



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:25 pm GMT

PDB ID : 1IR5
Title : Solution Structure of the 17mer TF1 Binding Site
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Deposited on : 2001-09-07

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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
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

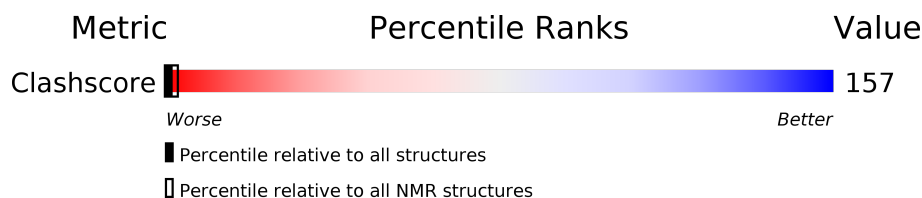
1 Overall quality at a glance

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	125131	11601

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	17	 12% 88%
2	B	17	 12% 88%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1079 atoms, of which 388 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	17	Total	C	H	N	O	P	0
			538	166	196	56	104	16	

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

Mol	Chain	Residues	Atoms						Trace
2	B	17	Total	C	H	N	O	P	0
			541	167	192	70	96	16	

4 Residue-property plots [i](#)

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.

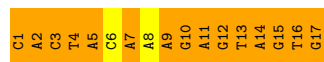
- Molecule 1: 5'-D(*CP*AP*CP*TP*AP*CP*TP*CP*TP*TP*TP*GP*TP*AP*GP*TP*G)-3',

Chain A: 



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

Chain B: 



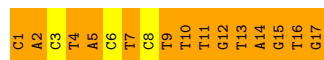
4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

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

Chain A: 



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

Chain B: 

C1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.2 Score per residue for model 2

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

Chain A:  12% 88%

C1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  6% 94%

C1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

4.2.3 Score per residue for model 3

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

Chain A:  18% 82%

C1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  12% 88%

C1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.4 Score per residue for model 4

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

Chain A:  12% 88%

C1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  6% 94%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.5 Score per residue for model 5

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

Chain A:  12% 88%

G1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  12% 88%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.6 Score per residue for model 6

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

Chain A:  12% 88%

G1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  12% 88%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.7 Score per residue for model 7

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

Chain A:  12% 88%

G1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  24% 76%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

4.2.8 Score per residue for model 8

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

Chain A:  12% 88%

G1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
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- Molecule 2: 5'-D(*CP*AP*CP*TP*AP*CP*AP*AP*AP*GP*AP*GP*TP*AP*GP*TP*G)-3

Chain B:  12% 88%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.9 Score per residue for model 9

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

Chain A:  12% 88%

G1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  12% 88%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.10 Score per residue for model 10

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

Chain A:  12% 88%



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

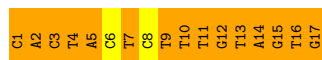
Chain B:  12% 88%



4.2.11 Score per residue for model 11

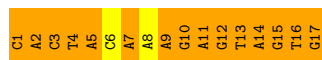
- Molecule 1: 5'-D(*CP*AP*CP*TP*AP*CP*TP*CP*TP*TP*TP*GP*TP*AP*GP*TP*G)-3',

Chain A:  12% 88%



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

Chain B:  12% 88%



4.2.12 Score per residue for model 12

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

Chain A:  12% 88%



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

Chain B:  12% 88%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.13 Score per residue for model 13

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

Chain A:  12% 88%

G1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  12% 88%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
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4.2.14 Score per residue for model 14

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

Chain A:  12% 88%

G1	A2	C3	T4	A5	C6	T7	C8	T9	T10	T11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain B:  12% 88%

G1	A2	C3	T4	A5	C6	A7	A8	A9	G10	A11	G12	T13	A14	G15	T16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

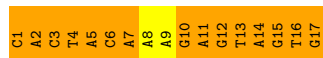
4.2.15 Score per residue for model 15

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

Chain A:  12% 88%

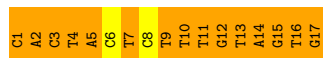


• Molecule 2: 5'-D(*CP*AP*CP*TP*AP*CP*AP*AP*AP*GP*AP*GP*TP*AP*GP*TP*G)-3',

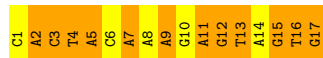


4.2.16 Score per residue for model 16

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

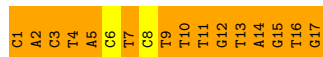


• Molecule 2: 5'-D(*CP*AP*CP*TP*AP*CP*AP*AP*AP*GP*AP*GP*TP*AP*GP*TP*G)-3',

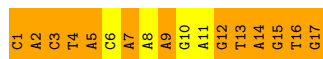


4.2.17 Score per residue for model 17

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



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



4.2.18 Score per residue for model 18

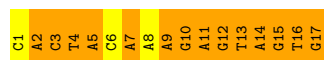
- Molecule 1: 5'-D(*CP*AP*CP*TP*AP*CP*TP*CP*TP*TP*TP*GP*TP*AP*GP*TP*G)-3',

Chain A:  12% 88%



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

Chain B:  18% 82%



4.2.19 Score per residue for model 19

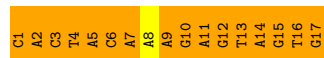
- Molecule 1: 5'-D(*CP*AP*CP*TP*AP*CP*TP*CP*TP*TP*TP*GP*TP*AP*GP*TP*G)-3',

Chain A:  12% 88%



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

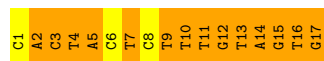
Chain B:  6% 94%



4.2.20 Score per residue for model 20

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

Chain A:  18% 82%



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



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
DISCOVER	refinement	3.1

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 5243
Number of chemical shift lists	1
Total number of shifts	363
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	363
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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](#)

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	1.60±0.00	7±0/381 (1.8±0.0%)	2.34±0.01	26±1/586 (4.4±0.2%)
2	B	1.52±0.00	3±0/393 (0.8±0.0%)	2.43±0.01	36±1/605 (5.9±0.2%)
All	All	1.56	200/15480 (1.3%)	2.39	1226/23820 (5.1%)

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	A	16	DT	C5-C7	5.87	1.53	1.50	9	20
2	B	16	DT	C5-C7	5.85	1.53	1.50	3	20
1	A	4	DT	C5-C7	5.82	1.53	1.50	20	20
1	A	11	DT	C5-C7	5.73	1.53	1.50	8	20
1	A	7	DT	C5-C7	5.70	1.53	1.50	12	20
1	A	13	DT	C5-C7	5.70	1.53	1.50	14	20
1	A	10	DT	C5-C7	5.69	1.53	1.50	2	20
2	B	4	DT	C5-C7	5.67	1.53	1.50	10	20
2	B	13	DT	C5-C7	5.67	1.53	1.50	16	20
1	A	9	DT	C5-C7	5.64	1.53	1.50	13	20

