



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:53 pm GMT

PDB ID : 1MSF
Title : SOLUTION STRUCTURE OF A SPECIFIC DNA COMPLEX OF THE MYB DNA-BINDING DOMAIN WITH COOPERATIVE RECOGNITION HELICES
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Deposited on : 1995-01-24

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
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

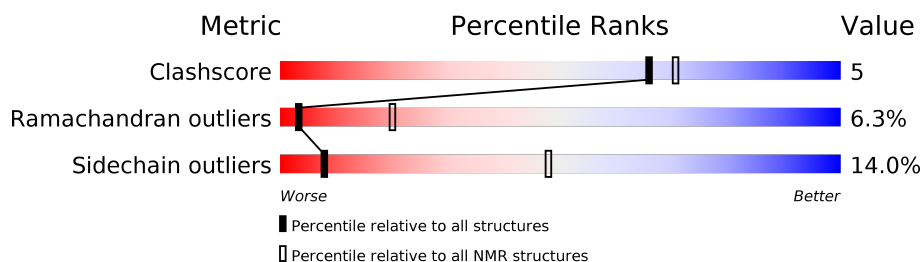
1 Overall quality at a glance

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
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	16	
2	B	16	
3	C	105	

2 Ensemble composition and analysis

This entry contains 25 models. Model 5 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	C:92-C:190 (99)	0.88	5

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 5, 7, 8, 9, 12, 16, 17, 18, 24, 25
2	1, 2, 4, 11, 14, 15, 19
3	6, 10, 13, 20, 21, 22, 23

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2513 atoms, of which 1172 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	11	Total	C	H	N	O	P	0
			343	106	124	41	62	10	

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

Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	P	0
			355	109	126	41	68	11	

- Molecule 3 is a protein called C-Myb DNA-Binding Domain.

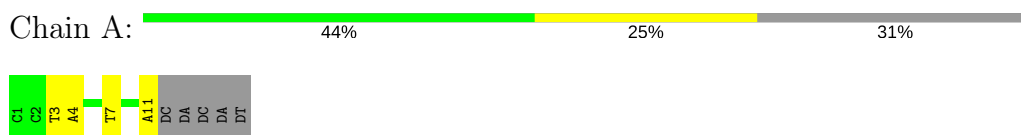
Mol	Chain	Residues	Atoms						Trace
3	C	105	Total	C	H	N	O	S	0
			1815	564	922	178	148	3	

4 Residue-property plots [i](#)

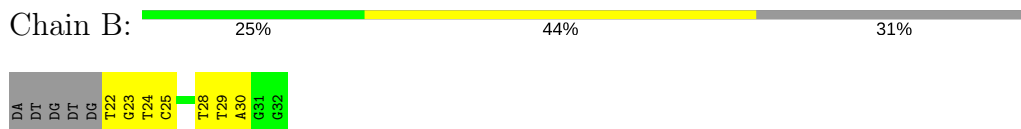
4.1 Average score per residue in the NMR ensemble

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.

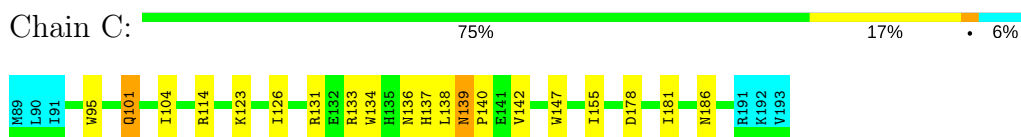
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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



- Molecule 3: C-Myb DNA-Binding Domain

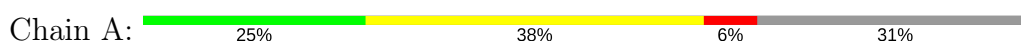


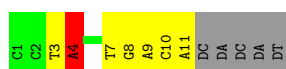
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

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





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



- Molecule 3: C-Myb DNA-Binding Domain



4.2.2 Score per residue for model 2

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



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



- Molecule 3: C-Myb DNA-Binding Domain



4.2.3 Score per residue for model 3

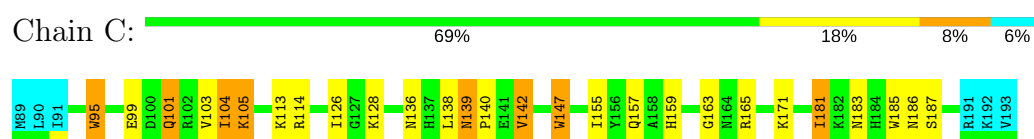
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

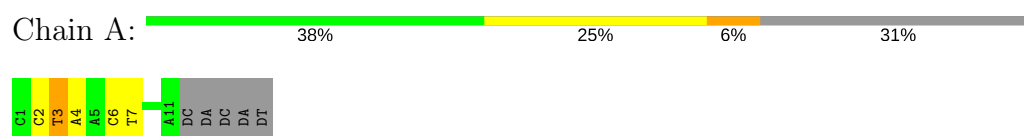


- Molecule 3: C-Myb DNA-Binding Domain

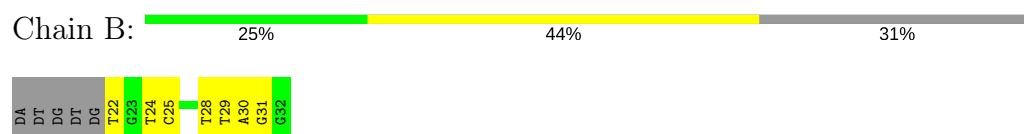


4.2.4 Score per residue for model 4

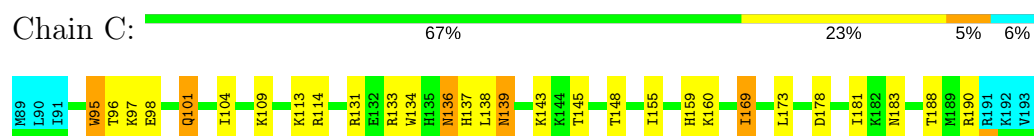
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

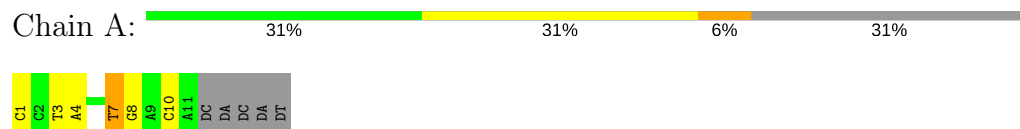


- Molecule 3: C-Myb DNA-Binding Domain

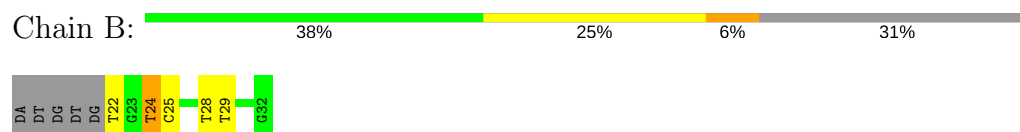


4.2.5 Score per residue for model 5 (medoid)

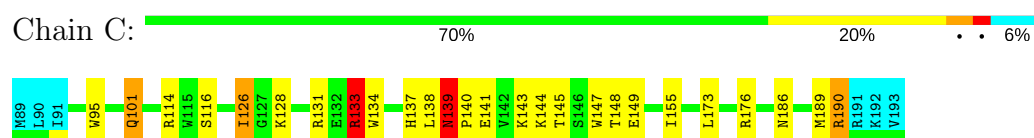
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

