



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 08:19 AM BST

PDB ID : 6IID  
Title : Human EXOG-H140A in complex with RNA-DNA chimeric duplex  
Authors : Wu, C.C.; Lin, J.L.J.; Yuan, H.S.  
Deposited on : 2018-10-04  
Resolution : 2.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.13.1  
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) : 2.13.1

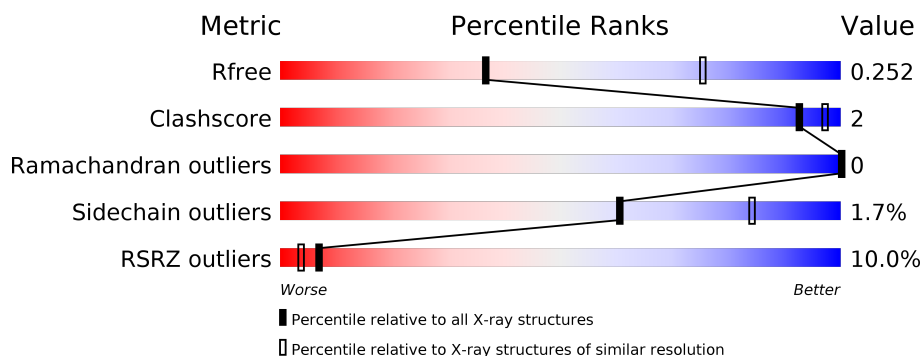
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	348	<div> <div>9%</div> <div>80% 5% 15%</div> </div>
1	B	348	<div> <div>7%</div> <div>79% 5% 17%</div> </div>
1	C	348	<div> <div>7%</div> <div>82% • 16%</div> </div>
1	D	348	<div> <div>9%</div> <div>76% 6% • 17%</div> </div>
2	E	12	<div> <div>8%</div> <div>67% 17% 17%</div> </div>
2	G	12	<div> <div>8%</div> <div>42% 17% 42%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	12	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>17%75%17%8%</div>
2	K	12	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>8%17%25%58%</div>
3	F	12	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>8%67%25%8%</div>
3	H	12	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>33%67%33%</div>
3	J	12	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>75%25%</div>
3	L	12	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>33%67%</div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20628 atoms, of which 9886 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 Nuclease EXOG, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	H	N	O	S	0	0	0
			4701	1510	2328	404	448	11			
1	B	290	Total	C	H	N	O	S	0	0	0
			4602	1483	2273	392	443	11			
1	C	291	Total	C	H	N	O	S	0	0	0
			4622	1485	2289	398	439	11			
1	D	288	Total	C	H	N	O	S	0	0	0
			4581	1474	2268	393	435	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	expression tag	UNP Q9Y2C4
A	22	GLY	-	expression tag	UNP Q9Y2C4
A	23	SER	-	expression tag	UNP Q9Y2C4
A	24	SER	-	expression tag	UNP Q9Y2C4
A	25	HIS	-	expression tag	UNP Q9Y2C4
A	26	HIS	-	expression tag	UNP Q9Y2C4
A	27	HIS	-	expression tag	UNP Q9Y2C4
A	28	HIS	-	expression tag	UNP Q9Y2C4
A	29	HIS	-	expression tag	UNP Q9Y2C4
A	30	HIS	-	expression tag	UNP Q9Y2C4
A	31	SER	-	expression tag	UNP Q9Y2C4
A	32	SER	-	expression tag	UNP Q9Y2C4
A	33	GLY	-	expression tag	UNP Q9Y2C4
A	34	LEU	-	expression tag	UNP Q9Y2C4
A	35	VAL	-	expression tag	UNP Q9Y2C4
A	36	PRO	-	expression tag	UNP Q9Y2C4
A	37	ARG	-	expression tag	UNP Q9Y2C4
A	38	GLY	-	expression tag	UNP Q9Y2C4
A	39	SER	-	expression tag	UNP Q9Y2C4
A	40	HIS	-	expression tag	UNP Q9Y2C4
A	41	MET	-	expression tag	UNP Q9Y2C4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ALA	HIS	engineered mutation	UNP Q9Y2C4