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	A	5	DA	N1-C6-N6	-9.15	113.11	118.60	18	20
2	B	5	DA	N1-C6-N6	-9.11	113.14	118.60	2	20
2	B	7	DA	N1-C6-N6	-9.07	113.16	118.60	16	20
1	A	2	DA	N1-C6-N6	-9.06	113.16	118.60	7	20
2	B	11	DA	N1-C6-N6	-9.04	113.18	118.60	18	20
2	B	14	DA	N1-C6-N6	-9.04	113.18	118.60	20	20
2	B	2	DA	N1-C6-N6	-8.99	113.21	118.60	14	20
1	A	14	DA	N1-C6-N6	-8.97	113.22	118.60	12	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	8	DA	N1-C6-N6	-8.86	113.28	118.60	3	20
2	B	9	DA	N1-C6-N6	-8.77	113.34	118.60	2	20
2	B	14	DA	C5-C6-N1	7.85	121.62	117.70	20	20
1	A	14	DA	C5-C6-N1	7.81	121.61	117.70	17	20
2	B	2	DA	C5-C6-N1	7.79	121.59	117.70	3	20
2	B	11	DA	C5-C6-N1	7.75	121.58	117.70	5	20
2	B	5	DA	C5-C6-N1	7.71	121.56	117.70	17	20
1	A	13	DT	C6-C5-C7	-7.68	118.29	122.90	16	20
2	B	9	DA	C5-C6-N1	7.68	121.54	117.70	8	20
1	A	2	DA	C5-C6-N1	7.68	121.54	117.70	7	20
2	B	7	DA	C5-C6-N1	7.67	121.54	117.70	2	20
2	B	8	DA	C5-C6-N1	7.63	121.52	117.70	3	20
1	A	7	DT	C6-C5-C7	-7.61	118.33	122.90	1	20
1	A	5	DA	C5-C6-N1	7.61	121.50	117.70	3	20
2	B	13	DT	C6-C5-C7	-7.60	118.34	122.90	18	20
1	A	16	DT	C6-C5-C7	-7.58	118.35	122.90	7	20
1	A	4	DT	C6-C5-C7	-7.54	118.38	122.90	18	20
2	B	4	DT	C6-C5-C7	-7.52	118.39	122.90	4	20
1	A	11	DT	C6-C5-C7	-7.33	118.50	122.90	5	20
1	A	10	DT	C6-C5-C7	-7.30	118.52	122.90	13	20
1	A	9	DT	C6-C5-C7	-7.28	118.53	122.90	2	20
2	B	16	DT	C6-C5-C7	-7.11	118.63	122.90	7	20
2	B	14	DA	C4-C5-C6	-6.91	113.54	117.00	19	20
1	A	14	DA	C4-C5-C6	-6.89	113.55	117.00	17	20
1	A	5	DA	C4-C5-C6	-6.85	113.58	117.00	7	20
2	B	11	DA	C4-C5-C6	-6.81	113.59	117.00	5	20
1	A	2	DA	C4-C5-C6	-6.79	113.60	117.00	7	20
2	B	2	DA	C4-C5-C6	-6.79	113.60	117.00	6	20
2	B	5	DA	C4-C5-C6	-6.77	113.61	117.00	14	20
2	B	7	DA	C4-C5-C6	-6.76	113.62	117.00	6	20
2	B	8	DA	C4-C5-C6	-6.75	113.62	117.00	9	20
2	B	9	DA	C4-C5-C6	-6.67	113.67	117.00	7	20
1	A	17	DG	N1-C6-O6	-6.41	116.06	119.90	2	20
2	B	17	DG	N1-C6-O6	-6.36	116.08	119.90	3	20
1	A	15	DG	N1-C6-O6	-6.33	116.10	119.90	17	20
2	B	15	DG	N1-C6-O6	-6.32	116.11	119.90	20	20
2	B	10	DG	N1-C6-O6	-6.29	116.13	119.90	20	20
2	B	12	DG	N1-C6-O6	-6.24	116.15	119.90	13	20
1	A	14	DA	O4'-C1'-N9	6.22	112.35	108.00	16	2
1	A	12	DG	N1-C6-O6	-6.20	116.18	119.90	13	20
2	B	1	DC	N3-C4-N4	-5.62	114.07	118.00	15	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1	DC	N3-C4-N4	-5.53	114.13	118.00	7	19
2	B	15	DG	C5-C6-N1	5.48	114.24	111.50	7	20
1	A	15	DG	C5-C6-N1	5.46	114.23	111.50	4	20
1	A	12	DG	C5-C6-N1	5.44	114.22	111.50	12	20
2	B	17	DG	C5-C6-N1	5.43	114.22	111.50	2	20
1	A	17	DG	C5-C6-N1	5.43	114.22	111.50	2	20
2	B	10	DG	C5-C6-N1	5.43	114.21	111.50	16	20
2	B	12	DG	C5-C6-N1	5.38	114.19	111.50	4	20
2	B	3	DC	N3-C4-N4	-5.29	114.30	118.00	13	20
2	B	14	DA	O4'-C1'-N9	5.28	111.70	108.00	12	9
2	B	3	DC	N3-C4-C5	5.22	123.99	121.90	6	14
1	A	3	DC	N3-C4-N4	-5.20	114.36	118.00	16	15
1	A	3	DC	N3-C4-C5	5.20	123.98	121.90	11	17
1	A	6	DC	N3-C4-C5	5.18	123.97	121.90	15	1
1	A	1	DC	N3-C4-C5	5.16	123.96	121.90	13	11
1	A	13	DT	C4-C5-C7	5.15	122.09	119.00	14	11
2	B	1	DC	N3-C4-C5	5.09	123.94	121.90	15	5
2	B	16	DT	O4'-C1'-N1	5.08	111.56	108.00	14	1
2	B	6	DC	N3-C4-C5	5.05	123.92	121.90	4	5

There are no chirality outliers.

There are no planarity outliers.

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	342	196	196	108±11
2	B	349	192	192	85±8
All	All	13820	7760	7758	3395