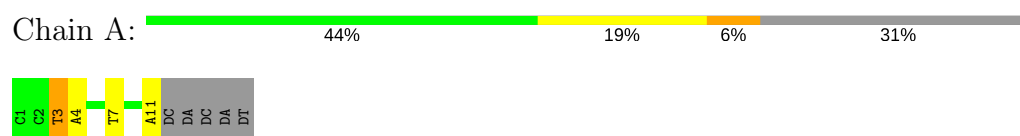


- Molecule 3: C-Myb DNA-Binding Domain

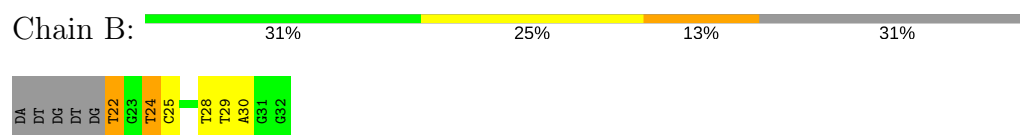


4.2.6 Score per residue for model 6

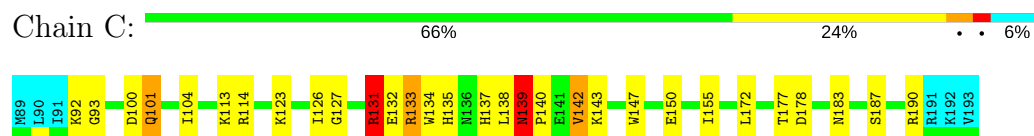
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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



- Molecule 3: C-Myb DNA-Binding Domain

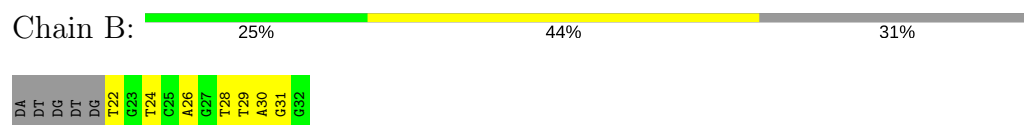


4.2.7 Score per residue for model 7

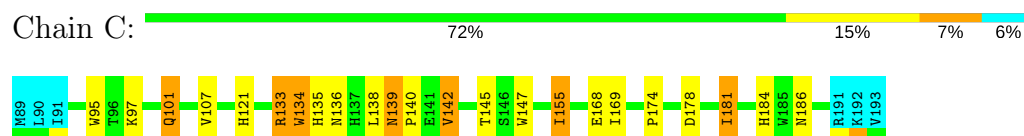
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

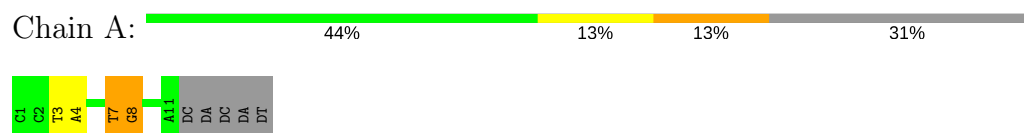


- Molecule 3: C-Myb DNA-Binding Domain

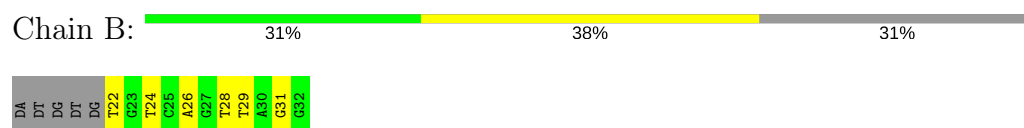


4.2.8 Score per residue for model 8

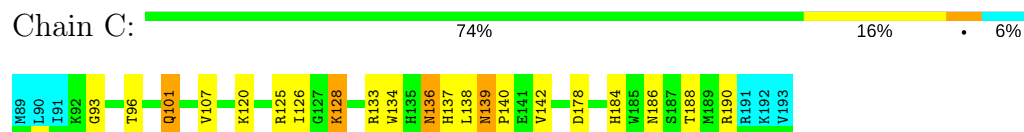
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

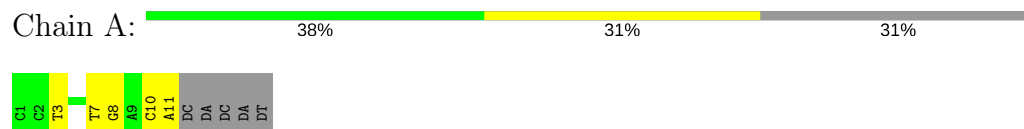


- Molecule 3: C-Myb DNA-Binding Domain

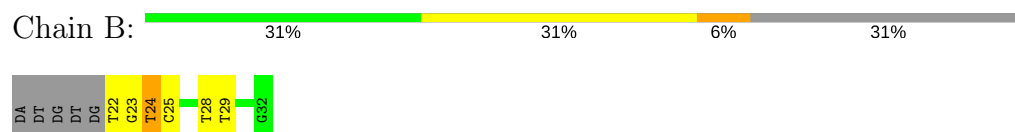


4.2.9 Score per residue for model 9

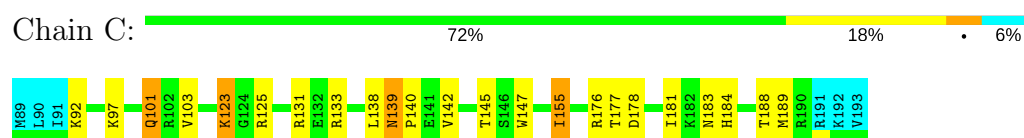
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

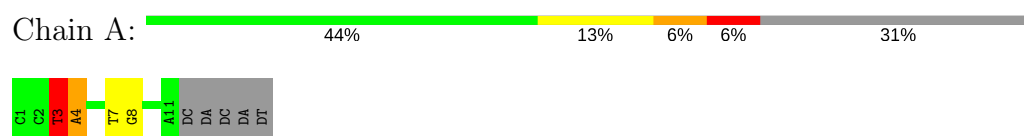


- Molecule 3: C-Myb DNA-Binding Domain

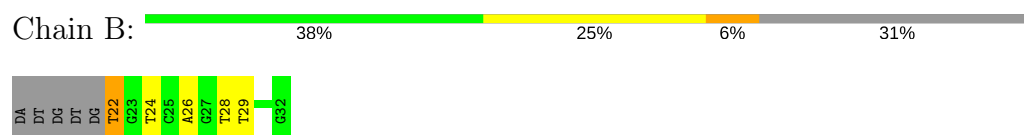


4.2.10 Score per residue for model 10

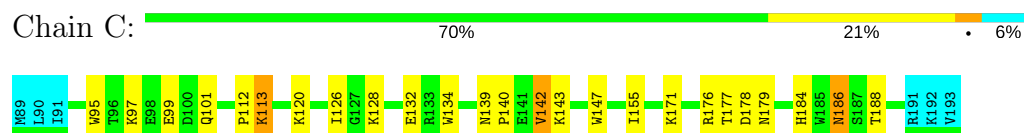
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

