



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:24 am BST

PDB ID : 5UK7  
Title : Escherichia coli Hfq bound to dsDNA  
Authors : Orans, J.; Kovach, A.R.; Brennan, R.G.  
Deposited on : 2017-01-20  
Resolution : 3.00 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.

---

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

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

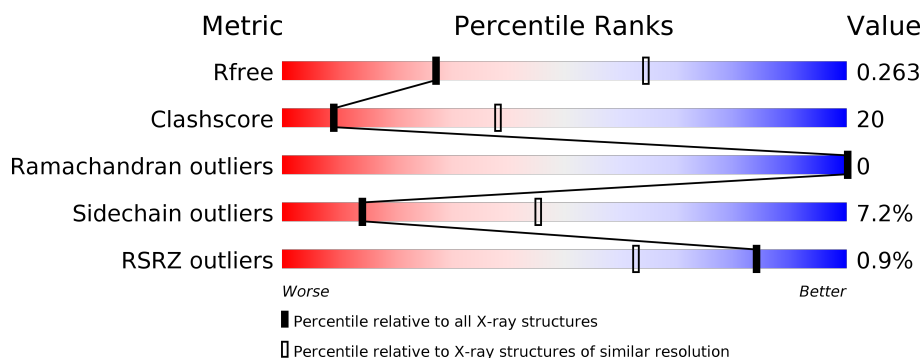
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	68	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>•</div> <div>6%</div> </div> </div>
1	B	68	<div> <div>74%</div> <div>18%</div> <div>•</div> <div>•</div> </div>
1	C	68	<div> <div>54%</div> <div>35%</div> <div>6%</div> <div>•</div> </div>
1	D	68	<div> <div>74%</div> <div>22%</div> <div>•</div> </div>
1	E	68	<div> <div>60%</div> <div>28%</div> <div>9%</div> <div>•</div> </div>
1	F	68	<div> <div>3%</div> <div>59%</div> <div>25%</div> <div>12%</div> <div>•</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	68	<div><div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div></div><div>65%</div><div>31%</div><div>• •</div></div>
1	H	68	<div><div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div></div><div>74%</div><div>18%</div><div>• •</div></div>
1	I	68	<div><div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div></div><div>65%</div><div>28%</div><div>• •</div></div>
1	J	68	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>72%</div><div>16%</div><div>7%</div><div>•</div></div>
1	K	68	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>66%</div><div>28%</div><div>• •</div></div>
1	L	68	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>60%</div><div>28%</div><div>9%</div><div>•</div></div>
2	N	20	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>40%</div><div>50%</div><div>10%</div></div>
2	Z	20	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>15%</div><div>65%</div><div>20%</div></div>
3	M	20	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>10%</div><div>55%</div><div>35%</div></div>
3	Y	20	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>15%</div><div>30%</div><div>55%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8044 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 RNA-binding protein Hfq.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			506	326	88	91	1			
1	B	67	Total	C	N	O	S	0	0	0
			531	342	94	94	1			
1	C	67	Total	C	N	O	S	0	0	0
			531	342	94	94	1			
1	D	67	Total	C	N	O	S	0	0	0
			531	342	94	94	1			
1	E	66	Total	C	N	O	S	0	0	0
			524	337	93	93	1			
1	F	65	Total	C	N	O	S	0	0	0
			517	332	92	92	1			
1	G	67	Total	C	N	O	S	0	0	0
			531	342	94	94	1			
1	H	65	Total	C	N	O	S	0	0	0
			517	333	91	92	1			
1	I	65	Total	C	N	O	S	0	0	0
			517	333	91	92	1			
1	J	65	Total	C	N	O	S	0	0	0
			511	329	89	92	1			
1	K	68	Total	C	N	O	S	0	0	0
			537	345	95	96	1			
1	L	66	Total	C	N	O	S	0	0	0
			522	335	93	93	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	20	Total	C	N	O	P	0	0	0
			416	196	92	108	20			
2	Z	20	Total	C	N	O	P	0	0	0
			416	196	92	108	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	20	Total	C	N	O	P	0	0	0
			404	196	56	132	20			
3	Y	20	Total	C	N	O	P	0	0	0
			404	196	56	132	20			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	8	Total	O	0	0
			8	8		