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 157.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:DA:C2	2:B:5:DA:N3	1.51	1.73	13	18
1:A:15:DG:C5	1:A:16:DT:H72	1.48	1.39	18	1
2:B:1:DC:N4	2:B:2:DA:C6	1.47	1.83	9	15
1:A:8:DC:H42	2:B:9:DA:N6	1.46	1.06	7	19
1:A:17:DG:N2	2:B:2:DA:C2	1.43	1.87	7	6
1:A:15:DG:N7	1:A:16:DT:H72	1.41	1.15	18	1
2:B:1:DC:N4	2:B:2:DA:N1	1.39	1.71	9	15
1:A:8:DC:N4	2:B:9:DA:N6	1.36	1.74	3	19
1:A:3:DC:C6	1:A:4:DT:H72	1.35	1.57	15	8
1:A:16:DT:N3	1:A:17:DG:C5	1.30	1.99	15	5
2:B:5:DA:C6	2:B:6:DC:N4	1.29	2.01	2	20
1:A:16:DT:O4	1:A:17:DG:C6	1.26	1.88	15	3
2:B:1:DC:C4	2:B:2:DA:C6	1.25	2.25	9	15
2:B:1:DC:C4	2:B:2:DA:C5	1.24	2.25	9	15
1:A:15:DG:C5	1:A:16:DT:C7	1.23	2.21	18	19
1:A:16:DT:O4	1:A:17:DG:O6	1.22	1.55	15	3
1:A:10:DT:C6	1:A:11:DT:H71	1.21	1.70	15	20
1:A:1:DC:N4	1:A:2:DA:C6	1.20	2.08	16	20
1:A:17:DG:C2	2:B:2:DA:C2	1.20	2.29	7	8
1:A:15:DG:C8	1:A:16:DT:H71	1.20	1.71	3	17
1:A:15:DG:N7	1:A:16:DT:C7	1.19	2.05	18	18
2:B:3:DC:C2	2:B:4:DT:C6	1.18	2.30	15	18
1:A:9:DT:C6	1:A:10:DT:H72	1.18	1.73	13	5
1:A:14:DA:C2	2:B:5:DA:C2	1.15	2.32	13	18
1:A:16:DT:C4	1:A:17:DG:C5	1.12	2.22	16	4
2:B:5:DA:C6	2:B:6:DC:C4	1.11	2.37	20	20
1:A:10:DT:C5	1:A:11:DT:H73	1.11	1.79	15	20
1:A:15:DG:O6	2:B:2:DA:N6	1.10	1.83	2	19
2:B:1:DC:N3	2:B:2:DA:C4	1.08	2.22	9	15
1:A:10:DT:C5	1:A:11:DT:C7	1.07	2.37	15	20
1:A:17:DG:C2	2:B:2:DA:N1	1.07	2.23	7	5
2:B:5:DA:N6	2:B:6:DC:N4	1.07	2.00	20	20
1:A:3:DC:N3	1:A:4:DT:C4	1.07	2.21	1	9
1:A:9:DT:C5	1:A:10:DT:H72	1.07	1.83	13	5
2:B:5:DA:N1	2:B:6:DC:C4	1.06	2.23	12	20
1:A:1:DC:C4	1:A:2:DA:C5	1.06	2.42	7	20
1:A:1:DC:N4	1:A:2:DA:N6	1.06	2.03	7	19
2:B:4:DT:O2	2:B:5:DA:O4'	1.04	1.76	12	20
1:A:1:DC:N4	2:B:17:DG:H1	1.04	1.49	18	19
1:A:10:DT:C6	1:A:11:DT:C7	1.03	2.42	15	20
1:A:2:DA:N6	1:A:3:DC:N4	1.02	2.05	16	11
1:A:15:DG:C8	1:A:16:DT:H72	1.02	1.89	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:DT:C4	1:A:11:DT:H73	1.02	1.89	15	16
1:A:2:DA:C6	1:A:3:DC:C4	1.02	2.48	16	18
1:A:3:DC:N1	1:A:4:DT:H72	1.02	1.68	15	8
1:A:3:DC:C2	1:A:4:DT:C5	1.02	2.47	19	19
2:B:1:DC:C2	2:B:2:DA:N7	1.02	2.28	16	5
2:B:1:DC:O2	2:B:2:DA:O4'	1.01	1.78	17	15
1:A:1:DC:N3	1:A:2:DA:C5	1.01	2.28	7	20
1:A:10:DT:N1	1:A:11:DT:H71	1.00	1.69	15	20
1:A:16:DT:O4	2:B:2:DA:N1	1.00	1.92	17	1
1:A:11:DT:O2	1:A:12:DG:C8	1.00	2.14	2	20
1:A:1:DC:C4	1:A:2:DA:N7	0.99	2.31	7	19
2:B:2:DA:C5	2:B:3:DC:C5	0.99	2.50	13	19
1:A:2:DA:C6	1:A:3:DC:N4	0.98	2.31	16	11
1:A:16:DT:N3	1:A:17:DG:C4	0.98	2.30	13	5
1:A:1:DC:C2	1:A:2:DA:C8	0.98	2.49	7	20
1:A:3:DC:C6	1:A:4:DT:H71	0.98	1.92	13	12
1:A:3:DC:C5	1:A:4:DT:H73	0.97	1.95	3	12
1:A:17:DG:N2	2:B:2:DA:N3	0.96	2.13	7	5
1:A:16:DT:C4	1:A:17:DG:C6	0.96	2.52	15	3
2:B:1:DC:N4	2:B:2:DA:C2	0.96	2.33	9	14
1:A:16:DT:C4	1:A:17:DG:N7	0.96	2.30	13	5
2:B:5:DA:C2	2:B:6:DC:C4	0.95	2.54	12	20
2:B:1:DC:H2'	2:B:2:DA:C8	0.95	1.96	16	5
1:A:15:DG:C8	1:A:16:DT:C7	0.94	2.49	18	18
1:A:2:DA:N6	2:B:15:DG:O6	0.94	1.99	8	15
1:A:10:DT:C4	1:A:11:DT:C7	0.94	2.51	15	20
1:A:3:DC:C6	1:A:4:DT:C7	0.94	2.50	13	20
1:A:15:DG:N7	1:A:16:DT:H73	0.93	1.78	13	17
1:A:13:DT:O2	1:A:14:DA:C8	0.93	2.22	13	17
1:A:14:DA:N1	2:B:5:DA:C2	0.93	2.36	13	4
1:A:8:DC:N4	2:B:9:DA:H62	0.92	1.58	3	13
2:B:16:DT:O4	2:B:17:DG:C6	0.92	2.21	18	19
2:B:3:DC:O2	2:B:4:DT:C6	0.92	2.21	15	3
2:B:3:DC:C6	2:B:4:DT:H71	0.92	2.00	2	20
1:A:5:DA:C6	2:B:14:DA:N6	0.92	2.36	8	9
1:A:8:DC:N4	2:B:9:DA:H61	0.92	1.55	4	19
1:A:14:DA:C2	2:B:5:DA:C4	0.92	2.58	13	6
1:A:14:DA:N1	2:B:5:DA:N3	0.91	2.17	13	5
1:A:10:DT:C2	1:A:11:DT:C6	0.91	2.58	15	20
2:B:2:DA:C6	2:B:3:DC:C4	0.91	2.58	4	18
2:B:3:DC:O2	2:B:4:DT:O4'	0.91	1.89	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:DC:H42	2:B:9:DA:H62	0.91	0.95	9	7
2:B:5:DA:C2	2:B:6:DC:N3	0.91	2.39	2	20
1:A:15:DG:C5	1:A:16:DT:C5	0.91	2.59	18	18
1:A:15:DG:N7	1:A:16:DT:H71	0.90	1.74	3	13
1:A:1:DC:N3	2:B:17:DG:N2	0.90	2.20	4	20
2:B:1:DC:C4	2:B:2:DA:C4	0.88	2.61	9	10
1:A:15:DG:C5	1:A:16:DT:H71	0.87	2.02	8	17
1:A:9:DT:C6	1:A:10:DT:C7	0.87	2.56	13	16
1:A:2:DA:C5	1:A:3:DC:C5	0.87	2.62	9	20
1:A:3:DC:C5	1:A:4:DT:H72	0.87	2.05	19	8
1:A:14:DA:C6	2:B:5:DA:C2	0.86	2.61	13	4
1:A:15:DG:C5	1:A:16:DT:H73	0.86	2.03	4	18
2:B:5:DA:C2	2:B:6:DC:C2	0.85	2.64	3	20
1:A:1:DC:N4	2:B:17:DG:N1	0.84	2.24	14	20
1:A:1:DC:H42	2:B:17:DG:H1	0.84	1.15	18	1
2:B:16:DT:O4	2:B:17:DG:O6	0.84	1.96	18	14
2:B:16:DT:C4	2:B:17:DG:C6	0.83	2.66	18	13
1:A:9:DT:C5	1:A:10:DT:C7	0.83	2.61	13	13
2:B:1:DC:HO5'	2:B:1:DC:H6	0.83	0.86	15	2
1:A:10:DT:C2	1:A:11:DT:C5	0.83	2.66	15	20
2:B:2:DA:C4	2:B:3:DC:C6	0.83	2.66	13	20
1:A:15:DG:C4	1:A:16:DT:H71	0.82	2.08	4	17
2:B:5:DA:C4	2:B:6:DC:C5	0.82	2.68	2	20
1:A:3:DC:C4	1:A:4:DT:O4	0.82	2.32	1	9
1:A:10:DT:N3	1:A:11:DT:C5	0.82	2.48	15	20
2:B:1:DC:O5'	2:B:1:DC:H6	0.82	1.57	13	1
2:B:5:DA:N1	2:B:6:DC:N3	0.81	2.28	20	20
1:A:6:DC:H42	2:B:11:DA:H61	0.81	1.13	20	9
2:B:1:DC:H2'	2:B:2:DA:H8	0.81	1.34	16	2
1:A:16:DT:N3	1:A:17:DG:C6	0.81	2.49	3	4
1:A:3:DC:C2	1:A:4:DT:C4	0.80	2.69	1	9
1:A:1:DC:N4	1:A:2:DA:C5	0.80	2.47	7	13
2:B:15:DG:N7	2:B:16:DT:C7	0.79	2.46	14	4
2:B:4:DT:C2	2:B:5:DA:C8	0.79	2.70	16	20
1:A:17:DG:N1	2:B:2:DA:C6	0.78	2.52	13	5
1:A:3:DC:N3	1:A:4:DT:O4	0.78	2.16	1	9
1:A:3:DC:C5	1:A:4:DT:C7	0.78	2.67	3	20