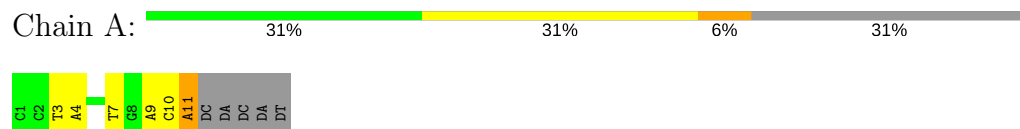


- Molecule 3: C-Myb DNA-Binding Domain

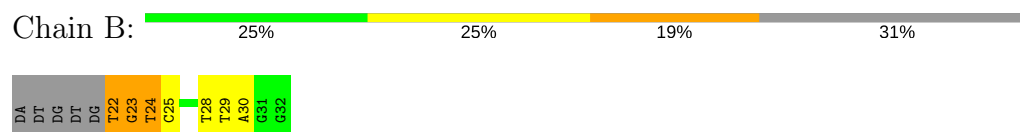


4.2.11 Score per residue for model 11

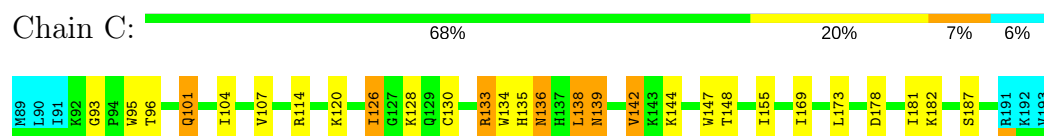
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

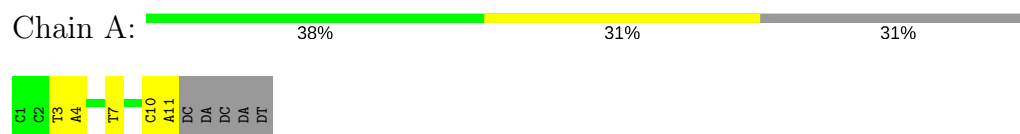


- Molecule 3: C-Myb DNA-Binding Domain

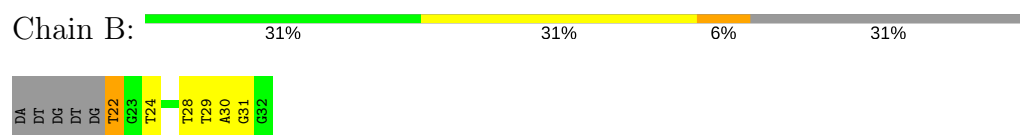


4.2.12 Score per residue for model 12

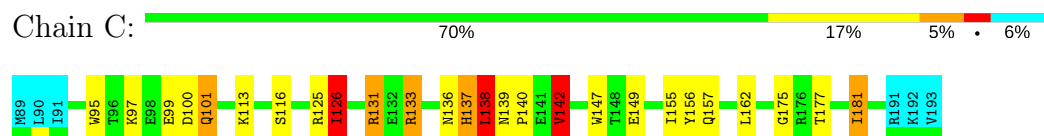
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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



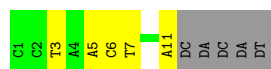
- Molecule 3: C-Myb DNA-Binding Domain



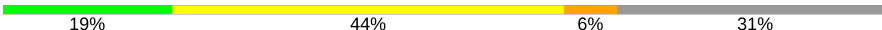
4.2.13 Score per residue for model 13

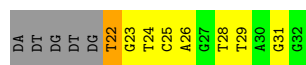
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')

Chain A: 



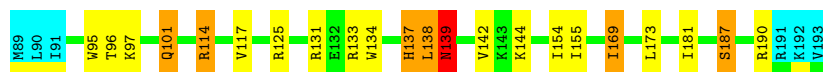
- Molecule 2: DNA (5'-D(*AP*TP*GP*TP*GP*TP*GP*TP*CP*AP*GP*TP*TP*AP*GP*G)-3')

Chain B: 



- Molecule 3: C-Myb DNA-Binding Domain

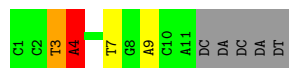
Chain C: 



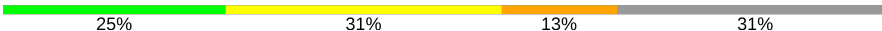
4.2.14 Score per residue for model 14

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

Chain A: 



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

Chain B: 



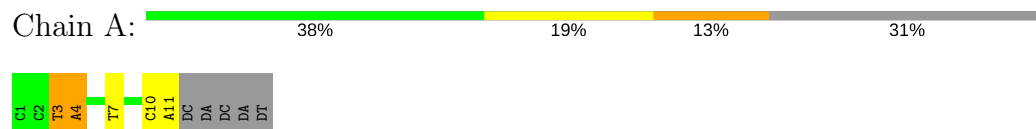
- Molecule 3: C-Myb DNA-Binding Domain

Chain C: 

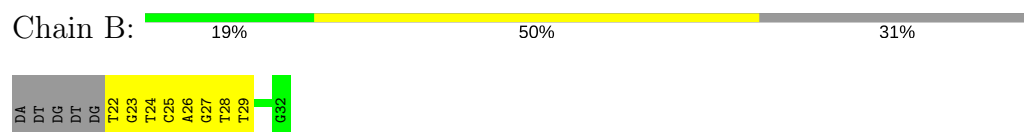


4.2.15 Score per residue for model 15

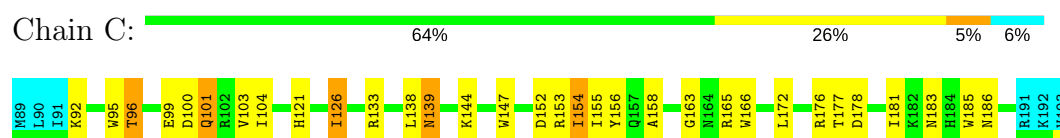
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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



