



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 09:56 PM UTC

PDB ID : 9TOY / pdb\_00009toy  
Title : Investigating the binding mechanism of Interferon Regulatory Factor 4 to DNA  
in the context of Multiple Myeloma  
Authors : Alamaniotis, C.; Roe, M.; Mancini, E.J.  
Deposited on : 2025-12-17  
Resolution : 2.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

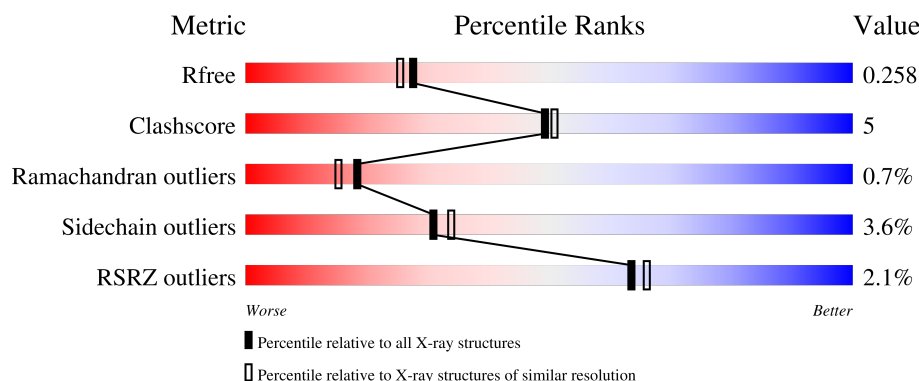
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 of 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	123	<div> <div>2%</div> <div>72% 16% 8%</div> </div>
1	B	123	<div> <div>3%</div> <div>77% 12% 7%</div> </div>
1	D	123	<div> <div>3%</div> <div>73% 15% 8%</div> </div>
1	F	123	<div> <div>%</div> <div>71% 15% 10%</div> </div>
2	C	20	<div> <div>50% 40% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	20	<div><div></div><div>55%</div><div>40%</div><div>5%</div></div>
3	E	20	<div><div></div><div>35%</div><div>60%</div><div>5%</div></div>
3	H	20	<div><div></div><div>30%</div><div>50%</div><div>20%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10086 atoms, of which 4585 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 Interferon regulatory factor 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	113	Total	C	H	N	O	S	14	0	0
			1857	601	919	165	171	1			
1	B	114	Total	C	H	N	O	S	16	0	0
			1862	603	922	165	171	1			
1	D	113	Total	C	H	N	O	S	14	0	0
			1864	604	923	165	171	1			
1	F	111	Total	C	H	N	O	S	14	0	0
			1843	597	913	163	169	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	expression tag	UNP Q15306
A	18	PRO	-	expression tag	UNP Q15306
A	19	GLY	-	expression tag	UNP Q15306
B	17	GLY	-	expression tag	UNP Q15306
B	18	PRO	-	expression tag	UNP Q15306
B	19	GLY	-	expression tag	UNP Q15306
D	17	GLY	-	expression tag	UNP Q15306
D	18	PRO	-	expression tag	UNP Q15306
D	19	GLY	-	expression tag	UNP Q15306
F	17	GLY	-	expression tag	UNP Q15306
F	18	PRO	-	expression tag	UNP Q15306
F	19	GLY	-	expression tag	UNP Q15306

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	20	Total	C	H	N	O	P	10	0	0
			637	196	224	83	114	20			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	20	Total	C	H	N	O	P	10	0	0
			637	196	224	83	114	20			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	20	Total	C	H	N	O	P	28	0	0
			637	196	230	65	126	20			
3	H	20	Total	C	H	N	O	P	28	0	0
			637	196	230	65	126	20			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	27	Total	O	0	0
			27	27		
5	C	6	Total	O	0	0
			6	6		
5	E	7	Total	O	0	0
			7	7		
5	D	14	Total	O	0	0
			14	14		
5	F	13	Total	O	0	0
			13	13		
5	G	5	Total	O	0	0
			5	5		