B	21	MET	-	expression tag	UNP Q9Y2C4
B	22	GLY	-	expression tag	UNP Q9Y2C4
B	23	SER	-	expression tag	UNP Q9Y2C4
B	24	SER	-	expression tag	UNP Q9Y2C4
B	25	HIS	-	expression tag	UNP Q9Y2C4
B	26	HIS	-	expression tag	UNP Q9Y2C4
B	27	HIS	-	expression tag	UNP Q9Y2C4
B	28	HIS	-	expression tag	UNP Q9Y2C4
B	29	HIS	-	expression tag	UNP Q9Y2C4
B	30	HIS	-	expression tag	UNP Q9Y2C4
B	31	SER	-	expression tag	UNP Q9Y2C4
B	32	SER	-	expression tag	UNP Q9Y2C4
B	33	GLY	-	expression tag	UNP Q9Y2C4
B	34	LEU	-	expression tag	UNP Q9Y2C4
B	35	VAL	-	expression tag	UNP Q9Y2C4
B	36	PRO	-	expression tag	UNP Q9Y2C4
B	37	ARG	-	expression tag	UNP Q9Y2C4
B	38	GLY	-	expression tag	UNP Q9Y2C4
B	39	SER	-	expression tag	UNP Q9Y2C4
B	40	HIS	-	expression tag	UNP Q9Y2C4
B	41	MET	-	expression tag	UNP Q9Y2C4
B	140	ALA	HIS	engineered mutation	UNP Q9Y2C4
C	21	MET	-	expression tag	UNP Q9Y2C4
C	22	GLY	-	expression tag	UNP Q9Y2C4
C	23	SER	-	expression tag	UNP Q9Y2C4
C	24	SER	-	expression tag	UNP Q9Y2C4
C	25	HIS	-	expression tag	UNP Q9Y2C4
C	26	HIS	-	expression tag	UNP Q9Y2C4
C	27	HIS	-	expression tag	UNP Q9Y2C4
C	28	HIS	-	expression tag	UNP Q9Y2C4
C	29	HIS	-	expression tag	UNP Q9Y2C4
C	30	HIS	-	expression tag	UNP Q9Y2C4
C	31	SER	-	expression tag	UNP Q9Y2C4
C	32	SER	-	expression tag	UNP Q9Y2C4
C	33	GLY	-	expression tag	UNP Q9Y2C4
C	34	LEU	-	expression tag	UNP Q9Y2C4
C	35	VAL	-	expression tag	UNP Q9Y2C4
C	36	PRO	-	expression tag	UNP Q9Y2C4
C	37	ARG	-	expression tag	UNP Q9Y2C4
C	38	GLY	-	expression tag	UNP Q9Y2C4
C	39	SER	-	expression tag	UNP Q9Y2C4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	40	HIS	-	expression tag	UNP Q9Y2C4
C	41	MET	-	expression tag	UNP Q9Y2C4
C	140	ALA	HIS	engineered mutation	UNP Q9Y2C4
D	21	MET	-	expression tag	UNP Q9Y2C4
D	22	GLY	-	expression tag	UNP Q9Y2C4
D	23	SER	-	expression tag	UNP Q9Y2C4
D	24	SER	-	expression tag	UNP Q9Y2C4
D	25	HIS	-	expression tag	UNP Q9Y2C4
D	26	HIS	-	expression tag	UNP Q9Y2C4
D	27	HIS	-	expression tag	UNP Q9Y2C4
D	28	HIS	-	expression tag	UNP Q9Y2C4
D	29	HIS	-	expression tag	UNP Q9Y2C4
D	30	HIS	-	expression tag	UNP Q9Y2C4
D	31	SER	-	expression tag	UNP Q9Y2C4
D	32	SER	-	expression tag	UNP Q9Y2C4
D	33	GLY	-	expression tag	UNP Q9Y2C4
D	34	LEU	-	expression tag	UNP Q9Y2C4
D	35	VAL	-	expression tag	UNP Q9Y2C4
D	36	PRO	-	expression tag	UNP Q9Y2C4
D	37	ARG	-	expression tag	UNP Q9Y2C4
D	38	GLY	-	expression tag	UNP Q9Y2C4
D	39	SER	-	expression tag	UNP Q9Y2C4
D	40	HIS	-	expression tag	UNP Q9Y2C4
D	41	MET	-	expression tag	UNP Q9Y2C4
D	140	ALA	HIS	engineered mutation	UNP Q9Y2C4