- Molecule 3: C-Myb DNA-Binding Domain

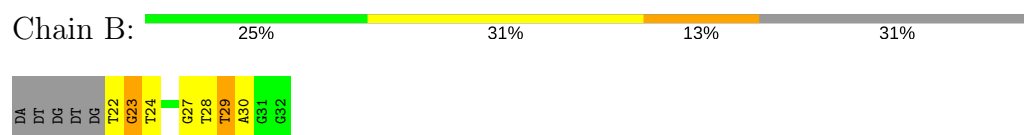


4.2.16 Score per residue for model 16

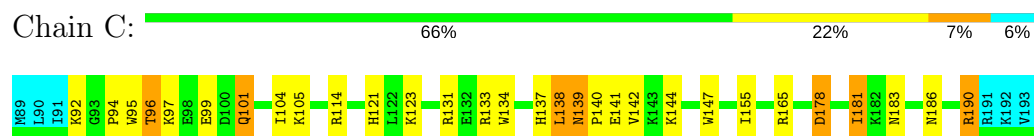
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

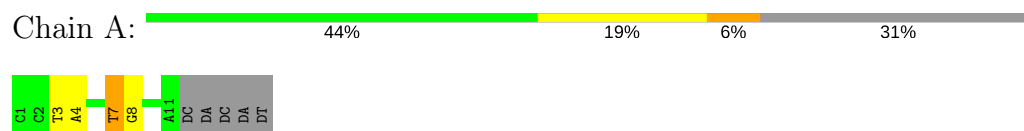


- Molecule 3: C-Myb DNA-Binding Domain



4.2.17 Score per residue for model 17

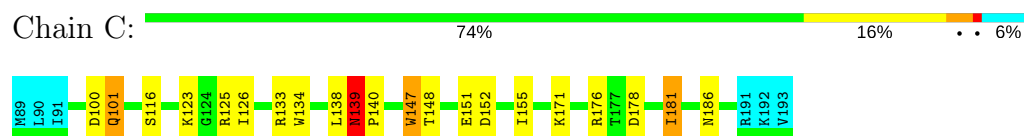
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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



- Molecule 3: C-Myb DNA-Binding Domain

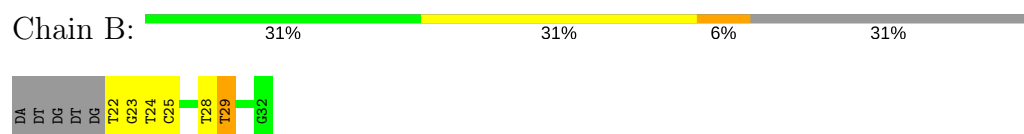


4.2.18 Score per residue for model 18

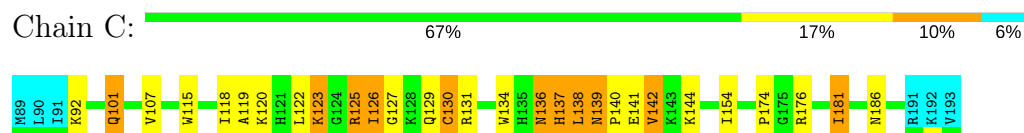
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

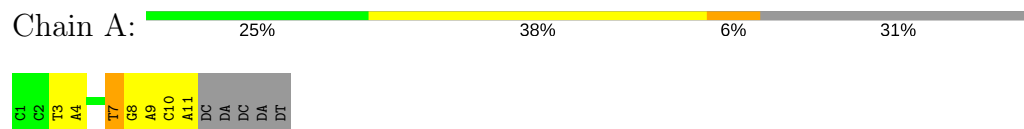


- Molecule 3: C-Myb DNA-Binding Domain

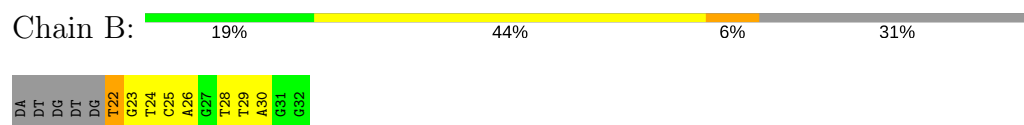


4.2.19 Score per residue for model 19

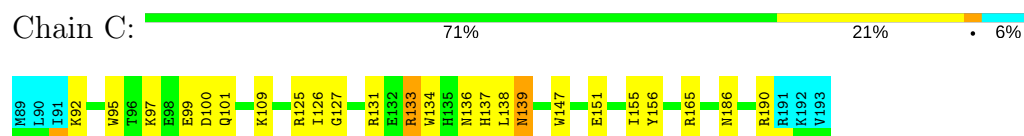
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

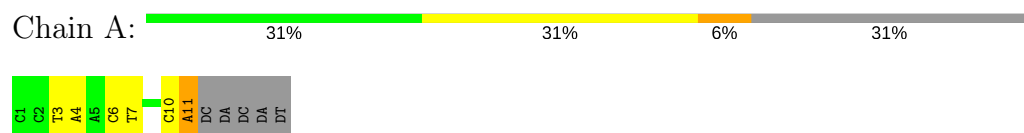


- Molecule 3: C-Myb DNA-Binding Domain

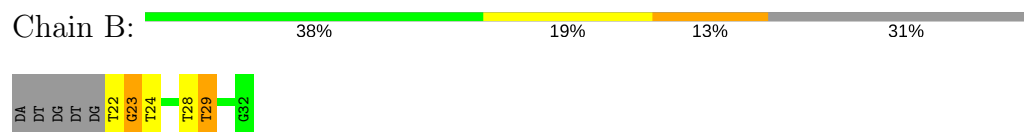


4.2.20 Score per residue for model 20

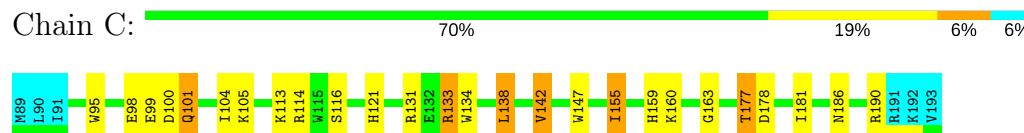
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

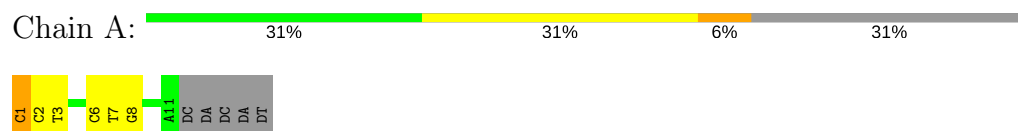


- Molecule 3: C-Myb DNA-Binding Domain

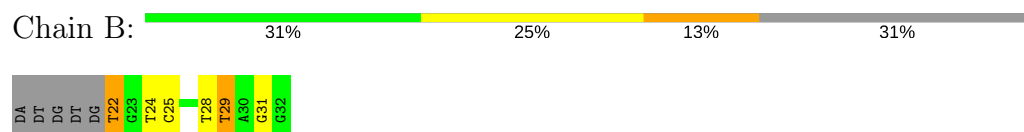


4.2.21 Score per residue for model 21

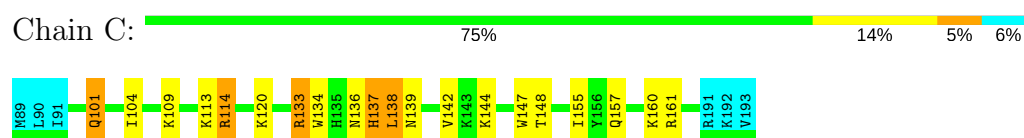
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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

