



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:28 am BST

PDB ID : 5AKN  
Title : THE CRYSTAL STRUCTURE OF I-DMOI Q42AK120M IN COMPLEX WITH ITS TARGET DNA NICKED IN THE non-CODING STRAND B AND IN THE PRESENCE OF 2MM MN  
Authors : Molina, R.; Marcaida, M.J.; Redondo, P.; Marenchino, M.; D'Abramo, M.; Montoya, G.; Prieto, J.  
Deposited on : 2015-03-04  
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

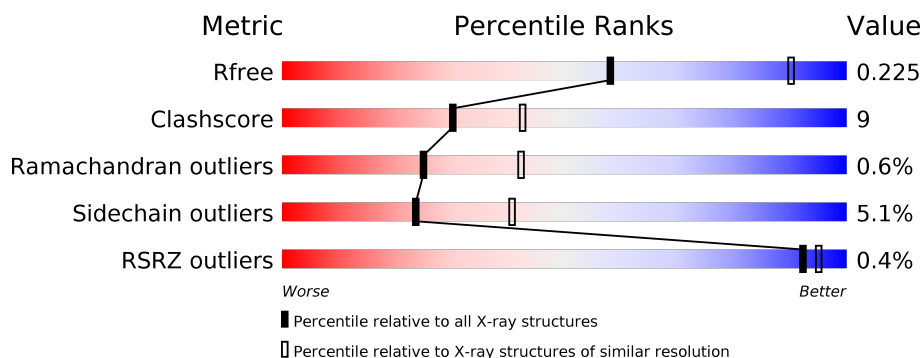
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

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.







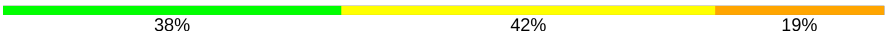
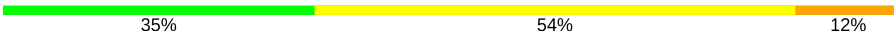

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	199	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	F	199	<div> <div>70%</div> <div>20%</div> <div>•</div> <div>8%</div> </div>
1	K	199	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	14	<div> <div>50%</div> <div>36%</div> <div>14%</div> </div>
2	G	14	<div> <div>50%</div> <div>36%</div> <div>14%</div> </div>
3	C	11	<div> <div>45%</div> <div>45%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	15	
5	E	10	
5	J	10	
5	O	10	
6	H	26	
6	M	26	
7	L	29	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7873 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HOMING ENDONUCLEASE I-DMOI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	6	0
			1508	976	275	252	5			
1	F	184	Total	C	N	O	S	8	6	0
			1554	1005	281	263	5			
1	K	183	Total	C	N	O	S	5	5	0
			1538	996	278	260	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP P21505
A	42	ALA	GLN	engineered mutation	UNP P21505
A	120	MET	LYS	engineered mutation	UNP P21505
A	189	ALA	-	expression tag	UNP P21505
A	190	ALA	-	expression tag	UNP P21505
A	191	ALA	-	expression tag	UNP P21505
A	192	LEU	-	expression tag	UNP P21505
A	193	GLU	-	expression tag	UNP P21505
A	194	HIS	-	expression tag	UNP P21505
A	195	HIS	-	expression tag	UNP P21505
A	196	HIS	-	expression tag	UNP P21505
A	197	HIS	-	expression tag	UNP P21505
A	198	HIS	-	expression tag	UNP P21505
A	199	HIS	-	expression tag	UNP P21505
F	1	ALA	-	expression tag	UNP P21505
F	42	ALA	GLN	engineered mutation	UNP P21505
F	120	MET	LYS	engineered mutation	UNP P21505
F	189	ALA	-	expression tag	UNP P21505
F	190	ALA	-	expression tag	UNP P21505
F	191	ALA	-	expression tag	UNP P21505
F	192	LEU	-	expression tag	UNP P21505
F	193	GLU	-	expression tag	UNP P21505
F	194	HIS	-	expression tag	UNP P21505