- Molecule 2 is DNA/RNA hybrid called DNA/RNA (5'-R(P\*CP\*GP\*GP\*GP\*A)-D(P\*T)-R(P\*G)-D(P\*T)-R(P\*CP\*AP\*CP\*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	10	Total	C	H	N	O	P	0	0	0
			323	98	112	40	63	10			
2	G	7	Total	C	H	N	O	P	0	0	0
			229	69	78	30	45	7			
2	I	11	Total	C	H	N	O	P	0	0	0
			353	107	123	43	69	11			
2	K	5	Total	C	H	N	O	P	0	0	0
			164	49	55	23	32	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	11	Total	C	H	N	O	P	0	0	0
			348	106	124	41	66	11			
3	H	8	Total	C	H	N	O	P	0	0	0
			250	76	90	29	47	8			
3	J	9	Total	C	H	N	O	P	0	0	0
			283	86	101	34	53	9			
3	L	4	Total	C	H	N	O	P	0	0	0
			124	37	45	14	24	4			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

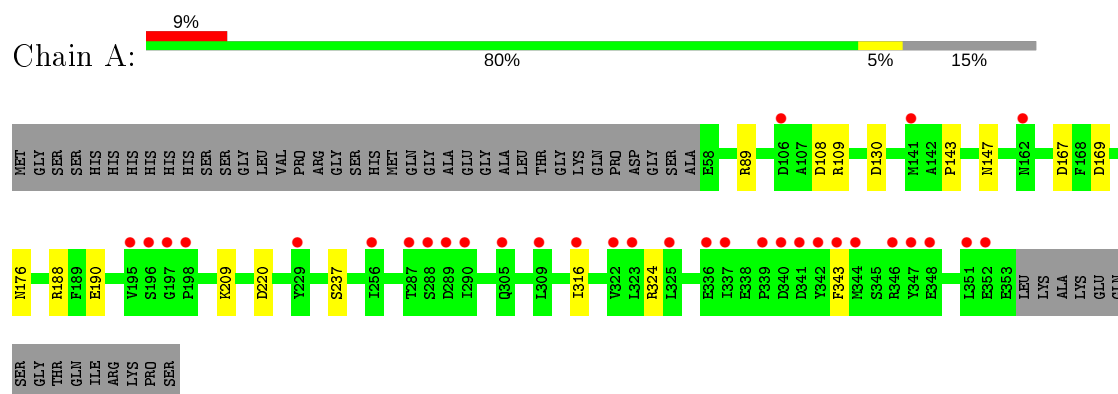
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	10	Total	O	0	0
			10	10		
5	C	11	Total	O	0	0
			11	11		
5	D	10	Total	O	0	0
			10	10		
5	E	1	Total	O	0	0
			1	1		
5	I	1	Total	O	0	0
			1	1		
5	J	1	Total	O	0	0
			1	1		

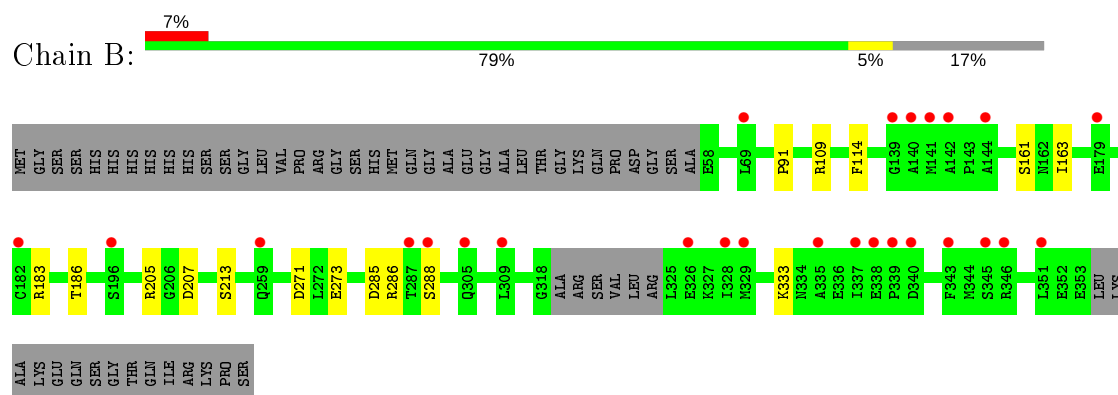
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

