



# Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 02:53 am BST

PDB ID : 3NIC  
Title : DNA binding and cleavage by the GIY-YIG endonuclease R.Eco29kI inactive variant Y49F  
Authors : Mak, A.N.S.; Lambert, A.R.; Stoddard, B.L.  
Deposited on : 2010-06-15  
Resolution : 2.80 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

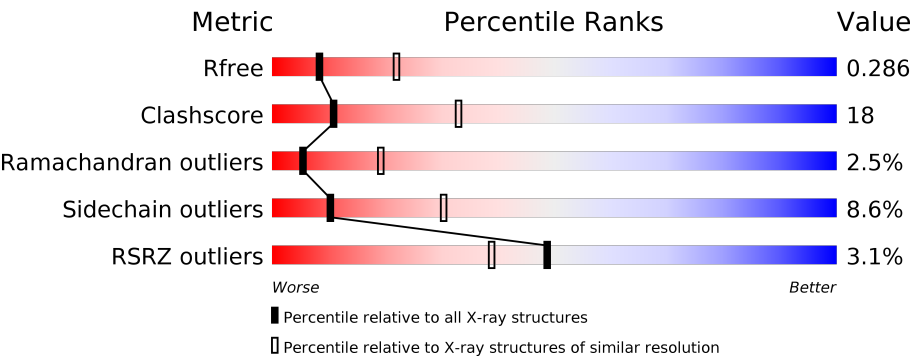
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	235	
1	B	235	
1	C	235	
1	D	235	
1	E	235	
1	F	235	

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Mol	Chain	Length	Quality of chain
1	G	235	
1	H	235	
2	I	22	
2	K	22	
2	M	22	
2	O	22	
3	J	22	
3	L	22	
3	N	22	
3	P	22	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	H	216	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17279 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 Eco29kIR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1671	1066	297	304	4			
1	B	210	Total	C	N	O	S	0	0	0
			1683	1072	299	308	4			
1	C	209	Total	C	N	O	S	0	0	0
			1635	1042	288	301	4			
1	D	209	Total	C	N	O	S	0	0	0
			1649	1053	290	302	4			
1	E	209	Total	C	N	O	S	0	0	0
			1631	1043	285	299	4			
1	F	209	Total	C	N	O	S	0	0	0
			1627	1038	285	300	4			
1	G	209	Total	C	N	O	S	0	0	0
			1612	1029	281	298	4			
1	H	209	Total	C	N	O	S	0	0	0
			1642	1050	286	302	4			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q46944
A	-19	ALA	-	EXPRESSION TAG	UNP Q46944
A	-18	SER	-	EXPRESSION TAG	UNP Q46944
A	-17	SER	-	EXPRESSION TAG	UNP Q46944
A	-16	HIS	-	EXPRESSION TAG	UNP Q46944
A	-15	HIS	-	EXPRESSION TAG	UNP Q46944
A	-14	HIS	-	EXPRESSION TAG	UNP Q46944
A	-13	HIS	-	EXPRESSION TAG	UNP Q46944
A	-12	HIS	-	EXPRESSION TAG	UNP Q46944
A	-11	HIS	-	EXPRESSION TAG	UNP Q46944
A	-10	SER	-	EXPRESSION TAG	UNP Q46944
A	-9	SER	-	EXPRESSION TAG	UNP Q46944
A	-8	GLY	-	EXPRESSION TAG	UNP Q46944

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	EXPRESSION TAG	UNP Q46944
A	-6	VAL	-	EXPRESSION TAG	UNP Q46944
A	-5	PRO	-	EXPRESSION TAG	UNP Q46944
A	-4	ARG	-	EXPRESSION TAG	UNP Q46944
A	-3	GLY	-	EXPRESSION TAG	UNP Q46944
A	-2	SER	-	EXPRESSION TAG	UNP Q46944
A	-1	SER	-	EXPRESSION TAG	UNP Q46944
A	0	MET	-	EXPRESSION TAG	UNP Q46944
A	1	GLY	-	EXPRESSION TAG	UNP Q46944
A	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
A	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944
B	-20	MET	-	EXPRESSION TAG	UNP Q46944
B	-19	ALA	-	EXPRESSION TAG	UNP Q46944
B	-18	SER	-	EXPRESSION TAG	UNP Q46944
B	-17	SER	-	EXPRESSION TAG	UNP Q46944
B	-16	HIS	-	EXPRESSION TAG	UNP Q46944
B	-15	HIS	-	EXPRESSION TAG	UNP Q46944
B	-14	HIS	-	EXPRESSION TAG	UNP Q46944
B	-13	HIS	-	EXPRESSION TAG	UNP Q46944
B	-12	HIS	-	EXPRESSION TAG	UNP Q46944
B	-11	HIS	-	EXPRESSION TAG	UNP Q46944
B	-10	SER	-	EXPRESSION TAG	UNP Q46944
B	-9	SER	-	EXPRESSION TAG	UNP Q46944
B	-8	GLY	-	EXPRESSION TAG	UNP Q46944
B	-7	LEU	-	EXPRESSION TAG	UNP Q46944
B	-6	VAL	-	EXPRESSION TAG	UNP Q46944
B	-5	PRO	-	EXPRESSION TAG	UNP Q46944
B	-4	ARG	-	EXPRESSION TAG	UNP Q46944
B	-3	GLY	-	EXPRESSION TAG	UNP Q46944
B	-2	SER	-	EXPRESSION TAG	UNP Q46944
B	-1	SER	-	EXPRESSION TAG	UNP Q46944
B	0	MET	-	EXPRESSION TAG	UNP Q46944
B	1	GLY	-	EXPRESSION TAG	UNP Q46944
B	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
B	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944
C	-20	MET	-	EXPRESSION TAG	UNP Q46944
C	-19	ALA	-	EXPRESSION TAG	UNP Q46944
C	-18	SER	-	EXPRESSION TAG	UNP Q46944
C	-17	SER	-	EXPRESSION TAG	UNP Q46944
C	-16	HIS	-	EXPRESSION TAG	UNP Q46944
C	-15	HIS	-	EXPRESSION TAG	UNP Q46944
C	-14	HIS	-	EXPRESSION TAG	UNP Q46944

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	EXPRESSION TAG	UNP Q46944
C	-12	HIS	-	EXPRESSION TAG	UNP Q46944
C	-11	HIS	-	EXPRESSION TAG	UNP Q46944
C	-10	SER	-	EXPRESSION TAG	UNP Q46944
C	-9	SER	-	EXPRESSION TAG	UNP Q46944
C	-8	GLY	-	EXPRESSION TAG	UNP Q46944
C	-7	LEU	-	EXPRESSION TAG	UNP Q46944
C	-6	VAL	-	EXPRESSION TAG	UNP Q46944
C	-5	PRO	-	EXPRESSION TAG	UNP Q46944
C	-4	ARG	-	EXPRESSION TAG	UNP Q46944
C	-3	GLY	-	EXPRESSION TAG	UNP Q46944
C	-2	SER	-	EXPRESSION TAG	UNP Q46944
C	-1	SER	-	EXPRESSION TAG	UNP Q46944
C	0	MET	-	EXPRESSION TAG	UNP Q46944
C	1	GLY	-	EXPRESSION TAG	UNP Q46944
C	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
C	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944
D	-20	MET	-	EXPRESSION TAG	UNP Q46944
D	-19	ALA	-	EXPRESSION TAG	UNP Q46944
D	-18	SER	-	EXPRESSION TAG	UNP Q46944
D	-17	SER	-	EXPRESSION TAG	UNP Q46944
D	-16	HIS	-	EXPRESSION TAG	UNP Q46944
D	-15	HIS	-	EXPRESSION TAG	UNP Q46944
D	-14	HIS	-	EXPRESSION TAG	UNP Q46944
D	-13	HIS	-	EXPRESSION TAG	UNP Q46944
D	-12	HIS	-	EXPRESSION TAG	UNP Q46944
D	-11	HIS	-	EXPRESSION TAG	UNP Q46944
D	-10	SER	-	EXPRESSION TAG	UNP Q46944
D	-9	SER	-	EXPRESSION TAG	UNP Q46944
D	-8	GLY	-	EXPRESSION TAG	UNP Q46944
D	-7	LEU	-	EXPRESSION TAG	UNP Q46944
D	-6	VAL	-	EXPRESSION TAG	UNP Q46944
D	-5	PRO	-	EXPRESSION TAG	UNP Q46944
D	-4	ARG	-	EXPRESSION TAG	UNP Q46944
D	-3	GLY	-	EXPRESSION TAG	UNP Q46944
D	-2	SER	-	EXPRESSION TAG	UNP Q46944
D	-1	SER	-	EXPRESSION TAG	UNP Q46944
D	0	MET	-	EXPRESSION TAG	UNP Q46944
D	1	GLY	-	EXPRESSION TAG	UNP Q46944
D	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
D	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944
E	-20	MET	-	EXPRESSION TAG	UNP Q46944

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	ALA	-	EXPRESSION TAG	UNP Q46944
E	-18	SER	-	EXPRESSION TAG	UNP Q46944
E	-17	SER	-	EXPRESSION TAG	UNP Q46944
E	-16	HIS	-	EXPRESSION TAG	UNP Q46944
E	-15	HIS	-	EXPRESSION TAG	UNP Q46944
E	-14	HIS	-	EXPRESSION TAG	UNP Q46944
E	-13	HIS	-	EXPRESSION TAG	UNP Q46944
E	-12	HIS	-	EXPRESSION TAG	UNP Q46944
E	-11	HIS	-	EXPRESSION TAG	UNP Q46944
E	-10	SER	-	EXPRESSION TAG	UNP Q46944
E	-9	SER	-	EXPRESSION TAG	UNP Q46944
E	-8	GLY	-	EXPRESSION TAG	UNP Q46944
E	-7	LEU	-	EXPRESSION TAG	UNP Q46944
E	-6	VAL	-	EXPRESSION TAG	UNP Q46944
E	-5	PRO	-	EXPRESSION TAG	UNP Q46944
E	-4	ARG	-	EXPRESSION TAG	UNP Q46944
E	-3	GLY	-	EXPRESSION TAG	UNP Q46944
E	-2	SER	-	EXPRESSION TAG	UNP Q46944
E	-1	SER	-	EXPRESSION TAG	UNP Q46944
E	0	MET	-	EXPRESSION TAG	UNP Q46944
E	1	GLY	-	EXPRESSION TAG	UNP Q46944
E	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
E	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944
F	-20	MET	-	EXPRESSION TAG	UNP Q46944
F	-19	ALA	-	EXPRESSION TAG	UNP Q46944
F	-18	SER	-	EXPRESSION TAG	UNP Q46944
F	-17	SER	-	EXPRESSION TAG	UNP Q46944
F	-16	HIS	-	EXPRESSION TAG	UNP Q46944
F	-15	HIS	-	EXPRESSION TAG	UNP Q46944
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F	-13	HIS	-	EXPRESSION TAG	UNP Q46944
F	-12	HIS	-	EXPRESSION TAG	UNP Q46944
F	-11	HIS	-	EXPRESSION TAG	UNP Q46944
F	-10	SER	-	EXPRESSION TAG	UNP Q46944
F	-9	SER	-	EXPRESSION TAG	UNP Q46944
F	-8	GLY	-	EXPRESSION TAG	UNP Q46944
F	-7	LEU	-	EXPRESSION TAG	UNP Q46944
F	-6	VAL	-	EXPRESSION TAG	UNP Q46944
F	-5	PRO	-	EXPRESSION TAG	UNP Q46944
F	-4	ARG	-	EXPRESSION TAG	UNP Q46944
F	-3	GLY	-	EXPRESSION TAG	UNP Q46944
F	-2	SER	-	EXPRESSION TAG	UNP Q46944

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	SER	-	EXPRESSION TAG	UNP Q46944
F	0	MET	-	EXPRESSION TAG	UNP Q46944
F	1	GLY	-	EXPRESSION TAG	UNP Q46944
F	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
F	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944
G	-20	MET	-	EXPRESSION TAG	UNP Q46944
G	-19	ALA	-	EXPRESSION TAG	UNP Q46944
G	-18	SER	-	EXPRESSION TAG	UNP Q46944
G	-17	SER	-	EXPRESSION TAG	UNP Q46944
G	-16	HIS	-	EXPRESSION TAG	UNP Q46944
G	-15	HIS	-	EXPRESSION TAG	UNP Q46944
G	-14	HIS	-	EXPRESSION TAG	UNP Q46944
G	-13	HIS	-	EXPRESSION TAG	UNP Q46944
G	-12	HIS	-	EXPRESSION TAG	UNP Q46944
G	-11	HIS	-	EXPRESSION TAG	UNP Q46944
G	-10	SER	-	EXPRESSION TAG	UNP Q46944
G	-9	SER	-	EXPRESSION TAG	UNP Q46944
G	-8	GLY	-	EXPRESSION TAG	UNP Q46944
G	-7	LEU	-	EXPRESSION TAG	UNP Q46944
G	-6	VAL	-	EXPRESSION TAG	UNP Q46944
G	-5	PRO	-	EXPRESSION TAG	UNP Q46944
G	-4	ARG	-	EXPRESSION TAG	UNP Q46944
G	-3	GLY	-	EXPRESSION TAG	UNP Q46944
G	-2	SER	-	EXPRESSION TAG	UNP Q46944
G	-1	SER	-	EXPRESSION TAG	UNP Q46944
G	0	MET	-	EXPRESSION TAG	UNP Q46944
G	1	GLY	-	EXPRESSION TAG	UNP Q46944
G	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
G	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944
H	-20	MET	-	EXPRESSION TAG	UNP Q46944
H	-19	ALA	-	EXPRESSION TAG	UNP Q46944
H	-18	SER	-	EXPRESSION TAG	UNP Q46944
H	-17	SER	-	EXPRESSION TAG	UNP Q46944
H	-16	HIS	-	EXPRESSION TAG	UNP Q46944
H	-15	HIS	-	EXPRESSION TAG	UNP Q46944
H	-14	HIS	-	EXPRESSION TAG	UNP Q46944
H	-13	HIS	-	EXPRESSION TAG	UNP Q46944
H	-12	HIS	-	EXPRESSION TAG	UNP Q46944
H	-11	HIS	-	EXPRESSION TAG	UNP Q46944
H	-10	SER	-	EXPRESSION TAG	UNP Q46944
H	-9	SER	-	EXPRESSION TAG	UNP Q46944
H	-8	GLY	-	EXPRESSION TAG	UNP Q46944

