



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 09:26 PM UTC

PDB ID : 2JPA / pdb_00002jpa
BMRB ID : 15533
Title : Structure of the Wilms Tumor Suppressor Protein Zinc Finger Domain Bound to DNA
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Deposited on : 2007-05-01

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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

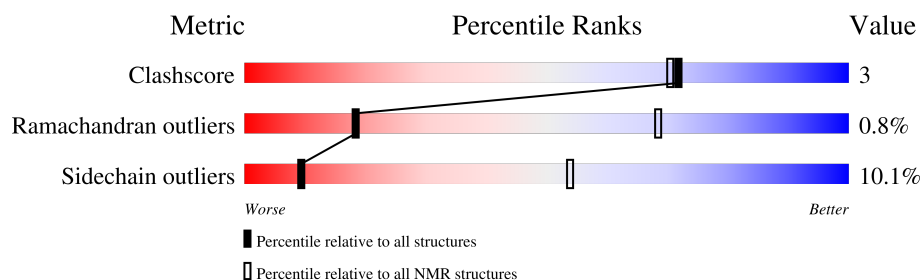
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 10%.

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	B	14	57% 36% 7%
2	C	14	79% 21%
3	A	119	79% 13% • 5%

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)	1.21	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*DGP*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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	4	Total	Zn
			4	4

4 Residue-property plots

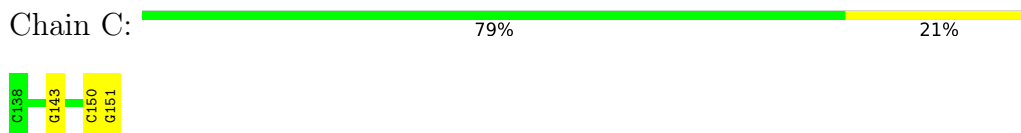
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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.

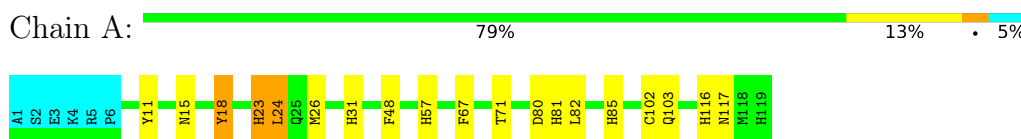
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')



- 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 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')





- 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*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')



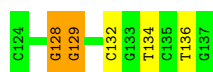
- Molecule 3: Wilms tumor 1



4.2.3 Score per residue for model 3

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

Chain B:  64% 21% 14%



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

Chain C:  57% 21% 21%



- Molecule 3: Wilms tumor 1

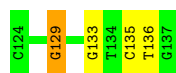
Chain A:  75% 15% 5% 5%



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:  71% 21% 7%



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

Chain C:  79% 21%



- Molecule 3: Wilms tumor 1

Chain A:  77% 11% 7% 5%



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')

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

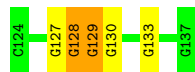
Chain A: 



4.2.6 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')

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: 



4.2.7 Score per residue for model 7

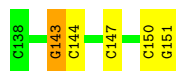
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B:  79% 21%



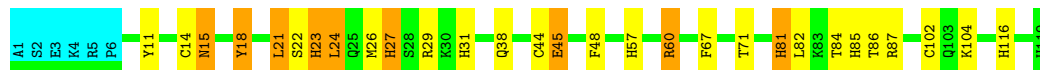
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:  64% 29% 7%



- Molecule 3: Wilms tumor 1

Chain A:  71% 17% 8% 5%



4.2.8 Score per residue for model 8

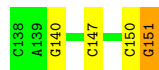
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B:  57% 36% 7%



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

Chain C:  71% 21% 7%



- Molecule 3: Wilms tumor 1

Chain A:  77% 13% • • 5%



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')

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

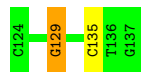
Chain A: 



4.2.10 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')

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: 