1:A:9:DT:C2	1:A:10:DT:C6	0.78	2.72	17	20
2:B:3:DC:C2	2:B:4:DT:C5	0.78	2.72	15	6
1:A:5:DA:N3	1:A:6:DC:C6	0.78	2.52	17	19
1:A:6:DC:O2	1:A:7:DT:O4'	0.78	2.02	12	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:DA:C4	1:A:6:DC:C5	0.77	2.73	17	20
1:A:15:DG:N9	1:A:16:DT:H71	0.77	1.94	5	17
2:B:2:DA:C5	2:B:3:DC:C4	0.77	2.73	4	18
1:A:8:DC:H42	2:B:9:DA:H61	0.77	1.20	13	3
1:A:14:DA:N1	2:B:5:DA:C4	0.77	2.53	13	2
2:B:15:DG:C8	2:B:16:DT:H71	0.76	2.16	14	4
2:B:2:DA:N6	2:B:3:DC:N4	0.76	2.34	4	12
2:B:1:DC:C5	2:B:2:DA:C5	0.76	2.72	9	7
2:B:15:DG:N7	2:B:16:DT:H71	0.76	1.96	16	4
2:B:2:DA:C6	2:B:3:DC:N4	0.76	2.54	4	8
1:A:1:DC:N3	1:A:2:DA:C4	0.75	2.54	16	14
1:A:9:DT:O2	1:A:10:DT:O4'	0.75	2.04	15	20
1:A:15:DG:C4	1:A:16:DT:C6	0.75	2.75	18	18
2:B:3:DC:N3	2:B:4:DT:C5	0.75	2.55	15	3
1:A:9:DT:C4	1:A:10:DT:C4	0.73	2.76	9	12
1:A:5:DA:C2	2:B:14:DA:C2	0.73	2.76	10	9
1:A:5:DA:N6	2:B:14:DA:N6	0.73	2.36	6	9
1:A:11:DT:C2	1:A:12:DG:C8	0.73	2.77	14	20
1:A:10:DT:C2	1:A:11:DT:C7	0.73	2.71	15	3
1:A:13:DT:C2	1:A:14:DA:C8	0.73	2.76	13	17
1:A:9:DT:C6	1:A:10:DT:H71	0.72	2.18	16	10
1:A:15:DG:C6	1:A:16:DT:C5	0.72	2.77	18	17
2:B:2:DA:C4	2:B:3:DC:C5	0.72	2.77	4	18
1:A:17:DG:N1	2:B:2:DA:N1	0.72	2.36	7	4
1:A:16:DT:N3	1:A:17:DG:N7	0.72	2.37	15	3
1:A:10:DT:C2	1:A:11:DT:H71	0.72	2.19	15	2
2:B:1:DC:O2	2:B:2:DA:C5	0.72	2.43	16	1
1:A:15:DG:C4	1:A:16:DT:C7	0.71	2.72	4	19
1:A:17:DG:N1	2:B:1:DC:N4	0.71	2.39	11	15
1:A:17:DG:N2	2:B:1:DC:N3	0.71	2.38	18	15
1:A:3:DC:C6	1:A:4:DT:H73	0.71	2.19	2	1
1:A:3:DC:N1	1:A:4:DT:C7	0.71	2.53	15	12
1:A:17:DG:N2	2:B:2:DA:N1	0.71	2.35	3	2
1:A:14:DA:C4	2:B:5:DA:C2	0.70	2.79	13	1
2:B:1:DC:C2	2:B:2:DA:C4	0.70	2.79	2	15
1:A:16:DT:C2	1:A:17:DG:C8	0.70	2.80	15	3
2:B:5:DA:N1	2:B:6:DC:N4	0.70	2.29	12	19
1:A:16:DT:C5	1:A:17:DG:N7	0.70	2.59	16	1
1:A:3:DC:C4	1:A:4:DT:C4	0.70	2.80	8	8
2:B:5:DA:C5	2:B:6:DC:C5	0.70	2.79	20	20
2:B:1:DC:C2	2:B:2:DA:C5	0.70	2.79	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:DC:H42	2:B:11:DA:N6	0.69	1.83	20	7
2:B:1:DC:N3	2:B:2:DA:C5	0.69	2.60	14	16
1:A:1:DC:O2	1:A:2:DA:O4'	0.69	2.11	16	19
2:B:16:DT:N3	2:B:17:DG:C5	0.69	2.61	18	6
2:B:16:DT:C4	2:B:17:DG:C5	0.69	2.81	20	15
1:A:3:DC:N1	1:A:4:DT:H71	0.69	2.01	13	12
2:B:4:DT:O2	2:B:5:DA:C1'	0.69	2.41	16	17
1:A:1:DC:N3	1:A:2:DA:N7	0.69	2.39	7	11
1:A:5:DA:C2	2:B:14:DA:N1	0.69	2.61	8	9
2:B:3:DC:C5	2:B:4:DT:C7	0.69	2.75	13	20
1:A:16:DT:O2	1:A:17:DG:O4'	0.68	2.10	19	13
1:A:5:DA:C4	1:A:6:DC:C6	0.68	2.81	16	19
1:A:5:DA:C5	1:A:6:DC:C5	0.68	2.81	16	19
2:B:1:DC:N4	2:B:2:DA:N6	0.68	2.41	9	13
1:A:14:DA:N3	2:B:5:DA:C2	0.67	2.61	13	2
2:B:1:DC:N3	2:B:2:DA:N3	0.67	2.42	9	14
1:A:9:DT:C5	1:A:10:DT:C5	0.67	2.81	9	9
1:A:5:DA:N1	2:B:14:DA:C6	0.67	2.63	8	9
1:A:2:DA:C4	1:A:3:DC:C5	0.67	2.83	11	11
2:B:3:DC:C6	2:B:4:DT:C7	0.67	2.78	13	20
1:A:16:DT:H2''	1:A:17:DG:H5'	0.66	1.64	16	1
2:B:3:DC:N3	2:B:4:DT:C6	0.66	2.64	15	3
1:A:2:DA:C5	1:A:3:DC:C4	0.66	2.84	11	11
1:A:3:DC:C4	1:A:4:DT:H73	0.66	2.25	2	11
1:A:1:DC:N3	1:A:2:DA:C8	0.66	2.64	7	11
1:A:3:DC:N4	1:A:4:DT:O4	0.66	2.28	8	8
1:A:3:DC:C2	1:A:4:DT:C7	0.65	2.79	15	8
1:A:5:DA:C5	1:A:6:DC:C4	0.65	2.85	15	1
1:A:6:DC:C2	1:A:7:DT:C6	0.64	2.84	12	19
1:A:3:DC:C2	1:A:4:DT:H72	0.64	2.26	15	6
2:B:13:DT:N3	2:B:14:DA:N7	0.64	2.46	20	9
2:B:13:DT:N3	2:B:14:DA:C5	0.63	2.66	12	9
2:B:4:DT:O2	2:B:5:DA:N9	0.63	2.31	16	14
2:B:3:DC:C5	2:B:4:DT:H73	0.63	2.28	2	18
1:A:5:DA:C6	2:B:12:DG:O6	0.63	2.51	13	7
1:A:15:DG:C8	1:A:16:DT:H73	0.63	2.29	18	1
2:B:5:DA:C5	2:B:6:DC:C4	0.62	2.86	20	20
1:A:9:DT:C4	1:A:10:DT:C5	0.62	2.87	13	12
1:A:3:DC:N3	1:A:4:DT:C5	0.62	2.65	1	9
2:B:5:DA:N6	2:B:6:DC:H42	0.62	1.88	20	18
2:B:3:DC:C4	2:B:4:DT:C5	0.62	2.87	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:DT:O2	1:A:11:DT:C6	0.62	2.53	15	8
2:B:15:DG:C5	2:B:16:DT:C5	0.62	2.88	14	4
1:A:14:DA:C5	2:B:5:DA:C2	0.62	2.87	13	1
1:A:16:DT:C2	1:A:17:DG:C4	0.62	2.88	15	4
1:A:15:DG:C4	1:A:16:DT:C5	0.61	2.88	6	18
1:A:10:DT:N3	1:A:11:DT:C7	0.61	2.63	15	2
1:A:14:DA:N3	2:B:5:DA:N3	0.61	2.41	13	1
1:A:1:DC:C4	1:A:2:DA:C6	0.61	2.84	15	2
2:B:3:DC:N1	2:B:4:DT:H71	0.61	2.09	12	20
1:A:1:DC:H41	1:A:2:DA:N6	0.61	1.93	16	3
1:A:8:DC:H2''	1:A:9:DT:H5'	0.61	1.72	15	19
1:A:16:DT:C4	2:B:2:DA:N1	0.61	2.69	17	1
1:A:9:DT:C7	1:A:10:DT:H72	0.60	2.25	13	5
1:A:5:DA:C6	1:A:6:DC:C4	0.60	2.90	15	2
1:A:6:DC:N3	1:A:7:DT:C4	0.59	2.70	17	19
1:A:3:DC:C2	1:A:4:DT:C6	0.59	2.90	2	12
2:B:1:DC:H41	2:B:2:DA:N6	0.59	1.95	9	5
2:B:10:DG:C6	2:B:11:DA:C5	0.59	2.90	6	13
2:B:1:DC:C5	2:B:2:DA:C6	0.59	2.88	9	1
2:B:13:DT:C2	2:B:14:DA:N7	0.59	2.70	20	9
1:A:15:DG:N3	1:A:16:DT:C6	0.59	2.71	1	15
2:B:1:DC:O2	2:B:2:DA:C1'	0.58	2.51	17	2
1:A:5:DA:C2	1:A:6:DC:C6	0.58	2.92	17	10
1:A:2:DA:N6	1:A:3:DC:H42	0.58	1.94	16	1
2:B:4:DT:O2	2:B:5:DA:C8	0.58	2.57	16	13
2:B:1:DC:C2	2:B:2:DA:N9	0.58	2.72	11	14
2:B:4:DT:N3	2:B:5:DA:C8	0.57	2.72	16	3
1:A:14:DA:H2	2:B:5:DA:N3	0.57	1.75	13	1
1:A:15:DG:C6	2:B:2:DA:N6	0.57	2.72	16	1
2:B:1:DC:O2	2:B:2:DA:N7	0.57	2.37	16	1
1:A:15:DG:C6	1:A:16:DT:C4	0.57	2.92	13	15
1:A:17:DG:N1	2:B:1:DC:C4	0.57	2.73	20	15
1:A:13:DT:O2	1:A:14:DA:N9	0.57	2.38	13	5
1:A:2:DA:C4	2:B:17:DG:N2	0.57	2.73	18	2
1:A:5:DA:C2	1:A:6:DC:C2	0.56	2.93	15	1
1:A:1:DC:C2	1:A:2:DA:N9	0.56	2.73	7	7
1:A:3:DC:H2'	1:A:4:DT:H71	0.56	1.75	2	1