*Continued on next page...*

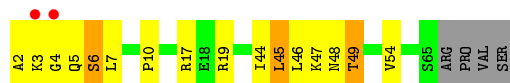
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	8	Total 8	O 8	0	0
5	D	11	Total 11	O 11	0	0
5	E	10	Total 10	O 10	0	0
5	F	11	Total 11	O 11	0	0
5	G	8	Total 8	O 8	0	0
5	H	12	Total 12	O 12	0	0
5	I	14	Total 14	O 14	0	0
5	J	9	Total 9	O 9	0	0
5	K	8	Total 8	O 8	0	0
5	L	11	Total 11	O 11	0	0
5	M	1	Total 1	O 1	0	0
5	Z	1	Total 1	O 1	0	0

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq

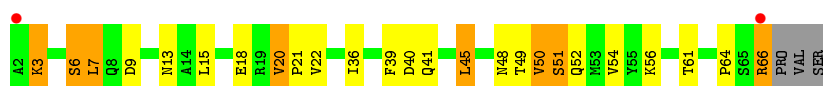


- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq





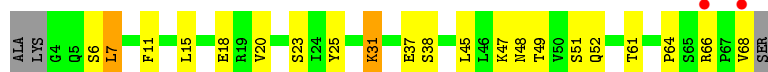
- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



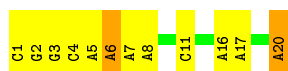
- Molecule 1: RNA-binding protein Hfq



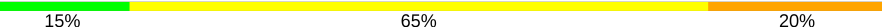
- Molecule 2: DNA (5'-D(P\*CP\*GP\*GP\*CP\*AP\*AP\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*CP\*AP\*A  
P\*AP\*AP\*AP\*A)-3')

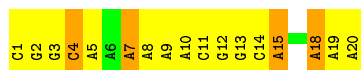


Chain N: 




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

Chain Z: 



- Molecule 3: DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*GP\*CP\*CP\*GP\*TP\*TP\*TP\*TP\*TP\*T P\*GP\*CP\*CP\*G)-3')

Chain M: 



- Molecule 3: DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*GP\*CP\*CP\*GP\*TP\*TP\*TP\*TP\*TP\*T P\*GP\*CP\*CP\*G)-3')

Chain Y: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.75Å 65.80Å 82.00Å 105.93° 92.28° 119.92°	Depositor
Resolution (Å)	25.68 – 3.00 42.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (25.68-3.00) 94.7 (42.68-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168, CNS	Depositor
R, $R_{free}$	0.210 , 0.260 0.219 , 0.263	Depositor DCC
$R_{free}$ test set	1063 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.076 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.14% 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: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/514	1.38	11/695 (1.6%)
1	B	0.27	0/540	0.97	6/731 (0.8%)
1	C	0.28	0/540	1.20	8/731 (1.1%)
1	D	0.25	0/540	0.95	6/731 (0.8%)
1	E	0.27	0/533	0.74	2/721 (0.3%)
1	F	0.26	0/525	0.97	8/709 (1.1%)
1	G	0.24	0/540	0.65	2/731 (0.3%)
1	H	0.39	1/526 (0.2%)	0.87	5/713 (0.7%)
1	I	0.27	0/526	1.03	6/713 (0.8%)
1	J	0.25	0/519	1.15	9/702 (1.3%)
1	K	0.31	0/546	0.86	5/739 (0.7%)
1	L	0.25	0/530	0.80	2/716 (0.3%)
2	N	1.03	0/471	1.24	3/724 (0.4%)
2	Z	1.07	0/471	1.42	5/724 (0.7%)
3	M	1.10	1/447 (0.2%)	1.85	17/688 (2.5%)
3	Y	1.16	2/447 (0.4%)	1.80	14/688 (2.0%)
All	All	0.57	4/8215 (0.0%)	1.16	109/11456 (1.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	3	DT	C1'-N1	10.04	1.62	1.49
3	Y	1	DT	C1'-N1	8.34	1.60	1.49
1	H	67	PRO	N-CD	5.33	1.55	1.47
3	M	15	DT	C1'-N1	5.14	1.55	1.49

