Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 05:32 PM EDT

PDB ID	:	2KN7
Title	:	Structure of the XPF-single strand DNA complex
Authors	:	Das, D.; Folkers, G.E.; van Dijk, M.; Jaspers, N.G.J.; Hoeijmakers, J.H.J.; Kaptein, R.; Boelens, R.
Deposited on	:	2009-08-16

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

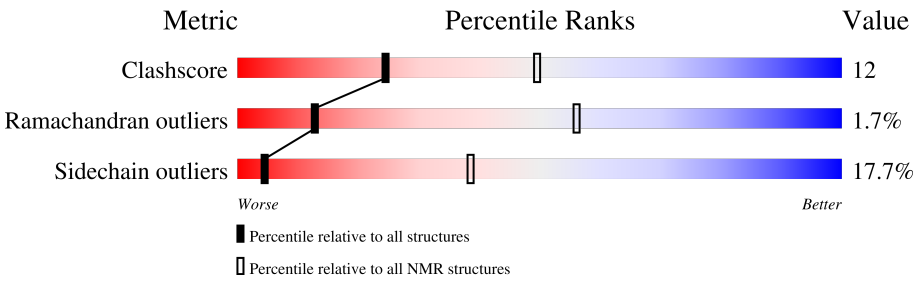
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	67	66% 25% • 7%
1	D	67	63% 22% • 12%
2	B	10	40% 50% 10%
2	C	10	40% 50% 10%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:12-A:73, D:115-D:173 (121)	0.29	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 5 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2720 atoms, of which 1268 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA repair endonuclease XPF.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	67	1041	329	520	90	99	3	0
1	D	67	1041	329	520	90	99	3	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	10	319	98	114	40	58	9	0
2	C	10	319	98	114	40	58	9	0

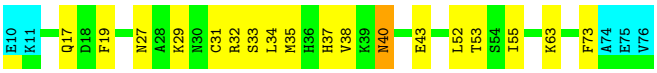
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: DNA repair endonuclease XPF

Chain A:

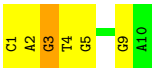


• Molecule 1: DNA repair endonuclease XPF

Chain D:

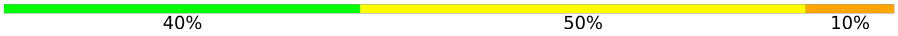
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

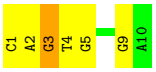
Chain B:



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

Chain C:





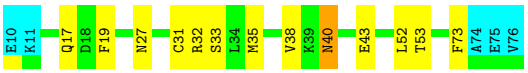
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: DNA repair endonuclease XPF

Chain A: 73% 18% • 7%



- Molecule 1: DNA repair endonuclease XPF

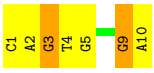
Chain D: 55% 28% • • 12%

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

Chain B: 40% 50% 10%

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

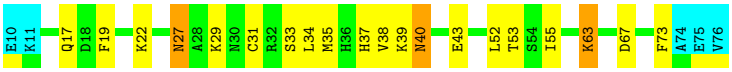
Chain C: 30% 50% 20%



4.2.2 Score per residue for model 2

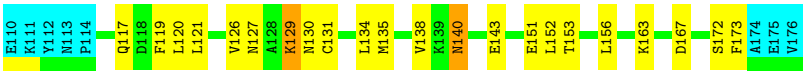
- Molecule 1: DNA repair endonuclease XPF

Chain A: 63% 25% • 7%



- Molecule 1: DNA repair endonuclease XPF

Chain D: 55% 30% • 12%

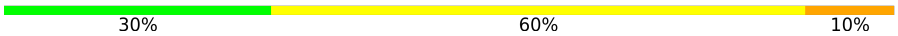


- Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 60% 30% 10%

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

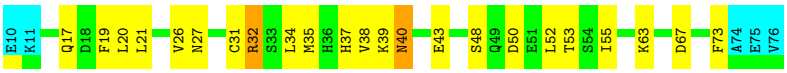
Chain C:



4.2.3 Score per residue for model 3

• Molecule 1: DNA repair endonuclease XPF

Chain A:

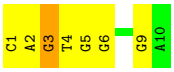


• Molecule 1: DNA repair endonuclease XPF

Chain D:

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

Chain B:



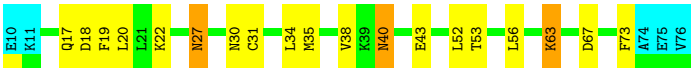
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain C:

4.2.4 Score per residue for model 4

• Molecule 1: DNA repair endonuclease XPF

Chain A:

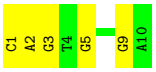


• Molecule 1: DNA repair endonuclease XPF

Chain D:

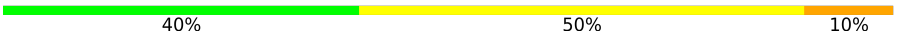
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

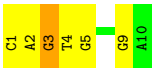
Chain B:



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

Chain C:

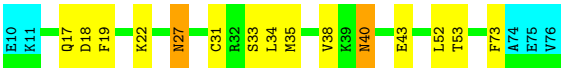




4.2.5 Score per residue for model 5 (medoid)

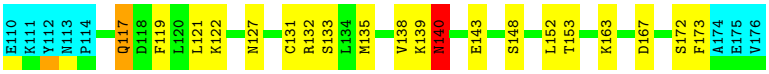
• Molecule 1: DNA repair endonuclease XPF

Chain A:



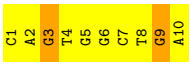
• Molecule 1: DNA repair endonuclease XPF

Chain D:



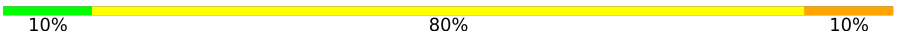
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

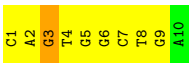
Chain B:



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

Chain C:

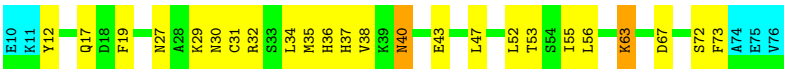




4.2.6 Score per residue for model 6

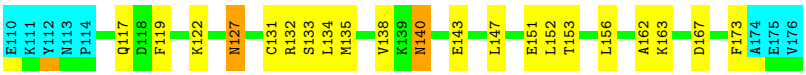
- Molecule 1: DNA repair endonuclease XPF

Chain A: 57% 33% • 7%



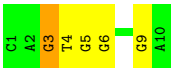
- Molecule 1: DNA repair endonuclease XPF

Chain D: 57% 28% • 12%



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

Chain B: 50% 40% 10%



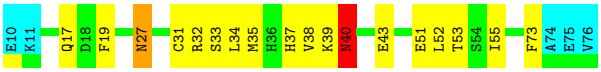
- Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain C: 30% 60% 10%

4.2.7 Score per residue for model 7

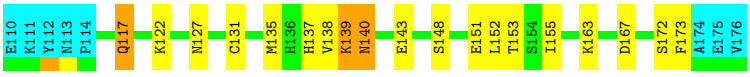
- Molecule 1: DNA repair endonuclease XPF

Chain A: 66% 24% •• 7%



- Molecule 1: DNA repair endonuclease XPF

Chain D: 60% 24% • 12%

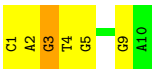


- Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 40% 50% 10%

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

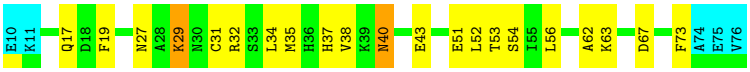
Chain C: 40% 50% 10%



4.2.8 Score per residue for model 8

• Molecule 1: DNA repair endonuclease XPF

Chain A: 61% 28% • 7%

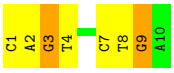


• Molecule 1: DNA repair endonuclease XPF

Chain D: 54% 28% • • 12%

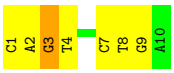
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 30% 50% 20%



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

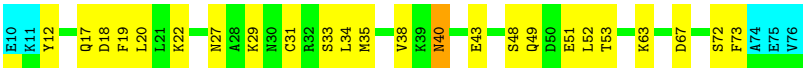
Chain C: 30% 60% 10%



4.2.9 Score per residue for model 9

• Molecule 1: DNA repair endonuclease XPF

Chain A: 57% 34% • 7%

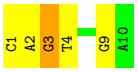


• Molecule 1: DNA repair endonuclease XPF

Chain D:

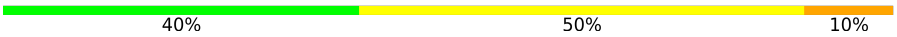
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

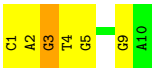
Chain B:



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

Chain C:

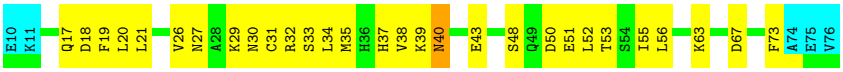




4.2.10 Score per residue for model 10

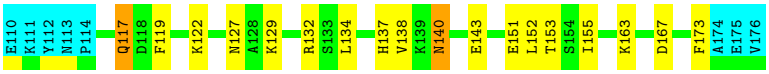
• Molecule 1: DNA repair endonuclease XPF

Chain A:



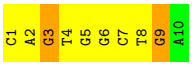
• Molecule 1: DNA repair endonuclease XPF

Chain D:



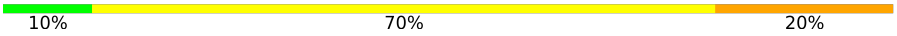
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

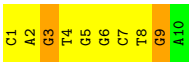
Chain B:



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

Chain C:

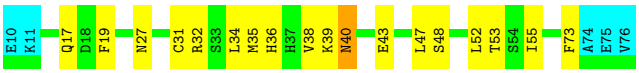




4.2.11 Score per residue for model 11

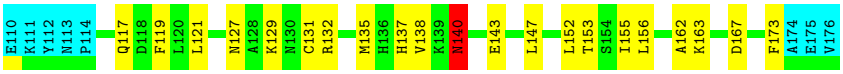
- Molecule 1: DNA repair endonuclease XPF

Chain A: 66% 25% • 7%



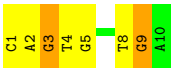
- Molecule 1: DNA repair endonuclease XPF

Chain D: 57% 30% • 12%



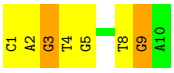
- Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 30% 50% 20%



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

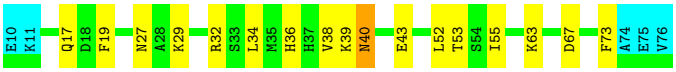
Chain C: 30% 50% 20%



4.2.12 Score per residue for model 12

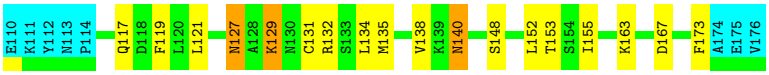
- Molecule 1: DNA repair endonuclease XPF

Chain A: 67% 24% • 7%



- Molecule 1: DNA repair endonuclease XPF

Chain D: 61% 22% • 12%

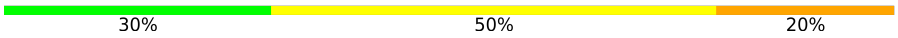


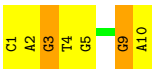
- Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 40% 50% 10%

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

Chain C:

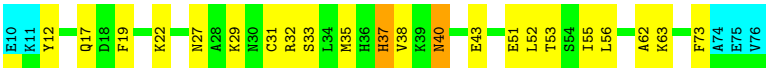




4.2.13 Score per residue for model 13

• Molecule 1: DNA repair endonuclease XPF

Chain A:

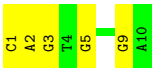


• Molecule 1: DNA repair endonuclease XPF

Chain D:

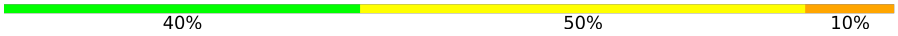
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B:



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

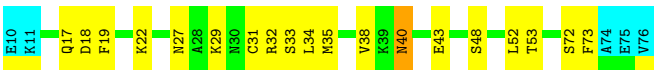
Chain C:



4.2.14 Score per residue for model 14

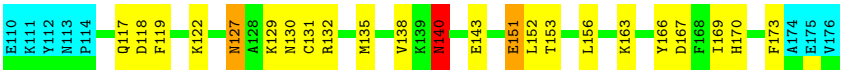
• Molecule 1: DNA repair endonuclease XPF

Chain A:



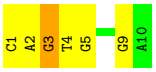
• Molecule 1: DNA repair endonuclease XPF

Chain D:



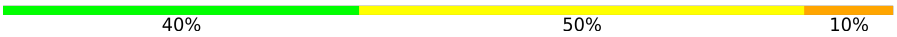
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

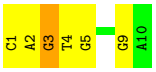
Chain B:



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

Chain C:

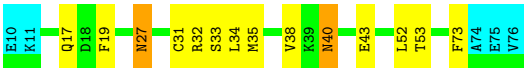




4.2.15 Score per residue for model 15

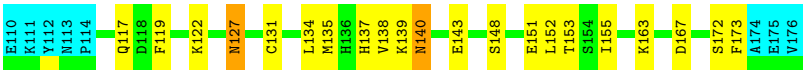
• Molecule 1: DNA repair endonuclease XPF

Chain A:



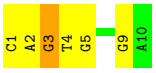
• Molecule 1: DNA repair endonuclease XPF

Chain D:



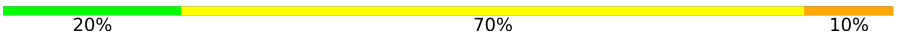
• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

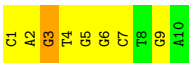
Chain B:



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

Chain C:

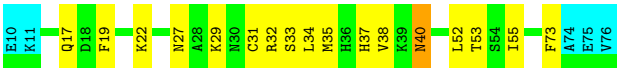




4.2.16 Score per residue for model 16

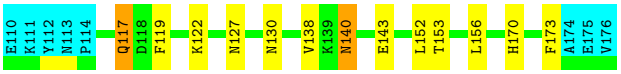
- Molecule 1: DNA repair endonuclease XPF

Chain A: 67% 24% • 7%



- Molecule 1: DNA repair endonuclease XPF

Chain D: 69% 16% • 12%

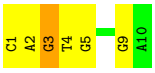


- Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 40% 50% 10%

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

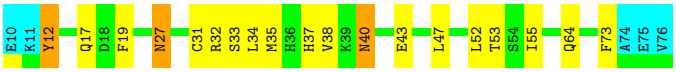
Chain C: 40% 50% 10%



4.2.17 Score per residue for model 17

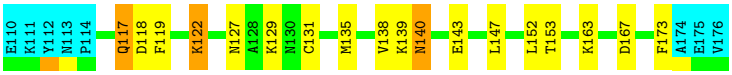
- Molecule 1: DNA repair endonuclease XPF

Chain A: 64% 24% • 7%



- Molecule 1: DNA repair endonuclease XPF

Chain D: 61% 22% • 12%

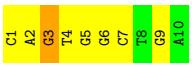


- Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 40% 50% 10%

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

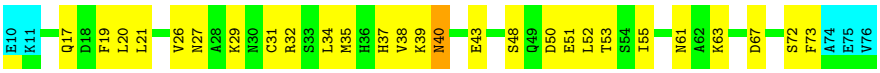
Chain C: 20% 70% 10%



4.2.18 Score per residue for model 18

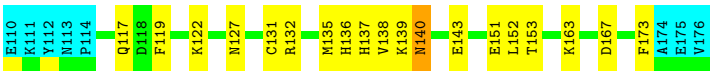
• Molecule 1: DNA repair endonuclease XPF

Chain A: 52% 39% • 7%



• Molecule 1: DNA repair endonuclease XPF

Chain D: 60% 27% • 12%

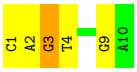


• Molecule 2: DNA (5'-D(*CP*AP*GP*TP*GP*GP*CP*TP*GP*A)-3')

