B	137	DG	C4'-O4'	-5.46	1.39	1.45	20	1
1	B	129	DG	N9-C4	5.44	1.42	1.38	18	1
1	B	129	DG	C5'-C4'	5.44	1.57	1.51	18	1
1	B	128	DG	P-O5'	5.44	1.65	1.59	5	1
1	B	133	DG	P-O5'	5.42	1.65	1.59	10	1
1	B	132	DC	O3'-P	5.40	1.67	1.61	10	1
1	B	129	DG	N3-C4	5.39	1.39	1.35	15	1
1	B	130	DG	C2-N3	5.38	1.37	1.32	19	1
1	B	127	DG	C2-N2	-5.33	1.29	1.34	7	1
1	B	136	DT	N1-C2	5.33	1.42	1.38	6	2
2	C	149	DG	C2-N2	-5.32	1.29	1.34	18	1
2	C	142	DC	C4-N4	-5.32	1.29	1.33	6	2
1	B	134	DT	C1'-N1	5.32	1.56	1.49	15	1
2	C	147	DC	C5'-C4'	5.28	1.57	1.51	5	1
1	B	126	DC	C4-N4	-5.26	1.29	1.33	16	2
2	C	148	DC	P-O5'	5.21	1.65	1.59	3	1
2	C	145	DC	P-O5'	5.16	1.65	1.59	19	1
2	C	139	DA	C4'-O4'	-5.16	1.39	1.45	18	1
2	C	144	DC	C4-N4	-5.15	1.29	1.33	18	1
1	B	127	DG	C5'-C4'	5.14	1.57	1.51	5	1
2	C	146	DC	P-O5'	5.14	1.64	1.59	13	2
2	C	144	DC	C4'-O4'	-5.13	1.40	1.45	7	1
2	C	143	DG	C5'-C4'	5.12	1.56	1.51	19	1
1	B	135	DC	C2-N3	5.12	1.39	1.35	4	1
1	B	128	DG	N3-C4	5.10	1.39	1.35	6	1
1	B	131	DG	C5'-C4'	5.08	1.56	1.51	6	1
1	B	134	DT	N1-C6	-5.06	1.34	1.38	15	1
2	C	148	DC	C4'-O4'	-5.04	1.40	1.45	18	1
1	B	131	DG	N3-C4	5.04	1.39	1.35	9	1
1	B	129	DG	C8-N7	-5.04	1.27	1.30	18	1
1	B	130	DG	C5-C4	-5.03	1.34	1.38	19	1
1	B	137	DG	C2-N2	-5.02	1.29	1.34	4	1
1	B	134	DT	C4-C5	5.01	1.49	1.45	12	1
2	C	142	DC	C4-C5	5.01	1.47	1.43	7	1
1	B	132	DC	C4'-O4'	-5.01	1.40	1.45	13	1

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
1	B	130	DG	O4'-C4'-C3'	16.80	116.08	106.00	6	9
1	B	128	DG	O4'-C1'-C2'	-15.30	93.66	105.90	5	1
2	C	143	DG	O4'-C4'-C3'	13.99	114.39	106.00	7	14
1	B	134	DT	O4'-C4'-C3'	12.86	113.71	106.00	14	10
1	B	137	DG	O4'-C4'-C3'	12.79	113.67	106.00	20	10
1	B	136	DT	O4'-C4'-C3'	12.66	113.59	106.00	2	7
1	B	135	DC	O4'-C4'-C3'	11.83	113.10	106.00	14	5
2	C	140	DG	O4'-C4'-C3'	11.40	112.84	106.00	14	6
1	B	133	DG	O4'-C4'-C3'	11.15	112.69	106.00	14	4
1	B	132	DC	O4'-C4'-C3'	10.58	112.35	106.00	8	11
2	C	150	DC	O4'-C4'-C3'	10.44	112.27	106.00	5	11
2	C	147	DC	O4'-C4'-C3'	9.98	111.99	106.00	16	11
2	C	144	DC	O4'-C4'-C3'	9.90	111.94	106.00	12	13
2	C	143	DG	C4'-C3'-C2'	-9.84	94.25	103.10	7	5
3	A	50	ARG	NE-CZ-NH2	-9.82	115.39	120.30	1	5
3	A	56	ARG	NE-CZ-NH1	9.65	125.12	120.30	10	15
1	B	130	DG	C4'-C3'-C2'	-9.64	94.42	103.10	6	3
2	C	146	DC	O4'-C1'-C2'	-9.60	98.22	105.90	12	3