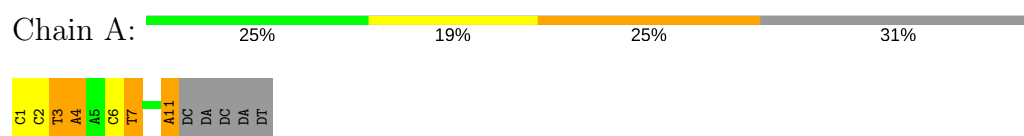


- Molecule 3: C-Myb DNA-Binding Domain

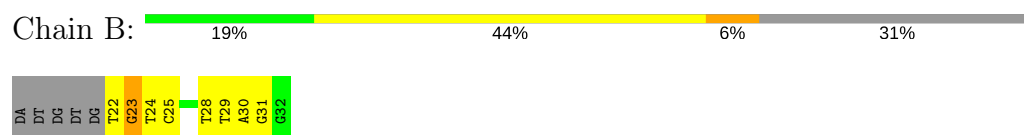


4.2.22 Score per residue for model 22

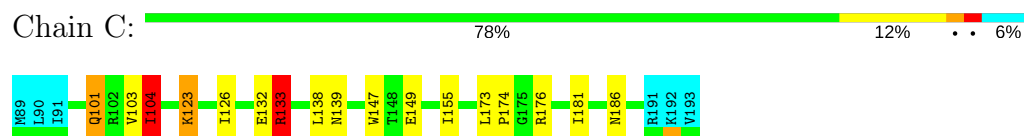
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')



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



- Molecule 3: C-Myb DNA-Binding Domain



4.2.23 Score per residue for model 23

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

Chain A: 



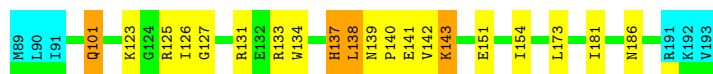
- Molecule 2: DNA (5'-D(*AP*TP*GP*TP*GP*TP*GP*TP*CP*AP*GP*TP*TP*AP*GP*G)-3')

Chain B: 



- Molecule 3: C-Myb DNA-Binding Domain

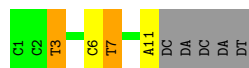
Chain C: 



4.2.24 Score per residue for model 24

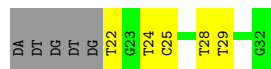
- Molecule 1: DNA (5'-D(*CP*CP*TP*AP*AP*CP*TP*GP*AP*CP*AP*CP*AP*CP*AP*T)-3')

Chain A: 



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

Chain B: 



- Molecule 3: C-Myb DNA-Binding Domain

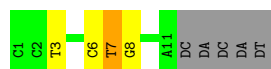
Chain C: 



4.2.25 Score per residue for model 25

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

Chain A: 



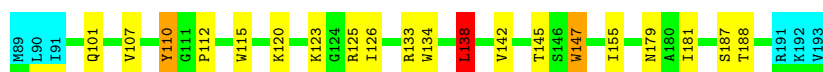
- Molecule 2: DNA (5'-D(*AP*TP*GP*TP*GP*TP*GP*TP*CP*AP*GP*TP*TP*AP*GP*G)-3')

Chain B: 



- Molecule 3: C-Myb DNA-Binding Domain

Chain C: 



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 25 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided. 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	1.12±0.02	0±0/245 (0.0±0.0%)	1.98±0.02	9±1/375 (2.3±0.2%)
2	B	1.20±0.03	0±0/256 (0.0±0.0%)	2.41±0.02	17±1/394 (4.2±0.2%)
3	C	0.61±0.01	0±0/864 (0.0±0.0%)	0.85±0.01	0±0/1163 (0.0±0.0%)
All	All	0.86	0/34125 (0.0%)	1.54	635/48300 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.9±1.4
2	B	0.0±0.0	2.9±1.4
3	C	0.0±0.0	1.0±0.9
All	All	0	172

There are no bond-length outliers.

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	3	DT	C6-C5-C7	-15.73	113.46	122.90	25	25
2	B	28	DT	C6-C5-C7	-15.64	113.52	122.90	16	25
2	B	22	DT	C6-C5-C7	-15.59	113.55	122.90	14	25
1	A	7	DT	C6-C5-C7	-15.56	113.56	122.90	11	25
2	B	24	DT	C6-C5-C7	-15.54	113.57	122.90	7	25
2	B	29	DT	C6-C5-C7	-15.46	113.62	122.90	22	25
2	B	24	DT	C4-C5-C6	8.50	123.10	118.00	7	25
2	B	28	DT	C4-C5-C6	8.47	123.08	118.00	16	25
1	A	3	DT	C4-C5-C6	8.16	122.90	118.00	9	25
1	A	7	DT	C4-C5-C6	8.13	122.88	118.00	4	25
1	A	3	DT	C4-C5-C7	8.04	123.83	119.00	4	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	22	DT	C4-C5-C6	8.02	122.81	118.00	1	25
2	B	22	DT	C4-C5-C7	7.99	123.79	119.00	20	25
2	B	29	DT	C4-C5-C6	7.97	122.78	118.00	9	25
1	A	7	DT	C4-C5-C7	7.89	123.74	119.00	11	25
2	B	28	DT	C4-C5-C7	7.85	123.71	119.00	10	25
2	B	29	DT	C4-C5-C7	7.80	123.68	119.00	13	25
2	B	24	DT	C4-C5-C7	7.76	123.65	119.00	1	25
1	A	4	DA	O4'-C1'-N9	5.96	112.17	108.00	14	12
2	B	24	DT	C5-C6-N1	-5.96	120.13	123.70	19	25
2	B	23	DG	O4'-C1'-N9	5.90	112.13	108.00	19	3
2	B	24	DT	O4'-C1'-N1	5.88	112.12	108.00	23	5
2	B	22	DT	C5-C6-N1	-5.83	120.20	123.70	25	24
1	A	3	DT	C5-C6-N1	-5.78	120.23	123.70	19	25
2	B	29	DT	C5-C6-N1	-5.73	120.26	123.70	14	24
1	A	8	DG	O4'-C1'-N9	5.54	111.88	108.00	21	1
2	B	28	DT	C5-C6-N1	-5.53	120.39	123.70	6	25
1	A	7	DT	C5-C6-N1	-5.51	120.39	123.70	8	25
2	B	29	DT	O4'-C1'-N1	5.41	111.79	108.00	11	3
2	B	22	DT	O4'-C1'-N1	5.39	111.78	108.00	25	2
2	B	26	DA	O4'-C1'-N9	5.33	111.73	108.00	7	2
1	A	3	DT	O4'-C1'-N1	5.25	111.68	108.00	17	3
2	B	22	DT	P-O3'-C3'	5.18	125.92	119.70	5	1
1	A	1	DC	O4'-C1'-N1	5.07	111.55	108.00	21	2
2	B	27	DG	O4'-C1'-N9	5.07	111.55	108.00	15	2
1	A	9	DA	O4'-C1'-N9	5.06	111.54	108.00	19	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)
2	B	25	DC	Sidechain	18
2	B	30	DA	Sidechain	12
1	A	11	DA	Sidechain	11
1	A	10	DC	Sidechain	11
3	C	133	ARG	Sidechain	10
2	B	22	DT	Sidechain	10
1	A	4	DA	Sidechain	10
1	A	8	DG	Sidechain	10
2	B	31	DG	Sidechain	8
1	A	7	DT	Sidechain	7