4.2.11 Score per residue for model 11 (medoid)

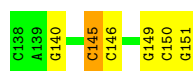
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

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

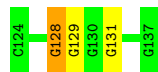
Chain A: 



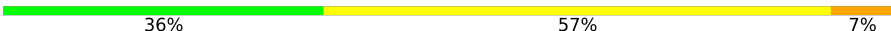
4.2.12 Score per residue for model 12

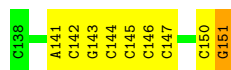
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



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

Chain C: 



- Molecule 3: Wilms tumor 1

Chain A: 



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')

Chain B:  64% 36%



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

Chain C:  86% 14%



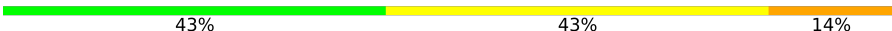
- Molecule 3: Wilms tumor 1

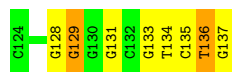
Chain A:  79% 13% • 5%



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:  43% 43% 14%



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

Chain C:  43% 36% 21%



- Molecule 3: Wilms tumor 1

Chain A:  73% 16% 6% 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: 



- 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

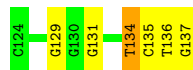
Chain A: 



4.2.16 Score per residue for model 16

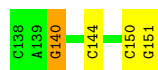
- Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DG)-3')

Chain B: 



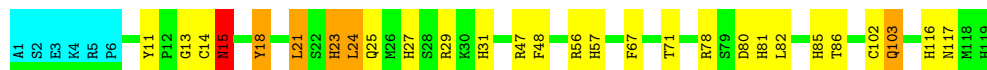
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

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:  79% 21%



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

Chain C:  79% 21%



- Molecule 3: Wilms tumor 1

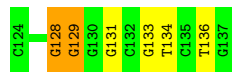
Chain A:  71% 16% 7% 5%



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')

Chain B:  57% 29% 14%



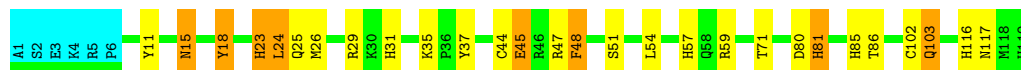
- Molecule 2: DNA (5'-D(P*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:  71% 21% 7%



- Molecule 3: Wilms tumor 1

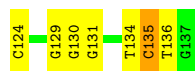
Chain A:  71% 17% 7% 5%



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')

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: 



4.2.20 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')

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: 



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)	working_cs.cif
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)	100%

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	0.85±0.07	0±0/327 (0.0± 0.0%)	1.29±0.09	4±2/504 (0.7± 0.3%)
2	C	0.79±0.06	0±0/315 (0.0± 0.0%)	1.19±0.08	2±2/482 (0.4± 0.3%)
3	A	0.96±0.01	0±0/992 (0.0± 0.0%)	1.21±0.03	7±2/1320 (0.5± 0.2%)
All	All	0.91	1/32680 (0.0%)	1.22	240/46120 (0.5%)