2:B:6:DC:H2''	2:B:7:DA:O5'	0.56	2.00	13	20
1:A:1:DC:C5	1:A:2:DA:N7	0.56	2.73	7	6
1:A:8:DC:H2''	1:A:9:DT:C5'	0.56	2.30	15	20
1:A:2:DA:C4	1:A:3:DC:C6	0.56	2.93	20	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:DG:C5	2:B:16:DT:C7	0.56	2.88	16	2
1:A:10:DT:C4	1:A:11:DT:C5	0.56	2.92	15	17
2:B:12:DG:C6	2:B:13:DT:C4	0.56	2.93	12	17
1:A:14:DA:H4'	1:A:15:DG:OP1	0.55	2.01	16	2
1:A:5:DA:C6	2:B:14:DA:C6	0.55	2.95	12	9
1:A:5:DA:C6	2:B:14:DA:N1	0.55	2.74	2	6
2:B:4:DT:N3	2:B:5:DA:C5	0.55	2.74	16	1
2:B:12:DG:C5	2:B:13:DT:C5	0.54	2.94	12	16
1:A:17:DG:N2	2:B:2:DA:C4	0.54	2.74	7	4
1:A:6:DC:N3	1:A:7:DT:C5	0.54	2.75	17	19
1:A:1:DC:H42	1:A:2:DA:N6	0.54	2.00	18	1
2:B:1:DC:C2'	2:B:2:DA:C8	0.54	2.83	16	1
2:B:1:DC:C4	2:B:2:DA:C2	0.54	2.93	9	3
1:A:5:DA:N1	2:B:12:DG:O6	0.54	2.41	3	6
2:B:12:DG:C6	2:B:13:DT:N3	0.53	2.76	10	17
1:A:2:DA:N1	1:A:3:DC:C4	0.53	2.77	16	4
2:B:2:DA:N7	2:B:3:DC:C5	0.53	2.77	13	9
1:A:15:DG:C2	1:A:16:DT:C6	0.53	2.97	19	9
1:A:2:DA:C2	2:B:17:DG:N2	0.53	2.77	18	1
1:A:6:DC:N4	2:B:11:DA:H61	0.53	1.94	20	1
2:B:5:DA:C2	2:B:6:DC:C5	0.53	2.97	12	4
1:A:16:DT:C2	1:A:17:DG:N9	0.53	2.77	15	2
2:B:2:DA:C6	2:B:3:DC:C5	0.53	2.94	13	1
1:A:9:DT:C6	1:A:10:DT:C5	0.52	2.97	9	5
1:A:5:DA:C2	2:B:14:DA:C6	0.52	2.96	8	1
2:B:10:DG:C6	2:B:11:DA:C6	0.52	2.97	18	9
2:B:14:DA:C5	2:B:15:DG:N7	0.52	2.78	3	1
2:B:10:DG:C4	2:B:11:DA:C8	0.52	2.98	12	5
1:A:5:DA:N1	2:B:14:DA:N1	0.52	2.58	1	6
2:B:3:DC:O2	2:B:4:DT:C1'	0.52	2.57	16	2
2:B:1:DC:N3	2:B:2:DA:N6	0.52	2.57	16	1
2:B:3:DC:C4	2:B:4:DT:C7	0.52	2.93	13	13
1:A:9:DT:C5	1:A:10:DT:H73	0.51	2.40	20	4
1:A:11:DT:N3	1:A:12:DG:N7	0.51	2.58	14	14
1:A:4:DT:N3	2:B:15:DG:N2	0.51	2.59	15	1
2:B:1:DC:H2''	2:B:2:DA:O5'	0.51	2.04	9	15
2:B:14:DA:H4'	2:B:15:DG:OP1	0.51	2.06	15	9
1:A:17:DG:C2	2:B:2:DA:C6	0.51	2.99	15	4
1:A:6:DC:N4	2:B:11:DA:N6	0.51	2.58	20	1
2:B:5:DA:N3	2:B:6:DC:C6	0.51	2.79	12	4
1:A:6:DC:C4	1:A:7:DT:C4	0.50	2.99	1	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:16:DT:N3	2:B:17:DG:C6	0.50	2.79	18	1
1:A:4:DT:C2	2:B:15:DG:N2	0.50	2.80	2	1
1:A:3:DC:C4	1:A:4:DT:C7	0.50	2.94	15	12
1:A:5:DA:N6	2:B:14:DA:H61	0.49	2.05	6	3
2:B:4:DT:N3	2:B:5:DA:N7	0.49	2.59	16	1
1:A:1:DC:C4	2:B:17:DG:N1	0.49	2.80	20	4
1:A:16:DT:C2'	1:A:17:DG:H5'	0.49	2.36	16	1
1:A:11:DT:C2	1:A:12:DG:N7	0.49	2.81	14	20
2:B:5:DA:N6	2:B:6:DC:H41	0.49	1.98	20	11
1:A:16:DT:H3	2:B:2:DA:H61	0.49	1.48	16	1
2:B:16:DT:H2''	2:B:17:DG:O5'	0.49	2.07	9	20
1:A:16:DT:H2''	1:A:17:DG:O5'	0.49	2.07	17	8
2:B:1:DC:N3	2:B:2:DA:C2	0.49	2.81	2	9
1:A:16:DT:C2'	1:A:17:DG:C5'	0.48	2.90	16	1
1:A:15:DG:N2	2:B:4:DT:C2	0.48	2.81	13	1
1:A:16:DT:N3	1:A:17:DG:C8	0.48	2.80	15	2
2:B:2:DA:N6	2:B:3:DC:C4	0.48	2.82	13	1
1:A:14:DA:C4	2:B:5:DA:H2	0.47	2.22	13	1
1:A:17:DG:C6	2:B:1:DC:N4	0.47	2.83	14	11
1:A:8:DC:H2'	1:A:9:DT:C6	0.47	2.43	6	12
1:A:5:DA:C6	1:A:6:DC:C5	0.47	3.02	16	9
2:B:13:DT:C2	2:B:14:DA:C5	0.47	3.02	20	8
2:B:1:DC:N3	2:B:2:DA:N7	0.47	2.60	16	1
2:B:12:DG:H2''	2:B:13:DT:O5'	0.47	2.09	7	19
1:A:12:DG:C6	2:B:7:DA:C2	0.47	3.02	16	5
1:A:5:DA:C2	1:A:6:DC:C5	0.47	3.03	17	6
2:B:1:DC:C2	2:B:2:DA:C8	0.46	3.01	16	2
2:B:16:DT:N3	2:B:17:DG:C4	0.46	2.83	18	3
2:B:5:DA:N3	2:B:6:DC:C5	0.46	2.84	12	2
2:B:15:DG:H2''	2:B:16:DT:O5'	0.46	2.11	4	7
1:A:17:DG:N1	2:B:2:DA:N6	0.46	2.63	16	1
2:B:9:DA:C6	2:B:10:DG:C6	0.46	3.04	9	2
2:B:10:DG:N3	2:B:11:DA:O4'	0.45	2.49	15	1
1:A:13:DT:C2	1:A:14:DA:N7	0.45	2.83	13	1
2:B:10:DG:C5	2:B:11:DA:C5	0.45	3.04	18	3
1:A:14:DA:C6	2:B:5:DA:N1	0.45	2.84	13	1
2:B:3:DC:C4	2:B:4:DT:H73	0.45	2.47	2	3
1:A:3:DC:H2'	1:A:4:DT:C6	0.45	2.47	20	6
1:A:8:DC:C4	2:B:9:DA:N6	0.45	2.56	5	2
1:A:2:DA:C2	1:A:3:DC:C2	0.45	3.05	17	2
2:B:12:DG:C5	2:B:13:DT:C4	0.45	3.05	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:3:DC:O2	2:B:4:DT:N1	0.45	2.50	16	2
2:B:5:DA:C6	2:B:6:DC:C5	0.44	3.01	12	1
1:A:16:DT:C2	1:A:17:DG:C5	0.44	3.00	7	2
1:A:12:DG:C8	1:A:13:DT:H71	0.44	2.47	6	9
2:B:13:DT:C2	2:B:14:DA:C8	0.44	3.04	12	2
2:B:2:DA:C8	2:B:3:DC:C5	0.44	3.05	6	9
1:A:1:DC:N4	1:A:2:DA:H62	0.44	2.01	7	1
2:B:11:DA:C2	2:B:12:DG:C4	0.44	3.05	15	5
1:A:5:DA:C6	1:A:6:DC:N4	0.44	2.86	15	1
1:A:2:DA:C2	2:B:17:DG:C2	0.44	3.06	3	1
1:A:6:DC:C2	1:A:7:DT:C5	0.43	3.06	17	1
1:A:2:DA:N1	1:A:3:DC:N3	0.43	2.66	16	4
2:B:13:DT:H2''	2:B:14:DA:O5'	0.43	2.13	18	9
2:B:1:DC:C5	2:B:2:DA:N7	0.43	2.86	9	1
2:B:15:DG:C5	2:B:16:DT:H71	0.42	2.48	16	1
1:A:9:DT:N1	1:A:10:DT:C6	0.42	2.87	9	4
2:B:14:DA:C6	2:B:15:DG:C5	0.42	3.08	3	1
2:B:4:DT:H2''	2:B:5:DA:O5'	0.42	2.15	17	3
2:B:1:DC:N3	2:B:2:DA:C6	0.42	2.88	7	1
1:A:16:DT:O2	1:A:17:DG:N9	0.42	2.52	15	1
1:A:6:DC:N4	1:A:7:DT:C4	0.42	2.88	1	1
1:A:15:DG:N2	2:B:4:DT:H1'	0.42	2.29	13	1
2:B:15:DG:C6	2:B:16:DT:C4	0.41	3.08	14	2
1:A:13:DT:N3	1:A:14:DA:N7	0.41	2.68	13	1
2:B:5:DA:C4	2:B:6:DC:C6	0.41	3.09	12	3
2:B:10:DG:O6	2:B:11:DA:C6	0.41	2.73	4	1
2:B:1:DC:C2	2:B:2:DA:O4'	0.41	2.71	9	1
2:B:12:DG:C4	2:B:13:DT:C6	0.41	3.09	12	1
1:A:6:DC:O2	1:A:7:DT:C6	0.41	2.73	17	1
2:B:13:DT:N3	2:B:14:DA:C6	0.41	2.89	10	3
1:A:16:DT:H3	2:B:2:DA:N6	0.41	2.13	16	1
1:A:17:DG:N2	2:B:2:DA:C6	0.40	2.89	3	1
1:A:4:DT:H2''	1:A:5:DA:O5'	0.40	2.16	3	1
2:B:15:DG:N7	2:B:16:DT:H73	0.40	2.31	11	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5243