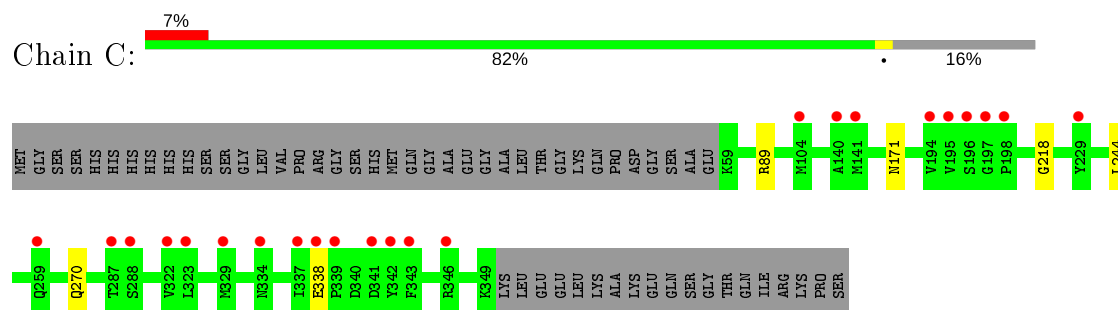
- Molecule 1: Nuclease EXOG, mitochondrial



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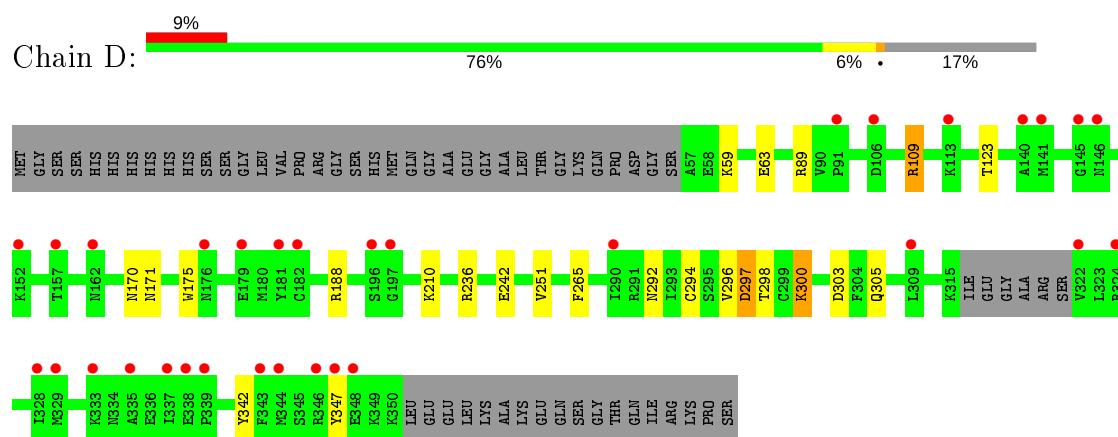