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.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	72	CYS	CA-C	5.69	1.55	1.52	5	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
3	A	23	HIS	CA-CB-CG	15.19	128.99	113.80	16	20
3	A	41	PHE	CA-CB-CG	9.82	123.62	113.80	17	2
1	B	133	DG	O3'-P-O5'	-9.56	89.66	104.00	5	9
1	B	135	DC	O3'-P-O5'	-8.70	90.95	104.00	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	128	DG	O4'-C1'-C2'	-8.49	93.66	106.40	5	1
1	B	136	DT	O3'-P-O5'	-7.61	92.59	104.00	14	9
3	A	15	ASN	CA-CB-CG	7.61	120.21	112.60	15	4
3	A	113	VAL	CA-CB-CG2	7.61	123.33	110.40	2	3
1	B	132	DC	O3'-P-O5'	-7.59	92.61	104.00	5	2
1	B	134	DT	C5'-C4'-C3'	-7.16	104.16	114.90	15	8
1	B	130	DG	O4'-C4'-C3'	7.12	116.08	105.40	6	1
1	B	134	DT	C4'-C3'-O3'	6.99	120.48	110.00	8	4
1	B	128	DG	C2'-C3'-O3'	-6.71	101.43	111.50	7	3
2	C	147	DC	O3'-P-O5'	-6.67	93.99	104.00	14	6
3	A	81	HIS	CA-CB-CG	6.59	120.39	113.80	8	8
3	A	80	ASP	CA-CB-CG	6.56	119.16	112.60	2	11
3	A	57	HIS	CB-CG-CD2	-6.50	122.75	131.20	17	5
3	A	61	HIS	CA-CB-CG	6.50	120.30	113.80	17	2
2	C	142	DC	O3'-P-O5'	-6.45	94.33	104.00	12	2
1	B	129	DG	C2'-C3'-O3'	6.45	121.17	111.50	6	1
2	C	143	DG	C5'-C4'-C3'	-6.39	105.32	114.90	19	2
2	C	144	DC	O3'-P-O5'	-6.23	94.66	104.00	7	2
1	B	136	DT	C1'-O4'-C4'	6.22	119.04	109.70	9	1
3	A	116	HIS	CB-CG-CD2	-6.15	123.21	131.20	9	20
1	B	135	DC	C5'-C4'-C3'	-6.12	105.72	114.90	11	1
1	B	131	DG	O3'-P-O5'	-6.10	94.85	104.00	19	6
1	B	135	DC	P-O3'-C3'	6.04	129.25	120.20	8	1
2	C	143	DG	O4'-C4'-C3'	6.00	114.39	105.40	7	1
2	C	146	DC	C5'-C4'-O4'	5.91	118.27	109.40	11	1
2	C	143	DG	O3'-P-O5'	-5.91	95.13	104.00	14	1
2	C	143	DG	C2'-C3'-O3'	5.90	120.34	111.50	5	2
3	A	32	THR	CA-CB-CG2	5.83	120.42	110.50	17	3
3	A	85	HIS	CB-CG-CD2	-5.82	123.64	131.20	12	16
1	B	134	DT	O3'-P-O5'	-5.81	95.29	104.00	1	2
3	A	25	GLN	OE1-CD-NE2	-5.81	116.79	122.60	14	2
3	A	52	ASP	CA-CB-CG	5.79	118.39	112.60	10	2
2	C	140	DG	O5'-C5'-C4'	5.79	119.48	110.80	4	3
3	A	110	ASP	CA-CB-CG	5.78	118.38	112.60	5	2
2	C	144	DC	C2'-C3'-O3'	5.68	120.02	111.50	3	1
3	A	84	THR	CA-CB-CG2	5.68	120.15	110.50	7	3
3	A	57	HIS	CA-CB-CG	-5.62	108.18	113.80	8	2
1	B	129	DG	C3'-C2'-C1'	-5.59	93.22	101.60	6	1
1	B	130	DG	C5'-C4'-C3'	-5.59	106.52	114.90	20	1
3	A	81	HIS	CB-CG-CD2	-5.58	123.95	131.20	11	8
3	A	86	THR	CA-CB-CG2	5.55	119.94	110.50	14	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	134	DT	O4'-C4'-C3'	5.54	113.71	105.40	14	1
1	B	137	DG	O4'-C4'-C3'	5.51	113.67	105.40	20	1
3	A	60	ARG	CA-CB-CG	5.49	125.08	114.10	7	1