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	LEU	-	EXPRESSION TAG	UNP Q46944
H	-6	VAL	-	EXPRESSION TAG	UNP Q46944
H	-5	PRO	-	EXPRESSION TAG	UNP Q46944
H	-4	ARG	-	EXPRESSION TAG	UNP Q46944
H	-3	GLY	-	EXPRESSION TAG	UNP Q46944
H	-2	SER	-	EXPRESSION TAG	UNP Q46944
H	-1	SER	-	EXPRESSION TAG	UNP Q46944
H	0	MET	-	EXPRESSION TAG	UNP Q46944
H	1	GLY	-	EXPRESSION TAG	UNP Q46944
H	49	PHE	TYR	ENGINEERED MUTATION	UNP Q46944
H	69	LYS	LEU	ENGINEERED MUTATION	UNP Q46944

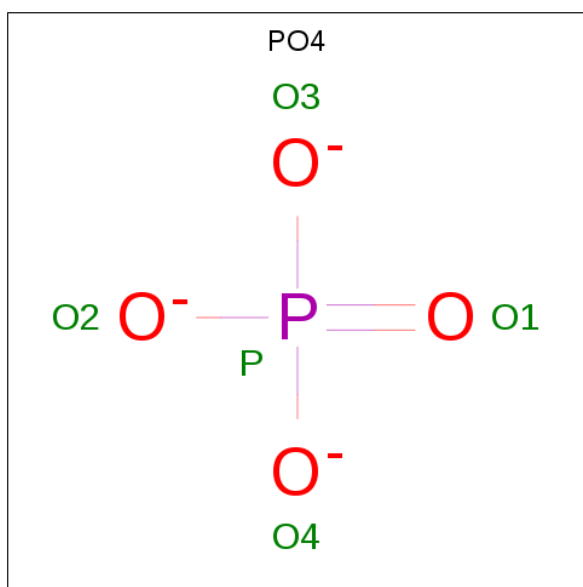
- Molecule 2 is a DNA chain called DNA (5'-D(P\*CP\*GP\*GP\*GP\*AP\*GP\*GP\*CP\*CP\*CP\*GP\*CP\*GP\*GP\*GP\*CP\*CP\*GP\*CP\*CP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	22	Total	C	N	O	P	0	0	0
			453	210	90	131	22			
2	I	22	Total	C	N	O	P	0	0	0
			453	210	90	131	22			
2	K	22	Total	C	N	O	P	0	0	0
			453	210	90	131	22			
2	O	22	Total	C	N	O	P	0	0	0
			453	210	90	131	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	22	Total	C	N	O	P	0	0	0
			449	209	85	133	22			
3	J	22	Total	C	N	O	P	0	0	0
			449	209	85	133	22			
3	L	22	Total	C	N	O	P	0	0	0
			449	209	85	133	22			
3	P	22	Total	C	N	O	P	0	0	0
			449	209	85	133	22			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		

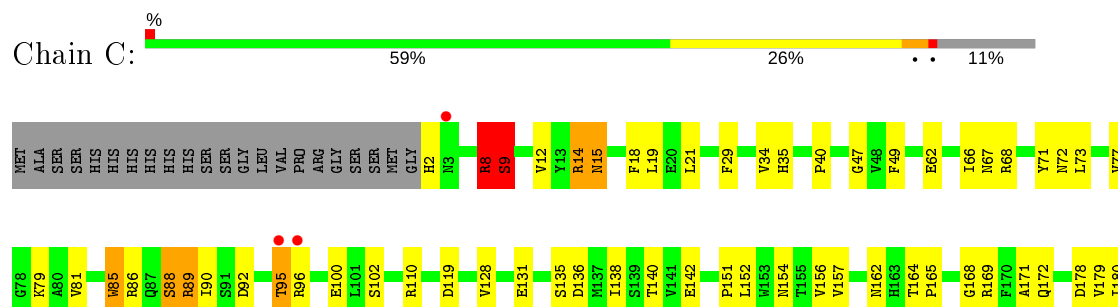
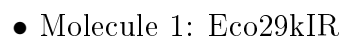
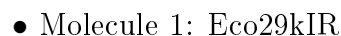
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	56	Total 56	O 56	0	0
5	C	60	Total 60	O 60	0	0
5	D	35	Total 35	O 35	0	0
5	E	46	Total 46	O 46	0	0
5	F	59	Total 59	O 59	0	0
5	G	37	Total 37	O 37	0	0
5	H	29	Total 29	O 29	0	0
5	M	11	Total 11	O 11	0	0
5	N	10	Total 10	O 10	0	0
5	I	5	Total 5	O 5	0	0
5	J	12	Total 12	O 12	0	0
5	K	11	Total 11	O 11	0	0
5	L	19	Total 19	O 19	0	0
5	O	7	Total 7	O 7	0	0
5	P	18	Total 18	O 18	0	0

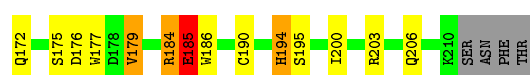
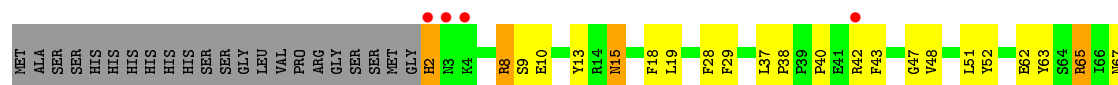


- Molecule 1: Eco29kIR





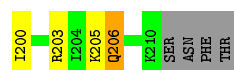
• Molecule 1: Eco29kIR



• Molecule 1: Eco29kIR

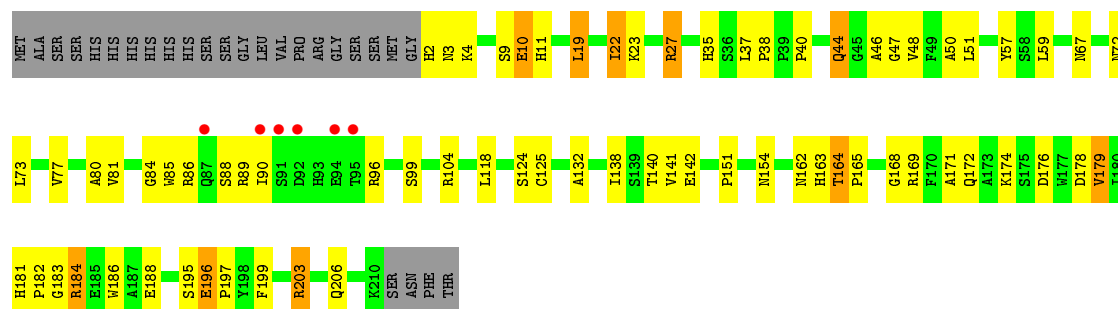


• Molecule 1: Eco29kIR

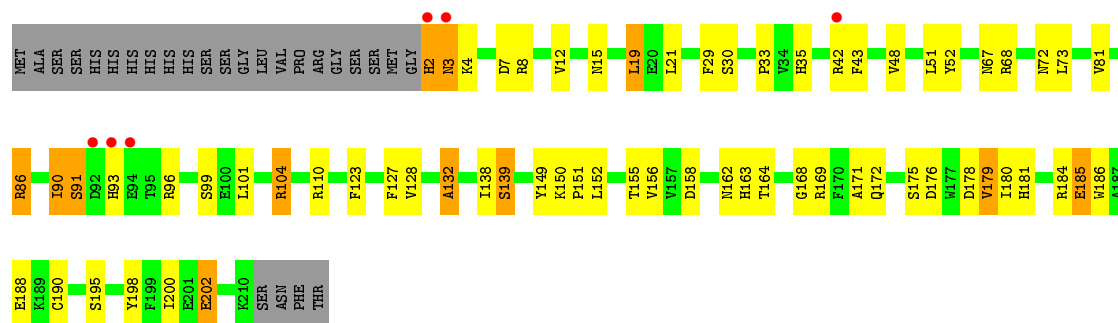


• Molecule 1: Eco29kIR

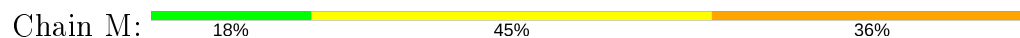




• Molecule 1: Eco29kIR



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



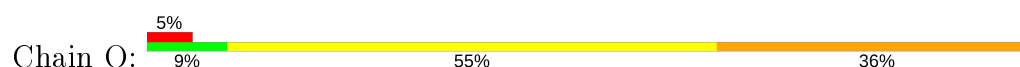
• Molecule 2: DNA (5'-D(P\*CP\*GP\*GP\*GP\*AP\*GP\*GP\*CP\*CP\*CP\*GP\*CP\*GP\*GP\*GP\*C  
P\*CP\*GP\*CP\*CP\*GP\*C)-3')

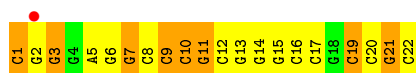


• Molecule 2: DNA (5'-D(P\*CP\*GP\*GP\*GP\*AP\*GP\*GP\*CP\*CP\*CP\*GP\*CP\*GP\*GP\*GP\*C  
P\*CP\*GP\*CP\*CP\*GP\*C)-3')

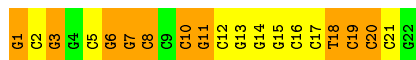


• Molecule 2: DNA (5'-D(P\*CP\*GP\*GP\*GP\*AP\*GP\*GP\*CP\*CP\*CP\*GP\*CP\*GP\*GP\*GP\*C  
P\*CP\*GP\*CP\*CP\*GP\*C)-3')





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



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.87Å 101.35Å 142.35Å 90.00° 109.59° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.80) 99.5 (49.93-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.58 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.206 , 0.279 0.213 , 0.286	Depositor DCC
$R_{free}$ test set	3347 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.832	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7645e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PO4

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	0.80	0/1720	0.82	2/2331 (0.1%)
1	B	0.83	0/1733	0.80	0/2347
1	C	0.83	0/1682	0.88	3/2280 (0.1%)
1	D	0.77	0/1698	0.82	0/2302
1	E	0.80	0/1680	0.81	1/2281 (0.0%)
1	F	0.85	1/1674 (0.1%)	0.85	0/2267
1	G	0.76	0/1659	0.85	2/2251 (0.1%)
1	H	0.73	1/1691 (0.1%)	0.82	2/2296 (0.1%)
2	I	1.34	2/508 (0.4%)	2.25	28/782 (3.6%)
2	K	1.30	2/508 (0.4%)	2.19	32/782 (4.1%)
2	M	1.30	1/508 (0.2%)	2.13	27/782 (3.5%)
2	O	1.33	2/508 (0.4%)	2.37	32/782 (4.1%)
3	J	1.37	3/502 (0.6%)	2.50	40/772 (5.2%)
3	L	1.28	1/502 (0.2%)	2.21	28/772 (3.6%)
3	N	1.43	2/502 (0.4%)	2.35	30/772 (3.9%)
3	P	1.31	2/502 (0.4%)	2.25	28/772 (3.6%)
All	All	0.95	17/17577 (0.1%)	1.36	255/24571 (1.0%)

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	H	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	9	DC	C3'-O3'	-9.98	1.30	1.44
2	M	12	DC	C3'-O3'	-7.86	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	11	DG	N7-C5	-7.29	1.34	1.39
3	P	9	DC	C3'-O3'	-6.57	1.35	1.44
2	K	9	DC	C3'-O3'	-6.54	1.35	1.44
2	K	1	DC	C3'-O3'	5.88	1.51	1.44
3	N	13	DG	C3'-O3'	-5.60	1.36	1.44
3	J	17	DC	C1'-N1	5.59	1.56	1.49
2	O	13	DG	C2-N3	5.59	1.37	1.32
3	P	15	DG	C3'-O3'	-5.42	1.36	1.44
3	J	15	DG	C3'-O3'	-5.29	1.37	1.44
3	J	9	DC	C3'-O3'	-5.24	1.37	1.44
2	I	10	DC	C3'-O3'	-5.22	1.37	1.44
2	O	15	DG	C3'-O3'	-5.12	1.37	1.44
3	L	10	DC	C3'-O3'	-5.10	1.37	1.44
1	H	104	ARG	CB-CG	-5.09	1.38	1.52
1	F	185	GLU	CG-CD	5.09	1.59	1.51