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Chain	Residue	Modelled	Actual	Comment	Reference
F	195	HIS	-	expression tag	UNP P21505
F	196	HIS	-	expression tag	UNP P21505
F	197	HIS	-	expression tag	UNP P21505
F	198	HIS	-	expression tag	UNP P21505
F	199	HIS	-	expression tag	UNP P21505
K	1	ALA	-	expression tag	UNP P21505
K	42	ALA	GLN	engineered mutation	UNP P21505
K	120	MET	LYS	engineered mutation	UNP P21505
K	189	ALA	-	expression tag	UNP P21505
K	190	ALA	-	expression tag	UNP P21505
K	191	ALA	-	expression tag	UNP P21505
K	192	LEU	-	expression tag	UNP P21505
K	193	GLU	-	expression tag	UNP P21505
K	194	HIS	-	expression tag	UNP P21505
K	195	HIS	-	expression tag	UNP P21505
K	196	HIS	-	expression tag	UNP P21505
K	197	HIS	-	expression tag	UNP P21505
K	198	HIS	-	expression tag	UNP P21505
K	199	HIS	-	expression tag	UNP P21505

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			285	136	53	83	13			
2	G	14	Total	C	N	O	P	0	0	0
			285	136	53	83	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	P	0	0	0
			227	106	41	69	11			

- Molecule 4 is a DNA chain called D(\*CP\*GP\*CP\*GP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*AP\*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			306	144	57	90	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	10	Total	C	N	O	P	0	0	0
			207	96	42	59	10			
5	J	10	Total	C	N	O	P	0	0	0
			207	96	42	59	10			
5	O	10	Total	C	N	O	P	0	0	0
			207	96	42	59	10			

- Molecule 6 is a DNA chain called 5'-D(\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*GP\*C  
P\*GP\*CP \*GP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*AP\*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	26	Total	C	N	O	P	0	0	0
			533	250	98	159	26			
6	M	26	Total	C	N	O	P	0	0	0
			533	250	98	159	26			

- Molecule 7 is a DNA chain called 5'-D(\*GP\*CP\*CP\*TP\*TP\*GP\*CP\*CP\*GP\*GP\*GP\*T  
P\*AP\*AP \*CP\*GP\*CP\*GP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	14	Total	C	N	O	P	0	0	0
			285	136	53	83	13			

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Mn	0	0
			2	2		
8	K	2	Total	Mn	0	0
			2	2		
8	F	2	Total	Mn	0	0
			2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	39	Total	O	0	0
			39	39		
9	B	7	Total	O	0	0
			7	7		

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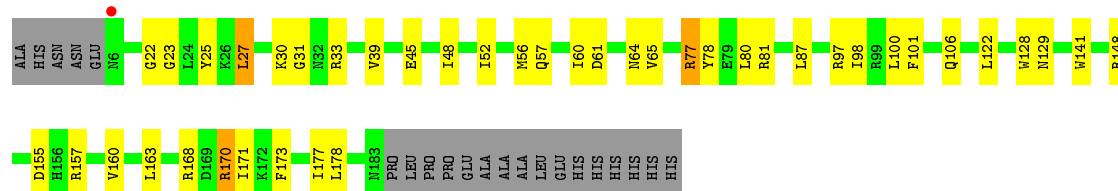
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	9	Total 9	O 9	0	0
9	D	6	Total 6	O 6	0	0
9	E	5	Total 5	O 5	0	0
9	F	32	Total 32	O 32	0	0
9	G	10	Total 10	O 10	0	0
9	H	11	Total 11	O 11	0	0
9	J	4	Total 4	O 4	0	0
9	K	35	Total 35	O 35	0	0
9	L	12	Total 12	O 12	0	0
9	M	19	Total 19	O 19	0	0
9	O	3	Total 3	O 3	0	0

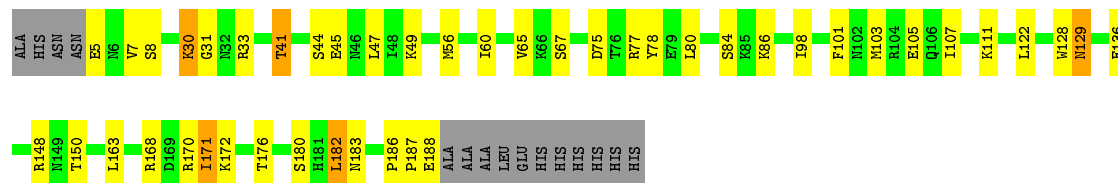
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