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	23	DG	Sidechain	7
1	A	6	DC	Sidechain	7
3	C	131	ARG	Sidechain	6
2	B	29	DT	Sidechain	6
1	A	3	DT	Sidechain	6
2	B	26	DA	Sidechain	5
1	A	9	DA	Sidechain	4
2	B	24	DT	Sidechain	4
1	A	1	DC	Sidechain	4
3	C	114	ARG	Sidechain	3
3	C	176	ARG	Sidechain	3
2	B	27	DG	Sidechain	2
3	C	125	ARG	Sidechain	2
3	C	165	ARG	Sidechain	2
1	A	2	DC	Sidechain	2
2	B	28	DT	Sidechain	1
1	A	5	DA	Sidechain	1

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	219	124	125	0±0
2	B	229	126	126	0±1
3	C	841	854	854	11±4
All	All	32225	27600	27625	284

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:147:TRP:CE3	3:C:155:ILE:HD11	0.85	2.06	22	5
3:C:155:ILE:HD12	3:C:181:ILE:HG22	0.84	1.45	12	1
3:C:147:TRP:CZ3	3:C:155:ILE:HD11	0.84	2.07	3	6
3:C:95:TRP:CE3	3:C:133:ARG:CD	0.81	2.63	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:155:ILE:CD1	3:C:181:ILE:HG22	0.80	2.06	12	1
3:C:147:TRP:CH2	3:C:181:ILE:HG23	0.79	2.12	12	3
3:C:133:ARG:HD3	3:C:138:LEU:HD11	0.70	1.62	22	1
3:C:134:TRP:CZ3	3:C:138:LEU:HD12	0.69	2.22	25	2
3:C:95:TRP:O	3:C:96:THR:HG23	0.67	1.89	16	1
3:C:169:ILE:HG22	3:C:181:ILE:HD13	0.67	1.67	7	1
3:C:101:GLN:N	3:C:101:GLN:HE21	0.67	1.88	21	5
3:C:133:ARG:CG	3:C:138:LEU:HD12	0.66	2.20	21	1
3:C:101:GLN:O	3:C:104:ILE:HG22	0.64	1.93	15	2
3:C:133:ARG:C	3:C:138:LEU:HD12	0.62	2.15	22	1
3:C:142:VAL:HG22	3:C:143:LYS:H	0.61	1.54	10	1
3:C:101:GLN:NE2	3:C:101:GLN:N	0.61	2.49	13	8
3:C:101:GLN:H	3:C:101:GLN:HE21	0.60	1.38	4	3
3:C:133:ARG:CD	3:C:138:LEU:HD13	0.59	2.27	11	1
3:C:184:HIS:CE1	3:C:188:THR:HG23	0.59	2.33	10	1
3:C:101:GLN:H	3:C:101:GLN:NE2	0.58	1.95	6	7
3:C:154:ILE:HD12	3:C:154:ILE:H	0.58	1.59	15	1
3:C:154:ILE:HG21	3:C:173:LEU:HD11	0.58	1.73	13	2
3:C:139:ASN:CB	3:C:140:PRO:CD	0.57	2.82	24	10
3:C:133:ARG:CD	3:C:138:LEU:HD11	0.57	2.29	22	1
3:C:101:GLN:HE21	3:C:101:GLN:N	0.57	1.97	8	4
3:C:115:TRP:O	3:C:119:ALA:HB3	0.56	2.00	18	1
3:C:142:VAL:HG13	3:C:142:VAL:O	0.56	2.00	6	2
3:C:133:ARG:HG3	3:C:138:LEU:HD12	0.56	1.76	21	1
3:C:148:THR:O	3:C:148:THR:HG22	0.56	2.01	4	1
3:C:134:TRP:CZ2	3:C:139:ASN:O	0.56	2.59	6	4
3:C:101:GLN:NE2	3:C:101:GLN:H	0.55	1.99	12	7
3:C:107:VAL:HG13	3:C:112:PRO:HA	0.55	1.77	25	1
3:C:95:TRP:CE3	3:C:133:ARG:HD2	0.55	2.35	4	1
3:C:101:GLN:HE21	3:C:101:GLN:H	0.55	1.45	22	2
3:C:101:GLN:N	3:C:101:GLN:NE2	0.55	2.54	2	12
3:C:95:TRP:CE3	3:C:133:ARG:HD3	0.54	2.37	15	3
3:C:139:ASN:O	3:C:141:GLU:N	0.54	2.40	23	3
3:C:155:ILE:CG2	3:C:156:TYR:N	0.54	2.70	12	1
3:C:107:VAL:HG11	3:C:134:TRP:CZ2	0.54	2.38	8	4
3:C:139:ASN:HB2	3:C:140:PRO:CD	0.53	2.33	9	4
3:C:95:TRP:CE3	3:C:99:GLU:HB3	0.53	2.39	16	6
3:C:154:ILE:HG21	3:C:173:LEU:CD1	0.53	2.32	13	2
3:C:173:LEU:CD2	3:C:181:ILE:HD12	0.53	2.32	4	1
3:C:155:ILE:HD11	3:C:181:ILE:O	0.53	2.02	12	1
3:C:155:ILE:HD12	3:C:155:ILE:H	0.53	1.62	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:154:ILE:N	3:C:154:ILE:HD12	0.53	2.19	18	1
3:C:169:ILE:HG23	3:C:181:ILE:HD13	0.52	1.80	4	2
3:C:154:ILE:O	3:C:158:ALA:HB3	0.52	2.05	15	1
3:C:184:HIS:CE1	3:C:188:THR:CG2	0.52	2.93	10	1
3:C:134:TRP:CE3	3:C:138:LEU:CD2	0.52	2.93	11	3
3:C:154:ILE:N	3:C:154:ILE:CD1	0.52	2.73	18	1
3:C:133:ARG:HD3	3:C:138:LEU:CD1	0.51	2.33	22	1
3:C:147:TRP:C	3:C:148:THR:HG23	0.51	2.25	5	1
3:C:103:VAL:O	3:C:103:VAL:HG12	0.50	2.05	22	1
3:C:133:ARG:HD2	3:C:138:LEU:HD13	0.50	1.82	11	1
3:C:103:VAL:HG12	3:C:103:VAL:O	0.50	2.06	3	1
3:C:142:VAL:O	3:C:142:VAL:HG13	0.49	2.07	7	1
3:C:95:TRP:CZ2	3:C:130:CYS:HA	0.49	2.43	11	1
3:C:169:ILE:CG2	3:C:181:ILE:HG21	0.49	2.36	13	2
3:C:134:TRP:CZ3	3:C:138:LEU:HD22	0.49	2.42	16	4
3:C:125:ARG:H	3:C:125:ARG:CD	0.49	2.20	18	1
3:C:101:GLN:O	3:C:104:ILE:CG2	0.49	2.60	15	1
3:C:155:ILE:N	3:C:155:ILE:HD13	0.48	2.24	7	2
3:C:177:THR:HG22	3:C:178:ASP:H	0.48	1.68	10	1
3:C:137:HIS:O	3:C:138:LEU:CB	0.48	2.60	23	1
3:C:95:TRP:CD2	3:C:133:ARG:CD	0.48	2.96	4	2
3:C:94:PRO:O	3:C:95:TRP:HB2	0.48	2.09	2	1
3:C:139:ASN:ND2	3:C:139:ASN:N	0.48	2.61	19	1
3:C:155:ILE:HD12	3:C:181:ILE:CG1	0.48	2.39	7	1
3:C:173:LEU:HD23	3:C:181:ILE:HD12	0.48	1.86	4	1
3:C:134:TRP:CE3	3:C:138:LEU:HD22	0.48	2.43	14	2
3:C:139:ASN:HB3	3:C:140:PRO:CD	0.47	2.39	24	3
3:C:95:TRP:O	3:C:96:THR:CG2	0.47	2.62	16	1