1	B	136	DT	O4'-C4'-C3'	5.46	113.59	105.40	2	1
1	B	129	DG	O3'-P-O5'	-5.46	95.82	104.00	14	2
2	C	146	DC	O4'-C1'-C2'	-5.45	98.22	106.40	12	1
1	B	127	DG	C5'-C4'-C3'	-5.44	106.74	114.90	9	1
2	C	144	DC	C3'-C2'-C1'	5.44	109.76	101.60	6	1
2	C	143	DG	C4'-C3'-C2'	-5.43	94.25	102.40	7	1
1	B	136	DT	P-O3'-C3'	5.43	128.34	120.20	13	1
3	A	88	THR	CA-CB-CG2	5.42	119.71	110.50	5	1
1	B	126	DC	O3'-P-O5'	-5.41	95.89	104.00	2	2
2	C	145	DC	C5'-C4'-C3'	-5.39	106.81	114.90	3	1
2	C	140	DG	O3'-P-O5'	-5.39	95.92	104.00	1	2
3	A	27	HIS	CB-CG-CD2	-5.36	124.23	131.20	4	2
1	B	128	DG	C5'-C4'-C3'	-5.36	106.86	114.90	12	1
3	A	61	HIS	CB-CG-CD2	-5.33	124.28	131.20	8	2
1	B	130	DG	C4'-C3'-C2'	-5.32	94.42	102.40	6	1
1	B	130	DG	C3'-C2'-C1'	5.32	109.57	101.60	15	2
1	B	134	DT	C5'-C4'-O4'	5.31	117.37	109.40	3	1
2	C	145	DC	O3'-P-O5'	-5.25	96.12	104.00	6	2
2	C	139	DA	O3'-P-O5'	-5.25	96.13	104.00	14	1
2	C	143	DG	C5'-C4'-O4'	5.21	117.22	109.40	7	1
3	A	115	HIS	CB-CG-CD2	-5.19	124.46	131.20	1	1
1	B	134	DT	P-O5'-C5'	5.16	127.75	120.00	3	1
1	B	134	DT	O5'-C5'-C4'	5.15	118.52	110.80	8	1
3	A	31	HIS	CA-CB-CG	-5.14	108.66	113.80	8	1
1	B	135	DC	O4'-C4'-C3'	5.13	113.10	105.40	14	1
1	B	130	DG	O3'-P-O5'	-5.13	96.31	104.00	19	1
1	B	136	DT	C2'-C3'-O3'	5.12	119.19	111.50	1	1
1	B	136	DT	O4'-C1'-C2'	-5.11	98.74	106.40	9	1
3	A	115	HIS	CA-CB-CG	-5.08	108.72	113.80	9	1
3	A	103	GLN	OE1-CD-NE2	-5.06	117.54	122.60	16	1
3	A	27	HIS	CA-CB-CG	-5.06	108.74	113.80	4	1
1	B	135	DC	O4'-C1'-C2'	-5.05	98.83	106.40	10	1
2	C	146	DC	O3'-P-O5'	-5.03	96.46	104.00	1	3
3	A	116	HIS	CA-CB-CG	5.03	118.83	113.80	15	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
1	B	127	DG	Sidechain	8
2	C	151	DG	Sidechain	8
3	A	48	PHE	Sidechain	8
2	C	143	DG	Sidechain	6
2	C	140	DG	Sidechain	5
3	A	47	ARG	Sidechain	4
1	B	128	DG	Sidechain	4
1	B	136	DT	Sidechain	3
3	A	74	ARG	Sidechain	3
1	B	135	DC	Sidechain	3
1	B	137	DG	Sidechain	3
1	B	130	DG	Sidechain	3
3	A	56	ARG	Sidechain	3
1	B	131	DG	Sidechain	3
1	B	124	DC	Sidechain	2
2	C	144	DC	Sidechain	2
2	C	145	DC	Sidechain	2
1	B	133	DG	Sidechain	2
3	A	41	PHE	Sidechain	2
3	A	98	ARG	Sidechain	2
2	C	149	DG	Sidechain	2
3	A	78	ARG	Sidechain	2
3	A	114	ARG	Sidechain	1
3	A	87	ARG	Sidechain	1
3	A	57	HIS	Sidechain	1
3	A	61	HIS	Sidechain	1
1	B	134	DT	Sidechain	1
3	A	60	ARG	Sidechain	1
2	C	141	DA	Sidechain	1
2	C	139	DA	Sidechain	1
2	C	150	DC	Sidechain	1
3	A	37	TYR	Sidechain	1
3	A	29	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	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	190

