



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 09:22 pm GMT

PDB ID : 3MQY  
Title : SgrAI with cleaved DNA and Magnesium bound  
Authors : Dunten, P.W.; Horton, N.C.; Little, E.J.  
Deposited on : 2010-04-28  
Resolution : 2.00 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 : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

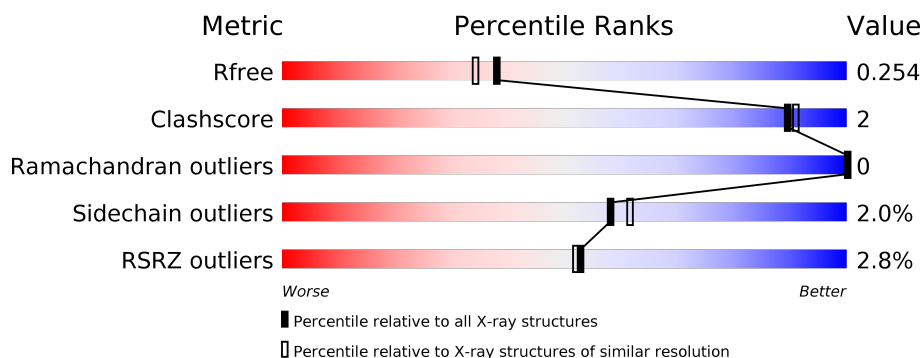
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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. 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	338	<div> <div>4%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	B	338	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>
2	C	7	<div> <div>43%</div> <div>57%</div> </div>
2	E	7	<div> <div>14%</div> <div>86%</div> </div>
3	D	11	<div> <div>18%</div> <div>64%</div> <div>18%</div> </div>
3	F	11	<div> <div>18%</div> <div>73%</div> <div>9%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6425 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 SgraIR restriction enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	3	0
			2687	1702	476	500	9			
1	B	338	Total	C	N	O	S	0	1	0
			2680	1695	477	499	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASP	ASN	ENGINEERED MUTATION	UNP Q9F6L0
B	63	ASP	ASN	ENGINEERED MUTATION	UNP Q9F6L0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	P	0	0	0
			141	68	28	39	6			
2	E	7	Total	C	N	O	P	0	0	0
			141	68	28	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			226	106	41	68	11			
3	F	11	Total	C	N	O	P	0	0	0
			226	106	41	68	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Mg 2	0	0
4	A	2	Total 2	Mg 2	0	0
4	D	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0

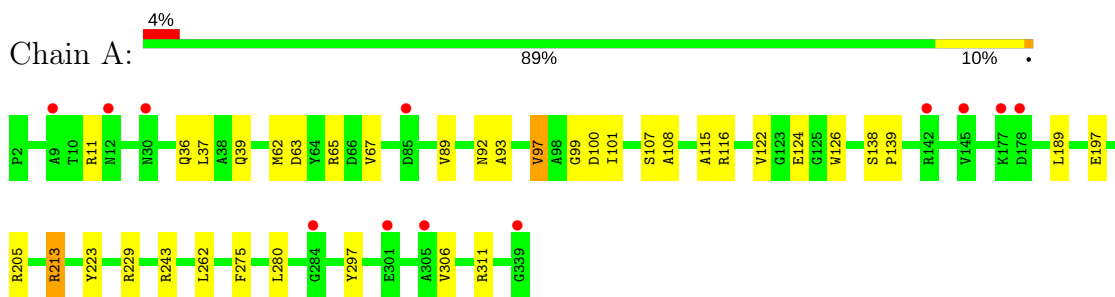
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total 147	O 147	0	0
5	B	136	Total 136	O 136	0	0
5	C	6	Total 6	O 6	0	0
5	D	12	Total 12	O 12	0	0
5	E	5	Total 5	O 5	0	0
5	F	12	Total 12	O 12	0	0