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	CB-CA-C	-14.17	82.05	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	SER	N-CA-C	-13.54	74.44	111.00
1	C	65	SER	CB-CA-C	13.19	135.17	110.10
1	J	48	ASN	N-CA-C	13.20	146.63	111.00
1	A	4	GLY	N-CA-C	13.01	145.62	113.10
1	J	47	LYS	N-CA-C	12.38	144.42	111.00
1	L	67	PRO	N-CA-CB	12.24	117.99	103.30
1	B	6	SER	CB-CA-C	11.84	132.59	110.10
1	I	47	LYS	N-CA-C	11.41	141.81	111.00
1	A	46	LEU	N-CA-C	-11.01	81.28	111.00
1	A	5	GLN	N-CA-CB	10.91	130.24	110.60
1	I	47	LYS	CB-CA-C	-10.77	88.86	110.40
1	A	46	LEU	CB-CA-C	10.37	129.91	110.20
1	D	6	SER	N-CA-C	-10.11	83.70	111.00
1	D	5	GLN	CB-CA-C	10.05	130.51	110.40
1	I	48	ASN	N-CA-C	10.03	138.08	111.00
1	C	66	ARG	N-CA-C	-10.01	83.98	111.00
1	H	65	SER	CB-CA-C	-9.76	91.56	110.10
3	M	1	DT	N1-C1'-C2'	9.59	130.81	112.60
1	A	6	SER	CB-CA-C	-9.23	92.56	110.10
1	B	47	LYS	CB-CA-C	-9.07	92.26	110.40
1	E	5	GLN	N-CA-CB	-8.43	95.43	110.60
1	J	48	ASN	N-CA-CB	-8.42	95.45	110.60
1	I	48	ASN	N-CA-CB	-8.39	95.51	110.60
1	K	46	LEU	CB-CA-C	8.29	125.95	110.20
3	Y	5	DT	C3'-C2'-C1'	-8.29	92.56	102.50
1	G	65	SER	CB-CA-C	-8.26	94.41	110.10
1	J	47	LYS	CB-CA-C	-8.08	94.25	110.40
1	A	45	LEU	CB-CA-C	7.97	125.35	110.20
1	C	6	SER	N-CA-CB	7.95	122.42	110.50
1	A	6	SER	N-CA-C	7.82	132.12	111.00
3	M	16	DT	O4'-C1'-C2'	-7.67	99.76	105.90
3	Y	7	DG	O4'-C1'-N9	7.48	113.23	108.00
1	D	5	GLN	N-CA-C	-7.42	90.97	111.00
3	M	15	DT	N1-C1'-C2'	7.27	126.42	112.60
1	C	6	SER	CB-CA-C	7.22	123.81	110.10
3	M	3	DT	N3-C4-O4	6.96	124.08	119.90
1	F	50	VAL	CB-CA-C	-6.86	98.36	111.40
1	F	51	SER	N-CA-CB	-6.84	100.23	110.50
1	B	48	ASN	N-CA-C	6.81	129.39	111.00
3	Y	5	DT	C4'-C3'-C2'	-6.81	96.97	103.10
1	H	65	SER	N-CA-C	6.81	129.38	111.00
1	D	6	SER	N-CA-CB	6.77	120.66	110.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	3	DT	N1-C1'-C2'	6.75	125.42	112.60
1	F	52	GLN	N-CA-CB	6.67	122.62	110.60
3	M	7	DG	O4'-C1'-C2'	-6.58	100.63	105.90
3	M	3	DT	C5-C4-O4	-6.54	120.32	124.90
3	M	13	DT	C5-C4-O4	-6.53	120.33	124.90
2	N	6	DA	N9-C1'-C2'	-6.47	100.31	112.60
3	M	16	DT	O4'-C1'-N1	6.38	112.46	108.00
1	A	47	LYS	N-CA-C	-6.30	93.98	111.00
3	M	16	DT	N3-C4-O4	6.29	123.68	119.90
1	B	47	LYS	N-CA-C	6.26	127.90	111.00
1	C	67	PRO	CB-CA-C	-6.25	96.37	112.00
1	H	49	THR	CB-CA-C	-6.24	94.74	111.60
3	M	15	DT	N3-C4-O4	6.21	123.62	119.90
1	A	46	LEU	N-CA-CB	6.19	122.78	110.40
1	G	66	ARG	N-CA-CB	6.13	121.64	110.60
1	K	6	SER	CB-CA-C	6.13	121.75	110.10
1	L	49	THR	N-CA-C	-6.06	94.64	111.00
1	C	5	GLN	N-CA-C	-6.01	94.77	111.00
1	J	49	THR	N-CA-C	-6.01	94.77	111.00
1	B	48	ASN	N-CA-CB	-5.98	99.84	110.60
1	F	7	LEU	CB-CA-C	-5.94	98.92	110.20
3	M	15	DT	C5-C4-O4	-5.92	120.75	124.90
1	K	7	LEU	CB-CA-C	-5.92	98.95	110.20
2	Z	4	DC	C6-N1-C1'	-5.91	113.70	120.80
1	J	7	LEU	CB-CA-C	-5.90	98.99	110.20
1	B	7	LEU	N-CA-CB	-5.90	98.61	110.40
1	J	16	ARG	CB-CA-C	-5.89	98.63	110.40
3	M	13	DT	N3-C4-O4	5.89	123.43	119.90
1	I	7	LEU	CB-CA-C	-5.87	99.06	110.20
2	Z	18	DA	O4'-C1'-N9	5.85	112.09	108.00
2	N	17	DA	O4'-C1'-N9	5.84	112.09	108.00
3	M	1	DT	O4'-C4'-C3'	-5.83	102.17	104.50
3	Y	14	DT	O4'-C1'-C2'	-5.82	101.25	105.90
1	J	48	ASN	CB-CA-C	-5.81	98.78	110.40
1	I	6	SER	N-CA-CB	-5.79	101.81	110.50
2	Z	4	DC	C6-N1-C2	5.78	122.61	120.30
2	N	20	DA	O4'-C1'-N9	-5.75	103.97	108.00
1	H	66	ARG	N-CA-C	-5.66	95.72	111.00
1	J	46	LEU	CB-CA-C	-5.66	99.44	110.20
3	Y	5	DT	O4'-C1'-C2'	-5.62	101.41	105.90
1	H	66	ARG	C-N-CD	5.60	140.17	128.40
3	Y	4	DT	P-O3'-C3'	5.58	126.40	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	64	PRO	CB-CA-C	-5.56	98.10	112.00
1	F	51	SER	N-CA-C	-5.53	96.07	111.00
3	Y	6	DT	C3'-C2'-C1'	-5.53	95.87	102.50
1	A	49	THR	CB-CA-C	-5.52	96.70	111.60
2	Z	7	DA	C3'-C2'-C1'	-5.46	95.95	102.50
3	Y	12	DT	C5-C4-O4	-5.46	121.08	124.90
1	D	68	VAL	N-CA-CB	5.44	123.47	111.50
1	F	51	SER	CB-CA-C	5.41	120.37	110.10
1	C	6	SER	N-CA-C	-5.38	96.49	111.00
3	Y	11	DT	C5-C4-O4	-5.34	121.16	124.90
3	Y	17	DG	O4'-C1'-N9	5.30	111.71	108.00
3	Y	16	DT	N3-C4-O4	5.29	123.08	119.90
3	M	13	DT	C3'-C2'-C1'	-5.28	96.16	102.50
3	M	4	DT	C5-C4-O4	-5.23	121.24	124.90
1	K	7	LEU	N-CA-C	5.22	125.09	111.00
1	K	47	LYS	N-CA-C	-5.20	96.95	111.00
3	M	16	DT	C2-N1-C1'	5.17	126.47	118.20
1	D	67	PRO	N-CA-C	-5.15	98.70	112.10
3	M	9	DC	O4'-C4'-C3'	-5.14	102.44	104.50
2	Z	15	DA	O4'-C1'-N9	5.14	111.60	108.00
3	Y	17	DG	O4'-C1'-C2'	-5.12	101.80	105.90
1	F	66	ARG	N-CA-C	5.12	124.82	111.00
3	Y	18	DC	P-O5'-C5'	-5.11	112.72	120.90
1	E	48	ASN	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	506	0	530	11	0
1	B	531	0	559	16	0
1	C	531	0	559	19	0
1	D	531	0	559	11	0
1	E	524	0	550	22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	517	0	543	23	0
1	G	531	0	559	16	0
1	H	517	0	541	10	0
1	I	517	0	541	11	0
1	J	511	0	532	15	0
1	K	537	0	564	18	0
1	L	522	0	544	18	0
2	N	416	0	221	15	0
2	Z	416	0	221	31	0
3	M	404	0	233	51	0
3	Y	404	0	233	62	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	5	0	0	0	0
5	B	8	0	0	0	0
5	C	8	0	0	1	0
5	D	11	0	0	3	0
5	E	10	0	0	1	0
5	F	11	0	0	1	0
5	G	8	0	0	0	0
5	H	12	0	0	1	0
5	I	14	0	0	0	0
5	J	9	0	0	0	0
5	K	8	0	0	1	0
5	L	11	0	0	0	0
5	M	1	0	0	1	0
5	Z	1	0	0	1	0
All	All	8044	0	7489	299	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 20.