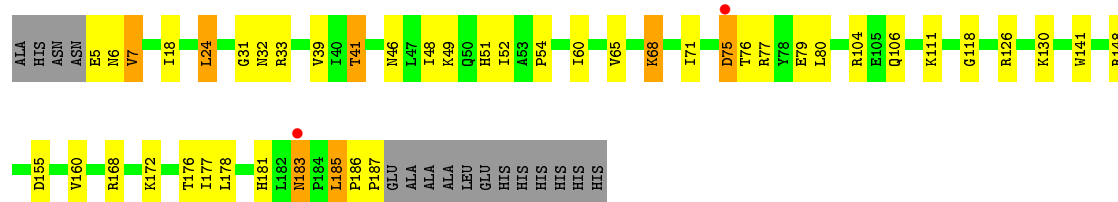
- Molecule 1: HOMING ENDONUCLEASE I-DMOI



- Molecule 1: HOMING ENDONUCLEASE I-DMOI



- Molecule 1: HOMING ENDONUCLEASE I-DMOI



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





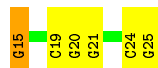
- Molecule 2: 5'-D(\*GP\*CP\*CP\*TP\*TP\*GP\*CP\*CP\*GP\*GP\*GP\*TP\*AP\*AP)-3'

Chain G: 



- Molecule 3: 5'-D(\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*GP)-3'

Chain C: 



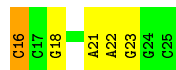
- Molecule 4: D(\*CP\*GP\*CP\*GP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*AP\*CP)-3'

Chain D: 



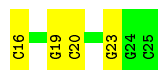
- Molecule 5: 5'-D(\*CP\*CP\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*CP)-3'

Chain E: 



- Molecule 5: 5'-D(\*CP\*CP\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*CP)-3'

Chain J: 

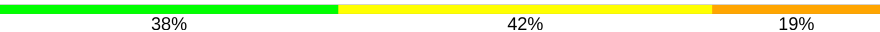


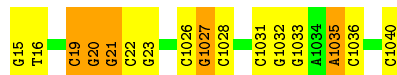
- Molecule 5: 5'-D(\*CP\*CP\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*CP)-3'

Chain O: 



- Molecule 6: 5'-D(\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*AP\*CP)-3'

Chain H: 




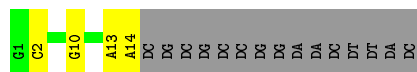
- Molecule 6: 5'-D(\*GP\*TP\*TP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*AP\*CP)-3'

Chain M:  35% 54% 12%



- Molecule 7: 5'-D(\*GP\*CP\*CP\*TP\*TP\*GP\*CP\*CP\*GP\*GP\*GP\*TP\*AP\*AP \*CP\*GP\*CP\*GP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*AP\*C)-3'