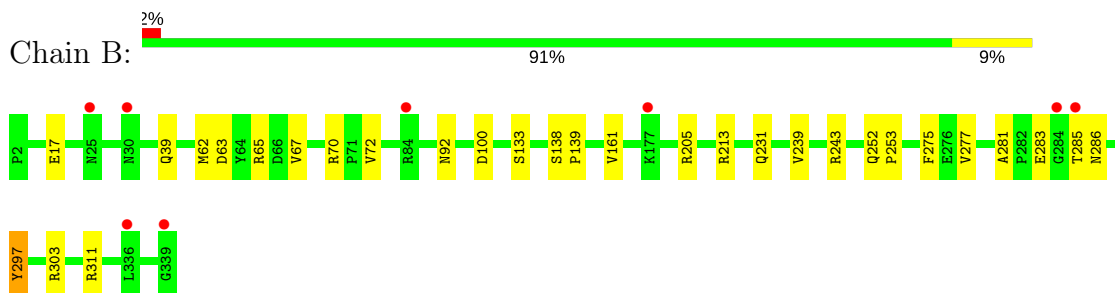
### 3 Residue-property plots

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.

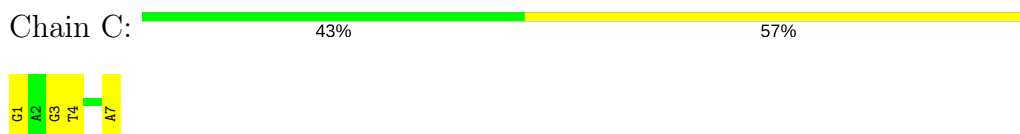
- Molecule 1: SgraIR restriction enzyme



- Molecule 1: SgraIR restriction enzyme



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



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

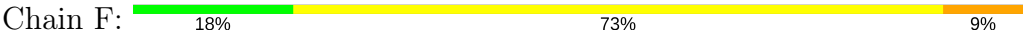


- Molecule 3: DNA (5'-D(P\*CP\*CP\*GP\*GP\*TP\*GP\*GP\*AP\*CP\*TP\*C)-3')