Chain B: 40% 50% 10%

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

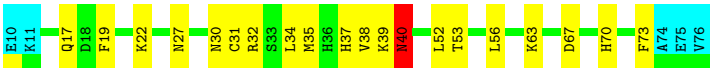
Chain C: 50% 40% 10%



4.2.19 Score per residue for model 19

• Molecule 1: DNA repair endonuclease XPF

Chain A: 63% 28% • 7%



• Molecule 1: DNA repair endonuclease XPF

Chain D: 67% 18% • 12%

E110 K111 Y112 N113 P114 Q117 D118 F119 N127 C131 R132 S133 L134 M135 V138 K139 N140 E143 S148 E151 L152 F173 A174 E175 V176

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

Chain B: 20% 70% 10%

C1 A2 G3 T4 G5 G6 C7 T8 G9 A10

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

Chain C: 40% 50% 10%

C1 A2 G3 T4 G5 G6 C7 T8 G9 A10

4.2.20 Score per residue for model 20

• Molecule 1: DNA repair endonuclease XPF

Chain A: 67% 22% • 7%

E10 K11 Q17 D18 F19 L20 N27 C31 L34 M35 V38 K39 N40 E43 L52 T53 K63 F68 T71 S72 F73 A74 E75 V76

• Molecule 1: DNA repair endonuclease XPF

Chain D: 46% 39% • 12%

E110 K111 Y112 N113 P114 Q117 D118 F119 L120 L121 V126 N127 A128 K129 N130 C131 R132 S133 L134 M135 H136 H137 V138 K139 N140 E143 S148 L152 T153 S154 I155 L156 A162 K163 D167 S172 F173 A174 E175 V176

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

Chain B: 40% 50% 10%

C1 A2 G3 T4 G5 G6 C7 T8 G9 A10

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

Chain C: 30% 50% 20%

C1 A2 G3 T4 G5 T8 G9 A10

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, torsion angle dynamics.*

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

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

Software name	Classification	Version
CYANA	structure solution	
CNS	refinement	

No chemical shift data was provided.

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	0.29±0.01	0±0/492 (0.0± 0.0%)	0.38±0.01	0±0/667 (0.0± 0.0%)
1	D	0.29±0.01	0±0/463 (0.0± 0.0%)	0.37±0.01	0±0/626 (0.0± 0.0%)
2	B	0.73±0.01	0±0/230 (0.0± 0.0%)	0.98±0.01	2±0/354 (0.6± 0.0%)
2	C	0.73±0.01	0±0/230 (0.0± 0.0%)	0.98±0.01	2±0/354 (0.6± 0.0%)
All	All	0.48	0/28300 (0.0%)	0.66	80/40020 (0.2%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	9	DG	N3-C2-N2	-6.39	115.42	119.90	12	20
2	C	9	DG	N3-C2-N2	-6.33	115.47	119.90	11	20
2	C	3	DG	N3-C2-N2	-5.77	115.86	119.90	19	20
2	B	3	DG	N3-C2-N2	-5.74	115.88	119.90	1	20

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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	481	479	476	10±3
1	D	454	457	454	11±2
2	B	205	114	114	7±3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	C	205	114	114	7±2
All	All	26900	23280	23160	591