Chain L:  34% 14% 52%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.10 Å   70.34 Å   107.17 Å 90.00°   119.81°   90.00°	Depositor
Resolution (Å)	46.49 – 2.75 46.49 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.49-2.75) 97.8 (46.49-2.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.77 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.175   ,   0.236 0.166   ,   0.225	Depositor DCC
$R_{free}$ test set	1777 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h-l,k,h 0.022 for l,k,-h-l 0.023 for h,-k,-h-l 0.017 for -h-l,-k,l 0.023 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7873	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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 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	0.40	0/1549	0.59	1/2080 (0.0%)
1	F	0.40	0/1599	0.56	0/2152
1	K	0.39	0/1579	0.57	0/2126
2	B	0.70	0/319	1.42	3/491 (0.6%)
2	G	1.88	15/319 (4.7%)	1.69	10/491 (2.0%)
3	C	0.95	1/253 (0.4%)	1.32	2/387 (0.5%)
4	D	0.91	1/342 (0.3%)	1.50	5/523 (1.0%)
5	E	0.97	1/232 (0.4%)	1.43	3/354 (0.8%)
5	J	0.95	1/232 (0.4%)	1.22	1/354 (0.3%)
5	O	0.95	1/232 (0.4%)	1.31	4/354 (1.1%)
6	H	0.90	2/595 (0.3%)	1.49	8/910 (0.9%)
6	M	0.93	2/595 (0.3%)	1.45	7/910 (0.8%)
7	L	0.68	0/319	1.44	4/491 (0.8%)
All	All	0.73	24/8165 (0.3%)	1.06	48/11623 (0.4%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	15	DG	OP3-P	-10.99	1.48	1.61
6	M	15	DG	OP3-P	-10.76	1.48	1.61
5	E	16	DC	OP3-P	-10.72	1.48	1.61
5	O	16	DC	OP3-P	-10.44	1.48	1.61
6	H	1026	DC	OP3-P	-10.29	1.48	1.61
6	M	1026	DC	OP3-P	-10.25	1.48	1.61
6	H	15	DG	OP3-P	-10.18	1.49	1.61
4	D	1	DC	OP3-P	-10.18	1.49	1.61
5	J	16	DC	OP3-P	-10.12	1.49	1.61
2	G	14	DA	P-O5'	-8.21	1.51	1.59
2	G	14	DA	N7-C5	-7.86	1.34	1.39
2	G	14	DA	C6-N1	-7.58	1.30	1.35
2	G	13	DA	C5-C4	-6.69	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	14	DA	C5-C4	-6.68	1.34	1.38
2	G	13	DA	C6-N1	-6.59	1.30	1.35
2	G	14	DA	C4'-O4'	-6.47	1.38	1.45
2	G	14	DA	C5-C6	-6.44	1.35	1.41
2	G	13	DA	N7-C5	-6.24	1.35	1.39
2	G	14	DA	C3'-O3'	-6.02	1.36	1.44
2	G	13	DA	N3-C4	-5.63	1.31	1.34
2	G	14	DA	C8-N7	-5.43	1.27	1.31
2	G	14	DA	N9-C8	-5.28	1.33	1.37
2	G	13	DA	O3'-P	-5.27	1.54	1.61
2	G	14	DA	N9-C4	-5.08	1.34	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	14	DA	O4'-C4'-C3'	-9.50	100.30	106.00
2	G	13	DA	O4'-C1'-C2'	-8.71	98.93	105.90
2	G	14	DA	C1'-O4'-C4'	-8.52	101.58	110.10
6	M	1033	DG	C1'-O4'-C4'	-8.25	101.85	110.10