3:C:139:ASN:HD22	3:C:139:ASN:N	0.47	2.07	15	1
3:C:154:ILE:CD1	3:C:154:ILE:H	0.47	2.22	15	1
3:C:147:TRP:CZ3	3:C:155:ILE:HD13	0.47	2.44	11	1
3:C:134:TRP:CE3	3:C:138:LEU:HD13	0.47	2.45	21	1
3:C:159:HIS:CD2	3:C:163:GLY:HA3	0.47	2.44	1	2
3:C:133:ARG:HG2	3:C:138:LEU:HD12	0.47	1.85	21	1
1:A:11:DA:C2	2:B:23:DG:C2	0.47	3.03	22	3
3:C:177:THR:HG22	3:C:178:ASP:N	0.46	2.26	10	1
3:C:95:TRP:CE3	3:C:133:ARG:HG3	0.46	2.44	2	2
3:C:133:ARG:CD	3:C:138:LEU:HD22	0.46	2.40	19	1
3:C:178:ASP:O	3:C:179:ASN:CB	0.46	2.63	14	1
1:A:4:DA:C2	2:B:30:DA:C2	0.46	3.04	23	2
3:C:139:ASN:H	3:C:139:ASN:ND2	0.46	2.09	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:139:ASN:CB	3:C:140:PRO:HD3	0.46	2.41	18	7
3:C:95:TRP:CD2	3:C:133:ARG:HD3	0.46	2.46	15	4
3:C:125:ARG:O	3:C:126:ILE:HG22	0.46	2.11	12	1
3:C:95:TRP:CD2	3:C:133:ARG:HG3	0.46	2.46	20	4
3:C:100:ASP:N	3:C:133:ARG:HH21	0.45	2.10	2	1
3:C:154:ILE:HG21	3:C:173:LEU:HD12	0.45	1.87	23	1
3:C:95:TRP:CZ3	3:C:133:ARG:NH1	0.45	2.84	5	1
3:C:95:TRP:CE3	3:C:133:ARG:NE	0.45	2.85	5	2
3:C:173:LEU:HD13	3:C:173:LEU:O	0.45	2.11	11	1
3:C:155:ILE:HD13	3:C:155:ILE:N	0.45	2.27	3	1
3:C:142:VAL:HG13	3:C:143:LYS:N	0.44	2.27	10	1
3:C:163:GLY:O	3:C:166:TRP:CE2	0.44	2.70	15	1
3:C:95:TRP:CE3	3:C:99:GLU:HB2	0.44	2.48	20	1
3:C:155:ILE:HD12	3:C:181:ILE:HG12	0.44	1.88	3	1
3:C:139:ASN:O	3:C:142:VAL:HG22	0.44	2.12	11	1
3:C:112:PRO:O	3:C:113:LYS:CB	0.44	2.66	10	1
3:C:133:ARG:CZ	3:C:138:LEU:CD1	0.44	2.95	12	1
3:C:126:ILE:C	3:C:126:ILE:HD12	0.44	2.32	19	1
3:C:155:ILE:HG22	3:C:156:TYR:N	0.44	2.28	15	1
3:C:140:PRO:HG2	3:C:142:VAL:HG13	0.44	1.89	12	1
3:C:142:VAL:HG22	3:C:143:LYS:N	0.43	2.27	10	1
3:C:125:ARG:N	3:C:125:ARG:CD	0.43	2.81	8	1
3:C:126:ILE:HG22	3:C:127:GLY:N	0.43	2.28	23	2
3:C:155:ILE:HD12	3:C:181:ILE:CD1	0.43	2.44	14	1
3:C:159:HIS:CE1	3:C:185:TRP:CZ2	0.43	3.07	3	1
3:C:101:GLN:HA	3:C:104:ILE:CG2	0.43	2.43	11	1
3:C:129:GLN:O	3:C:130:CYS:SG	0.43	2.77	18	1
1:A:2:DC:OP2	3:C:188:THR:HG23	0.43	2.14	4	1
3:C:139:ASN:ND2	3:C:139:ASN:H	0.43	2.10	14	1
2:B:26:DA:C6	2:B:27:DG:C6	0.43	3.07	23	1
3:C:98:GLU:N	3:C:101:GLN:NE2	0.43	2.66	2	1
3:C:147:TRP:CD2	3:C:184:HIS:CD2	0.43	3.07	2	1
3:C:95:TRP:CZ3	3:C:99:GLU:HB3	0.43	2.49	12	2
3:C:159:HIS:HA	3:C:163:GLY:CA	0.43	2.44	20	2
3:C:147:TRP:CD1	3:C:184:HIS:ND1	0.43	2.87	7	2
3:C:104:ILE:HG23	3:C:105:LYS:N	0.43	2.28	16	2
3:C:139:ASN:C	3:C:141:GLU:H	0.43	2.16	16	1
3:C:138:LEU:O	3:C:139:ASN:C	0.43	2.57	13	1
3:C:142:VAL:CG1	3:C:142:VAL:O	0.42	2.67	20	1
2:B:24:DT:H73	3:C:131:ARG:HD2	0.42	1.91	23	1
3:C:134:TRP:CZ3	3:C:138:LEU:CD2	0.42	3.02	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:121:HIS:C	3:C:123:LYS:H	0.42	2.18	16	1
3:C:126:ILE:HD13	3:C:126:ILE:N	0.42	2.30	15	1
3:C:155:ILE:O	3:C:159:HIS:CB	0.42	2.68	4	1
3:C:139:ASN:CB	3:C:140:PRO:HD2	0.42	2.45	24	3
3:C:189:MET:O	3:C:190:ARG:CB	0.42	2.67	5	1
3:C:101:GLN:C	3:C:104:ILE:HG22	0.42	2.35	20	2
3:C:142:VAL:O	3:C:142:VAL:CG1	0.42	2.68	6	1
3:C:114:ARG:C	3:C:116:SER:H	0.41	2.19	20	1
3:C:147:TRP:CH2	3:C:181:ILE:HG13	0.41	2.51	7	1
3:C:159:HIS:CD2	3:C:163:GLY:O	0.41	2.73	3	1
3:C:141:GLU:O	3:C:142:VAL:C	0.41	2.58	18	1
3:C:131:ARG:NE	3:C:135:HIS:CD2	0.41	2.88	6	1
3:C:134:TRP:O	3:C:135:HIS:C	0.41	2.57	7	1
3:C:134:TRP:CD1	3:C:139:ASN:HB3	0.41	2.50	10	1
3:C:98:GLU:N	3:C:101:GLN:HE22	0.41	2.13	2	1
3:C:138:LEU:HD23	3:C:139:ASN:N	0.41	2.31	2	1
3:C:136:ASN:OD1	3:C:137:HIS:N	0.41	2.54	12	1
3:C:147:TRP:HH2	3:C:181:ILE:HG23	0.41	1.65	12	1
3:C:184:HIS:CE1	3:C:188:THR:OG1	0.41	2.73	9	1
2:B:24:DT:H72	3:C:131:ARG:HE	0.41	1.76	5	1
1:A:8:DG:C2	2:B:26:DA:C2	0.41	3.09	8	1
1:A:3:DT:C2	1:A:4:DA:C8	0.41	3.08	14	2
3:C:142:VAL:O	3:C:142:VAL:CG2	0.41	2.69	14	1
3:C:169:ILE:HG21	3:C:181:ILE:CD1	0.41	2.46	11	1
3:C:155:ILE:HD12	3:C:189:MET:SD	0.41	2.56	9	1
3:C:139:ASN:HD22	3:C:139:ASN:H	0.41	1.59	15	1
3:C:177:THR:HG23	3:C:178:ASP:N	0.41	2.30	20	1
3:C:154:ILE:HG21	3:C:173:LEU:HD23	0.40	1.93	2	1
3:C:162:LEU:N	3:C:162:LEU:CD1	0.40	2.84	2	1
3:C:184:HIS:CE1	3:C:188:THR:HG21	0.40	2.51	8	1
3:C:104:ILE:CG2	3:C:105:LYS:N	0.40	2.84	3	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	C	99/105 (94%)	71±3 (72±3%)	21±2 (22±2%)	6±2 (6±2%)	3	20
All	All	2475/2625 (94%)	1784 (72%)	535 (22%)	156 (6%)	3	20