All (299) 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:J:47:LYS:O	1:J:47:LYS:CG	1.73	1.26
3:Y:3:DT:C6	3:Y:4:DT:H72	1.74	1.22
3:Y:1:DT:C2	3:Y:2:DT:C5	2.34	1.16
2:Z:3:DG:C2	2:Z:4:DC:C4	2.35	1.15
1:F:7:LEU:HD23	1:F:7:LEU:O	1.52	1.09
1:B:47:LYS:O	1:B:47:LYS:CG	1.99	1.04
1:E:3:LYS:O	1:F:40:ASP:HB2	1.58	1.03
2:N:20:DA:N1	3:M:1:DT:N3	2.05	1.03
1:B:47:LYS:HG3	1:B:47:LYS:O	1.23	1.02
2:N:20:DA:N6	3:M:1:DT:O4	1.93	1.00
3:Y:1:DT:C2	3:Y:2:DT:C6	2.52	0.97
2:N:16:DA:N6	3:M:5:DT:O4	2.00	0.94
3:Y:1:DT:O4	2:Z:20:DA:N6	2.01	0.94
3:Y:3:DT:O4	2:Z:18:DA:N6	2.02	0.93
2:Z:3:DG:N3	2:Z:4:DC:C5	2.37	0.93
1:I:7:LEU:O	1:I:7:LEU:HD23	1.69	0.93
3:Y:1:DT:N3	2:Z:20:DA:N1	2.15	0.92
3:Y:1:DT:C6	3:Y:2:DT:C7	2.52	0.92
2:Z:3:DG:N3	2:Z:4:DC:C4	2.38	0.91
3:Y:3:DT:N1	3:Y:4:DT:H72	1.85	0.90
3:Y:1:DT:O2	3:Y:2:DT:C6	2.25	0.90
3:Y:12:DT:O4	2:Z:9:DA:N6	2.03	0.89
2:Z:3:DG:C2	2:Z:4:DC:N3	2.41	0.88
3:Y:3:DT:C2	3:Y:4:DT:C5	2.62	0.87
1:F:3:LYS:O	1:J:40:ASP:HB2	1.74	0.87
3:Y:1:DT:N1	3:Y:2:DT:H71	1.94	0.83
3:Y:1:DT:C6	3:Y:2:DT:H73	2.14	0.82
3:Y:1:DT:C6	3:Y:2:DT:H71	2.15	0.81
3:Y:10:DG:C2	3:Y:11:DT:C4	2.68	0.81
3:M:15:DT:H2'	3:M:16:DT:H71	1.62	0.81
1:J:47:LYS:HG3	1:J:47:LYS:O	1.01	0.80
2:Z:3:DG:C6	2:Z:4:DC:N4	2.50	0.80
2:Z:3:DG:C4	2:Z:4:DC:C5	2.69	0.80
1:I:23:SER:HB3	1:I:31:LYS:HD2	1.64	0.80
1:K:6:SER:O	1:K:10:PRO:HG2	1.82	0.80
3:Y:1:DT:N1	3:Y:2:DT:C7	2.44	0.80
2:Z:3:DG:N2	2:Z:4:DC:C2	2.53	0.77
3:M:1:DT:H2'	3:M:2:DT:C6	2.19	0.77
3:Y:1:DT:C5	3:Y:2:DT:H73	2.20	0.77
3:M:2:DT:H2'	3:M:3:DT:H71	1.67	0.76
3:Y:1:DT:N3	3:Y:2:DT:C4	2.54	0.76
1:I:7:LEU:CD2	1:I:7:LEU:O	2.33	0.76