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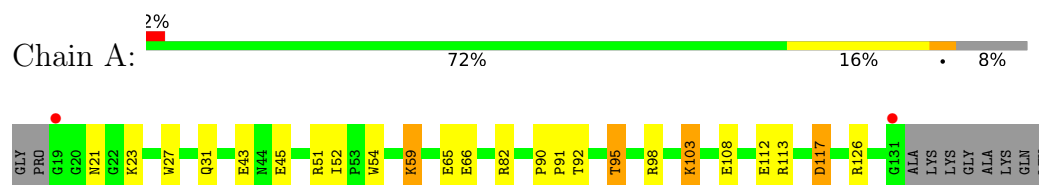
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	9	Total	O	0	0
			9	9		

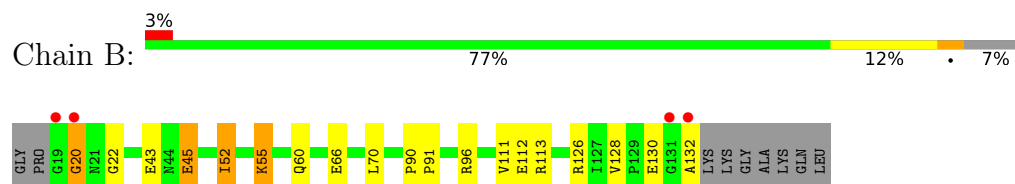
### 3 Residue-property plots [i](#)

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.

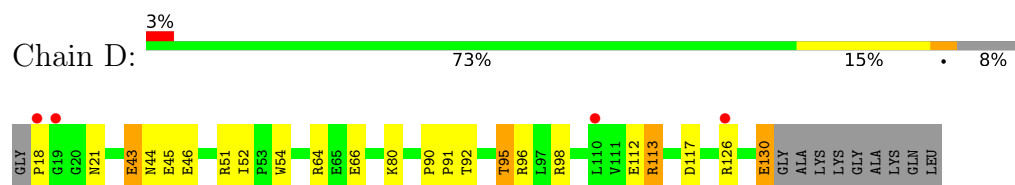
- Molecule 1: Interferon regulatory factor 4



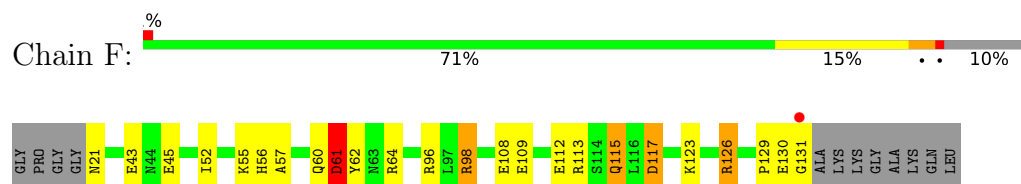
- Molecule 1: Interferon regulatory factor 4



- Molecule 1: Interferon regulatory factor 4



- Molecule 1: Interferon regulatory factor 4



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



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

Chain G:  55% 40% 5%



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

Chain E:  35% 60% 5%



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

Chain H:  30% 50% 20%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.51Å 65.12Å 70.69Å 89.86° 75.32° 66.79°	Depositor
Resolution (Å)	59.56 – 2.10 59.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (59.56-2.10) 98.2 (59.56-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, $R_{free}$	0.211 , 0.258 0.211 , 0.258	Depositor DCC
$R_{free}$ test set	1471 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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: CA

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	1.08	0/964	1.57	10/1300 (0.8%)
1	B	1.00	0/966	1.57	12/1303 (0.9%)
1	D	1.01	0/968	1.62	16/1306 (1.2%)
1	F	0.94	2/956 (0.2%)	1.54	17/1290 (1.3%)
2	C	0.74	0/465	1.74	14/715 (2.0%)
2	G	0.72	0/465	1.75	12/715 (1.7%)
3	E	0.72	0/453	1.84	16/697 (2.3%)
3	H	0.73	0/453	1.88	16/697 (2.3%)
All	All	0.93	2/5690 (0.0%)	1.66	113/8023 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	F	0	2
3	H	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	98	ARG	NE-CZ	-6.81	1.25	1.33
1	F	56	HIS	ND1-CE1	5.10	1.37	1.32