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.16Å 119.98Å 69.86Å 90.00° 102.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.00) 98.2 (19.97-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0031	Depositor
R, $R_{free}$	0.196 , 0.249 0.203 , 0.254	Depositor DCC
$R_{free}$ test set	3189 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6425	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	1.14	9/2747 (0.3%)	0.95	10/3729 (0.3%)
1	B	1.09	4/2740 (0.1%)	0.95	9/3720 (0.2%)
2	C	1.64	2/158 (1.3%)	2.03	6/242 (2.5%)
2	E	1.69	3/158 (1.9%)	2.18	9/242 (3.7%)
3	D	3.05	24/252 (9.5%)	3.02	39/385 (10.1%)
3	F	2.49	14/252 (5.6%)	2.69	31/385 (8.1%)
All	All	1.36	56/6307 (0.9%)	1.32	104/8703 (1.2%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	10	DG	P-O5'	11.40	1.71	1.59
3	D	8	DC	OP3-P	-11.38	1.47	1.61
3	D	9	DC	P-O5'	10.97	1.70	1.59
3	F	8	DC	P-O5'	10.95	1.70	1.59
3	F	8	DC	OP3-P	-10.76	1.48	1.61
3	D	9	DC	C5'-C4'	10.48	1.62	1.51
3	D	9	DC	C3'-O3'	9.51	1.56	1.44
1	A	93	ALA	CA-CB	9.48	1.72	1.52
3	D	8	DC	P-O5'	9.48	1.69	1.59
3	F	8	DC	N3-C4	8.21	1.39	1.33
3	D	8	DC	O3'-P	-7.96	1.51	1.61
3	D	9	DC	N3-C4	7.36	1.39	1.33
3	D	10	DG	N1-C2	7.36	1.43	1.37
3	F	12	DT	C5-C6	-7.24	1.29	1.34
3	F	13	DG	N7-C5	7.21	1.43	1.39
3	D	8	DC	C3'-O3'	7.18	1.53	1.44
3	D	13	DG	C2-N3	7.10	1.38	1.32
3	F	9	DC	P-O5'	-6.97	1.52	1.59
1	B	281	ALA	CA-CB	6.89	1.67	1.52
1	A	108	ALA	CA-CB	6.74	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	13	DG	P-O5'	6.72	1.66	1.59
3	D	13	DG	C8-N7	6.62	1.34	1.30
3	D	11	DG	P-O5'	6.48	1.66	1.59
2	E	7	DA	N9-C4	6.46	1.41	1.37
3	D	9	DC	N1-C6	6.43	1.41	1.37
1	B	17	GLU	CG-CD	6.42	1.61	1.51
3	D	11	DG	C6-O6	6.38	1.29	1.24
3	F	11	DG	C6-N1	6.29	1.44	1.39
3	D	13	DG	C4'-O4'	6.23	1.51	1.45
1	B	277	VAL	CB-CG1	6.19	1.65	1.52
3	D	10	DG	N7-C5	6.12	1.43	1.39
3	D	13	DG	N9-C4	6.09	1.42	1.38
3	D	11	DG	C8-N7	6.06	1.34	1.30
3	F	13	DG	C5-C6	-6.01	1.36	1.42
3	D	10	DG	N3-C4	6.01	1.39	1.35
1	A	39	GLN	CB-CG	-5.85	1.36	1.52
3	F	9	DC	P-OP2	5.77	1.58	1.49
3	D	8	DC	C5'-C4'	5.72	1.57	1.51
1	B	239	VAL	CB-CG1	5.69	1.64	1.52
1	A	223	TYR	CD1-CE1	-5.64	1.30	1.39
1	A	99	GLY	N-CA	5.63	1.54	1.46
2	E	7	DA	C2-N3	5.54	1.38	1.33
1	A	115	ALA	CA-CB	5.44	1.63	1.52
3	D	13	DG	C6-N1	5.42	1.43	1.39
3	F	10	DG	C6-N1	-5.41	1.35	1.39
3	D	13	DG	N3-C4	-5.37	1.31	1.35
2	C	7	DA	C8-N7	5.34	1.35	1.31
1	A	63	ASP	CB-CG	5.33	1.62	1.51
3	F	15	DA	C6-N1	-5.32	1.31	1.35
1	A	197	GLU	CG-CD	5.28	1.59	1.51
3	F	12	DT	C2-N3	-5.24	1.33	1.37
1	A	97	VAL	CA-CB	5.18	1.65	1.54
3	D	11	DG	P-OP1	-5.15	1.40	1.49
2	E	6	DC	O3'-P	-5.13	1.54	1.61
2	C	7	DA	N9-C4	5.07	1.40	1.37
3	F	8	DC	C4-C5	-5.02	1.39	1.43