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:3:DG:H2"	2:B:4:DT:O5'	0.94	1.62	10	18
2:C:3:DG:H2"	2:C:4:DT:O5'	0.91	1.63	18	20
2:B:5:DG:H5"	2:B:5:DG:N3	0.90	1.81	11	7
2:C:5:DG:H5"	2:C:5:DG:N3	0.89	1.82	11	5
1:A:55:ILE:HA	2:B:4:DT:OP2	0.73	1.84	2	7
2:C:5:DG:H5'	2:C:5:DG:N3	0.70	2.01	10	6
2:B:5:DG:N3	2:B:5:DG:H5'	0.69	2.00	19	4
2:B:1:DC:C5	2:B:2:DA:C8	0.67	2.83	15	16
1:D:155:ILE:HA	2:C:4:DT:OP2	0.64	1.93	11	3
1:D:138:VAL:HB	1:D:143:GLU:CB	0.63	2.24	4	14
1:A:37:HIS:CD2	1:A:55:ILE:HG12	0.62	2.30	10	5
2:C:1:DC:C5	2:C:2:DA:C8	0.62	2.88	18	16
2:C:1:DC:C5	2:C:2:DA:N7	0.61	2.69	13	9
1:D:121:LEU:HA	1:D:126:VAL:HG11	0.60	1.72	20	5
2:C:3:DG:N3	2:C:4:DT:H72	0.59	2.12	16	7
1:A:31:CYS:O	1:A:35:MET:HG2	0.59	1.97	5	19
2:B:1:DC:C5	2:B:2:DA:N7	0.59	2.70	13	12
1:A:38:VAL:HB	1:A:43:GLU:CB	0.59	2.27	17	13
2:C:3:DG:C2'	2:C:4:DT:O5'	0.57	2.49	18	11
1:D:167:ASP:HA	1:D:170:HIS:CE1	0.57	2.35	14	2
1:A:37:HIS:CG	1:A:55:ILE:HG12	0.57	2.34	13	1
2:B:1:DC:O5'	2:B:2:DA:H2'	0.57	1.98	13	2
1:D:131:CYS:O	1:D:135:MET:HG2	0.57	2.00	5	15
1:D:163:LYS:O	1:D:167:ASP:HB2	0.56	1.99	10	16
1:D:137:HIS:CD2	1:D:155:ILE:HG12	0.56	2.35	10	4
1:A:63:LYS:O	1:A:67:ASP:HB2	0.55	2.00	10	10
1:D:137:HIS:CG	1:D:155:ILE:HG12	0.55	2.35	20	1
2:B:1:DC:H5	2:B:2:DA:N7	0.54	1.99	17	2
1:D:120:LEU:O	1:D:126:VAL:HG11	0.54	2.02	2	3
1:D:138:VAL:HB	1:D:143:GLU:HB2	0.54	1.79	4	17
1:A:21:LEU:HA	1:A:26:VAL:HG11	0.54	1.78	10	3
2:B:3:DG:C2'	2:B:4:DT:O5'	0.54	2.54	3	12
2:B:3:DG:N3	2:B:4:DT:H72	0.53	2.19	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:DT:H73	2:B:6:DG:N7	0.53	2.19	6	1
1:A:39:LYS:CD	1:A:43:GLU:HG2	0.53	2.34	2	5
1:A:40:ASN:HA	1:D:173:PHE:CZ	0.53	2.38	1	20
1:A:18:ASP:O	1:A:22:LYS:HG2	0.52	2.04	4	4
1:D:156:LEU:HD12	1:D:162:ALA:HA	0.52	1.80	11	3
2:B:6:DG:H1'	2:B:7:DC:C5	0.52	2.39	19	4
1:A:38:VAL:HB	1:A:43:GLU:HB2	0.52	1.81	17	17
1:D:139:LYS:CD	1:D:143:GLU:HG2	0.52	2.35	15	5
1:A:34:LEU:O	1:A:38:VAL:HG22	0.52	2.05	2	18
1:D:121:LEU:HA	1:D:126:VAL:CG1	0.52	2.34	20	5
2:B:5:DG:N3	2:B:5:DG:H2'	0.51	2.20	2	4
2:B:5:DG:N3	2:B:5:DG:C5'	0.50	2.74	7	5
2:B:5:DG:C5'	2:B:5:DG:N3	0.50	2.75	5	3
2:B:5:DG:N3	2:B:5:DG:H5"	0.50	2.22	5	1
2:C:1:DC:C4	2:C:2:DA:N7	0.50	2.80	12	5
1:A:73:PHE:CZ	1:D:140:ASN:HA	0.49	2.42	6	16
1:A:21:LEU:HA	1:A:26:VAL:CG1	0.49	2.36	10	3
1:D:121:LEU:HD21	1:D:131:CYS:SG	0.49	2.47	12	3
1:A:29:LYS:HB3	2:B:7:DC:OP1	0.49	2.06	8	1
1:A:27:ASN:O	1:A:31:CYS:HB2	0.49	2.08	7	7
1:D:130:ASN:ND2	1:D:156:LEU:HD22	0.49	2.22	20	6
1:A:67:ASP:HA	1:A:70:HIS:CE1	0.49	2.42	19	1
1:D:127:ASN:HB2	1:D:129:LYS:HG2	0.49	1.85	4	3
2:C:5:DG:N3	2:C:5:DG:H2'	0.48	2.21	4	3
1:D:127:ASN:O	1:D:131:CYS:HB2	0.48	2.09	19	7
2:C:5:DG:N3	2:C:5:DG:C5'	0.48	2.76	1	10
1:A:29:LYS:HA	2:B:7:DC:OP1	0.47	2.09	10	1
1:A:32:ARG:HD2	2:B:6:DG:OP1	0.47	2.09	3	1
1:A:40:ASN:HA	1:D:173:PHE:CE2	0.47	2.44	7	14
2:C:9:DG:C4	2:C:10:DA:N7	0.47	2.82	1	2