3	A	78	ARG	NE-CZ-NH2	-9.33	115.63	120.30	19	1
3	A	23	HIS	CA-CB-CG	9.05	128.99	113.60	16	20
3	A	59	ARG	NE-CZ-NH1	8.99	124.80	120.30	10	17
1	B	136	DT	O4'-C1'-C2'	-8.95	98.74	105.90	9	3
1	B	136	DT	C1'-O4'-C4'	8.94	119.04	110.10	9	1
3	A	114	ARG	NE-CZ-NH1	8.93	124.77	120.30	1	5
2	C	145	DC	O4'-C4'-C3'	8.92	111.35	106.00	5	6
1	B	135	DC	O4'-C1'-C2'	-8.84	98.83	105.90	10	6
1	B	127	DG	O4'-C4'-C3'	8.65	111.19	106.00	20	8
2	C	147	DC	O4'-C1'-C2'	-8.60	99.02	105.90	18	5
3	A	108	ARG	NE-CZ-NH2	-8.58	116.01	120.30	3	1
2	C	149	DG	O4'-C4'-C3'	8.57	111.14	106.00	10	5
3	A	87	ARG	NE-CZ-NH1	8.44	124.52	120.30	20	20
3	A	108	ARG	NE-CZ-NH1	8.43	124.51	120.30	3	2
1	B	132	DC	O4'-C1'-C2'	-8.34	99.23	105.90	19	2
2	C	139	DA	O4'-C4'-C3'	8.34	111.00	106.00	16	5
1	B	134	DT	O4'-C1'-C2'	-8.33	99.24	105.90	9	5
3	A	113	VAL	CA-CB-CG2	8.29	123.33	110.90	2	3
2	C	151	DG	O4'-C4'-C3'	8.20	110.92	106.00	12	7
2	C	138	DC	O4'-C4'-C3'	8.13	110.88	106.00	11	2
3	A	78	ARG	NE-CZ-NH1	7.99	124.30	120.30	19	3
1	B	135	DC	P-O3'-C3'	7.96	129.25	119.70	8	2
2	C	148	DC	O4'-C4'-C3'	7.92	110.75	106.00	5	7
3	A	114	ARG	NE-CZ-NH2	-7.84	116.38	120.30	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	149	DG	O4'-C1'-C2'	-7.78	99.68	105.90	18	1
3	A	47	ARG	NE-CZ-NH1	7.75	124.17	120.30	20	16
1	B	129	DG	C3'-C2'-C1'	-7.74	93.22	102.50	6	1
1	B	129	DG	O4'-C4'-C3'	7.66	110.59	106.00	19	2
3	A	60	ARG	NE-CZ-NH1	7.59	124.10	120.30	9	16
1	B	131	DG	O4'-C1'-C2'	-7.57	99.84	105.90	2	1
1	B	133	DG	O3'-P-O5'	-7.55	89.66	104.00	5	3
3	A	46	ARG	NE-CZ-NH1	7.53	124.06	120.30	3	17
3	A	17	ARG	NE-CZ-NH1	7.51	124.06	120.30	7	13
1	B	125	DG	O4'-C4'-C3'	7.49	110.50	106.00	11	5
1	B	135	DC	C4'-C3'-C2'	-7.48	96.37	103.10	14	2
3	A	98	ARG	NE-CZ-NH1	7.45	124.02	120.30	3	11
1	B	131	DG	O4'-C4'-C3'	7.38	110.43	106.00	4	5
3	A	74	ARG	NE-CZ-NH1	7.31	123.95	120.30	2	7
1	B	133	DG	O4'-C1'-C2'	-7.28	100.08	105.90	13	2
3	A	56	ARG	NE-CZ-NH2	-7.21	116.70	120.30	10	1
1	B	136	DT	P-O3'-C3'	7.20	128.34	119.70	13	3
1	B	136	DT	C4'-C3'-C2'	-7.14	96.68	103.10	9	2
3	A	29	ARG	NE-CZ-NH1	7.09	123.84	120.30	8	11
1	B	135	DC	O3'-P-O5'	-6.87	90.95	104.00	19	1
1	B	128	DG	C3'-C2'-C1'	-6.84	94.29	102.50	6	1
2	C	141	DA	O4'-C4'-C3'	6.80	110.08	106.00	8	6
1	B	128	DG	O4'-C4'-C3'	6.75	110.05	106.00	20	2