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	DG	O4'-C1'-N9	21.01	122.70	108.00
3	N	13	DG	O4'-C1'-N9	18.28	120.79	108.00
3	L	13	DG	O4'-C1'-N9	17.96	120.57	108.00
3	P	1	DG	O4'-C1'-N9	17.57	120.30	108.00
2	K	13	DG	O4'-C1'-N9	15.35	118.74	108.00
3	N	10	DC	O4'-C1'-N1	15.00	118.50	108.00
2	M	13	DG	O4'-C1'-N9	14.35	118.05	108.00
3	P	13	DG	O4'-C1'-N9	12.94	117.06	108.00
2	O	13	DG	O4'-C1'-N9	11.34	115.94	108.00
3	J	9	DC	O4'-C4'-C3'	-10.72	99.57	106.00
2	O	5	DA	O4'-C1'-N9	-10.71	100.50	108.00
2	I	13	DG	O4'-C1'-N9	10.38	115.26	108.00
3	P	17	DC	P-O3'-C3'	10.28	132.04	119.70
2	O	1	DC	O4'-C1'-N1	10.18	115.13	108.00
3	P	15	DG	O4'-C1'-N9	-10.09	100.94	108.00
3	J	8	DC	O4'-C1'-C2'	-9.99	97.91	105.90
3	L	3	DG	O4'-C1'-N9	9.61	114.73	108.00
3	J	6	DG	O4'-C1'-N9	-9.45	101.39	108.00
3	N	18	DT	O4'-C1'-N1	-9.41	101.41	108.00
2	I	5	DA	O4'-C4'-C3'	-9.34	100.40	106.00
2	M	15	DG	O4'-C4'-C3'	-9.33	100.40	106.00
3	J	1	DG	P-O3'-C3'	9.22	130.76	119.70
3	J	13	DG	O4'-C1'-N9	9.18	114.42	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	21	DC	O4'-C1'-N1	9.03	114.32	108.00
3	J	4	DG	P-O3'-C3'	8.98	130.47	119.70
2	M	1	DC	P-O3'-C3'	8.83	130.29	119.70
2	K	1	DC	O3'-P-O5'	8.74	120.61	104.00
3	J	1	DG	O4'-C4'-C3'	8.68	111.21	106.00
3	P	7	DG	O4'-C1'-N9	-8.66	101.94	108.00
3	P	15	DG	O5'-P-OP2	-8.56	97.99	105.70
2	M	11	DG	O5'-P-OP2	-8.56	98.00	105.70
2	I	7	DG	P-O3'-C3'	8.51	129.91	119.70
3	P	4	DG	P-O3'-C3'	8.45	129.84	119.70
3	J	17	DC	P-O3'-C3'	8.44	129.83	119.70
2	K	8	DC	O4'-C1'-C2'	-8.44	99.15	105.90
3	N	11	DG	P-O5'-C5'	-8.36	107.52	120.90
3	J	8	DC	O4'-C4'-C3'	-8.31	101.02	106.00
2	K	14	DG	O4'-C1'-N9	-8.30	102.19	108.00
3	N	11	DG	C8-N9-C4	-8.23	103.11	106.40
3	N	1	DG	P-O3'-C3'	8.14	129.47	119.70
2	I	21	DG	O4'-C1'-N9	8.13	113.69	108.00
2	I	6	DG	O4'-C1'-N9	-8.12	102.31	108.00
2	O	1	DC	C1'-O4'-C4'	-7.98	102.12	110.10
3	P	18	DT	P-O3'-C3'	7.97	129.27	119.70
3	J	8	DC	P-O3'-C3'	-7.91	110.20	119.70
3	J	19	DC	P-O3'-C3'	7.86	129.13	119.70
3	N	20	DC	P-O3'-C3'	7.83	129.10	119.70
2	I	5	DA	C3'-C2'-C1'	-7.78	93.17	102.50
2	I	11	DG	P-O3'-C3'	7.76	129.01	119.70
3	N	11	DG	C6-C5-N7	-7.65	125.81	130.40
3	N	7	DG	C5-C6-O6	-7.60	124.04	128.60
2	O	7	DG	P-O3'-C3'	7.59	128.80	119.70
3	L	20	DC	P-O3'-C3'	7.58	128.80	119.70
3	L	16	DC	P-O3'-C3'	7.58	128.79	119.70
3	P	1	DG	C1'-O4'-C4'	-7.58	102.52	110.10
3	L	1	DG	P-O3'-C3'	7.41	128.59	119.70
3	L	13	DG	O4'-C1'-C2'	-7.33	100.03	105.90
3	N	8	DC	O4'-C1'-N1	-7.33	102.87	108.00
2	I	19	DC	P-O3'-C3'	7.31	128.47	119.70
2	M	10	DC	O4'-C1'-C2'	-7.30	100.06	105.90
2	M	6	DG	P-O3'-C3'	7.29	128.45	119.70
3	J	11	DG	N9-C4-C5	7.29	108.31	105.40
3	P	21	DC	O4'-C1'-N1	7.13	112.99	108.00
3	J	11	DG	P-O3'-C3'	7.10	128.22	119.70
2	M	10	DC	N1-C2-O2	7.07	123.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	11	DG	C8-N9-C4	-7.07	103.57	106.40
3	L	18	DT	O4'-C1'-N1	-7.06	103.06	108.00
3	J	2	DC	P-O3'-C3'	-7.03	111.27	119.70
2	O	19	DC	P-O3'-C3'	7.02	128.13	119.70
2	K	2	DG	O4'-C1'-C2'	-7.01	100.30	105.90
2	M	11	DG	O4'-C1'-N9	-6.95	103.13	108.00
2	I	11	DG	N3-C4-C5	-6.95	125.12	128.60
2	K	2	DG	O5'-P-OP1	-6.95	99.44	105.70
2	O	10	DC	P-O3'-C3'	6.95	128.03	119.70
3	P	2	DC	P-O3'-C3'	-6.94	111.37	119.70
2	O	16	DC	O4'-C4'-C3'	-6.87	101.75	104.50
2	K	15	DG	C5-N7-C8	-6.86	100.87	104.30
3	J	16	DC	P-O3'-C3'	6.80	127.86	119.70
2	K	17	DC	P-O3'-C3'	6.79	127.85	119.70
2	K	15	DG	C8-N9-C4	-6.77	103.69	106.40
3	P	14	DG	O4'-C1'-N9	-6.76	103.27	108.00
2	O	21	DG	N3-C4-N9	-6.73	121.96	126.00
3	L	18	DT	P-O3'-C3'	6.68	127.72	119.70
3	P	1	DG	P-O3'-C3'	6.68	127.72	119.70
3	J	9	DC	O4'-C1'-N1	-6.67	103.33	108.00
2	I	1	DC	C1'-O4'-C4'	-6.64	103.46	110.10
3	P	6	DG	O4'-C1'-N9	-6.64	103.35	108.00
2	K	10	DC	N1-C2-O2	6.60	122.86	118.90
3	L	7	DG	O4'-C1'-N9	6.59	112.61	108.00
2	I	3	DG	P-O3'-C3'	6.59	127.61	119.70
3	L	1	DG	C4'-C3'-C2'	-6.59	97.17	103.10
2	O	11	DG	N1-C2-N2	-6.59	110.27	116.20
3	L	5	DC	P-O3'-C3'	6.57	127.59	119.70
3	N	13	DG	C1'-O4'-C4'	-6.57	103.53	110.10
2	O	9	DC	N3-C4-C5	-6.55	119.28	121.90
3	N	3	DG	C3'-C2'-C1'	-6.55	94.64	102.50
2	M	16	DC	C3'-C2'-C1'	-6.54	94.65	102.50
2	O	6	DG	P-O3'-C3'	6.53	127.54	119.70
3	L	9	DC	N3-C4-C5	-6.50	119.30	121.90
1	H	19	LEU	CA-CB-CG	6.50	130.25	115.30
3	J	22	DG	O4'-C1'-N9	6.47	112.53	108.00
2	O	3	DG	O4'-C1'-N9	-6.46	103.48	108.00
3	N	10	DC	C6-N1-C2	6.45	122.88	120.30
2	K	13	DG	N7-C8-N9	6.45	116.33	113.10
3	L	12	DC	C1'-O4'-C4'	-6.44	103.66	110.10
3	N	11	DG	N1-C6-O6	6.43	123.76	119.90
1	E	176	ASP	CB-CG-OD2	6.41	124.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	16	DC	O4'-C1'-N1	6.39	112.48	108.00
2	K	10	DC	N3-C2-O2	-6.38	117.43	121.90
2	I	11	DG	N3-C4-N9	6.36	129.81	126.00
3	L	11	DG	O4'-C1'-N9	-6.33	103.57	108.00
3	J	21	DC	C1'-O4'-C4'	-6.30	103.80	110.10
2	K	6	DG	C1'-O4'-C4'	-6.30	103.80	110.10
3	N	11	DG	N7-C8-N9	6.28	116.24	113.10
2	K	6	DG	O4'-C1'-C2'	-6.27	100.88	105.90
3	P	1	DG	O4'-C4'-C3'	6.25	109.75	106.00
3	L	6	DG	N1-C6-O6	6.24	123.64	119.90
3	J	11	DG	C6-N1-C2	-6.23	121.36	125.10
1	A	203	ARG	NE-CZ-NH1	6.19	123.39	120.30
3	J	13	DG	P-O3'-C3'	6.14	127.07	119.70
2	O	6	DG	N3-C2-N2	-6.14	115.60	119.90
3	J	9	DC	N1-C1'-C2'	6.14	124.26	112.60
2	O	9	DC	C5-C4-N4	6.12	124.48	120.20
2	K	11	DG	O4'-C1'-N9	-6.11	103.72	108.00
2	M	20	DC	O4'-C1'-N1	6.11	112.28	108.00
2	I	5	DA	N1-C6-N6	6.10	122.26	118.60
2	O	11	DG	N3-C2-N2	6.10	124.17	119.90
2	O	13	DG	P-O3'-C3'	6.08	126.99	119.70
2	M	10	DC	N3-C2-O2	-6.08	117.65	121.90
2	M	13	DG	N7-C8-N9	6.05	116.12	113.10
2	O	9	DC	O4'-C4'-C3'	-6.04	102.08	104.50
2	K	15	DG	N7-C8-N9	6.03	116.11	113.10
3	J	1	DG	C1'-O4'-C4'	-6.02	104.08	110.10
2	O	13	DG	C5-C6-N1	6.00	114.50	111.50
3	N	19	DC	P-O3'-C3'	6.00	126.90	119.70
2	I	22	DC	C4-C5-C6	6.00	120.40	117.40
2	M	4	DG	O4'-C1'-N9	6.00	112.20	108.00
2	K	2	DG	C5'-C4'-O4'	5.99	120.68	109.30
3	N	15	DG	O4'-C1'-N9	-5.98	103.81	108.00
2	K	13	DG	C5-C6-O6	-5.98	125.01	128.60
2	K	6	DG	O4'-C4'-C3'	-5.96	102.11	104.50
2	M	6	DG	N3-C4-C5	5.96	131.58	128.60
3	J	12	DC	N3-C4-C5	-5.95	119.52	121.90
2	M	13	DG	O4'-C1'-C2'	-5.91	101.17	105.90
3	P	12	DC	O3'-P-O5'	-5.89	92.80	104.00
1	C	136	ASP	CB-CG-OD1	5.89	123.60	118.30
3	N	18	DT	N3-C4-O4	5.89	123.44	119.90
2	M	18	DG	P-O3'-C3'	5.88	126.76	119.70
2	O	3	DG	P-O3'-C3'	5.88	126.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	9	DC	O4'-C4'-C3'	-5.87	102.15	104.50
3	J	11	DG	C8-N9-C4	-5.83	104.07	106.40
2	K	18	DG	O4'-C4'-C3'	-5.82	102.17	104.50
3	J	8	DC	C3'-C2'-C1'	-5.81	95.53	102.50
3	L	4	DG	P-O3'-C3'	5.81	126.67	119.70
3	L	9	DC	C2-N3-C4	5.79	122.79	119.90
2	O	13	DG	N3-C4-C5	-5.79	125.71	128.60
3	J	8	DC	C2-N3-C4	5.79	122.79	119.90
3	L	6	DG	C5-C6-O6	-5.77	125.14	128.60
2	I	8	DC	O4'-C1'-C2'	-5.76	101.29	105.90
2	K	15	DG	C4-C5-N7	5.75	113.10	110.80
3	L	18	DT	N3-C2-O2	-5.72	118.87	122.30
2	I	10	DC	OP2-P-O3'	5.72	117.78	105.20
3	P	11	DG	P-O3'-C3'	5.70	126.54	119.70
2	I	13	DG	C1'-O4'-C4'	-5.70	104.41	110.10
3	J	8	DC	C5-C6-N1	5.69	123.84	121.00
2	M	16	DC	N3-C4-C5	5.69	124.17	121.90
3	J	7	DG	O4'-C4'-C3'	-5.68	102.23	104.50
3	L	7	DG	P-O3'-C3'	5.67	126.51	119.70
2	M	12	DC	O4'-C1'-C2'	-5.63	101.40	105.90
3	P	16	DC	P-O3'-C3'	5.63	126.45	119.70
2	I	9	DC	C3'-C2'-C1'	-5.62	95.76	102.50
1	G	184	ARG	NE-CZ-NH2	-5.61	117.49	120.30
2	O	13	DG	O4'-C1'-C2'	-5.61	101.42	105.90
3	L	15	DG	C5-N7-C8	-5.60	101.50	104.30
2	O	17	DC	P-O3'-C3'	5.59	126.41	119.70
2	M	17	DC	O4'-C1'-N1	5.56	111.89	108.00
3	N	7	DG	C4-C5-N7	5.55	113.02	110.80
2	I	16	DC	O4'-C1'-C2'	-5.54	101.47	105.90
3	L	21	DC	P-O3'-C3'	5.53	126.33	119.70
1	G	184	ARG	NE-CZ-NH1	5.53	123.06	120.30
3	J	10	DC	O4'-C4'-C3'	-5.53	102.29	104.50
3	N	6	DG	N1-C6-O6	5.51	123.21	119.90
2	O	12	DC	OP2-P-O3'	5.51	117.32	105.20
3	P	20	DC	O4'-C1'-N1	5.50	111.85	108.00
2	O	5	DA	O4'-C4'-C3'	-5.49	102.30	104.50
2	M	13	DG	C8-N9-C4	-5.46	104.22	106.40
2	M	4	DG	C5-C6-O6	-5.45	125.33	128.60
3	P	19	DC	P-O3'-C3'	5.45	126.24	119.70
3	N	11	DG	C5-N7-C8	-5.45	101.58	104.30
2	I	13	DG	O4'-C1'-C2'	-5.45	101.54	105.90
3	J	1	DG	C4'-C3'-C2'	-5.44	98.20	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	11	DG	N1-C6-O6	-5.44	116.64	119.90
2	K	8	DC	O4'-C1'-N1	-5.43	104.20	108.00
3	N	12	DC	C1'-O4'-C4'	-5.43	104.67	110.10
3	P	3	DG	O4'-C1'-N9	5.42	111.80	108.00
2	M	6	DG	N3-C4-N9	-5.41	122.75	126.00
3	N	6	DG	C5-C6-O6	-5.41	125.35	128.60
3	L	15	DG	C4-C5-N7	5.41	112.97	110.80
2	K	13	DG	C1'-O4'-C4'	-5.41	104.69	110.10
2	O	6	DG	O4'-C1'-N9	-5.41	104.21	108.00
3	J	16	DC	C4'-C3'-O3'	-5.41	96.18	109.70
2	O	21	DG	C8-N9-C1'	5.40	134.02	127.00
1	A	203	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	8	ARG	NE-CZ-NH1	-5.38	117.61	120.30
3	P	8	DC	N1-C2-O2	5.38	122.12	118.90
3	P	12	DC	OP2-P-O3'	5.37	117.01	105.20
2	O	10	DC	O4'-C1'-N1	-5.36	104.25	108.00
1	H	110	ARG	NE-CZ-NH1	-5.36	117.62	120.30
3	N	3	DG	O4'-C1'-C2'	-5.35	101.62	105.90
3	N	11	DG	O4'-C1'-N9	-5.35	104.25	108.00
1	C	119	ASP	CB-CG-OD1	-5.32	113.52	118.30
2	O	14	DG	OP2-P-O3'	5.32	116.89	105.20
3	L	6	DG	P-O3'-C3'	5.30	126.06	119.70
3	N	16	DC	P-O3'-C3'	5.29	126.05	119.70
3	N	14	DG	N1-C2-N3	-5.29	120.72	123.90
2	I	5	DA	O4'-C1'-N9	-5.29	104.30	108.00
2	M	11	DG	N9-C4-C5	5.28	107.51	105.40
3	J	20	DC	O4'-C1'-N1	5.28	111.70	108.00
3	L	10	DC	C4-C5-C6	5.28	120.04	117.40
2	O	15	DG	C2-N3-C4	-5.28	109.26	111.90
2	I	15	DG	O4'-C4'-C3'	-5.28	102.39	104.50
3	P	22	DG	O4'-C1'-N9	5.28	111.69	108.00
3	J	21	DC	C6-N1-C2	5.27	122.41	120.30
2	O	5	DA	C3'-C2'-C1'	-5.25	96.20	102.50
3	P	11	DG	N7-C8-N9	5.22	115.71	113.10
2	O	21	DG	N3-C4-C5	5.22	131.21	128.60
3	N	10	DC	O4'-C1'-C2'	5.21	110.07	105.90
2	K	13	DG	C5-N7-C8	-5.21	101.69	104.30
2	K	2	DG	C8-N9-C4	-5.21	104.32	106.40
2	K	4	DG	O4'-C1'-N9	5.21	111.64	108.00
2	M	19	DC	O4'-C1'-N1	5.20	111.64	108.00
3	J	13	DG	C1'-O4'-C4'	-5.20	104.90	110.10
2	I	11	DG	N1-C2-N2	-5.18	111.54	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	DG	N7-C8-N9	5.18	115.69	113.10
2	K	13	DG	C8-N9-C4	-5.18	104.33	106.40
3	P	8	DC	O4'-C1'-C2'	-5.17	101.76	105.90
2	M	11	DG	N1-C6-O6	-5.17	116.80	119.90
2	I	9	DC	N3-C4-C5	-5.16	119.83	121.90
3	N	20	DC	O4'-C1'-N1	5.16	111.61	108.00
2	I	12	DC	N1-C2-O2	-5.14	115.81	118.90
3	J	13	DG	O4'-C4'-C3'	5.11	109.07	106.00
2	M	3	DG	O4'-C1'-N9	5.11	111.58	108.00
3	J	13	DG	C5-C6-N1	5.11	114.05	111.50
2	I	14	DG	C8-N9-C4	-5.10	104.36	106.40
2	K	16	DC	C3'-C2'-C1'	-5.09	96.39	102.50
3	J	3	DG	O4'-C1'-N9	5.09	111.56	108.00
3	N	11	DG	C5-C6-N1	-5.09	108.96	111.50
3	P	8	DC	C3'-C2'-C1'	-5.08	96.41	102.50
2	M	8	DC	O4'-C1'-C2'	-5.08	101.84	105.90
2	I	8	DC	O3'-P-O5'	-5.08	94.36	104.00
2	I	6	DG	N9-C1'-C2'	5.06	122.22	112.60
2	K	6	DG	N3-C2-N2	-5.02	116.39	119.90
2	K	8	DC	N1-C1'-C2'	5.02	122.13	112.60
3	L	14	DG	C5-N7-C8	-5.01	101.79	104.30
2	K	6	DG	O4'-C1'-N9	-5.01	104.49	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	162	ASN	Peptide
1	H	4	LYS	Peptide