- Molecule 1: Nuclease EXOG, mitochondrial

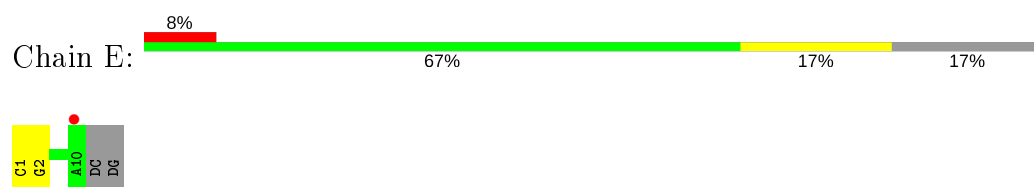


- Molecule 1: Nuclease EXOG, mitochondrial

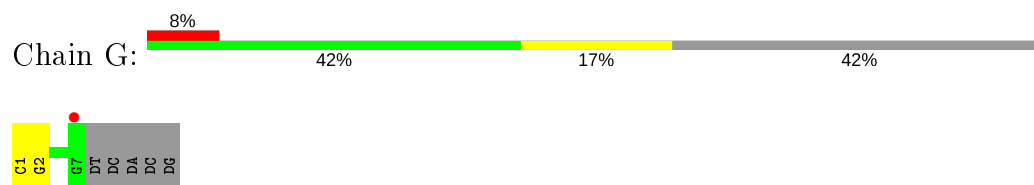




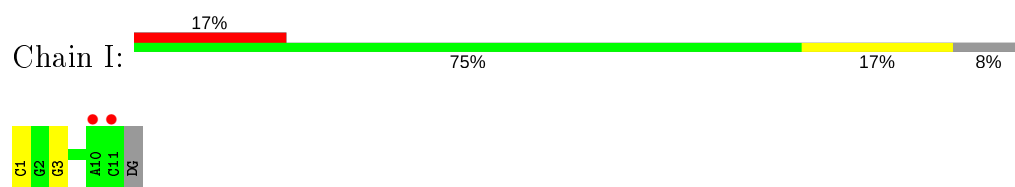
- Molecule 2: DNA/RNA (5'-R(P\*CP\*GP\*GP\*GP\*A)-D(P\*T)-R(P\*G)-D(P\*T)-R(P\*CP\*AP\*CP\*G)-3')



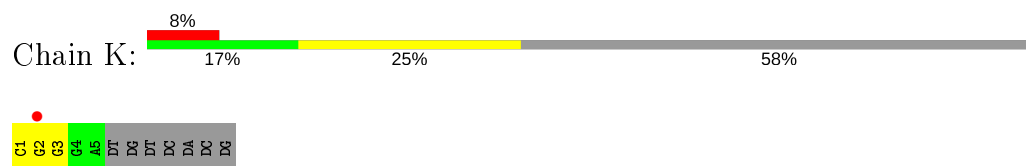
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- Molecule 2: DNA/RNA (5'-R(P\*CP\*GP\*GP\*GP\*A)-D(P\*T)-R(P\*G)-D(P\*T)-R(P\*CP\*AP\*CP\*G)-3')

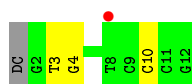


- Molecule 2: DNA/RNA (5'-R(P\*CP\*GP\*GP\*GP\*A)-D(P\*T)-R(P\*G)-D(P\*T)-R(P\*CP\*AP\*CP\*G)-3')

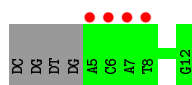


- Molecule 3: DNA (5'-D(\*CP\*GP\*TP\*GP\*AP\*CP\*AP\*TP\*CP\*CP\*CP\*G)-3')





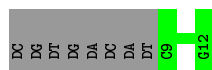
- Molecule 3: DNA (5'-D(\*CP\*GP\*TP\*GP\*AP\*CP\*AP\*TP\*CP\*CP\*CP\*G)-3')



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.71Å 75.95Å 81.15Å 72.96° 90.01° 70.75°	Depositor
Resolution (Å)	29.83 – 2.99 29.83 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.83-2.99) 95.9 (29.83-2.99)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.199 , 0.252 0.199 , 0.252	Depositor DCC
$R_{free}$ test set	1562 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 64.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.70% 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: MG

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	0.26	0/2429	0.41	0/3287
1	B	0.26	0/2384	0.41	0/3225
1	C	0.26	0/2389	0.41	0/3234
1	D	0.25	0/2368	0.41	0/3204
2	E	0.80	1/236 (0.4%)	0.78	0/362
2	G	0.90	1/169 (0.6%)	0.74	0/259
2	I	0.82	1/257 (0.4%)	0.89	0/394
2	K	1.02	1/122 (0.8%)	0.65	0/186
3	F	0.56	0/250	0.88	0/383
3	H	0.51	0/178	0.82	0/271
3	J	0.52	0/203	0.81	0/310
3	L	0.49	0/87	0.76	0/131
All	All	0.36	4/11072 (0.0%)	0.49	0/15246

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	C	OP3-P	-10.66	1.48	1.61
2	E	1	C	OP3-P	-10.61	1.48	1.61
2	G	1	C	OP3-P	-10.55	1.48	1.61
2	I	1	C	OP3-P	-10.50	1.48	1.61

There are no bond angle outliers.