1	B	133	DG	C4'-C3'-C2'	-6.71	97.06	103.10	13	2
2	C	139	DA	P-O3'-C3'	6.64	127.67	119.70	5	7
1	B	134	DT	C4'-C3'-C2'	-6.64	97.12	103.10	14	5
1	B	126	DC	O4'-C1'-C2'	-6.61	100.61	105.90	18	2
1	B	129	DG	C4'-C3'-C2'	6.56	109.01	103.10	6	2
1	B	134	DT	C6-C5-C7	-6.54	118.97	122.90	14	1
1	B	134	DT	C1'-O4'-C4'	-6.53	103.58	110.10	6	3
2	C	150	DC	C4'-C3'-C2'	-6.39	97.35	103.10	5	1
1	B	130	DG	O4'-C1'-C2'	6.35	110.98	105.90	11	1
2	C	146	DC	O4'-C4'-C3'	6.33	109.80	106.00	7	5
2	C	138	DC	P-O3'-C3'	6.31	127.28	119.70	17	5
2	C	151	DG	C4'-C3'-C2'	-6.30	97.43	103.10	12	1
1	B	126	DC	C3'-C2'-C1'	-6.30	94.94	102.50	5	3
1	B	137	DG	O4'-C1'-C2'	6.28	110.92	105.90	2	2
2	C	145	DC	O4'-C1'-C2'	-6.22	100.92	105.90	13	1
2	C	145	DC	P-O3'-C3'	6.22	127.16	119.70	11	3
2	C	145	DC	C4'-C3'-C2'	-6.21	97.51	103.10	13	1
2	C	142	DC	O4'-C4'-C3'	6.20	109.72	106.00	17	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	134	DT	C5-C6-N1	-6.08	120.05	123.70	8	5
2	C	144	DC	C3'-C2'-C1'	6.05	109.76	102.50	6	1
1	B	134	DT	C4-C5-C6	6.05	121.63	118.00	6	2
1	B	136	DT	O3'-P-O5'	-6.01	92.59	104.00	14	5
1	B	132	DC	O3'-P-O5'	-6.00	92.61	104.00	5	1
2	C	140	DG	C4'-C3'-C2'	-5.96	97.74	103.10	14	1
1	B	126	DC	C1'-O4'-C4'	-5.92	104.18	110.10	20	4
1	B	130	DG	C3'-C2'-C1'	5.89	109.57	102.50	15	2
1	B	136	DT	C5-C6-N1	-5.86	120.18	123.70	20	4
1	B	126	DC	P-O3'-C3'	5.82	126.68	119.70	9	1
3	A	9	CYS	CA-CB-SG	-5.82	103.53	114.00	12	3
2	C	151	DG	O4'-C1'-C2'	5.82	110.55	105.90	11	2
3	A	50	ARG	NE-CZ-NH1	5.79	123.19	120.30	5	4
3	A	32	THR	CA-CB-CG2	5.73	120.42	112.40	17	2
1	B	130	DG	C1'-O4'-C4'	-5.72	104.38	110.10	6	1
1	B	129	DG	O4'-C1'-C2'	5.71	110.47	105.90	6	3
1	B	129	DG	P-O3'-C3'	5.67	126.50	119.70	10	2
1	B	124	DC	O4'-C4'-C3'	5.55	109.33	106.00	18	2
3	A	84	THR	CA-CB-CG2	5.54	120.15	112.40	7	2
1	B	134	DT	C5'-C4'-C3'	-5.52	104.16	114.10	15	1
2	C	151	DG	C1'-O4'-C4'	-5.52	104.58	110.10	11	2
1	B	128	DG	C1'-O4'-C4'	-5.47	104.63	110.10	10	1
2	C	143	DG	P-O3'-C3'	5.42	126.21	119.70	19	1
1	B	136	DT	C4-C5-C6	5.42	121.25	118.00	13	2
2	C	149	DG	C8-N9-C4	-5.41	104.24	106.40	18	1
3	A	86	THR	CA-CB-CG2	5.39	119.94	112.40	14	1
3	A	17	ARG	NE-CZ-NH2	-5.36	117.62	120.30	7	1
1	B	132	DC	C4'-C3'-C2'	-5.34	98.29	103.10	19	1
3	A	46	ARG	CD-NE-CZ	5.33	131.07	123.60	6	1