All 42 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	142	VAL	13
3	C	136	ASN	12
3	C	137	HIS	10
3	C	139	ASN	10
3	C	126	ILE	9
3	C	114	ARG	8
3	C	187	SER	8
3	C	123	LYS	7
3	C	178	ASP	7
3	C	190	ARG	5
3	C	147	TRP	4
3	C	144	LYS	4
3	C	113	LYS	4
3	C	92	LYS	3
3	C	186	ASN	3
3	C	93	GLY	3
3	C	127	GLY	3
3	C	138	LEU	3
3	C	96	THR	3
3	C	179	ASN	3
3	C	95	TRP	3
3	C	97	LYS	3
3	C	128	LYS	2
3	C	99	GLU	2
3	C	100	ASP	2
3	C	145	THR	2
3	C	148	THR	2
3	C	115	TRP	2
3	C	135	HIS	2
3	C	104	ILE	2
3	C	175	GLY	1
3	C	140	PRO	1
3	C	94	PRO	1
3	C	130	CYS	1
3	C	98	GLU	1
3	C	150	GLU	1

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Mol	Chain	Res	Type	Models (Total)
3	C	110	TYR	1
3	C	151	GLU	1
3	C	149	GLU	1
3	C	143	LYS	1
3	C	181	ILE	1
3	C	134	TRP	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	C	88/94 (94%)	76±3 (86±3%)	12±3 (14±3%)	8	48
All	All	2200/2350 (94%)	1891 (86%)	309 (14%)	8	48

All 69 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	C	101	GLN	21
3	C	138	LEU	17
3	C	133	ARG	14
3	C	181	ILE	14
3	C	139	ASN	13
3	C	186	ASN	11
3	C	155	ILE	10
3	C	125	ARG	7
3	C	131	ARG	7
3	C	96	THR	7
3	C	176	ARG	7
3	C	126	ILE	6
3	C	183	ASN	6
3	C	177	THR	6
3	C	100	ASP	6
3	C	120	LYS	6
3	C	137	HIS	6
3	C	113	LYS	6
3	C	97	LYS	6

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Mol	Chain	Res	Type	Models (Total)
3	C	190	ARG	5
3	C	144	LYS	5
3	C	142	VAL	5
3	C	123	LYS	5
3	C	160	LYS	5
3	C	145	THR	5
3	C	171	LYS	5
3	C	132	GLU	4
3	C	178	ASP	4
3	C	165	ARG	4
3	C	128	LYS	4
3	C	148	THR	4
3	C	95	TRP	4
3	C	149	GLU	4
3	C	143	LYS	4
3	C	136	ASN	4
3	C	104	ILE	4
3	C	173	LEU	3
3	C	121	HIS	3
3	C	174	PRO	3
3	C	92	LYS	3
3	C	103	VAL	3
3	C	109	LYS	3
3	C	116	SER	3
3	C	98	GLU	3
3	C	157	GLN	3
3	C	172	LEU	2
3	C	153	ARG	2
3	C	151	GLU	2
3	C	152	ASP	2
3	C	169	ILE	2
3	C	179	ASN	2
3	C	114	ARG	2
3	C	140	PRO	1
3	C	182	LYS	1
3	C	156	TYR	1
3	C	94	PRO	1
3	C	168	GLU	1
3	C	150	GLU	1
3	C	110	TYR	1
3	C	105	LYS	1
3	C	122	LEU	1

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Mol	Chain	Res	Type	Models (Total)
3	C	162	LEU	1
3	C	118	ILE	1
3	C	117	VAL	1
3	C	188	THR	1
3	C	187	SER	1
3	C	161	ARG	1
3	C	102	ARG	1
3	C	154	ILE	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 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

No chemical shift data were provided