4	D	8	DG	C1'-O4'-C4'	-8.22	101.88	110.10
4	D	8	DG	O4'-C4'-C3'	-8.12	101.13	106.00
2	G	14	DA	P-O5'-C5'	-7.38	109.10	120.90
7	L	10	DG	O4'-C1'-N9	-7.35	102.86	108.00
6	M	16	DT	O4'-C1'-N1	-7.28	102.90	108.00
6	H	16	DT	O4'-C1'-N1	-7.21	102.95	108.00
5	J	23	DG	C1'-O4'-C4'	-6.85	103.25	110.10
6	M	1028	DC	P-O5'-C5'	-6.76	110.08	120.90
6	M	1033	DG	P-O5'-C5'	-6.67	110.22	120.90
7	L	13	DA	O4'-C1'-N9	6.62	112.63	108.00
6	H	19	DC	O4'-C1'-N1	6.59	112.61	108.00
5	E	16	DC	O4'-C1'-N1	-6.48	103.46	108.00
6	H	1035	DA	O4'-C1'-N9	-6.39	103.53	108.00
2	G	2	DC	O4'-C1'-N1	6.38	112.47	108.00
2	B	2	DC	C1'-O4'-C4'	-6.32	103.78	110.10
2	G	14	DA	O4'-C1'-C2'	-6.29	100.87	105.90
5	E	18	DG	O4'-C1'-N9	6.29	112.40	108.00
6	M	1034	DA	O4'-C1'-N9	6.24	112.36	108.00
4	D	13	DT	C5-C4-O4	-6.14	120.60	124.90
6	M	16	DT	N3-C4-O4	6.13	123.58	119.90
7	L	2	DC	C1'-O4'-C4'	-6.12	103.98	110.10
1	A	27	LEU	CA-CB-CG	6.09	129.31	115.30
4	D	13	DT	N3-C4-O4	5.93	123.46	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	DG	O4'-C1'-N9	-5.86	103.90	108.00
2	G	12	DT	O4'-C1'-N1	-5.75	103.98	108.00
3	C	21	DG	C1'-O4'-C4'	-5.69	104.41	110.10
5	O	16	DC	O4'-C1'-N1	-5.67	104.03	108.00
3	C	21	DG	O4'-C1'-N9	5.66	111.96	108.00
4	D	15	DC	C3'-C2'-C1'	-5.57	95.81	102.50
5	O	21	DA	C3'-C2'-C1'	-5.55	95.84	102.50
5	E	21	DA	C3'-C2'-C1'	-5.50	95.90	102.50
6	H	1040	DC	C3'-C2'-C1'	-5.49	95.91	102.50
6	H	1027	DG	O4'-C1'-N9	-5.30	104.29	108.00
6	H	20	DG	O4'-C1'-N9	5.25	111.68	108.00
5	O	18	DG	O4'-C1'-C2'	-5.24	101.71	105.90
2	G	8	DC	O4'-C1'-N1	5.19	111.64	108.00
6	H	1033	DG	O4'-C1'-N9	-5.19	104.36	108.00
2	G	8	DC	C1'-O4'-C4'	-5.15	104.95	110.10
6	M	16	DT	C5-C4-O4	-5.13	121.31	124.90
7	L	2	DC	O4'-C4'-C3'	-5.10	102.46	104.50
6	H	21	DG	O4'-C1'-N9	5.02	111.52	108.00
5	O	18	DG	O4'-C1'-N9	5.02	111.51	108.00
2	B	4	DT	N3-C4-O4	5.01	122.91	119.90
2	G	14	DA	O4'-C1'-N9	-5.01	104.49	108.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1508	0	1604	29	0
1	F	1554	0	1637	35	0
1	K	1538	0	1626	35	0
2	B	285	0	159	3	0
2	G	285	0	159	4	0
3	C	227	0	124	6	0
4	D	306	0	168	5	0
5	E	207	0	111	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	207	0	111	1	0
5	O	207	0	111	1	0
6	H	533	0	292	7	0
6	M	533	0	292	14	0
7	L	285	0	159	5	0
8	A	2	0	0	0	0
8	F	2	0	0	0	0
8	K	2	0	0	0	0
9	A	39	0	0	0	0
9	B	7	0	0	0	0
9	C	9	0	0	0	0
9	D	6	0	0	0	0
9	E	5	0	0	0	0
9	F	32	0	0	0	0
9	G	10	0	0	0	0
9	H	11	0	0	0	0
9	J	4	0	0	0	0
9	K	35	0	0	2	0
9	L	12	0	0	0	0
9	M	19	0	0	0	0
9	O	3	0	0	0	0
All	All	7873	0	6553	132	0