## 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	1671	0	1573	62	0
1	B	1683	0	1585	78	1
1	C	1635	0	1522	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1649	0	1540	73	0
1	E	1631	0	1513	54	0
1	F	1627	0	1516	62	1
1	G	1612	0	1480	67	0
1	H	1642	0	1526	57	0
2	I	453	0	243	27	0
2	K	453	0	243	25	0
2	M	453	0	243	13	0
2	O	453	0	243	15	0
3	J	449	0	244	18	0
3	L	449	0	244	17	0
3	N	449	0	244	18	0
3	P	449	0	244	18	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	D	10	0	0	2	0
4	E	5	0	0	0	0
4	F	10	0	0	1	0
4	G	5	0	0	0	0
4	H	10	0	0	3	0
5	A	51	0	0	1	0
5	B	56	0	0	2	0
5	C	60	0	0	8	0
5	D	35	0	0	3	0
5	E	46	0	0	3	0
5	F	59	0	0	9	0
5	G	37	0	0	1	0
5	H	29	0	0	2	0
5	I	5	0	0	0	0
5	J	12	0	0	0	0
5	K	11	0	0	1	0
5	L	19	0	0	5	0
5	M	11	0	0	1	0
5	N	10	0	0	2	0
5	O	7	0	0	2	0
5	P	18	0	0	2	0
All	All	17279	0	14203	559	1

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 18.