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	9	DC	O3'-P-O5'	-10.63	88.05	104.00
3	H	11	DG	O3'-P-O5'	10.21	119.32	104.00
3	H	4	DT	O3'-P-O5'	-9.71	89.44	104.00
1	F	98	ARG	CD-NE-CZ	9.60	137.84	124.40
1	B	43	GLU	CG-CD-OE1	8.62	138.22	118.40
3	E	18	DT	O3'-P-O5'	8.61	116.91	104.00
3	E	4	DT	O3'-P-O5'	-8.08	91.88	104.00
1	B	43	GLU	CB-CA-C	8.03	125.14	109.72
3	E	9	DC	O3'-P-O5'	-8.00	92.00	104.00
1	A	66	GLU	CB-CG-CD	7.95	126.12	112.60
1	B	112	GLU	CB-CG-CD	7.77	125.81	112.60
3	H	8	DT	O5'-P-OP1	-7.59	86.23	109.00
2	C	20	DC	C2'-C3'-O3'	7.46	122.70	111.50
1	D	130	GLU	N-CA-CB	7.41	123.09	110.50
1	B	96	ARG	CB-CA-C	7.37	122.45	110.88
3	E	5	DT	O3'-P-O5'	-7.36	92.96	104.00
1	D	95	THR	CA-CB-OG1	-7.35	98.58	109.60
1	D	43	GLU	N-CA-CB	-7.29	99.90	110.47
1	F	43	GLU	N-CA-CB	-7.25	99.08	110.46
1	D	112	GLU	CB-CG-CD	7.24	124.91	112.60
1	F	61	ASP	CB-CA-C	-7.17	96.16	110.42
1	A	112	GLU	CB-CG-CD	7.14	124.74	112.60
3	H	3	DC	C4'-C3'-O3'	7.08	120.62	110.00
3	E	14	DT	C2'-C3'-O3'	-7.00	100.99	111.50
3	H	1	DA	O3'-P-O5'	-6.86	93.71	104.00
2	G	16	DA	C4'-C3'-O3'	-6.84	99.75	110.00
1	F	117	ASP	CA-CB-CG	6.64	119.24	112.60
2	C	2	DC	O3'-P-O5'	-6.56	94.16	104.00
2	C	9	DA	C4-N9-C1'	-6.55	117.23	127.05
2	G	19	DG	O3'-P-O5'	-6.50	94.25	104.00
1	D	46	GLU	CB-CG-CD	-6.49	101.57	112.60
1	A	23	LYS	N-CA-CB	-6.47	102.44	110.98
1	F	115	GLN	N-CA-CB	-6.44	100.96	110.49
1	A	95	THR	CA-CB-OG1	-6.38	100.02	109.60
3	H	14	DT	C2'-C3'-O3'	-6.37	101.94	111.50
1	F	98	ARG	NE-CZ-NH2	-6.32	113.52	119.20
1	D	80	LYS	CB-CG-CD	6.30	125.79	111.30
1	A	43	GLU	N-CA-CB	-6.29	101.18	110.49
3	E	3	DC	C2'-C3'-O3'	-6.27	102.09	111.50
2	G	9	DA	C4'-C3'-O3'	-6.23	100.66	110.00
3	H	18	DT	O5'-P-OP1	-6.19	90.43	109.00
2	C	4	DA	O3'-P-O5'	-6.17	94.75	104.00
1	F	112	GLU	CB-CG-CD	6.17	123.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	14	DA	OP1-P-O3'	-6.15	89.55	108.00
2	G	2	DC	C4'-C3'-O3'	-6.12	100.81	110.00
1	D	117	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	55	LYS	CB-CG-CD	6.08	125.29	111.30
1	D	96	ARG	CD-NE-CZ	-6.08	115.89	124.40
1	D	45	GLU	CB-CG-CD	6.03	122.84	112.60
1	F	64	ARG	CG-CD-NE	-6.00	98.81	112.00
1	D	113	ARG	CD-NE-CZ	-5.95	116.06	124.40
1	A	108	GLU	CB-CA-C	5.95	120.07	109.65
1	B	43	GLU	CG-CD-OE2	-5.95	104.72	118.40
1	A	51	ARG	CB-CA-C	-5.93	99.52	109.48
3	H	8	DT	C4'-C3'-O3'	-5.92	101.13	110.00
2	C	9	DA	C4'-C3'-O3'	-5.89	101.17	110.00
1	A	117	ASP	CA-CB-CG	5.88	118.48	112.60