1:A:56:LEU:HD12	1:A:62:ALA:HA	0.47	1.85	8	2
2:C:3:DG:H2"	2:C:4:DT:C5'	0.47	2.39	10	2
1:A:73:PHE:CE2	1:D:140:ASN:HA	0.47	2.43	11	9
2:B:1:DC:C4	2:B:2:DA:N7	0.47	2.83	8	4
2:B:5:DG:H2'	2:B:5:DG:N3	0.47	2.24	14	2
2:C:2:DA:H4'	2:C:3:DG:OP1	0.46	2.09	5	1
1:D:139:LYS:HA	2:C:1:DC:C4	0.46	2.44	18	3
1:D:139:LYS:HB3	2:C:1:DC:C2	0.46	2.46	17	1
2:C:2:DA:C4'	2:C:3:DG:OP1	0.46	2.64	5	1
2:C:8:DT:H2"	2:C:9:DG:H5"	0.46	1.88	10	2
2:B:3:DG:H4'	2:B:4:DT:OP1	0.46	2.11	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:8:DT:H2"	2:B:9:DG:H5"	0.46	1.88	11	2
1:A:20:LEU:O	1:A:26:VAL:HG11	0.45	2.12	10	3
1:D:118:ASP:O	1:D:122:LYS:HG2	0.45	2.12	14	2
2:C:1:DC:H3'	2:C:2:DA:C5'	0.45	2.41	14	7
1:A:39:LYS:HG2	1:A:43:GLU:HG2	0.45	1.89	3	1
1:D:129:LYS:HB3	2:C:7:DC:OP1	0.45	2.12	8	2
1:D:143:GLU:O	1:D:147:LEU:HG	0.45	2.12	11	4
1:A:39:LYS:HA	2:B:1:DC:C4	0.45	2.47	3	5
2:C:7:DC:H3'	2:C:8:DT:H71	0.45	1.88	5	1
2:C:6:DG:H1'	2:C:7:DC:C5	0.44	2.46	10	5
2:C:8:DT:H4'	2:C:9:DG:C8	0.44	2.47	20	1
1:D:134:LEU:O	1:D:138:VAL:HG22	0.44	2.12	15	9
2:B:7:DC:H3'	2:B:8:DT:H71	0.44	1.90	5	1
2:C:9:DG:C5	2:C:10:DA:N7	0.44	2.86	1	2
2:B:7:DC:OP2	2:B:8:DT:C7	0.44	2.66	10	1
1:A:37:HIS:ND1	1:A:55:ILE:HG23	0.44	2.27	13	1
1:D:139:LYS:HG2	1:D:143:GLU:HG2	0.44	1.89	15	1
1:A:73:PHE:CE2	1:D:138:VAL:HG23	0.44	2.48	3	1
1:D:166:TYR:HA	1:D:169:ILE:HD12	0.43	1.90	14	1
1:A:30:ASN:ND2	1:A:56:LEU:HD22	0.43	2.28	6	4
1:A:73:PHE:CE1	1:D:120:LEU:HD11	0.43	2.48	9	1
2:B:9:DG:C4	2:B:10:DA:N7	0.43	2.86	5	1
1:A:43:GLU:O	1:A:47:LEU:HG	0.43	2.14	11	3
2:B:1:DC:H3'	2:B:2:DA:C5'	0.43	2.44	1	6
2:B:1:DC:O5'	2:B:2:DA:C2'	0.43	2.67	13	1
1:A:20:LEU:HD11	1:D:173:PHE:CE1	0.43	2.49	9	3
2:C:5:DG:N3	2:C:5:DG:H5"	0.42	2.29	5	2
1:D:148:SER:H	1:D:151:GLU:HB2	0.42	1.75	9	1
1:A:36:HIS:ND1	2:B:3:DG:N7	0.42	2.68	12	1
2:B:8:DT:H4'	2:B:9:DG:C8	0.42	2.50	8	1
1:D:136:HIS:ND1	2:C:3:DG:N7	0.41	2.68	18	2
2:B:1:DC:H3'	2:B:2:DA:H5'	0.41	1.92	11	1
1:D:129:LYS:HG3	1:D:130:ASN:OD1	0.41	2.14	8	1
1:A:12:TYR:CE1	1:A:35:MET:SD	0.41	3.14	13	1
2:C:3:DG:H4'	2:C:4:DT:OP1	0.41	2.16	15	1
2:C:7:DC:C2'	2:C:8:DT:H72	0.41	2.46	8	1
1:A:12:TYR:HA	1:D:173:PHE:O	0.41	2.16	9	1
1:A:40:ASN:HA	1:D:173:PHE:CE1	0.41	2.51	19	1
1:A:73:PHE:HE2	1:D:138:VAL:HG23	0.41	1.75	3	1
1:D:151:GLU:HA	1:D:151:GLU:OE1	0.41	2.16	14	1
1:D:139:LYS:CG	1:D:143:GLU:HG2	0.41	2.45	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:4:DT:H73	2:C:6:DG:N7	0.41	2.31	6	1
2:C:1:DC:H3'	2:C:2:DA:H5'	0.41	1.92	9	1
1:D:133:SER:O	1:D:137:HIS:HB2	0.41	2.16	20	1
1:D:132:ARG:HD3	1:D:133:SER:N	0.40	2.31	8	1
1:D:129:LYS:HA	2:C:7:DC:OP1	0.40	2.16	3	1
1:A:37:HIS:O	2:B:1:DC:C6	0.40	2.74	13	1
1:A:68:PHE:HA	1:A:71:THR:OG1	0.40	2.16	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	62/67 (93%)	58±1 (94±1%)	3±1 (4±1%)	1±0 (2±0%)	13	56
1	D	59/67 (88%)	57±1 (96±1%)	1±1 (2±1%)	1±0 (2±0%)	13	56
All	All	2420/2680 (90%)	2295 (95%)	84 (3%)	41 (2%)	13	56