All (559) 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:171:ALA:CB	1:G:168:GLY:HA2	1.76	1.15
2:I:22:DC:H5	2:K:1:DC:O5'	1.29	1.14
1:C:171:ALA:HB3	1:G:168:GLY:HA2	1.17	1.10
3:J:1:DG:H2"	3:J:2:DC:H5	1.12	1.09
1:G:196:GLU:HG3	1:G:197:PRO:HD2	1.31	1.07
1:D:86:ARG:HG2	1:D:86:ARG:HH11	1.20	1.07
3:N:10:DC:H4'	3:N:11:DG:OP1	1.59	1.03
1:G:27:ARG:HG2	1:G:27:ARG:HH11	1.18	1.03
3:J:1:DG:H2"	3:J:2:DC:C5	1.93	1.03
1:H:86:ARG:HH11	1:H:86:ARG:HG2	1.24	1.01
1:E:40:PRO:HG3	1:F:2:HIS:CE1	1.96	1.00
1:B:67:ASN:HD21	1:B:73:LEU:H	1.00	0.98
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.28	0.97
3:P:1:DG:H2"	3:P:2:DC:H5	1.26	0.96
1:F:77:VAL:H	1:F:154:ASN:HD21	1.10	0.96
2:I:22:DC:C5	2:K:1:DC:O5'	2.17	0.96
1:C:14:ARG:HH11	1:C:14:ARG:HG2	1.30	0.95
1:C:171:ALA:HB3	1:G:168:GLY:CA	1.95	0.95
1:C:8:ARG:HG3	1:C:8:ARG:HH11	1.29	0.94
1:A:67:ASN:HD21	1:A:73:LEU:H	0.97	0.93
1:E:169:ARG:HE	1:F:172:GLN:NE2	1.67	0.93
1:B:2:HIS:HB3	1:B:3:ASN:CA	2.00	0.92
2:I:21:DG:C8	2:K:1:DC:OP1	2.22	0.92
1:C:9:SER:HA	1:C:12:VAL:HG23	1.53	0.91
1:E:40:PRO:HG3	1:F:2:HIS:HE1	1.34	0.90
3:P:1:DG:H2"	3:P:2:DC:C5	2.05	0.90
1:C:77:VAL:H	1:C:154:ASN:HD21	1.15	0.90
1:B:15:ASN:HD21	1:B:17:SER:HB3	1.39	0.88
1:E:44:GLN:HA	1:E:99:SER:HB3	1.57	0.87
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.38	0.87
1:F:2:HIS:CE1	5:F:430:HOH:O	2.27	0.87
1:F:67:ASN:HD21	1:F:73:LEU:H	1.19	0.86
1:E:77:VAL:H	1:E:154:ASN:HD21	1.21	0.86
1:G:59:LEU:HD22	5:G:259:HOH:O	1.76	0.85
1:F:162:ASN:HD22	3:P:12:DC:H5	1.19	0.85
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.40	0.85
1:G:196:GLU:HG3	1:G:197:PRO:CD	2.07	0.85
1:G:104:ARG:NH1	1:G:163:HIS:NE2	2.25	0.84
1:B:77:VAL:H	1:B:154:ASN:HD21	1.22	0.84
1:C:168:GLY:HA2	1:G:171:ALA:HB3	1.60	0.81
1:E:169:ARG:HE	1:F:172:GLN:HE22	1.24	0.81
1:D:67:ASN:HD21	1:D:73:LEU:H	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:GLU:HG2	5:H:281:HOH:O	1.81	0.80
1:E:2:HIS:CE1	1:F:35:HIS:HD2	2.00	0.79
1:G:27:ARG:CG	1:G:27:ARG:HH11	1.93	0.79
1:B:171:ALA:HB3	1:D:168:GLY:HA2	1.64	0.79
1:A:87:GLN:O	1:H:155:THR:HG22	1.83	0.79
1:C:14:ARG:HH11	1:C:14:ARG:CG	1.95	0.79
1:C:168:GLY:HA2	1:G:171:ALA:CB	2.13	0.78
1:H:195:SER:HB2	4:H:216:PO4:O4	1.82	0.78
1:G:27:ARG:HG2	1:G:27:ARG:NH1	1.92	0.78
1:H:90:ILE:HG13	1:H:91:SER:H	1.49	0.78
2:I:2:DG:H2''	2:I:3:DG:OP2	1.83	0.78
1:C:8:ARG:HH11	1:C:8:ARG:CG	1.98	0.77
1:B:35:HIS:HD2	1:D:2:HIS:ND1	1.81	0.77
1:A:77:VAL:H	1:A:154:ASN:HD21	1.31	0.77
1:A:169:ARG:HG2	1:H:169:ARG:HG2	1.65	0.77
1:A:35:HIS:HD2	1:H:2:HIS:ND1	1.82	0.77
1:E:172:GLN:HE22	1:F:169:ARG:HH21	1.33	0.77
3:N:17:DC:H2''	3:N:18:DT:OP2	1.82	0.77
1:E:69:LYS:HE3	5:E:328:HOH:O	1.84	0.76
1:H:86:ARG:NH1	1:H:86:ARG:HG2	1.96	0.76
3:N:1:DG:H1'	3:N:2:DC:C5	2.19	0.76
1:E:168:GLY:HA2	1:F:171:ALA:HB3	1.67	0.76
1:E:67:ASN:HD21	1:E:73:LEU:H	1.34	0.76
2:I:1:DC:O2	3:J:22:DG:N1	2.19	0.75
1:A:14:ARG:CG	1:A:14:ARG:HH11	1.98	0.75
1:B:81:VAL:HG11	1:B:85:TRP:CD1	2.21	0.74
2:I:21:DG:H2''	2:K:1:DC:H5'	1.68	0.74
1:H:67:ASN:HD21	1:H:73:LEU:H	1.33	0.74
1:C:67:ASN:HD21	1:C:73:LEU:H	1.34	0.74
1:G:44:GLN:HA	1:G:99:SER:HB3	1.69	0.74
3:L:8:DC:H5'	5:L:155:HOH:O	1.88	0.73
3:L:22:DG:N2	5:L:454:HOH:O	2.16	0.73
1:H:158:ASP:HB2	5:H:348:HOH:O	1.88	0.72
1:B:172:GLN:HE22	1:D:169:ARG:HH21	1.36	0.72
1:C:8:ARG:O	1:C:9:SER:HB3	1.87	0.72
1:B:89:ARG:NH2	1:D:155:THR:HB	2.03	0.72
1:C:172:GLN:NE2	1:G:169:ARG:HE	1.87	0.72
1:B:67:ASN:HD21	1:B:73:LEU:N	1.81	0.72
3:N:3:DG:OP2	3:N:3:DG:H2'	1.90	0.72
1:B:171:ALA:CB	1:D:168:GLY:HA2	2.20	0.71
2:O:21:DG:N2	3:P:2:DC:O2	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:DC:H4'	2:K:2:DG:OP2	1.89	0.71
3:P:6:DG:H2''	3:P:7:DG:OP2	1.88	0.71
1:G:67:ASN:HD21	1:G:73:LEU:H	1.38	0.71
3:N:1:DG:H1'	3:N:2:DC:C6	2.25	0.71
1:A:67:ASN:HD21	1:A:73:LEU:N	1.80	0.71
1:C:165:PRO:HD3	1:C:186:TRP:CE3	2.25	0.70
1:D:96:ARG:CA	1:D:97:ALA:HB3	2.21	0.70
1:B:168:GLY:HA2	1:D:171:ALA:HB3	1.74	0.70
2:I:22:DC:H42	3:J:1:DG:H1	1.40	0.70
2:O:20:DC:H2''	2:O:21:DG:C8	2.25	0.70
3:N:10:DC:C4'	3:N:11:DG:OP1	2.35	0.70
1:B:15:ASN:C	1:B:15:ASN:HD22	1.95	0.70
1:B:40:PRO:HD3	1:D:2:HIS:HE1	1.56	0.70
1:B:169:ARG:HE	1:D:172:GLN:NE2	1.90	0.70
3:L:17:DC:H2''	3:L:18:DT:OP2	1.91	0.69
2:K:19:DC:H2''	2:K:20:DC:OP2	1.93	0.69
1:H:195:SER:CB	4:H:216:PO4:O4	2.40	0.69
1:C:2:HIS:CE1	5:C:460:HOH:O	2.45	0.69
1:E:59:LEU:HD21	1:E:201:GLU:HG2	1.75	0.68
1:A:67:ASN:ND2	1:A:73:LEU:H	1.81	0.68
3:L:3:DG:N3	5:L:286:HOH:O	2.27	0.68
2:O:20:DC:OP2	2:O:20:DC:H2'	1.93	0.68
1:C:162:ASN:HD22	3:J:12:DC:H5	1.41	0.68
1:A:168:GLY:HA2	1:H:171:ALA:HB3	1.74	0.68
2:K:2:DG:O6	3:L:21:DC:N4	2.19	0.67
1:C:2:HIS:HE1	1:G:40:PRO:HG3	1.58	0.67
3:P:1:DG:H4'	3:P:2:DC:OP1	1.94	0.67
1:A:171:ALA:CB	1:H:168:GLY:HA2	2.24	0.67
1:E:171:ALA:HB3	1:F:168:GLY:HA2	1.76	0.67
1:B:40:PRO:HD3	1:D:2:HIS:CE1	2.29	0.67
1:F:185:GLU:CD	1:F:185:GLU:H	1.98	0.67
1:C:8:ARG:HG3	1:C:8:ARG:NH1	2.04	0.66
2:O:1:DC:H1'	2:O:2:DG:N7	2.10	0.66
1:C:171:ALA:HB1	1:G:168:GLY:HA2	1.77	0.66
1:B:29:PHE:CD1	1:B:128:VAL:HG23	2.30	0.65
1:B:67:ASN:ND2	1:B:72:ASN:H	1.94	0.65
1:A:171:ALA:HB3	1:H:168:GLY:HA2	1.77	0.65
1:D:65:ARG:HH22	1:E:195:SER:HB3	1.61	0.65
1:D:86:ARG:CG	1:D:86:ARG:HH11	2.04	0.65
3:J:6:DG:H1'	3:J:7:DG:H5'	1.80	0.64
1:B:89:ARG:NH1	1:D:155:THR:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:VAL:N	1:F:154:ASN:HD21	1.90	0.64
2:I:18:DG:H2'	2:I:18:DG:OP2	1.97	0.64
1:D:43:PHE:O	1:D:99:SER:HB2	1.98	0.64
1:F:139:SER:HB2	5:F:239:HOH:O	1.96	0.64
1:C:95:THR:CG2	1:C:96:ARG:H	2.11	0.64
1:C:169:ARG:HH21	1:G:172:GLN:HE22	1.46	0.64
3:L:1:DG:H1'	3:L:2:DC:C5	2.32	0.64
1:E:65:ARG:HD3	5:E:285:HOH:O	1.98	0.64
2:M:20:DC:H2''	2:M:21:DG:C8	2.33	0.64
1:B:169:ARG:O	1:B:172:GLN:HG2	1.97	0.64
1:B:21:LEU:HD11	1:D:15:ASN:OD1	1.98	0.64
1:E:40:PRO:CG	1:F:2:HIS:HE1	2.10	0.64
2:K:2:DG:C8	2:K:2:DG:OP1	2.51	0.64
1:C:8:ARG:NH1	1:C:8:ARG:CG	2.56	0.63
1:D:77:VAL:H	1:D:154:ASN:HD21	1.46	0.63
1:G:77:VAL:H	1:G:154:ASN:HD21	1.45	0.63
1:A:44:GLN:HA	1:A:99:SER:HB3	1.79	0.63
1:F:164:THR:HG22	1:F:166:GLY:H	1.62	0.63
1:B:160:PHE:O	1:B:184:ARG:NH2	2.31	0.63
1:B:81:VAL:HG12	1:B:82:PRO:O	1.99	0.63
1:H:185:GLU:HG2	1:H:186:TRP:N	2.13	0.63
1:C:2:HIS:CG	5:C:460:HOH:O	2.52	0.63
1:F:178:ASP:OD1	1:F:184:ARG:HD2	1.98	0.63
1:C:62:GLU:OE2	1:C:62:GLU:HA	1.98	0.63
1:F:205:LYS:HE3	5:F:439:HOH:O	1.99	0.63
1:E:59:LEU:CD2	1:E:201:GLU:HG2	2.28	0.63
1:E:169:ARG:NE	1:F:172:GLN:HE22	1.96	0.63
2:K:2:DG:N1	3:L:21:DC:N3	2.33	0.63
2:M:2:DG:OP2	5:M:420:HOH:O	2.15	0.63
3:N:10:DC:H2''	3:N:11:DG:C8	2.33	0.63
1:C:8:ARG:O	1:C:9:SER:CB	2.47	0.62
1:E:168:GLY:HA2	1:F:171:ALA:CB	2.28	0.62
2:I:1:DC:H1'	2:I:2:DG:N7	2.13	0.62
3:N:8:DC:C5'	5:N:246:HOH:O	2.46	0.62
3:N:8:DC:H5''	5:N:246:HOH:O	1.99	0.62
1:B:42:ARG:NH2	5:B:445:HOH:O	2.32	0.62
1:B:44:GLN:O	1:D:8:ARG:NH2	2.32	0.62
1:D:65:ARG:HH22	1:E:195:SER:CB	2.12	0.62
1:F:176:ASP:HA	1:F:179:VAL:HG13	1.81	0.62
1:F:2:HIS:CD2	5:F:430:HOH:O	2.53	0.62
2:O:20:DC:H2''	2:O:21:DG:H8	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:HIS:CD2	1:D:2:HIS:N	2.68	0.61
1:H:29:PHE:CD1	1:H:128:VAL:HG23	2.36	0.61
1:D:172:GLN:O	1:D:190:CYS:HB3	1.99	0.61
1:F:43:PHE:O	1:F:99:SER:HB2	1.99	0.61
1:B:77:VAL:H	1:B:154:ASN:ND2	1.96	0.61
2:K:15:DG:H2'	5:K:431:HOH:O	2.00	0.61
1:C:172:GLN:HE22	1:G:169:ARG:HE	1.48	0.60
1:C:135:SER:O	1:C:138:ILE:HG13	2.01	0.60
1:C:199:PHE:O	1:C:203:ARG:HG2	2.01	0.60
1:G:84:GLY:N	1:G:85:TRP:HA	2.16	0.60
3:P:8:DC:H5'	5:P:290:HOH:O	2.00	0.60
1:B:79:LYS:HD3	1:B:142:GLU:OE2	2.02	0.60
1:A:169:ARG:HE	1:H:172:GLN:NE2	1.99	0.60
1:C:169:ARG:HE	1:G:172:GLN:NE2	1.99	0.60
1:B:67:ASN:HD22	1:B:72:ASN:H	1.50	0.60
3:J:6:DG:H2''	3:J:7:DG:OP2	2.02	0.60
1:D:86:ARG:HG2	1:D:86:ARG:NH1	2.00	0.60
1:C:2:HIS:ND1	5:C:460:HOH:O	2.32	0.59
1:C:79:LYS:HD3	1:C:142:GLU:OE2	2.02	0.59
3:J:2:DC:H2''	3:J:3:DG:C8	2.37	0.59