1	B	124	DC	O4'-C1'-C2'	5.33	110.16	105.90	18	1
3	A	60	ARG	CA-CB-CG	5.31	125.08	113.40	7	1
1	B	135	DC	C1'-O4'-C4'	-5.27	104.83	110.10	14	1
2	C	147	DC	O3'-P-O5'	-5.27	93.99	104.00	14	1
2	C	150	DC	C1'-O4'-C4'	-5.27	104.83	110.10	4	1
1	B	133	DG	C8-N9-C4	-5.26	104.29	106.40	16	1
2	C	141	DA	O4'-C1'-C2'	-5.26	101.69	105.90	19	1
3	A	88	THR	CA-CB-CG2	5.22	119.71	112.40	5	1
3	A	98	ARG	NE-CZ-NH2	-5.22	117.69	120.30	8	1
1	B	125	DG	P-O3'-C3'	5.18	125.92	119.70	19	1
2	C	143	DG	C1'-O4'-C4'	-5.18	104.92	110.10	7	1
1	B	127	DG	O4'-C1'-C2'	5.14	110.01	105.90	20	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	148	DC	O4'-C1'-C2'	5.12	109.99	105.90	3	1
3	A	41	PHE	CB-CG-CD1	-5.11	117.22	120.80	8	1
1	B	126	DC	O4'-C4'-C3'	5.10	109.06	106.00	20	1
2	C	142	DC	O3'-P-O5'	-5.09	94.33	104.00	12	1
1	B	125	DG	C4'-C3'-C2'	5.08	107.67	103.10	19	1
2	C	147	DC	C4'-C3'-C2'	-5.07	98.54	103.10	16	1
3	A	64	VAL	CA-CB-CG2	5.06	118.49	110.90	3	1
1	B	129	DG	C8-N9-C4	-5.05	104.38	106.40	7	1
2	C	143	DG	C8-N9-C4	-5.05	104.38	106.40	19	1
2	C	139	DA	O4'-C1'-C2'	-5.05	101.86	105.90	9	1
1	B	131	DG	C4'-C3'-C2'	-5.05	98.56	103.10	6	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)
3	A	18	TYR	Sidechain	20
1	B	129	DG	Sidechain	9
2	C	151	DG	Sidechain	8
3	A	48	PHE	Sidechain	8
1	B	127	DG	Sidechain	8
2	C	143	DG	Sidechain	6
2	C	140	DG	Sidechain	5
1	B	128	DG	Sidechain	4
3	A	47	ARG	Sidechain	4
1	B	135	DC	Sidechain	3
3	A	56	ARG	Sidechain	3
1	B	131	DG	Sidechain	3
1	B	137	DG	Sidechain	3
1	B	136	DT	Sidechain	3
3	A	74	ARG	Sidechain	3
1	B	130	DG	Sidechain	3
2	C	149	DG	Sidechain	2
1	B	133	DG	Sidechain	2
2	C	145	DC	Sidechain	2
3	A	41	PHE	Sidechain	2
3	A	98	ARG	Sidechain	2
2	C	144	DC	Sidechain	2
1	B	124	DC	Sidechain	2
3	A	78	ARG	Sidechain	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
3	A	87	ARG	Sidechain	1
3	A	60	ARG	Sidechain	1
3	A	114	ARG	Sidechain	1
2	C	150	DC	Sidechain	1
3	A	57	HIS	Sidechain	1
3	A	37	TYR	Sidechain	1
2	C	139	DA	Sidechain	1
1	B	134	DT	Sidechain	1
3	A	29	ARG	Sidechain	1
2	C	141	DA	Sidechain	1
3	A	61	HIS	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	B	292	156	157	2±1
2	C	282	154	153	1±0
3	A	964	932	932	8±2
All	All	30840	24840	24835	188