1	F	52	ILE	CB-CA-C	5.86	117.02	110.52
1	A	51	ARG	CG-CD-NE	-5.85	99.12	112.00
1	F	96	ARG	CB-CA-C	5.84	120.06	110.88
2	G	17	DA	O5'-P-OP2	5.83	125.49	108.00
2	C	20	DC	C4'-C3'-O3'	-5.83	101.25	110.00
2	C	16	DA	C4'-C3'-O3'	-5.78	101.33	110.00
3	E	11	DG	O3'-P-O5'	5.75	112.63	104.00
1	B	55	LYS	CG-CD-CE	5.73	124.48	111.30
3	E	19	DT	C4'-C3'-O3'	-5.72	101.42	110.00
3	H	19	DT	C4'-C3'-O3'	-5.71	101.44	110.00
2	G	2	DC	C2'-C3'-O3'	5.70	120.05	111.50
1	D	96	ARG	CB-CA-C	5.68	119.87	110.90
3	H	18	DT	C4'-C3'-O3'	-5.67	101.50	110.00
1	B	52	ILE	CB-CA-C	5.63	116.77	110.52
1	F	109	GLU	CG-CD-OE1	-5.59	105.53	118.40
3	H	18	DT	C4-C5-C7	-5.59	114.02	122.40
2	C	17	DA	O5'-P-OP2	5.58	124.73	108.00
1	D	66	GLU	CB-CG-CD	-5.58	103.12	112.60
2	C	12	DT	O3'-P-O5'	5.56	112.35	104.00
1	F	60	GLN	CA-C-N	5.55	132.14	121.54
1	F	60	GLN	C-N-CA	5.55	132.14	121.54
3	E	4	DT	C4'-C3'-O3'	-5.54	101.69	110.00
2	G	5	DC	C2'-C3'-O3'	-5.43	103.36	111.50
3	E	3	DC	C1'-O4'-C4'	-5.41	101.59	109.70
3	H	14	DT	P-O5'-C5'	-5.37	111.95	120.00
1	B	52	ILE	CA-C-O	5.33	124.56	119.98
3	H	19	DT	C2'-C3'-O3'	5.31	119.47	111.50
2	G	9	DA	C2'-C3'-O3'	5.31	119.47	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	THR	OG1-CB-CG2	-5.30	98.70	109.30
1	A	92	THR	OG1-CB-CG2	-5.29	98.72	109.30
2	C	9	DA	C8-N9-C1'	5.29	134.98	127.05
1	D	51	ARG	CB-CA-C	-5.27	100.63	109.48
1	B	45	GLU	CB-CG-CD	5.23	121.50	112.60
2	C	8	DA	O3'-P-O5'	5.21	111.82	104.00
2	G	16	DA	O5'-P-OP2	-5.21	92.37	108.00
1	D	45	GLU	CG-CD-OE1	5.20	130.35	118.40
1	F	112	GLU	CG-CD-OE1	5.19	130.34	118.40
2	G	1	DT	C2'-C3'-O3'	-5.19	103.72	111.50
1	F	123	LYS	CG-CD-CE	5.18	123.22	111.30
1	D	52	ILE	CB-CA-C	5.16	116.25	110.52
2	G	12	DT	P-O5'-C5'	-5.15	112.28	120.00
1	F	21	ASN	CB-CA-C	5.15	119.88	110.10
1	F	56	HIS	CB-CA-C	5.14	118.81	110.22
2	C	10	DA	OP1-P-O3'	-5.14	92.58	108.00
1	B	113	ARG	CA-CB-CG	-5.13	103.83	114.10
3	E	8	DT	O5'-P-OP1	-5.12	93.64	109.00
3	H	3	DC	C1'-O4'-C4'	-5.08	102.08	109.70
2	C	8	DA	OP1-P-O3'	-5.07	92.80	108.00
3	E	14	DT	P-O5'-C5'	-5.07	112.40	120.00
3	E	8	DT	O5'-P-OP2	5.06	123.19	108.00
2	C	10	DA	O5'-C5'-C4'	-5.05	103.22	110.80
3	E	18	DT	C2'-C3'-O3'	5.05	119.07	111.50
3	H	10	DA	C4-N9-C1'	-5.02	119.52	127.05
1	B	126	ARG	NE-CZ-NH2	-5.02	114.68	119.20
3	E	6	DT	O3'-P-O5'	-5.02	96.47	104.00
3	E	3	DC	O4'-C4'-C3'	-5.01	97.89	105.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	82	ARG	Sidechain
1	F	113	ARG	Sidechain
1	F	126	ARG	Sidechain
3	H	12	DT	Sidechain