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	363
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	363
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 363 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	3	DC	H42	6.79	0.01	1
UNMAPPED	32	DG	H4'	4.39	0.01	1
UNMAPPED	14	DA	H3'	5.04	0.01	1
UNMAPPED	7	DT	H1'	6.02	0.01	1
UNMAPPED	14	DA	H2''	2.88	0.01	2
UNMAPPED	33	DT	H5''	4.1	0.01	1
UNMAPPED	25	DA	H2	7.04	0.01	1
UNMAPPED	2	DA	H4'	4.44	0.01	1
UNMAPPED	1	DC	H5	5.87	0.01	1
UNMAPPED	28	DA	H4'	4.44	0.01	1
UNMAPPED	17	DG	H4'	4.39	0.01	1
UNMAPPED	12	DG	H5''	4.14	0.01	2
UNMAPPED	33	DT	H1'	5.84	0.01	1
UNMAPPED	12	DG	H1'	5.88	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	9	DT	H2'	2.19	0.01	1
UNMAPPED	1	DC	H4'	4.05	0.01	1
UNMAPPED	2	DA	H61	7.65	0.01	2
UNMAPPED	2	DA	H3'	5.03	0.01	1
UNMAPPED	22	DA	H3'	5.0	0.01	1
UNMAPPED	7	DT	H6	7.41	0.01	1
UNMAPPED	12	DG	H8	7.88	0.01	1
UNMAPPED	21	DT	H71	1.59	0.01	1
UNMAPPED	19	DA	H2''	2.92	0.01	2
UNMAPPED	11	DT	H71	1.68	0.01	1
UNMAPPED	33	DT	H73	1.38	0.01	1
UNMAPPED	33	DT	H2'	1.89	0.01	2
UNMAPPED	13	DT	H73	1.41	0.01	1
UNMAPPED	26	DA	H5'	4.17	0.01	1
UNMAPPED	13	DT	H1'	5.62	0.01	1
UNMAPPED	16	DT	H72	1.38	0.01	1
UNMAPPED	8	DC	H42	7.03	0.01	2
UNMAPPED	5	DA	H4'	4.43	0.01	1
UNMAPPED	1	DC	H1'	5.6	0.01	1
UNMAPPED	21	DT	H2''	2.46	0.01	1
UNMAPPED	31	DA	H62	7.75	0.01	2
UNMAPPED	25	DA	H2'	2.58	0.01	2
UNMAPPED	6	DC	H41	7.9	0.01	2
UNMAPPED	21	DT	H2'	2.1	0.01	1
UNMAPPED	30	DT	H72	1.25	0.01	1
UNMAPPED	1	DC	H3'	4.69	0.01	1
UNMAPPED	11	DT	H3	13.45	0.01	1
UNMAPPED	19	DA	H61	7.65	0.01	2
UNMAPPED	17	DG	H2''	2.61	0.01	2
UNMAPPED	30	DT	H6	7.14	0.01	1
UNMAPPED	7	DT	H71	1.51	0.01	1
UNMAPPED	9	DT	H71	1.59	0.01	1
UNMAPPED	2	DA	H1'	6.26	0.01	1
UNMAPPED	21	DT	H6	7.37	0.01	1
UNMAPPED	3	DC	H2''	2.45	0.01	1
UNMAPPED	10	DT	H73	1.59	0.01	1
UNMAPPED	17	DG	H1'	6.13	0.01	1
UNMAPPED	4	DT	H73	1.59	0.01	1
UNMAPPED	16	DT	H5'	4.1	0.01	1
UNMAPPED	14	DA	H4'	4.39	0.01	1
UNMAPPED	20	DC	H6	7.33	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	24	DA	H5'	4.09	0.01	2
UNMAPPED	7	DT	H4'	4.22	0.01	1
UNMAPPED	33	DT	H3	13.86	0.01	1
UNMAPPED	29	DG	H3'	4.83	0.01	1
UNMAPPED	32	DG	H1'	5.84	0.01	1
UNMAPPED	17	DG	H5''	4.09	0.01	2
UNMAPPED	8	DC	H5	5.55	0.01	1
UNMAPPED	10	DT	H2''	2.58	0.01	2
UNMAPPED	10	DT	H3'	4.89	0.01	1
UNMAPPED	6	DC	H5''	4.22	0.01	1
UNMAPPED	7	DT	H2'	2.19	0.01	1
UNMAPPED	28	DA	H2'	2.59	0.01	2
UNMAPPED	28	DA	H3'	5.0	0.01	1
UNMAPPED	7	DT	H3'	4.86	0.01	1
UNMAPPED	5	DA	H2''	2.83	0.01	2
UNMAPPED	2	DA	H8	8.37	0.01	1
UNMAPPED	10	DT	H2'	2.17	0.01	2
UNMAPPED	5	DA	H3'	5.04	0.01	1
UNMAPPED	26	DA	H2	7.3	0.01	1
UNMAPPED	16	DT	H4'	4.18	0.01	1
UNMAPPED	20	DC	H42	6.79	0.01	2
UNMAPPED	10	DT	H5'	4.09	0.01	1
UNMAPPED	9	DT	H3	14.08	0.01	1
UNMAPPED	23	DC	H3'	4.75	0.01	1
UNMAPPED	11	DT	H72	1.68	0.01	1
UNMAPPED	23	DC	H2''	2.18	0.01	2
UNMAPPED	28	DA	H2	7.53	0.01	1
UNMAPPED	13	DT	H5''	4.13	0.01	1
UNMAPPED	24	DA	H2'	2.62	0.01	2
UNMAPPED	5	DA	H61	5.67	0.01	2
UNMAPPED	8	DC	H2'	2.2	0.01	1
UNMAPPED	28	DA	H62	7.5	0.01	2
UNMAPPED	16	DT	H71	1.38	0.01	1
UNMAPPED	27	DG	H1'	5.42	0.01	1
UNMAPPED	8	DC	H41	8.26	0.01	2
UNMAPPED	20	DC	H2''	2.45	0.01	2
UNMAPPED	29	DG	H5'	4.19	0.01	1
UNMAPPED	19	DA	H5'	4.13	0.01	2
UNMAPPED	1	DC	H6	7.65	0.01	1
UNMAPPED	15	DG	H2'	2.45	0.01	1
UNMAPPED	8	DC	H1'	6.03	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	DG	H4'	4.39	0.01	1
UNMAPPED	16	DT	H2''	2.35	0.01	2
UNMAPPED	34	DG	H1	12.9	0.01	1
UNMAPPED	8	DC	H2''	2.54	0.01	1
UNMAPPED	28	DA	H1'	6.03	0.01	1
UNMAPPED	30	DT	H71	1.25	0.01	1
UNMAPPED	27	DG	H8	7.47	0.01	1
UNMAPPED	21	DT	H4'	4.17	0.01	1
UNMAPPED	19	DA	H2'	2.8	0.01	2
UNMAPPED	22	DA	H5''	4.09	0.01	2
UNMAPPED	30	DT	H4'	4.17	0.01	1
UNMAPPED	8	DC	H5'	4.09	0.01	1
UNMAPPED	31	DA	H8	8.22	0.01	1
UNMAPPED	23	DC	H5'	4.09	0.01	1
UNMAPPED	31	DA	H2	7.19	0.01	1
UNMAPPED	27	DG	H3'	4.91	0.01	1
UNMAPPED	27	DG	H2''	2.62	0.01	2
UNMAPPED	4	DT	H5''	4.09	0.01	1
UNMAPPED	2	DA	H5''	4.02	0.01	2
UNMAPPED	9	DT	H5''	4.09	0.01	1
UNMAPPED	16	DT	H5''	4.1	0.01	1
UNMAPPED	27	DG	H2'	2.4	0.01	2
UNMAPPED	24	DA	H5''	3.96	0.01	2
UNMAPPED	25	DA	H3'	4.99	0.01	1