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	DC	O5'-P-OP1	-11.56	95.30	105.70
3	F	12	DT	C5-C4-O4	-11.13	117.11	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	11	DG	C5-C6-O6	-10.15	122.51	128.60
2	E	5	DC	O4'-C1'-N1	-9.98	101.01	108.00
3	F	12	DT	C6-C5-C7	9.81	128.79	122.90
2	C	4	DT	C4-C5-C7	9.78	124.87	119.00
3	D	9	DC	O5'-P-OP2	-9.60	97.06	105.70
2	E	3	DG	O4'-C1'-N9	9.40	114.58	108.00
3	D	11	DG	C2-N3-C4	9.39	116.59	111.90
3	D	13	DG	N9-C4-C5	8.77	108.91	105.40
3	F	8	DC	O4'-C1'-N1	8.76	114.13	108.00
3	F	12	DT	N3-C4-O4	8.72	125.14	119.90
3	D	10	DG	N3-C4-C5	8.64	132.92	128.60
1	A	243	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	C	3	DG	O4'-C1'-N9	8.53	113.97	108.00
2	E	6	DC	O4'-C4'-C3'	-8.46	100.92	106.00
2	C	4	DT	C6-C5-C7	-8.33	117.90	122.90
3	D	10	DG	O5'-P-OP2	-8.17	98.35	105.70
3	D	13	DG	C5-C6-O6	-8.16	123.70	128.60
3	D	12	DT	O4'-C1'-C2'	7.63	112.00	105.90
3	F	13	DG	C4-C5-N7	7.51	113.80	110.80
3	D	13	DG	C8-N9-C4	-7.46	103.42	106.40
3	F	13	DG	OP1-P-OP2	7.46	130.79	119.60
3	D	13	DG	N1-C6-O6	7.35	124.31	119.90
2	E	4	DT	O4'-C1'-N1	-7.32	102.87	108.00
3	F	13	DG	C5-C6-O6	-7.18	124.29	128.60
3	D	10	DG	C5-N7-C8	-7.10	100.75	104.30
3	F	13	DG	C5-N7-C8	-7.07	100.77	104.30
3	D	9	DC	OP2-P-O3'	7.04	120.70	105.20
3	F	18	DC	O4'-C4'-C3'	-7.00	101.70	104.50
1	B	243	ARG	NE-CZ-NH1	6.98	123.79	120.30
3	D	8	DC	C6-N1-C2	-6.97	117.51	120.30
3	F	11	DG	C2-N3-C4	6.94	115.37	111.90
3	D	15	DA	N1-C6-N6	-6.88	114.47	118.60
3	D	12	DT	O5'-P-OP1	-6.87	99.52	105.70
1	A	205	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	F	16	DC	O4'-C1'-N1	6.74	112.72	108.00
1	A	243	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	70	ARG	NE-CZ-NH1	6.66	123.63	120.30
3	F	12	DT	C5-C6-N1	6.62	127.67	123.70
3	F	11	DG	N1-C6-O6	6.57	123.84	119.90
3	F	8	DC	P-O3'-C3'	6.55	127.56	119.70
3	D	9	DC	O4'-C4'-C3'	-6.54	101.88	104.50
3	D	17	DT	O4'-C1'-N1	-6.49	103.45	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	ARG	NE-CZ-NH1	6.49	123.54	120.30
3	F	16	DC	O4'-C4'-C3'	-6.46	101.92	104.50
1	A	63	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	213	ARG	NE-CZ-NH1	6.46	123.53	120.30
3	D	8	DC	OP2-P-O3'	6.43	119.34	105.20
3	F	8	DC	O5'-P-OP1	-6.42	99.92	105.70
3	D	11	DG	N1-C2-N3	-6.37	120.08	123.90