## 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	938	919	917	12	0
1	B	940	922	918	8	0
1	D	941	923	922	15	0
1	F	930	913	911	4	2
2	C	413	224	224	5	0
2	G	413	224	224	3	0
3	E	407	230	230	5	0
3	H	407	230	230	11	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	G	1	0	0	0	0
5	A	26	0	0	4	2
5	B	27	0	0	0	0
5	C	6	0	0	0	0
5	D	14	0	0	2	0
5	E	7	0	0	1	0
5	F	13	0	0	1	0
5	G	5	0	0	0	0
5	H	9	0	0	0	0
All	All	5501	4585	4576	53	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (53) 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:A:59:LYS:HD2	5:E:106:HOH:O	1.54	1.06
2:C:1:DT:H6	2:C:1:DT:P	1.95	0.90
2:G:1:DT:H6	2:G:1:DT:P	1.97	0.88
1:D:64:ARG:HD3	5:D:213:HOH:O	1.78	0.82
2:C:1:DT:P	2:C:1:DT:C6	2.81	0.73
1:A:45:GLU:OE1	5:A:301:HOH:O	2.06	0.73
1:A:98:ARG:NH1	5:A:303:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:NH2	5:A:302:HOH:O	2.23	0.70
2:G:1:DT:P	2:G:1:DT:C6	2.87	0.67
1:D:18:PRO:HB3	3:H:2:DG:H4'	1.77	0.66
1:B:111:VAL:HG22	1:D:44:ASN:HA	1.82	0.62
3:E:1:DA:H2'	3:E:1:DA:N3	2.17	0.59
3:H:15:DC:H2'	3:H:16:DA:C8	2.39	0.58
3:H:1:DA:H2'	3:H:1:DA:N3	2.18	0.57
1:D:18:PRO:HA	3:H:3:DC:C4'	2.35	0.55
1:A:45:GLU:CD	5:A:301:HOH:O	2.46	0.55
1:B:130:GLU:HA	1:B:130:GLU:OE1	2.08	0.54
1:A:91:PRO:O	1:A:95:THR:HG23	2.08	0.53
1:D:18:PRO:HB3	3:H:2:DG:C4'	2.38	0.53
1:D:18:PRO:HA	3:H:3:DC:H4'	1.91	0.53
3:E:15:DC:H2'	3:E:16:DA:C8	2.44	0.53
3:H:11:DG:H2''	3:H:12:DT:H5'	1.90	0.52
3:E:15:DC:H2''	3:E:16:DA:H5'	1.90	0.52
1:F:108:GLU:OE1	1:F:126:ARG:NH1	2.44	0.50
1:F:98:ARG:NH1	5:F:201:HOH:O	2.34	0.48
1:B:20:GLY:O	1:B:22:GLY:N	2.39	0.48
1:F:129:PRO:O	1:F:131:GLY:N	2.47	0.47
1:B:111:VAL:HG21	1:D:43:GLU:O	2.14	0.47
2:C:8:DA:OP1	1:D:113:ARG:HG2	2.15	0.47
3:E:1:DA:H3'	3:E:1:DA:OP2	2.15	0.46
1:D:98:ARG:NH2	5:D:204:HOH:O	2.48	0.46
1:D:126:ARG:HH11	1:D:126:ARG:HG3	1.79	0.46
2:C:1:DT:C6	2:C:1:DT:OP1	2.69	0.46
1:D:91:PRO:O	1:D:95:THR:HG23	2.16	0.46
2:G:1:DT:C6	2:G:1:DT:OP1	2.70	0.45
1:B:111:VAL:CG2	1:D:44:ASN:HA	2.45	0.45
1:A:126:ARG:HH11	1:A:126:ARG:HG3	1.81	0.45
1:D:54:TRP:CH2	1:D:98:ARG:HB2	2.52	0.45
1:B:90:PRO:HB2	1:B:91:PRO:HD3	2.00	0.44
1:D:90:PRO:HB2	1:D:91:PRO:HD3	2.00	0.44
3:H:15:DC:H2''	3:H:16:DA:H5'	2.00	0.43
1:D:18:PRO:HB3	3:H:2:DG:O3'	2.19	0.43
1:F:57:ALA:HA	1:F:62:TYR:CD1	2.54	0.42
1:B:52:ILE:HD11	1:B:70:LEU:HD23	2.00	0.42
3:H:1:DA:H3'	3:H:1:DA:OP2	2.19	0.42
1:A:52:ILE:HD13	1:A:52:ILE:HG21	1.83	0.42
3:H:11:DG:H2''	3:H:12:DT:C5'	2.50	0.41
1:A:103:LYS:HE3	3:E:6:DT:O4	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:CG1	1:B:132:ALA:HB3	2.49	0.41
1:A:54:TRP:CH2	1:A:98:ARG:HB2	2.55	0.41
1:A:90:PRO:HB2	1:A:91:PRO:HD3	2.02	0.41
2:C:9:DA:H2'	2:C:9:DA:O5'	2.21	0.41
1:A:27:TRP:O	1:A:31:GLN:HG2	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:GLN:OE1	5:A:301:HOH:O[1_554]	2.09	0.11
1:F:117:ASP:OD1	5:A:301:HOH:O[1_554]	2.10	0.10