3:P:18:DT:H1'	3:P:19:DC:H5'	1.84	0.59
1:C:14:ARG:NH1	1:C:14:ARG:CG	2.65	0.59
1:F:162:ASN:ND2	3:P:12:DC:H5	1.97	0.59
1:D:62:GLU:OE1	1:E:196:GLU:CA	2.50	0.59
2:I:1:DC:O2	3:J:22:DG:C2	2.55	0.59
1:C:95:THR:HG23	1:C:96:ARG:H	1.68	0.59
3:L:3:DG:H2'	3:L:3:DG:OP2	2.03	0.59
1:B:103:ASN:ND2	5:B:236:HOH:O	2.35	0.58
1:F:82:PRO:O	1:F:83:ALA:O	2.21	0.58
3:L:2:DC:H2''	3:L:3:DG:C8	2.39	0.58
3:N:2:DC:H2''	3:N:3:DG:C8	2.39	0.58
1:G:118:LEU:HD11	1:G:181:HIS:CE1	2.39	0.58
1:H:43:PHE:O	1:H:99:SER:HB2	2.04	0.58
2:M:19:DC:H2''	2:M:20:DC:OP2	2.02	0.58
1:B:95:THR:CB	1:B:96:ARG:HA	2.33	0.57
1:A:29:PHE:CD1	1:A:128:VAL:HG23	2.40	0.57
1:H:90:ILE:HG13	1:H:91:SER:N	2.19	0.57
1:B:137:MET:HE1	1:D:15:ASN:HB3	1.86	0.57
1:B:15:ASN:ND2	1:B:17:SER:HB3	2.15	0.57
1:B:37:LEU:HD12	1:B:38:PRO:HA	1.87	0.57
2:I:22:DC:N4	3:J:1:DG:H1	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:PRO:HB2	1:B:154:ASN:HD22	1.68	0.57
2:K:12:DC:H2"	2:K:13:DG:O5'	2.04	0.57
1:C:40:PRO:HD3	1:G:2:HIS:CE1	2.40	0.56
1:F:2:HIS:CG	5:F:430:HOH:O	2.58	0.56
1:F:80:ALA:HB2	1:F:104:ARG:HG3	1.88	0.56
1:D:176:ASP:HA	1:D:179:VAL:HG13	1.86	0.56
1:E:171:ALA:CB	1:F:168:GLY:HA2	2.34	0.56
1:C:47:GLY:HA2	1:C:138:ILE:HD13	1.88	0.56
1:C:178:ASP:OD1	1:C:184:ARG:HD2	2.06	0.56
1:B:178:ASP:OD2	1:B:184:ARG:NH1	2.39	0.56
1:E:155:THR:HB	1:F:86:ARG:HA	1.88	0.56
1:E:168:GLY:CA	1:F:171:ALA:HB3	2.36	0.56
3:P:13:DG:H4'	3:P:14:DG:OP1	2.06	0.56
1:B:195:SER:HB2	1:B:200:ILE:HD11	1.87	0.56
1:F:162:ASN:HD21	3:P:11:DG:H2'	1.70	0.56
2:I:22:DC:H5	2:K:1:DC:P	2.28	0.56
1:B:2:HIS:NE2	1:D:40:PRO:HG3	2.22	0.55
1:E:57:TYR:HE2	1:E:59:LEU:HD12	1.71	0.55
1:E:40:PRO:CG	1:F:2:HIS:CE1	2.82	0.55
1:B:169:ARG:HG2	1:D:169:ARG:HG2	1.87	0.55
1:D:81:VAL:O	1:D:100:GLU:HG3	2.06	0.55
1:F:83:ALA:HB1	1:F:84:GLY:O	2.06	0.55
5:C:460:HOH:O	1:G:35:HIS:HD2	1.89	0.55
2:M:3:DG:C5	2:M:4:DG:C6	2.94	0.55
1:A:27:ARG:CG	1:A:27:ARG:HH11	2.14	0.55
1:B:159:GLY:HA3	1:B:175:SER:HB2	1.88	0.55
1:G:176:ASP:HA	1:G:179:VAL:HG13	1.88	0.55
1:G:48:VAL:HG23	1:G:138:ILE:HG23	1.88	0.55
1:F:2:HIS:NE2	5:F:430:HOH:O	2.32	0.55
1:A:67:ASN:ND2	1:A:72:ASN:H	2.05	0.55
5:C:460:HOH:O	1:G:35:HIS:CD2	2.59	0.55
1:H:67:ASN:ND2	1:H:72:ASN:H	2.05	0.55
1:A:169:ARG:O	1:A:172:GLN:HG2	2.07	0.55
1:G:178:ASP:OD1	1:G:184:ARG:HD2	2.07	0.55
2:I:17:DC:H2'	2:I:17:DC:OP2	2.07	0.54
1:D:110:ARG:NH2	3:L:6:DG:OP1	2.40	0.54
2:I:20:DC:H2"	2:I:21:DG:C8	2.43	0.54
1:C:168:GLY:CA	1:G:171:ALA:HB3	2.34	0.54
1:B:7:ASP:HB3	1:B:10:GLU:HB2	1.89	0.54
1:D:95:THR:C	5:D:447:HOH:O	2.46	0.54
1:G:57:TYR:HE2	1:G:59:LEU:HD12	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:N	1:A:151:PRO:HD3	2.23	0.54
1:E:28:PHE:CE2	1:F:13:TYR:HB2	2.43	0.54
1:F:135:SER:O	1:F:138:ILE:HG13	2.08	0.54
3:N:6:DG:H1'	3:N:7:DG:H5'	1.88	0.54
1:B:168:GLY:HA2	1:D:171:ALA:CB	2.37	0.54
1:A:37:LEU:HD12	1:A:38:PRO:HA	1.90	0.53
1:C:169:ARG:HE	1:G:172:GLN:HE21	1.54	0.53
2:O:8:DC:H5"	5:O:240:HOH:O	2.07	0.53
1:C:196:GLU:HG3	1:C:197:PRO:HD2	1.89	0.53
1:D:47:GLY:HA2	1:D:138:ILE:HD13	1.90	0.53
1:E:77:VAL:N	1:E:154:ASN:HD21	1.99	0.53
1:H:164:THR:CG2	3:N:8:DC:C6	2.92	0.53
1:B:44:GLN:HA	1:B:99:SER:HB3	1.91	0.53
1:F:195:SER:HB2	1:F:200:ILE:HD11	1.89	0.53
1:G:80:ALA:HB2	1:G:104:ARG:HG3	1.90	0.53
2:K:5:DA:H2"	2:K:6:DG:C8	2.44	0.53
1:A:51:LEU:HD22	1:A:76:TYR:HD2	1.73	0.53
1:D:96:ARG:CA	1:D:97:ALA:CB	2.86	0.53
1:C:172:GLN:HE22	1:G:169:ARG:HH21	1.56	0.53
1:C:9:SER:HA	1:C:12:VAL:CG2	2.35	0.53
1:D:63:TYR:C	1:D:65:ARG:H	2.12	0.53
3:P:2:DC:H2"	3:P:3:DG:C8	2.43	0.53
1:C:35:HIS:HA	1:G:2:HIS:HA	1.91	0.53
1:G:84:GLY:HA2	1:G:85:TRP:CB	2.39	0.53
1:B:29:PHE:HD1	1:B:128:VAL:CG2	2.22	0.52
1:B:67:ASN:ND2	1:B:72:ASN:N	2.57	0.52
1:H:96:ARG:HD3	1:H:132:ALA:HB2	1.90	0.52
1:D:8:ARG:HD2	5:D:299:HOH:O	2.09	0.52
1:E:164:THR:HB	1:E:186:TRP:CD1	2.45	0.52
3:L:1:DG:H1'	3:L:2:DC:C6	2.44	0.52
1:A:195:SER:HB2	1:A:200:ILE:HD11	1.90	0.52
1:F:169:ARG:O	1:F:172:GLN:HG2	2.10	0.52
1:C:2:HIS:CE1	1:G:40:PRO:HD3	2.45	0.52
1:E:53:TYR:CZ	1:E:55:GLY:HA3	2.44	0.52
1:F:206:GLN:HG2	5:F:319:HOH:O	2.08	0.52
1:A:169:ARG:HG2	1:H:169:ARG:CG	2.37	0.52
1:E:176:ASP:HA	1:E:179:VAL:HG13	1.91	0.52
1:A:137:MET:O	1:A:138:ILE:C	2.48	0.52
1:A:18:PHE:HA	1:A:21:LEU:HD12	1.92	0.52
1:E:67:ASN:ND2	1:E:73:LEU:H	2.05	0.52
1:F:175:SER:O	1:F:179:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PRO:HB2	1:A:154:ASN:HD22	1.74	0.51
1:E:2:HIS:HE1	1:F:40:PRO:HG3	1.75	0.51
1:E:10:GLU:HG2	1:F:33:PRO:HG3	1.93	0.51
2:I:19:DC:H2''	2:I:20:DC:OP2	2.10	0.51
2:M:3:DG:H2''	2:M:4:DG:OP2	2.09	0.51
1:D:29:PHE:HD1	1:D:128:VAL:HG23	1.74	0.51
1:G:48:VAL:CG2	1:G:138:ILE:HG23	2.40	0.51
1:G:57:TYR:CE2	1:G:59:LEU:HD12	2.45	0.51
2:O:21:DG:N1	3:P:2:DC:N3	2.47	0.51
1:D:29:PHE:CD1	1:D:128:VAL:HG23	2.46	0.51
2:I:20:DC:OP2	2:I:20:DC:H2'	2.10	0.51
2:I:3:DG:H2''	2:I:4:DG:OP2	2.10	0.51
1:C:162:ASN:ND2	3:J:12:DC:H5	2.07	0.51
2:K:19:DC:H1'	2:K:20:DC:H5'	1.93	0.51
1:G:50:ALA:O	1:G:125:CYS:HA	2.09	0.51
3:J:17:DC:H2''	3:J:18:DT:OP2	2.10	0.51
2:M:9:DC:H2'	2:M:10:DC:C6	2.45	0.51
1:F:151:PRO:HB2	1:F:154:ASN:HD22	1.76	0.51
1:C:77:VAL:H	1:C:154:ASN:ND2	1.95	0.51
1:H:198:TYR:O	1:H:202:GLU:HB2	2.11	0.51
2:I:21:DG:H2''	2:K:1:DC:C5'	2.40	0.50
2:M:1:DC:H1'	2:M:2:DG:N7	2.26	0.50
1:E:204:ILE:O	1:E:205:LYS:C	2.50	0.50
1:H:52:TYR:O	1:H:123:PHE:HA	2.12	0.50
1:B:2:HIS:CB	1:B:3:ASN:CA	2.80	0.50
3:J:20:DC:H2'	3:J:20:DC:OP2	2.11	0.50
1:C:66:ILE:HG23	1:H:198:TYR:CZ	2.47	0.50
1:C:95:THR:CG2	1:C:96:ARG:N	2.75	0.49
1:G:141:VAL:O	1:G:142:GLU:C	2.49	0.49
3:P:19:DC:H2''	3:P:20:DC:OP2	2.12	0.49
1:F:162:ASN:ND2	5:F:252:HOH:O	2.44	0.49
1:C:2:HIS:CE1	1:G:40:PRO:HG3	2.44	0.49
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.76	0.49
1:C:185:GLU:CD	1:C:185:GLU:H	2.15	0.49
2:O:8:DC:C5'	5:O:240:HOH:O	2.60	0.49
1:D:162:ASN:HD21	2:K:11:DG:H2'	1.77	0.49
3:J:4:DG:H1'	3:J:5:DC:C6	2.47	0.49
2:I:21:DG:H8	2:K:1:DC:OP1	1.89	0.49
1:C:34:VAL:HG11	1:C:71:TYR:CE2	2.48	0.49
1:B:49:PHE:CZ	1:B:78:GLY:HA3	2.48	0.49
1:D:203:ARG:NH1	4:D:216:PO4:O3	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:5:DC:H2''	3:N:6:DG:OP2	2.11	0.49
2:O:1:DC:H1'	2:O:2:DG:C8	2.46	0.49
1:B:29:PHE:HD1	1:B:128:VAL:HG23	1.73	0.49
1:C:85:TRP:HA	5:C:461:HOH:O	2.12	0.49
1:B:178:ASP:CG	1:B:184:ARG:HH11	2.16	0.49
1:H:180:ILE:CG2	1:H:200:ILE:HG21	2.43	0.49
1:H:101:LEU:HD21	1:H:127:PHE:HB2	1.94	0.48
1:D:162:ASN:ND2	2:K:11:DG:H2'	2.28	0.48
1:H:152:LEU:HD12	1:H:156:VAL:HB	1.94	0.48
1:G:85:TRP:CB	2:I:15:DG:OP1	2.61	0.48
2:K:13:DG:H4'	2:K:14:DG:OP1	2.12	0.48
1:C:195:SER:HB2	1:C:200:ILE:HD11	1.95	0.48
1:F:164:THR:HG22	1:F:166:GLY:N	2.26	0.48
1:G:19:LEU:HA	1:G:22:ILE:HD11	1.93	0.48
1:H:29:PHE:HD1	1:H:128:VAL:HG23	1.76	0.48
3:N:20:DC:H2''	3:N:21:DC:C6	2.48	0.48
1:B:44:GLN:HA	1:B:99:SER:CB	2.43	0.48
2:K:15:DG:H2''	2:K:16:DC:OP2	2.13	0.48
2:M:1:DC:H4'	2:M:2:DG:O5'	2.13	0.48
3:N:19:DC:OP2	3:N:19:DC:H2'	2.12	0.48
1:A:81:VAL:HG11	1:A:85:TRP:CD1	2.48	0.48
1:H:176:ASP:OD2	1:H:195:SER:OG	2.26	0.48
2:M:19:DC:H1'	2:M:20:DC:H5'	1.96	0.48
1:A:119:ASP:OD2	1:A:121:CYS:HB2	2.14	0.48
1:A:67:ASN:HD22	1:A:72:ASN:H	1.62	0.48
3:J:3:DG:H2'	3:J:3:DG:OP2	2.14	0.48
2:M:1:DC:O4'	2:M:1:DC:O2	2.31	0.48
1:H:164:THR:HG23	3:N:8:DC:C6	2.48	0.48
1:A:106:ARG:NH1	1:A:106:ARG:HG2	2.28	0.48
1:C:169:ARG:O	1:C:172:GLN:HG2	2.14	0.48
2:K:3:DG:H2''	2:K:4:DG:OP2	2.14	0.48
1:A:181:HIS:O	1:A:182:PRO:C	2.49	0.48
1:A:49:PHE:CZ	1:A:78:GLY:HA3	2.48	0.48
1:B:137:MET:HE1	1:D:13:TYR:HE1	1.79	0.48
1:D:2:HIS:HD2	1:D:2:HIS:N	2.10	0.48
1:B:178:ASP:OD1	1:B:184:ARG:HD2	2.14	0.47
1:B:176:ASP:O	1:B:179:VAL:HG13	2.13	0.47
1:A:168:GLY:HA2	1:H:171:ALA:CB	2.43	0.47
1:C:196:GLU:HG3	5:C:412:HOH:O	2.14	0.47
2:M:17:DC:H2''	2:M:18:DG:C8	2.49	0.47
1:F:7:ASP:OD1	1:F:9:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3:DG:H1'	2:I:4:DG:H5'	1.96	0.47