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	40	ASN	20
1	D	140	ASN	20
1	A	12	TYR	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	52/56 (93%)	43±2 (83±4%)	9±2 (17±4%)	5	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	49/56 (88%)	40±1 (82±3%)	9±1 (18±3%)	4 37
All	All	2020/2240 (90%)	1663 (82%)	357 (18%)	4 38

All 43 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)
1	A	17	GLN	20
1	A	19	PHE	20
1	A	27	ASN	20
1	A	52	LEU	20
1	A	53	THR	20
1	D	117	GLN	20
1	D	127	ASN	20
1	D	119	PHE	19
1	D	152	LEU	19
1	D	153	THR	19
1	A	32	ARG	15
1	D	132	ARG	15
1	D	129	LYS	12
1	A	33	SER	11
1	D	151	GLU	10
1	D	122	LYS	10
1	A	29	LYS	9
1	A	37	HIS	7
1	D	172	SER	7
1	D	140	ASN	6
1	A	48	SER	6
1	D	148	SER	6
1	A	51	GLU	6
1	A	63	LYS	5
1	A	22	LYS	4
1	A	72	SER	4
1	D	133	SER	3
1	A	50	ASP	3
1	D	137	HIS	3
1	D	139	LYS	2
1	A	36	HIS	2
1	A	40	ASN	2
1	D	118	ASP	2
1	A	54	SER	1
1	D	167	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	49	GLN	1
1	D	136	HIS	1
1	A	18	ASP	1
1	D	163	LYS	1
1	D	170	HIS	1
1	A	64	GLN	1
1	A	39	LYS	1
1	A	61	ASN	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 monosaccharides 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 (i)

No chemical shift data were provided