## 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	111/123 (90%)	105 (95%)	6 (5%)	0	100	100
1	B	112/123 (91%)	104 (93%)	7 (6%)	1 (1%)	14	10
1	D	111/123 (90%)	107 (96%)	4 (4%)	0	100	100
1	F	109/123 (89%)	103 (94%)	4 (4%)	2 (2%)	6	3
All	All	443/492 (90%)	419 (95%)	21 (5%)	3 (1%)	18	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLY
1	F	61	ASP
1	F	130	GLU



### 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	98/104 (94%)	93 (95%)	5 (5%)	21	21
1	B	97/104 (93%)	93 (96%)	4 (4%)	27	29
1	D	99/104 (95%)	97 (98%)	2 (2%)	48	56
1	F	98/104 (94%)	95 (97%)	3 (3%)	35	39
All	All	392/416 (94%)	378 (96%)	14 (4%)	31	34

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	59	LYS
1	A	65	GLU
1	A	103	LYS
1	A	117	ASP
1	B	45	GLU
1	B	55	LYS
1	B	60	GLN
1	B	66	GLU
1	D	21	ASN
1	D	130	GLU
1	F	45	GLU
1	F	55	LYS
1	F	61	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	GLN

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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	113/123 (91%)	-0.16	2 (1%) 67 70	36, 46, 77, 98	0
1	B	114/123 (92%)	-0.04	4 (3%) 47 49	30, 51, 86, 120	0
1	D	113/123 (91%)	0.22	4 (3%) 47 49	38, 55, 86, 124	0
1	F	111/123 (90%)	0.17	1 (0%) 81 83	35, 62, 89, 103	0
2	C	20/20 (100%)	-0.90	0 100 100	34, 47, 65, 72	0
2	G	20/20 (100%)	-0.92	0 100 100	36, 49, 66, 73	0
3	E	20/20 (100%)	-0.95	0 100 100	36, 46, 67, 75	0
3	H	20/20 (100%)	-0.89	0 100 100	35, 53, 75, 79	0
All	All	531/572 (92%)	-0.10	11 (2%) 63 66	30, 53, 86, 124	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	ALA	6.6
1	A	131	GLY	4.7
1	F	131	GLY	3.5
1	A	19	GLY	3.3
1	B	19	GLY	3.0
1	B	20	GLY	3.0
1	B	131	GLY	2.6
1	D	110	LEU	2.6
1	D	126	ARG	2.6
1	D	19	GLY	2.5
1	D	18	PRO	2.2

### 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 oligosaccharides 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	CA	A	202	1/1	0.92	0.15	89,89,89,89	0
4	CA	C	101	1/1	0.93	0.07	75,75,75,75	0
4	CA	B	201	1/1	0.94	0.09	75,75,75,75	0
4	CA	A	201	1/1	0.94	0.16	85,85,85,85	0
4	CA	G	101	1/1	0.96	0.05	84,84,84,84	0

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

There are no such residues in this entry.