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:18:TYR:CD2	3:A:24:LEU:HD23	0.74	2.18	3	15
3:A:18:TYR:CD1	3:A:24:LEU:HD23	0.65	2.25	13	5
1:B:128:DG:C8	3:A:81:HIS:CE1	0.64	2.86	5	7
3:A:67:PHE:HB3	3:A:82:LEU:HD13	0.61	1.73	19	11
3:A:37:TYR:HB3	3:A:54:LEU:HD22	0.56	1.77	20	6
3:A:21:LEU:HD13	3:A:21:LEU:H	0.56	1.61	7	2
3:A:48:PHE:CZ	3:A:57:HIS:CG	0.56	2.94	17	17
3:A:41:PHE:CE2	3:A:61:HIS:CD2	0.55	2.95	1	1
3:A:11:TYR:CD2	3:A:31:HIS:CE1	0.54	2.95	18	13
3:A:21:LEU:H	3:A:21:LEU:HD13	0.53	1.64	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:109:SER:O	3:A:113:VAL:HG13	0.52	2.05	14	3
3:A:102:CYS:SG	3:A:104:LYS:HE2	0.51	2.46	11	2
1:B:129:DG:H5''	3:A:60:ARG:CG	0.51	2.36	10	1
3:A:21:LEU:HD22	3:A:22:SER:H	0.50	1.67	7	1
2:C:150:DC:H2''	2:C:151:DG:C8	0.50	2.41	19	19
3:A:18:TYR:CE2	3:A:27:HIS:CD2	0.49	3.00	7	3
3:A:41:PHE:CE1	3:A:61:HIS:CE1	0.49	3.01	6	1
3:A:14:CYS:SG	3:A:15:ASN:N	0.49	2.85	3	4
3:A:41:PHE:CE1	3:A:61:HIS:CD2	0.48	3.02	8	1
1:B:129:DG:H3'	3:A:60:ARG:HD3	0.48	1.86	10	1
1:B:129:DG:N7	3:A:81:HIS:CE1	0.48	2.82	14	19
3:A:102:CYS:SG	3:A:103:GLN:N	0.47	2.87	5	10
3:A:24:LEU:O	3:A:24:LEU:HD22	0.46	2.11	4	9
1:B:134:DT:C2	1:B:135:DC:C4	0.46	3.04	19	1
1:B:129:DG:N7	3:A:81:HIS:HE1	0.45	2.09	9	10
1:B:129:DG:H3'	3:A:60:ARG:CD	0.45	2.41	10	1
3:A:9:CYS:HB3	3:A:14:CYS:SG	0.45	2.52	4	1
1:B:127:DG:C6	1:B:128:DG:C6	0.44	3.06	6	1
3:A:30:LYS:HE3	3:A:31:HIS:CE1	0.44	2.47	2	3
3:A:102:CYS:SG	3:A:104:LYS:HE3	0.43	2.53	2	1
3:A:97:CYS:HA	3:A:112:LEU:HD11	0.43	1.90	3	1
3:A:24:LEU:HD22	3:A:24:LEU:O	0.43	2.13	8	4
1:B:134:DT:H2''	1:B:135:DC:C5	0.43	2.47	16	1
3:A:44:CYS:SG	3:A:45:GLU:N	0.43	2.92	9	3
1:B:129:DG:H5''	3:A:60:ARG:HG3	0.42	1.91	10	1
3:A:72:CYS:SG	3:A:73:GLN:N	0.42	2.93	2	2
1:B:129:DG:H5''	3:A:60:ARG:HD3	0.42	1.90	17	1
3:A:18:TYR:CE1	3:A:27:HIS:CD2	0.41	3.08	5	1
3:A:44:CYS:HB2	3:A:61:HIS:CE1	0.41	2.51	1	1
3:A:48:PHE:CE2	3:A:57:HIS:CD2	0.41	3.08	17	1
2:C:144:DC:H2''	2:C:145:DC:C6	0.40	2.51	12	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	A	112/119 (94%)	104±2 (93±2%)	7±2 (6±2%)	1±1 (1±1%)	29 74
All	All	2240/2380 (94%)	2083 (93%)	139 (6%)	18 (1%)	29 74

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	101	SER	5
3	A	102	CYS	4
3	A	73	GLN	2
3	A	103	GLN	2
3	A	99	TRP	1
3	A	64	VAL	1
3	A	13	GLY	1
3	A	12	PRO	1
3	A	15	ASN	1