1	A	205	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	D	14	DG	N3-C4-N9	-6.33	122.20	126.00
3	D	13	DG	C8-N9-C1'	6.29	135.17	127.00
3	D	8	DC	N3-C4-C5	-6.24	119.41	121.90
1	B	100	ASP	CB-CG-OD2	-6.22	112.70	118.30
3	D	12	DT	C6-N1-C1'	6.21	129.71	120.40
3	F	15	DA	O4'-C1'-N9	-6.19	103.67	108.00
3	F	11	DG	OP1-P-OP2	6.16	128.84	119.60
3	D	11	DG	N3-C4-C5	-6.15	125.53	128.60
2	C	7	DA	O4'-C4'-C3'	-6.13	102.05	104.50
2	E	6	DC	C4'-C3'-C2'	6.10	108.59	103.10
3	F	9	DC	N3-C4-C5	-6.03	119.49	121.90
2	E	6	DC	O4'-C1'-N1	-5.94	103.84	108.00
3	D	14	DG	N1-C6-O6	5.93	123.46	119.90
3	D	9	DC	C6-N1-C2	5.92	122.67	120.30
3	D	12	DT	C2-N1-C1'	-5.92	108.73	118.20
3	F	10	DG	C6-N1-C2	5.92	128.65	125.10
3	F	12	DT	C4-C5-C6	-5.92	114.45	118.00
2	C	1	DG	O4'-C4'-C3'	-5.76	102.19	104.50
3	D	13	DG	C4-C5-N7	-5.75	108.50	110.80
1	A	100	ASP	CB-CG-OD1	5.74	123.47	118.30
2	E	2	DA	O4'-C1'-N9	5.73	112.01	108.00
3	D	11	DG	C5-C6-O6	-5.70	125.18	128.60
3	F	12	DT	OP1-P-OP2	5.69	128.14	119.60
3	F	9	DC	C4-C5-C6	5.69	120.24	117.40
3	F	10	DG	C5-C6-O6	5.60	131.96	128.60
3	F	11	DG	O3'-P-O5'	-5.60	93.37	104.00
1	B	205	ARG	NE-CZ-NH2	-5.59	117.50	120.30
3	D	14	DG	N3-C4-C5	5.57	131.38	128.60
3	F	11	DG	O5'-P-OP2	-5.54	100.71	105.70
3	F	9	DC	C6-N1-C2	-5.49	118.11	120.30
3	D	9	DC	OP1-P-OP2	5.43	127.75	119.60
3	D	12	DT	C4-C5-C7	5.42	122.25	119.00
3	D	9	DC	P-O5'-C5'	-5.41	112.24	120.90
3	F	11	DG	N1-C2-N2	5.38	121.04	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	13	DG	N1-C6-O6	5.36	123.11	119.90
1	B	100	ASP	CB-CG-OD1	5.31	123.08	118.30
3	D	10	DG	C2-N3-C4	-5.28	109.26	111.90
1	A	213	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	F	13	DG	N3-C4-C5	5.24	131.22	128.60
3	D	14	DG	C2-N3-C4	-5.20	109.30	111.90
3	D	9	DC	O4'-C1'-C2'	5.18	110.04	105.90
1	A	213	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	229	ARG	NE-CZ-NH2	-5.15	117.72	120.30
3	D	9	DC	C4'-C3'-C2'	5.13	107.72	103.10
1	A	311	ARG	NE-CZ-NH2	-5.11	117.74	120.30
3	D	13	DG	N3-C4-N9	-5.10	122.94	126.00
2	C	1	DG	N1-C6-O6	-5.09	116.85	119.90
1	B	205	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	E	7	DA	C4-C5-C6	5.05	119.52	117.00
2	E	4	DT	N3-C4-O4	5.04	122.92	119.90
1	B	303	ARG	NE-CZ-NH2	-5.01	117.80	120.30
3	D	14	DG	C5-N7-C8	-5.00	101.80	104.30