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 9.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:1031:DC:H2"	6:H:1032:DG:H5'	1.55	0.86
1:K:111:LYS:HD3	1:K:186:PRO:HG3	1.60	0.83
1:K:111:LYS:HE2	1:K:177:ILE:O	1.79	0.83
6:H:1027:DG:H2"	6:H:1028:DC:H5"	1.62	0.81
1:K:178:LEU:O	1:K:186:PRO:HG2	1.87	0.75
1:K:41:THR:CG2	7:L:14:DA:H5"	2.16	0.75
1:F:5:GLU:HB3	1:F:8:SER:OG	1.87	0.74
1:F:148:ARG:HH21	1:F:168:ARG:HD2	1.54	0.73
1:F:33:ARG:NH1	6:H:21:DG:O6	2.24	0.71
1:A:45:GLU:HB2	1:A:78:TYR:CE2	2.25	0.71
1:A:148:ARG:HH21	1:A:168:ARG:HB3	1.56	0.71
2:G:8:DC:H2"	2:G:9:DG:C8	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:GLU:HG3	1:F:7:VAL:HG12	1.72	0.70
3:C:24:DC:H2''	3:C:25:DG:C8	2.28	0.68
1:F:111:LYS:HD2	1:F:186:PRO:HD3	1.76	0.67
1:K:5:GLU:HG3	1:K:7:VAL:HG13	1.77	0.67
3:C:19:DC:H2'	3:C:20:DG:C8	2.30	0.66
1:F:56:MET:O	1:F:60:ILE:HG12	1.98	0.64
1:K:18:ILE:HG21	1:K:24:LEU:HD13	1.79	0.64
4:D:15:DC:O3'	5:E:16:DC:OP2	2.15	0.64
1:K:106:GLN:HG2	1:K:141:TRP:CD2	2.34	0.62
1:A:45:GLU:HB2	1:A:78:TYR:CD2	2.33	0.62
1:K:111:LYS:CD	1:K:186:PRO:HG3	2.30	0.62
1:F:45:GLU:OE2	1:F:49:LYS:HE3	2.00	0.62
1:F:80:LEU:HD23	1:F:80:LEU:C	2.22	0.60
4:D:5:DC:H2''	4:D:6:DC:O5'	2.02	0.60
1:F:45:GLU:HB2	1:F:78:TYR:CE1	2.37	0.60
1:K:41:THR:HG23	7:L:14:DA:H5''	1.84	0.59
6:M:1027:DG:H2''	6:M:1028:DC:H5''	1.84	0.59
1:A:77:ARG:HD3	1:A:77:ARG:N	2.19	0.58
4:D:2:DG:H2''	4:D:3:DC:H5''	1.84	0.58
1:A:177:ILE:HG22	1:A:178:LEU:HD23	1.86	0.58
6:M:18:DC:H2''	6:M:19:DC:H5'	1.86	0.58
1:F:172:LYS:O	1:F:176:THR:HB	2.04	0.57
1:A:22:GLY:HA3	1:A:39:VAL:O	2.05	0.57
1:F:128:TRP:O	1:F:129:ASN:HB2	2.03	0.57
1:F:41:THR:HG22	2:G:14:DA:H5''	1.86	0.57
6:H:22:DC:H2'	6:H:23:DG:C8	2.40	0.56
6:M:19:DC:H2''	6:M:20:DG:H5'	1.87	0.56
1:K:41:THR:HG22	7:L:14:DA:H5''	1.87	0.56
1:K:106:GLN:HG2	1:K:141:TRP:CE2	2.41	0.56
1:A:122:LEU:O	1:A:170:ARG:NH2	2.39	0.55
1:F:98:ILE:HA	1:F:101:PHE:CE1	2.41	0.55
6:M:24:DC:H2''	6:M:25:DG:C8	2.41	0.55
1:A:30:LYS:O	1:A:30:LYS:HG3	2.05	0.55
1:K:41:THR:HG21	7:L:14:DA:H2'	1.89	0.55
3:C:19:DC:H2''	3:C:20:DG:H5'	1.88	0.55
1:K:48[B]:ILE:HD13	1:K:52:ILE:HD12	1.90	0.53
1:A:155:ASP:HB3	1:A:160:VAL:HB	1.91	0.53
1:K:80:LEU:HD23	1:K:80:LEU:C	2.29	0.53
4:D:13:DT:H4'	4:D:14:DA:OP1	2.09	0.53
1:K:5:GLU:O	1:K:6:ASN:HB3	2.08	0.53
1:K:68:LYS:HE3	6:M:1032:DG:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:19:DG:C4	5:J:20:DC:C5	2.97	0.52
1:F:150:THR:HG21	2:G:6:DG:OP1	2.10	0.52
1:K:118:GLY:HA2	1:K:126:ARG:O	2.10	0.52
1:K:148:ARG:HD2	1:K:168:ARG:HH21	1.74	0.51
3:C:24:DC:C2'	3:C:25:DG:C8	2.94	0.51
1:A:48[A]:ILE:HD13	1:A:52:ILE:HD12	1.92	0.51
1:K:130:LYS:HB2	6:M:1040:DC:OP2	2.10	0.50
1:F:101:PHE:CD2	1:F:105:GLU:HB3	2.46	0.50
1:K:181:HIS:ND1	1:K:185:LEU:HD11	2.26	0.50
6:H:19:DC:H2'	6:H:20:DG:C8	2.46	0.50
1:A:60[B]:ILE:HG23	1:A:65:VAL:HB	1.93	0.50
1:F:163:LEU:HD23	1:F:163:LEU:C	2.32	0.49
1:F:31:GLY:HA2	1:F:33:ARG:H	1.75	0.49
2:B:4:DT:H2''	2:B:5:DT:O5'	2.12	0.49
1:F:47:LEU:HD11	1:F:187:PRO:HG2	1.93	0.49