UNMAPPED	32	DG	H2'	2.45	0.01	2
UNMAPPED	31	DA	H5''	4.05	0.01	2
UNMAPPED	19	DA	H3'	5.03	0.01	1
UNMAPPED	21	DT	H3	13.68	0.01	1
UNMAPPED	9	DT	H72	1.59	0.01	1
UNMAPPED	25	DA	H8	8.08	0.01	1
UNMAPPED	10	DT	H72	1.59	0.01	1
UNMAPPED	4	DT	H72	1.59	0.01	1
UNMAPPED	3	DC	H2'	1.97	0.01	1
UNMAPPED	31	DA	H1'	6.06	0.01	1
UNMAPPED	20	DC	H5	5.32	0.01	1
UNMAPPED	18	DC	H3'	4.69	0.01	1
UNMAPPED	26	DA	H61	6.03	0.01	2
UNMAPPED	6	DC	H2'	1.98	0.01	1
UNMAPPED	33	DT	H3'	4.84	0.01	1
UNMAPPED	18	DC	H1'	5.6	0.01	1
UNMAPPED	13	DT	H3	13.45	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	31	DA	H3'	5.04	0.01	1
UNMAPPED	24	DA	H2	6.99	0.01	1
UNMAPPED	17	DG	H2'	2.17	0.01	2
UNMAPPED	11	DT	H3'	4.91	0.01	1
UNMAPPED	5	DA	H5'	4.17	0.01	1
UNMAPPED	11	DT	H2''	2.51	0.01	1
UNMAPPED	24	DA	H3'	4.99	0.01	1
UNMAPPED	24	DA	H61	6.03	0.01	2
UNMAPPED	15	DG	H4'	4.39	0.01	1
UNMAPPED	22	DA	H8	8.27	0.01	1
UNMAPPED	4	DT	H2'	2.1	0.01	1
UNMAPPED	10	DT	H6	7.49	0.01	1
UNMAPPED	26	DA	H2''	2.8	0.01	2
UNMAPPED	29	DG	H1	12.79	0.01	1
UNMAPPED	22	DA	H2	7.3	0.01	1
UNMAPPED	18	DC	H4'	4.05	0.01	1
UNMAPPED	18	DC	H5'	3.72	0.01	1
UNMAPPED	25	DA	H1'	5.75	0.01	1
UNMAPPED	20	DC	H4'	4.31	0.01	1
UNMAPPED	2	DA	H2'	2.8	0.01	1
UNMAPPED	5	DA	H2'	2.71	0.01	2
UNMAPPED	14	DA	H2	7.19	0.01	1
UNMAPPED	34	DG	H1'	6.13	0.01	1
UNMAPPED	9	DT	H3'	4.86	0.01	1
UNMAPPED	13	DT	H2'	2.09	0.01	2
UNMAPPED	21	DT	H73	1.59	0.01	1
UNMAPPED	11	DT	H73	1.68	0.01	1
UNMAPPED	13	DT	H71	1.41	0.01	1
UNMAPPED	34	DG	H5''	4.09	0.01	2
UNMAPPED	33	DT	H5'	4.1	0.01	1
UNMAPPED	6	DC	H5	5.2	0.01	1
UNMAPPED	18	DC	H5	5.87	0.01	1
UNMAPPED	7	DT	H2''	2.54	0.01	1
UNMAPPED	3	DC	H5	5.32	0.01	1
UNMAPPED	23	DC	H5''	4.09	0.01	1
UNMAPPED	21	DT	H5'	4.05	0.01	1
UNMAPPED	32	DG	H8	7.65	0.01	1
UNMAPPED	4	DT	H5'	4.09	0.01	1
UNMAPPED	23	DC	H42	6.48	0.01	2
UNMAPPED	4	DT	H1'	5.71	0.01	1
UNMAPPED	12	DG	H5'	4.17	0.01	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	6	DC	H4'	4.25	0.01	1
UNMAPPED	9	DT	H5'	4.09	0.01	1
UNMAPPED	21	DT	H1'	5.66	0.01	1
UNMAPPED	15	DG	H5''	4.17	0.01	1
UNMAPPED	13	DT	H3'	4.86	0.01	1
UNMAPPED	31	DA	H5'	4.17	0.01	2
UNMAPPED	4	DT	H3'	4.86	0.01	1
UNMAPPED	1	DC	H5'	3.72	0.01	1
UNMAPPED	17	DG	H5'	4.17	0.01	2
UNMAPPED	25	DA	H62	5.88	0.01	1
UNMAPPED	28	DA	H5''	4.09	0.01	2
UNMAPPED	30	DT	H2''	2.45	0.01	2
UNMAPPED	30	DT	H3'	4.87	0.01	1
UNMAPPED	33	DT	H71	1.38	0.01	1
UNMAPPED	33	DT	H4'	4.18	0.01	1
UNMAPPED	7	DT	H5''	4.09	0.01	2
UNMAPPED	26	DA	H1'	5.86	0.01	1
UNMAPPED	34	DG	H2'	2.17	0.01	2
UNMAPPED	27	DG	H4'	4.33	0.01	1
UNMAPPED	17	DG	H3'	4.69	0.01	1
UNMAPPED	11	DT	H4'	4.17	0.01	1
UNMAPPED	3	DC	H5''	4.18	0.01	1
UNMAPPED	9	DT	H73	1.59	0.01	1
UNMAPPED	3	DC	H1'	5.84	0.01	1
UNMAPPED	10	DT	H4'	4.22	0.01	1
UNMAPPED	18	DC	H2'	1.9	0.01	1
UNMAPPED	26	DA	H62	7.45	0.01	2
UNMAPPED	9	DT	H4'	4.22	0.01	1
UNMAPPED	30	DT	H5''	4.09	0.01	1
UNMAPPED	29	DG	H2''	2.67	0.01	2
UNMAPPED	12	DG	H2'	2.59	0.01	2
UNMAPPED	15	DG	H1	12.71	0.01	1
UNMAPPED	2	DA	H62	5.88	0.01	2
UNMAPPED	17	DG	H8	7.89	0.01	1
UNMAPPED	14	DA	H5'	4.17	0.01	2
UNMAPPED	2	DA	H2	7.9	0.01	1
UNMAPPED	21	DT	H72	1.59	0.01	1
UNMAPPED	29	DG	H2'	2.37	0.01	2
UNMAPPED	28	DA	H8	7.92	0.01	1
UNMAPPED	15	DG	H2''	2.67	0.01	1
UNMAPPED	22	DA	H2'	2.64	0.01	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	DG	H1	12.36	0.01	1
UNMAPPED	8	DC	H4'	4.22	0.01	1
UNMAPPED	20	DC	H3'	4.68	0.01	1
UNMAPPED	6	DC	H6	7.34	0.01	1
UNMAPPED	14	DA	H62	7.3	0.01	2
UNMAPPED	20	DC	H2'	1.97	0.01	2
UNMAPPED	34	DG	H2''	2.61	0.01	2
UNMAPPED	6	DC	H42	6.74	0.01	2
UNMAPPED	21	DT	H5''	4.05	0.01	1
UNMAPPED	28	DA	H5'	4.17	0.01	2
UNMAPPED	6	DC	H5'	4.22	0.01	1
UNMAPPED	23	DC	H2'	1.83	0.01	2
UNMAPPED	19	DA	H62	5.88	0.01	2
UNMAPPED	11	DT	H6	7.36	0.01	1
UNMAPPED	16	DT	H1'	5.84	0.01	1
UNMAPPED	29	DG	H1'	5.78	0.01	1
UNMAPPED	3	DC	H5'	4.18	0.01	1
UNMAPPED	12	DG	H3'	4.95	0.01	1
UNMAPPED	25	DA	H61	5.88	0.01	1
UNMAPPED	19	DA	H2	7.9	0.01	1
UNMAPPED	12	DG	H2''	2.75	0.01	2
UNMAPPED	23	DC	H5	5.32	0.01	1
UNMAPPED	19	DA	H8	8.37	0.01	1
UNMAPPED	26	DA	H5''	4.17	0.01	1
UNMAPPED	33	DT	H72	1.38	0.01	1
UNMAPPED	30	DT	H3	13.45	0.01	1
UNMAPPED	7	DT	H72	1.51	0.01	1
UNMAPPED	11	DT	H5''	4.12	0.01	1