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	2687	0	2636	13	0
1	B	2680	0	2637	9	0
2	C	141	0	80	0	0
2	E	141	0	80	0	0
3	D	226	0	123	2	0
3	F	226	0	124	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	147	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	136	0	0	2	0
5	C	6	0	0	0	0
5	D	12	0	0	0	0
5	E	5	0	0	1	0
5	F	12	0	0	0	0
All	All	6425	0	5680	22	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.

All (22) 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:306:VAL:HG13	1:A:306:VAL:O	1.90	0.72
1:B:297[A]:TYR:HB3	5:B:355:HOH:O	1.97	0.63
1:B:63:ASP:OD1	1:B:65:ARG:HB2	2.05	0.56
1:A:92:ASN:HB3	3:D:11:DG:N3	2.23	0.53
1:A:262:LEU:HG	1:A:297:TYR:CD1	2.47	0.50
1:A:97:VAL:O	1:A:101:ILE:HG12	2.11	0.50
1:A:65[A]:ARG:HA	1:A:280:LEU:HD13	1.94	0.49
1:A:306:VAL:O	1:A:306:VAL:CG1	2.59	0.48
1:A:122:VAL:HG23	1:A:124:GLU:HG3	1.96	0.47
1:B:62:MET:HG3	1:B:67:VAL:HG23	1.96	0.47
1:A:107:SER:OG	1:A:189:LEU:HD12	2.17	0.45
1:A:62:MET:HG3	1:A:67:VAL:HG23	1.99	0.45
1:A:138:SER:HA	1:A:139:PRO:HD3	1.83	0.44
1:A:116:ARG:HG2	1:A:126:TRP:CZ3	2.52	0.43
1:A:65[B]:ARG:HA	1:A:280:LEU:HD13	1.99	0.43
1:B:72:VAL:HG23	5:B:393:HOH:O	2.19	0.43
1:B:285:THR:HA	5:E:297:HOH:O	2.20	0.42
1:A:37:LEU:O	3:D:13:DG:H5"	2.21	0.41
1:B:161:VAL:HG11	1:B:231:GLN:NE2	2.36	0.41
1:B:92:ASN:HB3	3:F:11:DG:N3	2.36	0.40
1:B:252:GLN:HB3	1:B:253:PRO:HD3	2.03	0.40
1:B:138:SER:HA	1:B:139:PRO:HD3	1.92	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	339/338 (100%)	327 (96%)	12 (4%)	0	100	100
1	B	337/338 (100%)	329 (98%)	8 (2%)	0	100	100
All	All	676/676 (100%)	656 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	281/282 (100%)	275 (98%)	6 (2%)	56	60
1	B	282/282 (100%)	275 (98%)	7 (2%)	50	52
All	All	563/564 (100%)	550 (98%)	13 (2%)	58	56

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11[A]	ARG
1	A	11[B]	ARG
1	A	36	GLN
1	A	89	VAL
1	A	213	ARG
1	A	275	PHE
1	B	39	GLN
1	B	133	SER

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Mol	Chain	Res	Type
1	B	275	PHE
1	B	283	GLU
1	B	286	ASN
1	B	297[A]	TYR
1	B	297[B]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	74	ASN
1	A	215	ASN
1	A	307	HIS
1	B	74	ASN
1	B	231	GLN

### 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 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](#)

There are no chain breaks in this entry.



## 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	338/338 (100%)	0.03	12 (3%) 42 42	23, 38, 56, 65	0
1	B	338/338 (100%)	-0.01	8 (2%) 59 58	26, 40, 57, 69	0
2	C	7/7 (100%)	0.20	0 100 100	38, 49, 67, 69	0
2	E	7/7 (100%)	0.34	0 100 100	36, 49, 75, 78	0
3	D	11/11 (100%)	-0.42	0 100 100	24, 32, 55, 64	0
3	F	11/11 (100%)	-0.32	0 100 100	29, 32, 66, 68	0
All	All	712/712 (100%)	0.00	20 (2%) 53 52	23, 39, 58, 78	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	LEU	3.9
1	A	177	LYS	3.3
1	A	145	VAL	3.2
1	B	284	GLY	3.0
1	A	339	GLY	3.0
1	B	339	GLY	2.9
1	B	285	THR	2.9
1	B	177	LYS	2.8
1	A	301	GLU	2.7
1	A	178	ASP	2.6
1	B	84	ARG	2.5
1	A	9	ALA	2.4
1	A	30	ASN	2.3
1	A	142	ARG	2.3
1	B	25	ASN	2.2
1	B	30	ASN	2.2
1	A	305	ALA	2.2
1	A	12	ASN	2.1
1	A	85	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	284	GLY	2.1

## 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 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(Å <sup>2</sup> )	Q<0.9
4	MG	D	502	1/1	0.74	0.10	63,63,63,63	0
4	MG	A	501	1/1	0.93	0.09	43,43,43,43	0
4	MG	B	501	1/1	0.95	0.14	56,56,56,56	0
4	MG	B	500	1/1	0.95	0.08	23,23,23,23	0
4	MG	F	502	1/1	0.97	0.07	38,38,38,38	0
4	MG	A	500	1/1	0.98	0.05	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.