1:A:60[A]:ILE:HG22	1:A:61:ASP:N	2.28	0.48
1:F:111:LYS:HD2	1:F:186:PRO:CD	2.43	0.48
1:F:170:ARG:HG2	1:F:171:ILE:N	2.28	0.48
1:F:171:ILE:HD12	1:F:172:LYS:H	1.79	0.48
6:M:21:DG:H2''	6:M:22:DC:O5'	2.13	0.48
6:M:22:DC:H2''	6:M:23:DG:C8	2.49	0.47
1:A:170:ARG:HG2	1:A:171:ILE:N	2.29	0.47
1:A:31:GLY:HA2	1:A:33:ARG:H	1.80	0.47
1:A:128:TRP:O	1:A:129:ASN:HB2	2.15	0.47
1:F:180:SER:HB2	1:F:182:LEU:CD1	2.45	0.47
1:F:65:VAL:HG22	1:F:86:LYS:HD3	1.97	0.46
1:A:170:ARG:CG	1:A:171:ILE:N	2.78	0.46
1:F:182:LEU:HD12	1:F:182:LEU:H	1.79	0.46
1:A:80:LEU:HD23	1:A:81:ARG:N	2.31	0.46
4:D:9:DA:H2''	4:D:10:DA:C8	2.50	0.46
1:F:103:MET:O	1:F:107:ILE:HG12	2.16	0.46
1:A:77:ARG:NH1	3:C:15:DG:N7	2.64	0.46
1:K:172:LYS:O	1:K:176:THR:HB	2.15	0.46
1:F:111:LYS:HD2	1:F:186:PRO:HG3	1.98	0.46
6:M:1027:DG:C2'	6:M:1028:DC:H5''	2.46	0.46
1:K:49:LYS:HG2	1:K:71:ILE:HD13	1.98	0.45
1:A:48[A]:ILE:HD12	1:A:80:LEU:HB2	1.98	0.45
1:A:163:LEU:C	1:A:163:LEU:HD23	2.37	0.45
1:F:111:LYS:HG3	1:F:186:PRO:HG3	1.99	0.45
1:K:75:ASP:HB3	9:K:2019:HOH:O	2.16	0.45
6:H:1031:DC:C2'	6:H:1032:DG:H5'	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:ASP:HB3	1:K:160:VAL:HB	1.99	0.45
6:M:15:DG:C8	6:M:16:DT:H72	2.52	0.45
6:H:1035:DA:C2	6:H:1036:DC:C2	3.06	0.44
1:F:111:LYS:CG	1:F:186:PRO:HG3	2.47	0.44
1:F:41:THR:HG21	2:G:14:DA:H2'	1.99	0.44
1:K:185:LEU:HA	1:K:186:PRO:HD3	1.84	0.44
5:O:23:DG:H2''	5:O:24:DG:O5'	2.16	0.44
1:F:180:SER:HB2	1:F:182:LEU:HD12	1.98	0.43
6:M:18:DC:C2'	6:M:19:DC:H5'	2.47	0.43
1:A:23:GLY:HA3	1:A:25:TYR:CZ	2.52	0.43
1:A:57:GLN:HA	1:A:60[B]:ILE:HD12	2.01	0.43
3:C:15:DG:OP3	3:C:15:DG:H4'	2.18	0.43
1:A:173:PHE:O	1:A:177:ILE:HB	2.18	0.43
1:A:56:MET:O	1:A:60[B]:ILE:HG13	2.18	0.43
5:E:22:DA:H1'	5:E:23:DG:H5'	2.01	0.43
1:A:155:ASP:OD1	1:A:157:ARG:HB2	2.18	0.43
1:K:60[B]:ILE:HG23	1:K:65:VAL:HB	2.00	0.42
2:B:6:DG:H2''	2:B:7:DC:O5'	2.18	0.42
1:K:5:GLU:N	1:K:104:ARG:NH1	2.66	0.42
1:K:51:HIS:O	1:K:54:PRO:HD2	2.18	0.42
1:K:7:VAL:HG12	9:K:2001:HOH:O	2.18	0.42
1:A:77:ARG:H	1:A:77:ARG:HD3	1.85	0.42
1:F:187:PRO:O	1:F:188:GLU:C	2.58	0.42
1:F:30:LYS:O	1:F:30:LYS:HG2	2.19	0.42
1:K:186:PRO:HA	1:K:187:PRO:HD3	1.92	0.42
1:F:111:LYS:HD2	1:F:186:PRO:CG	2.50	0.42
6:M:22:DC:H2''	6:M:23:DG:H8	1.84	0.42
1:A:98:ILE:HA	1:A:101:PHE:CE1	2.55	0.42
1:A:106:GLN:HG2	1:A:141:TRP:CD2	2.55	0.42
1:K:130:LYS:N	6:M:1040:DC:OP2	2.53	0.41
1:K:33:ARG:NH1	6:M:21:DG:O6	2.53	0.41
1:A:60[A]:ILE:HD11	1:A:87:LEU:HD22	2.01	0.41
1:K:39:VAL:HG13	1:K:79:GLU:HG3	2.03	0.41
1:F:111:LYS:CD	1:F:186:PRO:HG3	2.51	0.41
1:F:67:SER:OG	1:F:84:SER:HB2	2.21	0.41
2:B:2:DC:H2''	2:B:3:DC:O5'	2.20	0.41
1:K:41:THR:HG22	7:L:14:DA:C5'	2.49	0.40
1:K:31:GLY:HA2	1:K:32:ASN:HA	1.81	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	182/199 (92%)	172 (94%)	10 (6%)	0	100	100
1	F	188/199 (94%)	178 (95%)	8 (4%)	2 (1%)	14	25
1	K	186/199 (94%)	172 (92%)	13 (7%)	1 (0%)	29	47
All	All	556/597 (93%)	522 (94%)	31 (6%)	3 (0%)	25	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	122	LEU
1	F	129	ASN
1	K	183	ASN