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	2373	2328	2326	8	0
1	B	2329	2273	2273	6	0
1	C	2333	2289	2288	2	0
1	D	2313	2268	2268	13	0
2	E	211	112	113	2	0
2	G	151	78	79	1	0
2	I	230	123	124	1	0
2	K	109	55	56	2	0
3	F	224	124	124	3	0
3	H	160	90	90	0	0
3	J	182	101	101	0	0
3	L	79	45	45	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	K	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	11	0	0	0	0
5	D	10	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
All	All	10742	9886	9887	30	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 2.

The worst 5 of 30 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)
1:C:218:GLY:O	1:D:210:LYS:NZ	2.30	0.65
1:B:91:PRO:HG3	1:B:161:SER:O	2.06	0.55
1:D:298:THR:HB	1:D:300:LYS:HB3	1.92	0.52
1:D:109:ARG:NE	2:K:2:G:OP2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ARG:NH2	3:F:10:DC:OP1	2.41	0.50

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 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	294/348 (84%)	282 (96%)	12 (4%)	0	100	100
1	B	286/348 (82%)	273 (96%)	13 (4%)	0	100	100
1	C	289/348 (83%)	279 (96%)	10 (4%)	0	100	100
1	D	284/348 (82%)	276 (97%)	8 (3%)	0	100	100
All	All	1153/1392 (83%)	1110 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 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	261/302 (86%)	257 (98%)	4 (2%)	65	86
1	B	257/302 (85%)	252 (98%)	5 (2%)	57	82
1	C	257/302 (85%)	253 (98%)	4 (2%)	62	85
1	D	255/302 (84%)	250 (98%)	5 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1030/1208 (85%)	1012 (98%)	18 (2%)	60 84

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	333	LYS
1	C	89	ARG
1	D	297	ASP
1	B	213	SER
1	B	271	ASP

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	296/348 (85%)	0.61	32 (10%) 5 3	38, 64, 128, 143	0
1	B	290/348 (83%)	0.47	26 (8%) 9 5	35, 55, 114, 135	0
1	C	291/348 (83%)	0.44	23 (7%) 12 6	33, 53, 113, 126	0
1	D	288/348 (82%)	0.57	32 (11%) 5 3	34, 58, 118, 134	0
2	E	10/12 (83%)	0.49	1 (10%) 7 4	63, 101, 125, 125	0
2	G	7/12 (58%)	0.99	1 (14%) 2 1	60, 63, 106, 116	0
2	I	11/12 (91%)	0.54	2 (18%) 1 0	48, 71, 113, 120	0
2	K	5/12 (41%)	0.90	1 (20%) 1 0	62, 66, 85, 100	0
3	F	11/12 (91%)	0.77	1 (9%) 9 5	86, 117, 126, 130	0
3	H	8/12 (66%)	2.14	4 (50%) 0 0	73, 105, 116, 118	0
3	J	9/12 (75%)	0.15	0 100 100	69, 106, 115, 116	0
3	L	4/12 (33%)	0.24	0 100 100	91, 103, 105, 111	0
All	All	1230/1488 (82%)	0.53	123 (10%) 7 4	33, 59, 119, 143	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	LEU	5.4
1	D	343	PHE	5.1
3	H	7	DA	4.8
1	A	346	ARG	4.8
1	A	341	ASP	4.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
4	MG	B	401	1/1	0.89	0.45	40,40,40,40	0
4	MG	E	101	1/1	0.96	0.27	40,40,40,40	0
4	MG	C	401	1/1	0.96	0.32	35,35,35,35	0
4	MG	K	101	1/1	0.98	0.56	50,50,50,50	0

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

There are no such residues in this entry.