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:H	3:A:21:LEU:HD13	0.56	1.61	7	4
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: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	13
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
3:A:30:LYS:HE3	3:A:31:HIS:CE1	0.44	2.47	2	3
1:B:127:DG:C6	1:B:128:DG:C6	0.44	3.06	6	1
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:C:144:DC:C5	3:A:80:ASP:CG	0.41	2.98	1	2
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 [i](#)

6.3.1 Protein backbone [i](#)

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%)	18	68
All	All	2240/2380 (94%)	2083 (93%)	139 (6%)	18 (1%)	18	68

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	12	PRO	1
3	A	15	ASN	1
3	A	99	TRP	1
3	A	13	GLY	1
3	A	64	VAL	1

6.3.2 Protein sidechains [i](#)

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%)	96±2 (90±2%)	11±2 (10±2%)	9	54
All	All	2140/2240 (96%)	1924 (90%)	216 (10%)	9	54

All 42 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	15	ASN	12
3	A	26	MET	11
3	A	51	SER	10
3	A	70	LYS	9
3	A	25	GLN	8
3	A	103	GLN	8
3	A	98	ARG	6
3	A	32	THR	5
3	A	35	LYS	5
3	A	42	LYS	5
3	A	45	GLU	5
3	A	38	GLN	4
3	A	21	LEU	4
3	A	104	LYS	4
3	A	29	ARG	4
3	A	59	ARG	4
3	A	73	GLN	3
3	A	30	LYS	3
3	A	16	LYS	3
3	A	47	ARG	3
3	A	17	ARG	3
3	A	55	LYS	3
3	A	37	TYR	2
3	A	39	CYS	2
3	A	60	ARG	2
3	A	46	ARG	2
3	A	52	ASP	2
3	A	57	HIS	2
3	A	96	SER	1

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Mol	Chain	Res	Type	Models (Total)
3	A	105	LYS	1
3	A	74	ARG	1
3	A	9	CYS	1
3	A	88	THR	1
3	A	53	GLN	1
3	A	68	GLN	1
3	A	93	LYS	1
3	A	34	GLU	1
3	A	64	VAL	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](#)

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

The completeness of assignment taking into account all chemical shift lists is 10% for the well-defined parts and 10% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	108	-0.10 ± 0.25	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 230 atoms were assigned a chemical shift out of a possible 2206. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	210/559 (38%)	105/225 (47%)	0/226 (0%)	105/108 (97%)
Sidechain	18/883 (2%)	12/558 (2%)	0/261 (0%)	6/64 (9%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	2/196 (1%)	1/102 (1%)	0/82 (0%)	1/12 (8%)
Sugar	0/336 (0%)	0/196 (0%)	0/140 (0%)	0/0 (—%)
Base	0/232 (0%)	0/148 (0%)	0/44 (0%)	0/40 (0%)
Overall	230/2206 (10%)	118/1229 (10%)	0/753 (0%)	112/224 (50%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 236 atoms were assigned a chemical shift out of a possible 2288. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	216/587 (37%)	108/236 (46%)	0/238 (0%)	108/113 (96%)
Sidechain	18/937 (2%)	12/592 (2%)	0/277 (0%)	6/68 (9%)
Aromatic	2/196 (1%)	1/102 (1%)	0/82 (0%)	1/12 (8%)
Sugar	0/336 (0%)	0/196 (0%)	0/140 (0%)	0/0 (—%)
Base	0/232 (0%)	0/148 (0%)	0/44 (0%)	0/40 (0%)
Overall	236/2288 (10%)	121/1274 (9%)	0/781 (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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