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	166/177 (94%)	159 (96%)	7 (4%)	30	49
1	F	172/177 (97%)	163 (95%)	9 (5%)	23	39
1	K	170/177 (96%)	160 (94%)	10 (6%)	19	34
All	All	508/531 (96%)	482 (95%)	26 (5%)	24	41

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	64	ASN
1	A	77	ARG
1	A	97[A]	ARG
1	A	97[B]	ARG
1	A	100	LEU
1	A	170	ARG
1	F	30	LYS
1	F	41	THR
1	F	44	SER
1	F	75	ASP
1	F	77	ARG
1	F	136	GLU
1	F	171	ILE
1	F	182	LEU
1	F	183	ASN
1	K	7	VAL
1	K	24	LEU
1	K	41	THR
1	K	46	ASN
1	K	68	LYS
1	K	75	ASP
1	K	76	THR
1	K	77	ARG
1	K	183	ASN
1	K	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	H	1
6	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	25:DG	O3'	1026:DC	P	16.82
1	M	25:DG	O3'	1026:DC	P	16.75

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	178/199 (89%)	-0.26	1 (0%) 89 92	21, 39, 76, 120	0
1	F	184/199 (92%)	-0.26	0 100 100	20, 42, 81, 102	0
1	K	183/199 (91%)	-0.19	2 (1%) 80 86	19, 37, 88, 161	0
2	B	14/14 (100%)	-0.76	0 100 100	40, 52, 67, 68	0
2	G	14/14 (100%)	-0.47	0 100 100	45, 73, 104, 110	0
3	C	11/11 (100%)	-0.71	0 100 100	37, 51, 77, 81	0
4	D	15/15 (100%)	-0.48	0 100 100	33, 58, 86, 87	0
5	E	10/10 (100%)	-0.83	0 100 100	36, 59, 71, 71	0
5	J	10/10 (100%)	0.21	0 100 100	42, 85, 112, 117	0
5	O	10/10 (100%)	-0.23	0 100 100	39, 70, 79, 81	0
6	H	26/26 (100%)	-0.58	0 100 100	33, 51, 73, 86	0
6	M	26/26 (100%)	-0.53	0 100 100	34, 55, 73, 79	0
7	L	14/29 (48%)	-0.48	0 100 100	43, 55, 70, 76	0
All	All	695/762 (91%)	-0.30	3 (0%) 92 95	19, 44, 86, 161	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	183	ASN	3.3
1	K	75	ASP	3.0
1	A	6	ASN	2.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MN	F	1189	1/1	0.92	0.09	56,56,56,56	0
8	MN	A	1185	1/1	0.96	0.12	59,59,59,59	0
8	MN	A	1184	1/1	0.97	0.11	52,52,52,52	0
8	MN	K	1188	1/1	0.97	0.10	71,71,71,71	0
8	MN	F	1190	1/1	0.97	0.08	61,61,61,61	0
8	MN	K	1189	1/1	0.99	0.11	49,49,49,49	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.