3:J:1:DG:H4'	3:J:2:DC:OP1	2.14	0.47
1:C:168:GLY:HA2	1:G:171:ALA:HB1	1.95	0.47
1:B:137:MET:CE	1:D:15:ASN:HB3	2.44	0.47
1:H:149:TYR:O	1:H:150:LYS:C	2.50	0.47
1:B:27:ARG:HH11	1:B:27:ARG:CG	2.17	0.47
1:A:131:GLU:HG3	1:H:12:VAL:HG13	1.96	0.47
2:I:22:DC:H3'	2:K:2:DG:H5'	1.95	0.47
1:C:95:THR:HG23	1:C:96:ARG:N	2.29	0.47
1:A:73:LEU:HD12	1:A:74:PRO:HD2	1.96	0.46
1:C:199:PHE:O	1:C:203:ARG:CG	2.62	0.46
1:B:169:ARG:HE	1:D:172:GLN:HE22	1.60	0.46
2:K:17:DC:H2''	2:K:18:DG:C8	2.51	0.46
1:A:14:ARG:CG	1:A:14:ARG:NH1	2.67	0.46
1:A:14:ARG:NH1	1:A:14:ARG:HG2	2.08	0.46
1:B:15:ASN:ND2	1:B:15:ASN:C	2.66	0.46
1:C:49:PHE:CD1	1:C:49:PHE:C	2.88	0.46
1:C:88:SER:O	1:C:89:ARG:HG2	2.15	0.46
1:E:57:TYR:CE2	1:E:59:LEU:HD12	2.51	0.46
1:G:9:SER:O	1:G:11:HIS:N	2.47	0.46
1:D:114:LYS:NZ	1:D:185:GLU:OE2	2.46	0.46
1:E:164:THR:HA	1:E:165:PRO:HD3	1.76	0.46
1:B:29:PHE:CD1	1:B:128:VAL:CG2	2.97	0.46
1:C:2:HIS:HA	1:G:35:HIS:HA	1.97	0.46
1:D:152:LEU:HD12	1:D:156:VAL:HB	1.97	0.46
1:E:135:SER:O	1:E:136:ASP:C	2.54	0.46
1:G:67:ASN:HD22	1:G:72:ASN:H	1.64	0.46
1:G:67:ASN:ND2	1:G:72:ASN:H	2.13	0.46
1:A:171:ALA:HB3	1:H:168:GLY:CA	2.43	0.46
1:F:164:THR:N	4:F:216:PO4:O1	2.49	0.46
2:I:1:DC:H1'	2:I:2:DG:C8	2.51	0.46
1:A:11:HIS:CE1	1:H:33:PRO:HD2	2.51	0.46
1:G:164:THR:HA	1:G:165:PRO:HD3	1.80	0.46
1:G:46:ALA:HB1	1:G:80:ALA:O	2.16	0.46
1:B:77:VAL:N	1:B:154:ASN:HD21	2.02	0.46
1:G:9:SER:C	1:G:11:HIS:H	2.19	0.45
1:A:137:MET:HE1	1:H:15:ASN:HB3	1.99	0.45
1:B:95:THR:CB	1:B:96:ARG:CA	2.94	0.45
1:G:151:PRO:HB2	1:G:154:ASN:HD22	1.80	0.45
1:D:28:PHE:O	1:D:29:PHE:C	2.54	0.45
1:E:48:VAL:HG23	1:E:138:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:ILE:HG13	1:H:181:HIS:CD2	2.52	0.45
3:P:3:DG:H2'	3:P:3:DG:OP2	2.16	0.45
1:A:23:LYS:O	1:A:27:ARG:HB2	2.17	0.45
1:B:87:GLN:O	1:D:155:THR:HG22	2.16	0.45
1:D:110:ARG:NH2	3:L:6:DG:P	2.89	0.45
1:C:140:THR:OG1	1:G:140:THR:OG1	2.28	0.45
1:D:29:PHE:HD1	1:D:128:VAL:CG2	2.30	0.45
2:K:5:DA:H2''	2:K:6:DG:H8	1.82	0.45
1:D:86:ARG:HD2	3:L:12:DC:H5'	1.99	0.45
1:F:29:PHE:CD1	1:F:128:VAL:HG23	2.52	0.45
1:A:77:VAL:H	1:A:154:ASN:ND2	2.07	0.44
1:H:29:PHE:HD1	1:H:128:VAL:CG2	2.30	0.44
1:D:67:ASN:ND2	1:D:73:LEU:H	2.06	0.44
1:H:48:VAL:HG23	1:H:138:ILE:HG23	1.99	0.44
1:F:162:ASN:ND2	3:P:11:DG:H2'	2.31	0.44
1:D:184:ARG:O	1:D:185:GLU:C	2.55	0.44
1:B:37:LEU:HD12	1:B:38:PRO:CA	2.46	0.44
1:C:203:ARG:HG3	1:C:203:ARG:NH1	2.33	0.44
1:D:101:LEU:HD21	1:D:127:PHE:HB2	1.98	0.44
1:F:49:PHE:C	1:F:49:PHE:CD1	2.91	0.44
1:G:165:PRO:HD3	1:G:186:TRP:CE3	2.52	0.44
3:N:1:DG:C1'	3:N:2:DC:C5	2.96	0.44
1:E:199:PHE:O	1:E:203:ARG:HG3	2.17	0.44
1:D:104:ARG:NH1	5:D:318:HOH:O	2.50	0.44
1:D:15:ASN:HD21	1:D:18:PHE:H	1.66	0.44
2:O:21:DG:C2	2:O:22:DC:C2	3.06	0.44
1:A:62:GLU:O	1:A:65:ARG:HB3	2.18	0.44
1:B:46:ALA:HB1	1:B:80:ALA:O	2.18	0.44
1:E:155:THR:HB	1:F:86:ARG:CA	2.47	0.44
1:G:84:GLY:CA	1:G:85:TRP:CB	2.95	0.44
1:B:165:PRO:HD3	1:B:186:TRP:CE3	2.53	0.44
1:C:169:ARG:NH2	1:G:172:GLN:HE22	2.14	0.44
3:L:5:DC:H5'	5:L:249:HOH:O	2.17	0.44
1:E:172:GLN:NE2	1:F:169:ARG:HE	2.16	0.43
1:F:165:PRO:CD	1:F:186:TRP:CE3	3.01	0.43
1:D:47:GLY:HA2	1:D:138:ILE:CD1	2.48	0.43
2:K:3:DG:H2'	2:K:3:DG:OP2	2.17	0.43
1:A:48:VAL:HG12	1:A:49:PHE:N	2.34	0.43
1:B:60:TYR:HB3	1:B:63:TYR:HD2	1.83	0.43
1:H:195:SER:HB3	4:H:216:PO4:O4	2.17	0.43
1:B:51:LEU:HD22	1:B:76:TYR:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ALA:CB	1:A:101:LEU:HA	2.48	0.43
1:E:204:ILE:O	1:E:207:TYR:N	2.51	0.43
1:A:185:GLU:H	1:A:185:GLU:CD	2.22	0.43
1:B:47:GLY:HA3	1:B:128:VAL:O	2.18	0.43
1:B:84:GLY:HA3	1:B:90:ILE:HD13	2.00	0.43
1:H:178:ASP:OD1	1:H:184:ARG:HD2	2.18	0.43
1:C:110:ARG:NH2	2:I:6:DG:OP2	2.52	0.43
3:P:8:DC:C5'	5:P:290:HOH:O	2.62	0.43
1:A:200:ILE:O	1:A:204:ILE:HG13	2.19	0.43
1:H:150:LYS:N	1:H:151:PRO:HD3	2.34	0.43
1:E:34:VAL:HG22	1:E:126:ARG:HG3	2.01	0.43
1:G:81:VAL:HG11	1:G:86:ARG:CB	2.49	0.43
2:I:15:DG:H2'	2:I:15:DG:O5'	2.19	0.42
1:A:2:HIS:HA	1:H:35:HIS:HA	2.00	0.42
1:E:57:TYR:O	1:E:58:SER:C	2.58	0.42
1:H:7:ASP:O	1:H:8:ARG:C	2.57	0.42
1:D:164:THR:CG2	3:L:8:DC:C5	3.02	0.42
1:D:167:ALA:C	1:D:169:ARG:H	2.23	0.42
1:D:175:SER:O	1:D:179:VAL:HG12	2.18	0.42
1:D:37:LEU:HD12	1:D:38:PRO:HA	2.01	0.42
1:H:175:SER:O	1:H:176:ASP:C	2.57	0.42
1:C:34:VAL:HG11	1:C:71:TYR:CD2	2.55	0.42
1:E:101:LEU:HD21	1:E:127:PHE:HB2	2.00	0.42
1:H:180:ILE:HG21	1:H:200:ILE:HG21	2.01	0.42
3:P:6:DG:H1'	3:P:7:DG:H5'	2.01	0.42
1:C:40:PRO:HD3	1:G:2:HIS:HE1	1.83	0.42
1:E:48:VAL:HG12	1:E:49:PHE:N	2.34	0.42
1:F:45:GLY:H	1:F:99:SER:HA	1.84	0.42
1:G:2:HIS:HB2	1:G:3:ASN:H	1.63	0.42
3:J:2:DC:H2''	3:J:3:DG:OP2	2.19	0.42
2:O:19:DC:H2''	2:O:20:DC:OP2	2.20	0.42
1:A:176:ASP:HA	1:A:179:VAL:CG1	2.49	0.42
1:C:29:PHE:CD1	1:C:128:VAL:HG23	2.54	0.42
1:C:62:GLU:CA	1:C:62:GLU:OE2	2.64	0.42
1:F:2:HIS:ND1	5:F:430:HOH:O	2.40	0.42
1:G:182:PRO:HA	1:G:183:GLY:HA2	1.90	0.42
2:O:9:DC:H2''	2:O:10:DC:H5'	2.01	0.42
1:B:80:ALA:CB	1:B:101:LEU:HA	2.50	0.42
1:D:194:HIS:CD2	1:D:194:HIS:C	2.93	0.42
1:H:185:GLU:OE1	1:H:185:GLU:N	2.53	0.42
1:A:131:GLU:O	1:A:132:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLU:O	1:B:197:PRO:C	2.56	0.42
1:C:15:ASN:HD22	1:C:15:ASN:C	2.23	0.42
1:E:83:ALA:HB2	5:E:228:HOH:O	2.20	0.42
1:E:86:ARG:O	1:E:88:SER:N	2.53	0.42
2:M:3:DG:H8	2:M:3:DG:OP2	2.03	0.42
1:A:103:ASN:ND2	5:A:302:HOH:O	2.53	0.41
1:A:151:PRO:O	1:A:154:ASN:HB2	2.20	0.41
1:A:35:HIS:O	1:A:124:SER:HB3	2.20	0.41
1:C:67:ASN:HD22	1:C:72:ASN:H	1.68	0.41
1:D:48:VAL:HG23	1:D:138:ILE:HG23	2.01	0.41
1:B:159:GLY:HA3	1:B:175:SER:CB	2.51	0.41
1:D:52:TYR:O	1:D:123:PHE:HA	2.20	0.41
1:F:37:LEU:HA	1:F:38:PRO:HA	1.90	0.41
1:B:182:PRO:HA	1:B:183:GLY:HA2	1.87	0.41
1:H:104:ARG:HH12	1:H:163:HIS:CE1	2.37	0.41
1:D:42:ARG:NH1	3:L:5:DC:OP1	2.53	0.41
1:C:157:VAL:HG11	1:C:180:ILE:HD11	2.03	0.41
1:E:132:ALA:O	1:E:133:THR:OG1	2.30	0.41
1:H:67:ASN:HD22	1:H:72:ASN:H	1.66	0.41
2:I:20:DC:H2''	2:I:21:DG:H8	1.83	0.41
3:J:7:DG:H2'	3:J:7:DG:O5'	2.20	0.41
2:O:7:DG:H1'	2:O:8:DC:H5'	2.03	0.41
1:B:28:PHE:O	1:B:32:THR:HG23	2.21	0.41
1:C:152:LEU:HD12	1:C:156:VAL:HB	2.03	0.41
1:H:2:HIS:O	1:H:3:ASN:CB	2.68	0.41
1:C:151:PRO:HG2	1:C:154:ASN:HD22	1.85	0.41
1:D:65:ARG:HB3	1:D:65:ARG:HE	1.63	0.41
1:G:22:ILE:HD12	1:G:23:LYS:H	1.85	0.41
1:A:169:ARG:HE	1:H:172:GLN:HE22	1.67	0.41
1:D:63:TYR:C	1:D:65:ARG:N	2.73	0.41
1:G:199:PHE:O	1:G:203:ARG:CG	2.68	0.41
1:A:115:THR:OG1	1:A:118:LEU:HB2	2.21	0.41
1:A:27:ARG:CG	1:A:27:ARG:NH1	2.80	0.41
1:B:202:GLU:O	1:B:203:ARG:C	2.59	0.41
1:D:165:PRO:HD2	1:D:186:TRP:CE3	2.56	0.41
1:G:10:GLU:OE1	1:G:10:GLU:HA	2.21	0.41
1:B:35:HIS:O	1:B:124:SER:HB3	2.21	0.41
1:E:2:HIS:CE1	1:F:40:PRO:HG3	2.55	0.41
3:L:8:DC:C5'	5:L:155:HOH:O	2.56	0.41
1:B:137:MET:HE1	1:D:13:TYR:CE1	2.57	0.40
1:D:177:TRP:HZ3	1:D:184:ARG:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:LEU:HD12	1:G:38:PRO:HA	2.02	0.40
1:B:89:ARG:HE	1:B:89:ARG:HA	1.87	0.40
1:C:47:GLY:HA3	1:C:128:VAL:O	2.21	0.40
1:A:137:MET:CE	1:H:15:ASN:HB3	2.51	0.40
1:E:158:ASP:HB3	2:O:11:DG:H5"	2.04	0.40
2:O:2:DG:H2"	2:O:3:DG:OP2	2.21	0.40
1:C:206:GLN:NE2	5:C:320:HOH:O	2.54	0.40
1:D:195:SER:HB2	1:D:200:ILE:HD11	2.03	0.40
1:D:194:HIS:HE1	4:D:215:PO4:O3	2.03	0.40
1:F:165:PRO:HD3	1:F:186:TRP:CZ3	2.56	0.40
1:F:83:ALA:HA	1:F:84:GLY:HA3	1.78	0.40
1:H:172:GLN:O	1:H:190:CYS:HB3	2.21	0.40
1:G:162:ASN:HD22	2:I:12:DC:H5	1.69	0.40
2:M:2:DG:H2"	2:M:3:DG:OP2	2.21	0.40
1:A:162:ASN:HD22	1:A:162:ASN:N	2.19	0.40
1:A:29:PHE:CD1	1:A:128:VAL:CG2	3.04	0.40
1:A:67:ASN:ND2	1:A:72:ASN:N	2.69	0.40
1:F:199:PHE:O	1:F:203:ARG:HG2	2.22	0.40
1:H:175:SER:O	1:H:179:VAL:HG12	2.21	0.40
1:B:7:ASP:O	1:B:11:HIS:HD2	2.05	0.40
1:E:182:PRO:HA	1:E:183:GLY:HA2	1.84	0.40
1:E:22:ILE:HA	1:E:22:ILE:HD12	1.84	0.40
1:F:203:ARG:HG3	1:F:203:ARG:NH1	2.36	0.40
1:G:47:GLY:HA2	1:G:138:ILE:HG12	2.03	0.40
1:H:42:ARG:NH1	3:N:5:DC:OP1	2.54	0.40