UNMAPPED	13	DT	H4'	4.17	0.01	1
UNMAPPED	29	DG	H4'	4.38	0.01	1
UNMAPPED	10	DT	H1'	6.1	0.01	1
UNMAPPED	25	DA	H2''	2.8	0.01	2
UNMAPPED	30	DT	H5'	4.09	0.01	1
UNMAPPED	21	DT	H3'	4.86	0.01	1
UNMAPPED	11	DT	H1'	5.83	0.01	1
UNMAPPED	33	DT	H2''	2.35	0.01	2
UNMAPPED	18	DC	H5''	3.72	0.01	1
UNMAPPED	16	DT	H6	7.14	0.01	1
UNMAPPED	14	DA	H5''	4.05	0.01	2
UNMAPPED	19	DA	H5''	4.02	0.01	2
UNMAPPED	14	DA	H1'	6.03	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	26	DA	H4'	4.39	0.01	1
UNMAPPED	18	DC	H2''	2.37	0.01	1
UNMAPPED	24	DA	H8	8.12	0.01	1
UNMAPPED	33	DT	H6	7.14	0.01	1
UNMAPPED	16	DT	H3'	4.84	0.01	1
UNMAPPED	8	DC	H6	7.62	0.01	1
UNMAPPED	2	DA	H2''	2.92	0.01	1
UNMAPPED	31	DA	H2''	2.9	0.01	2
UNMAPPED	25	DA	H5''	4.08	0.01	2
UNMAPPED	26	DA	H2'	2.5	0.01	2
UNMAPPED	24	DA	H2''	2.8	0.01	2
UNMAPPED	9	DT	H2''	2.54	0.01	1
UNMAPPED	14	DA	H8	8.21	0.01	1
UNMAPPED	26	DA	H3'	4.99	0.01	1
UNMAPPED	22	DA	H2''	2.83	0.01	2
UNMAPPED	4	DT	H2''	2.46	0.01	1
UNMAPPED	20	DC	H41	8.06	0.01	2
UNMAPPED	2	DA	H5'	4.13	0.01	2
UNMAPPED	9	DT	H6	7.44	0.01	1
UNMAPPED	8	DC	H5''	4.09	0.01	1
UNMAPPED	17	DG	H1	12.9	0.01	1
UNMAPPED	4	DT	H6	7.35	0.01	1
UNMAPPED	5	DA	H62	7.3	0.01	2
UNMAPPED	1	DC	H2'	1.9	0.01	1
UNMAPPED	28	DA	H61	5.77	0.01	2
UNMAPPED	22	DA	H61	5.83	0.01	2
UNMAPPED	20	DC	H5''	4.18	0.01	1
UNMAPPED	14	DA	H61	5.67	0.01	2
UNMAPPED	5	DA	H1'	6.13	0.01	1
UNMAPPED	9	DT	H1'	6.02	0.01	1
UNMAPPED	1	DC	H2''	2.37	0.01	1
UNMAPPED	27	DG	H1	12.54	0.01	1
UNMAPPED	13	DT	H2''	2.45	0.01	2
UNMAPPED	5	DA	H5''	4.09	0.01	1
UNMAPPED	25	DA	H4'	4.39	0.01	1
UNMAPPED	3	DC	H4'	4.31	0.01	1
UNMAPPED	11	DT	H5'	4.12	0.01	1
UNMAPPED	10	DT	H5''	4.09	0.01	1
UNMAPPED	11	DT	H2'	2.19	0.01	1
UNMAPPED	31	DA	H2'	2.74	0.01	2
UNMAPPED	23	DC	H6	7.24	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	3	DC	H41	8.06	0.01	1
UNMAPPED	32	DG	H5''	4.17	0.01	1
UNMAPPED	13	DT	H5'	4.13	0.01	1
UNMAPPED	6	DC	H3'	4.56	0.01	1
UNMAPPED	6	DC	H2''	2.45	0.01	1
UNMAPPED	7	DT	H73	1.51	0.01	1
UNMAPPED	34	DG	H8	7.89	0.01	1
UNMAPPED	31	DA	H4'	4.39	0.01	1
UNMAPPED	3	DC	H3'	4.68	0.01	1
UNMAPPED	34	DG	H5'	4.17	0.01	2
UNMAPPED	15	DG	H8	7.65	0.01	1
UNMAPPED	10	DT	H71	1.59	0.01	1
UNMAPPED	29	DG	H5''	4.19	0.01	1
UNMAPPED	4	DT	H71	1.59	0.01	1
UNMAPPED	16	DT	H3	13.86	0.01	1
UNMAPPED	25	DA	H5'	4.2	0.01	2
UNMAPPED	6	DC	H1'	5.75	0.01	1
UNMAPPED	32	DG	H3'	4.91	0.01	1
UNMAPPED	4	DT	H4'	4.17	0.01	1
UNMAPPED	32	DG	H2''	2.67	0.01	2
UNMAPPED	19	DA	H4'	4.44	0.01	1
UNMAPPED	22	DA	H5'	4.13	0.01	2
UNMAPPED	13	DT	H6	7.22	0.01	1
UNMAPPED	24	DA	H62	7.7	0.01	2
UNMAPPED	29	DG	H8	7.47	0.01	1
UNMAPPED	5	DA	H2	7.3	0.01	1
UNMAPPED	14	DA	H2'	2.71	0.01	2
UNMAPPED	10	DT	H3	13.96	0.01	1
UNMAPPED	5	DA	H8	8.3	0.01	1
UNMAPPED	19	DA	H1'	6.26	0.01	1
UNMAPPED	15	DG	H5'	4.17	0.01	1
UNMAPPED	30	DT	H1'	5.67	0.01	1
UNMAPPED	1	DC	H5''	3.72	0.01	1
UNMAPPED	28	DA	H2''	2.88	0.01	2
UNMAPPED	20	DC	H5'	4.18	0.01	1
UNMAPPED	26	DA	H8	7.94	0.01	1
UNMAPPED	24	DA	H4'	4.32	0.01	1
UNMAPPED	4	DT	H3	13.68	0.01	1
UNMAPPED	13	DT	H72	1.41	0.01	1
UNMAPPED	34	DG	H4'	4.39	0.01	1
UNMAPPED	15	DG	H3'	4.91	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	7	DT	H5'	4.08	0.01	2
UNMAPPED	16	DT	H73	1.38	0.01	1
UNMAPPED	22	DA	H62	7.7	0.01	2
UNMAPPED	22	DA	H4'	4.39	0.01	1
UNMAPPED	16	DT	H2'	1.89	0.01	2
UNMAPPED	20	DC	H1'	5.84	0.01	1
UNMAPPED	18	DC	H6	7.65	0.01	1
UNMAPPED	15	DG	H1'	5.84	0.01	1
UNMAPPED	23	DC	H4'	4.39	0.01	1
UNMAPPED	31	DA	H61	5.62	0.01	2
UNMAPPED	8	DC	H3'	4.81	0.01	1
UNMAPPED	3	DC	H6	7.33	0.01	1
UNMAPPED	23	DC	H1'	5.25	0.01	1
UNMAPPED	34	DG	H3'	4.69	0.01	1
UNMAPPED	23	DC	H41	8.21	0.01	2
UNMAPPED	30	DT	H73	1.25	0.01	1
UNMAPPED	30	DT	H2'	2.04	0.01	2
UNMAPPED	22	DA	H1'	6.13	0.01	1
UNMAPPED	32	DG	H1	12.71	0.01	1
UNMAPPED	32	DG	H5'	4.17	0.01	1
UNMAPPED	24	DA	H1'	5.72	0.01	1

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 667. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/667 (0%)	0/395 (0%)	0/231 (0%)	0/41 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 667.

0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/667 (0%)	0/395 (0%)	0/231 (0%)	0/41 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.