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	A	107/112 (96%)	94±2 (88±2%)	13±2 (12±2%)	11 54
All	All	2140/2240 (96%)	1889 (88%)	251 (12%)	11 54

All 46 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	A	23	HIS	20
3	A	24	LEU	20
3	A	71	THR	19
3	A	117	ASN	13
3	A	26	MET	12
3	A	51	SER	10
3	A	25	GLN	9
3	A	98	ARG	9
3	A	15	ASN	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
3	A	17	ARG	8
3	A	30	LYS	8
3	A	103	GLN	8
3	A	47	ARG	8
3	A	70	LYS	8
3	A	29	ARG	8
3	A	46	ARG	7
3	A	42	LYS	6
3	A	35	LYS	5
3	A	32	THR	5
3	A	45	GLU	5
3	A	59	ARG	5
3	A	104	LYS	5
3	A	21	LEU	4
3	A	38	GLN	3
3	A	52	ASP	3
3	A	73	GLN	3
3	A	93	LYS	3
3	A	60	ARG	3
3	A	16	LYS	3
3	A	37	TYR	2
3	A	57	HIS	2
3	A	39	CYS	2
3	A	8	MET	2
3	A	68	GLN	2
3	A	53	GLN	1
3	A	34	GLU	1
3	A	20	LYS	1
3	A	105	LYS	1
3	A	9	CYS	1
3	A	88	THR	1
3	A	64	VAL	1
3	A	55	LYS	1
3	A	19	PHE	1
3	A	96	SER	1
3	A	74	ARG	1
3	A	92	GLU	1

6.3.3 RNA ⓘ

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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 11% for the well-defined parts and 11% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15533

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	236
Number of shifts mapped to atoms	236
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	—
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
^{15}N	108	-0.10 ± 0.47	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 11%, i.e. 230 atoms were assigned a chemical shift out of a possible 2139. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	210/555 (38%)	105/221 (48%)	0/226 (0%)	105/108 (97%)
Sidechain	18/831 (2%)	12/506 (2%)	0/261 (0%)	6/64 (9%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/185 (1%)	1/102 (1%)	0/71 (0%)	1/12 (8%)
Overall	230/2139 (11%)	118/1173 (10%)	0/742 (0%)	112/224 (50%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 236 atoms were assigned a chemical shift out of a possible 2219. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	216/583 (37%)	108/232 (47%)	0/238 (0%)	108/113 (96%)
Sidechain	18/883 (2%)	12/538 (2%)	0/277 (0%)	6/68 (9%)
Aromatic	2/185 (1%)	1/102 (1%)	0/71 (0%)	1/12 (8%)
Overall	236/2219 (11%)	121/1216 (10%)	0/770 (0%)	115/233 (49%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