All (1) 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:B:61:ASP:OD1	1:F:133:THR:OG1[2_656]	2.16	0.04

## 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	208/235 (88%)	183 (88%)	21 (10%)	4 (2%)	8	26
1	B	208/235 (88%)	189 (91%)	16 (8%)	3 (1%)	11	34
1	C	207/235 (88%)	182 (88%)	20 (10%)	5 (2%)	6	20
1	D	207/235 (88%)	183 (88%)	20 (10%)	4 (2%)	8	26
1	E	207/235 (88%)	183 (88%)	18 (9%)	6 (3%)	4	15
1	F	207/235 (88%)	183 (88%)	18 (9%)	6 (3%)	4	15
1	G	207/235 (88%)	184 (89%)	16 (8%)	7 (3%)	3	13
1	H	207/235 (88%)	176 (85%)	24 (12%)	7 (3%)	3	13
All	All	1658/1880 (88%)	1463 (88%)	153 (9%)	42 (2%)	5	19

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ALA
1	B	90	ILE
1	B	132	ALA
1	C	90	ILE
1	D	10	GLU
1	D	185	GLU
1	E	83	ALA
1	E	87	GLN
1	F	83	ALA
1	F	94	GLU
1	G	10	GLU
1	G	88	SER
1	G	96	ARG
1	G	132	ALA
1	C	9	SER
1	E	3	ASN
1	E	91	SER
1	F	95	THR
1	H	3	ASN
1	H	91	SER
1	B	93	HIS
1	C	86	ARG
1	E	84	GLY
1	E	86	ARG

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Mol	Chain	Res	Type
1	G	89	ARG
1	H	93	HIS
1	H	132	ALA
1	H	139	SER
1	H	185	GLU
1	A	17	SER
1	A	95	THR
1	C	88	SER
1	D	132	ALA
1	F	85	TRP
1	F	89	ARG
1	G	4	LYS
1	C	85	TRP
1	D	89	ARG
1	F	90	ILE
1	G	90	ILE
1	H	90	ILE
1	A	138	ILE

### 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	171/201 (85%)	160 (94%)	11 (6%)	17	45
1	B	174/201 (87%)	157 (90%)	17 (10%)	8	24
1	C	165/201 (82%)	147 (89%)	18 (11%)	6	19
1	D	167/201 (83%)	147 (88%)	20 (12%)	5	15
1	E	163/201 (81%)	150 (92%)	13 (8%)	12	34
1	F	164/201 (82%)	153 (93%)	11 (7%)	16	43
1	G	160/201 (80%)	146 (91%)	14 (9%)	10	29
1	H	166/201 (83%)	155 (93%)	11 (7%)	16	44
All	All	1330/1608 (83%)	1215 (91%)	115 (9%)	10	30

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	9	SER
1	A	14	ARG
1	A	27	ARG
1	A	51	LEU
1	A	81	VAL
1	A	90	ILE
1	A	124	SER
1	A	179	VAL
1	A	184	ARG
1	A	205	LYS
1	B	10	GLU
1	B	14	ARG
1	B	15	ASN
1	B	21	LEU
1	B	27	ARG
1	B	51	LEU
1	B	68	ARG
1	B	85	TRP
1	B	89	ARG
1	B	90	ILE
1	B	119	ASP
1	B	133	THR
1	B	179	VAL
1	B	188	GLU
1	B	197	PRO
1	B	205	LYS
1	B	210	LYS
1	C	8	ARG
1	C	9	SER
1	C	14	ARG
1	C	15	ASN
1	C	18	PHE
1	C	19	LEU
1	C	21	LEU
1	C	68	ARG
1	C	81	VAL
1	C	89	ARG
1	C	92	ASP
1	C	95	THR
1	C	100	GLU
1	C	102	SER
1	C	131	GLU

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Mol	Chain	Res	Type
1	C	164	THR
1	C	179	VAL
1	C	188	GLU
1	D	2	HIS
1	D	8	ARG
1	D	9	SER
1	D	15	ASN
1	D	19	LEU
1	D	51	LEU
1	D	65	ARG
1	D	81	VAL
1	D	85	TRP
1	D	86	ARG
1	D	110	ARG
1	D	116	SER
1	D	139	SER
1	D	158	ASP
1	D	164	THR
1	D	179	VAL
1	D	184	ARG
1	D	185	GLU
1	D	194	HIS
1	D	206	GLN
1	E	2	HIS
1	E	10	GLU
1	E	15	ASN
1	E	27	ARG
1	E	65	ARG
1	E	104	ARG
1	E	133	THR
1	E	135	SER
1	E	139	SER
1	E	164	THR
1	E	179	VAL
1	E	185	GLU
1	E	209	SER
1	F	14	ARG
1	F	18	PHE
1	F	65	ARG
1	F	68	ARG
1	F	81	VAL
1	F	104	ARG

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Mol	Chain	Res	Type
1	F	107	GLU
1	F	179	VAL
1	F	185	GLU
1	F	195	SER
1	F	206	GLN
1	G	19	LEU
1	G	22	ILE
1	G	27	ARG
1	G	44	GLN
1	G	51	LEU
1	G	124	SER
1	G	164	THR
1	G	174	LYS
1	G	179	VAL
1	G	188	GLU
1	G	195	SER
1	G	196	GLU
1	G	203	ARG
1	G	206	GLN
1	H	2	HIS
1	H	19	LEU
1	H	21	LEU
1	H	30	SER
1	H	51	LEU
1	H	68	ARG
1	H	81	VAL
1	H	86	ARG
1	H	139	SER
1	H	179	VAL
1	H	202	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	44	GLN
1	A	67	ASN
1	A	103	ASN
1	A	154	ASN
1	A	162	ASN
1	A	172	GLN
1	B	15	ASN

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Mol	Chain	Res	Type
1	B	35	HIS
1	B	67	ASN
1	B	103	ASN
1	B	154	ASN
1	B	162	ASN
1	B	172	GLN
1	C	2	HIS
1	C	15	ASN
1	C	35	HIS
1	C	44	GLN
1	C	67	ASN
1	C	103	ASN
1	C	154	ASN
1	C	162	ASN
1	C	172	GLN
1	C	206	GLN
1	D	44	GLN
1	D	67	ASN
1	D	103	ASN
1	D	154	ASN
1	D	162	ASN
1	D	172	GLN
1	D	194	HIS
1	E	2	HIS
1	E	15	ASN
1	E	35	HIS
1	E	44	GLN
1	E	67	ASN
1	E	103	ASN
1	E	154	ASN
1	E	162	ASN
1	E	172	GLN
1	F	2	HIS
1	F	35	HIS
1	F	44	GLN
1	F	67	ASN
1	F	154	ASN
1	F	162	ASN
1	F	172	GLN
1	G	35	HIS
1	G	44	GLN
1	G	67	ASN

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Mol	Chain	Res	Type
1	G	103	ASN
1	G	154	ASN
1	G	162	ASN
1	G	172	GLN
1	G	206	GLN
1	H	15	ASN
1	H	44	GLN
1	H	56	HIS
1	H	67	ASN
1	H	103	ASN
1	H	162	ASN
1	H	172	GLN
1	H	206	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](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PO4	D	215	-	4,4,4	0.92	0	6,6,6	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PO4	B	215	-	4,4,4	0.83	0	6,6,6	0.45	0
4	PO4	F	216	-	4,4,4	0.78	0	6,6,6	0.60	0
4	PO4	B	216	-	4,4,4	1.04	0	6,6,6	0.67	0
4	PO4	D	216	-	4,4,4	1.22	0	6,6,6	0.46	0
4	PO4	E	215	-	4,4,4	0.79	0	6,6,6	0.61	0
4	PO4	A	215	-	4,4,4	1.03	0	6,6,6	0.54	0
4	PO4	G	215	-	4,4,4	1.01	0	6,6,6	0.50	0
4	PO4	H	216	-	4,4,4	1.10	0	6,6,6	0.87	0
4	PO4	H	215	-	4,4,4	0.92	0	6,6,6	0.70	0
4	PO4	F	215	-	4,4,4	0.90	0	6,6,6	0.54	0

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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	215	PO4	1	0
4	F	216	PO4	1	0
4	D	216	PO4	1	0
4	H	216	PO4	3	0

## 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	210/235 (89%)	-0.13	10 (4%) 30 21	21, 36, 79, 99	0
1	B	210/235 (89%)	-0.10	6 (2%) 51 41	18, 34, 75, 106	0
1	C	209/235 (88%)	-0.04	3 (1%) 75 70	20, 33, 69, 102	0
1	D	209/235 (88%)	0.02	8 (3%) 40 30	22, 45, 77, 94	0
1	E	209/235 (88%)	0.04	10 (4%) 30 21	22, 38, 76, 123	0
1	F	209/235 (88%)	-0.04	6 (2%) 51 41	20, 32, 77, 95	0
1	G	209/235 (88%)	-0.01	6 (2%) 51 41	21, 38, 73, 103	0
1	H	209/235 (88%)	0.00	6 (2%) 51 41	29, 48, 77, 97	0
2	I	22/22 (100%)	-0.08	0 100 100	22, 69, 113, 127	0
2	K	22/22 (100%)	-0.02	0 100 100	26, 58, 109, 125	0
2	M	22/22 (100%)	0.12	0 100 100	30, 64, 111, 134	0
2	O	22/22 (100%)	0.06	1 (4%) 33 23	23, 69, 135, 146	0
3	J	22/22 (100%)	0.06	0 100 100	21, 64, 121, 139	0
3	L	22/22 (100%)	0.01	0 100 100	21, 60, 98, 122	0
3	N	22/22 (100%)	0.00	0 100 100	23, 63, 114, 134	0
3	P	22/22 (100%)	0.08	1 (4%) 33 23	25, 64, 123, 140	0
All	All	1850/2056 (89%)	-0.03	57 (3%) 49 39	18, 38, 91, 146	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	HIS	9.3
1	C	95	THR	7.3
1	E	93	HIS	6.9
1	E	88	SER	6.6
1	D	3	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
1	G	92	ASP	6.4
1	B	92	ASP	5.9
1	H	93	HIS	5.6
1	C	96	ARG	5.0
1	D	92	ASP	5.0
1	H	3	ASN	4.9
1	F	3	ASN	4.8
1	E	95	THR	4.8
1	G	95	THR	4.8
1	F	93	HIS	4.8
1	F	94	GLU	4.7
1	A	91	SER	4.7
1	E	90	ILE	4.2
1	E	91	SER	4.2
1	E	92	ASP	4.1
1	D	2	HIS	4.0
1	A	95	THR	3.9
1	E	89	ARG	3.8
1	E	1	GLY	3.8
1	D	93	HIS	3.7
1	C	3	ASN	3.4
1	A	4	LYS	3.3
1	B	96	ARG	3.3
1	G	91	SER	3.3
1	G	87	GLN	3.3
1	G	94	GLU	3.1
1	A	92	ASP	3.0
1	H	2	HIS	3.0
1	F	90	ILE	2.9
1	D	4	LYS	2.9
1	A	94	GLU	2.8
1	G	90	ILE	2.8
1	A	93	HIS	2.8
1	B	94	GLU	2.7
1	B	95	THR	2.7
3	P	22	DG	2.6
1	H	92	ASP	2.6
1	D	91	SER	2.5
1	F	2	HIS	2.5
1	A	3	ASN	2.4
1	H	94	GLU	2.4
1	A	211	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	97	ALA	2.4
1	D	42	ARG	2.3
1	H	42	ARG	2.2
1	E	96	ARG	2.2
1	F	88	SER	2.2
1	E	94	GLU	2.1
2	O	2	DG	2.1
1	B	211	SER	2.1
1	A	10	GLU	2.0
1	A	7	ASP	2.0

## 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	PO4	B	215	5/5	0.70	0.40	109,110,110,110	0
4	PO4	F	215	5/5	0.84	0.29	115,115,115,115	0
4	PO4	E	215	5/5	0.87	0.31	100,100,101,101	0
4	PO4	G	215	5/5	0.87	0.26	101,101,101,102	0
4	PO4	D	215	5/5	0.87	0.21	100,101,101,101	0
4	PO4	F	216	5/5	0.88	0.38	104,104,105,105	0
4	PO4	A	215	5/5	0.88	0.22	75,76,77,78	0
4	PO4	H	216	5/5	0.89	0.16	66,66,67,68	0
4	PO4	D	216	5/5	0.92	0.16	75,75,76,77	0
4	PO4	H	215	5/5	0.93	0.21	89,89,90,91	0
4	PO4	B	216	5/5	0.94	0.15	73,73,74,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.