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:16:DT:H2''	3:M:17:DG:C8	2.20	0.76
3:Y:3:DT:C6	3:Y:4:DT:C7	2.64	0.76
2:Z:3:DG:N2	2:Z:4:DC:N3	2.34	0.76
3:M:7:DG:C4	3:M:8:DC:C5	2.74	0.74
2:Z:3:DG:C5	2:Z:4:DC:N4	2.55	0.74
1:A:45:LEU:HG	1:I:7:LEU:HD21	1.70	0.74
1:H:16:ARG:NH2	2:N:8:DA:OP1	2.22	0.73
1:A:44:ILE:HG22	1:A:45:LEU:O	1.89	0.72
3:Y:6:DT:H1'	3:Y:7:DG:C8	2.24	0.72
1:C:63:VAL:HG23	1:G:52:GLN:HB3	1.69	0.72
3:M:14:DT:C2	3:M:15:DT:C5	2.78	0.72
2:Z:3:DG:C4	2:Z:4:DC:C4	2.77	0.72
1:D:20:VAL:HG21	1:D:68:VAL:HG11	1.69	0.72
3:M:2:DT:OP1	5:M:101:HOH:O	2.08	0.71
2:N:5:DA:H2	3:M:16:DT:H3	1.39	0.70
3:Y:5:DT:H2''	3:Y:6:DT:H71	1.73	0.70
1:D:15:LEU:HD21	1:D:64:PRO:HB3	1.75	0.69
5:D:201:HOH:O	1:L:8:GLN:OE1	2.10	0.68
1:K:7:LEU:O	1:K:7:LEU:HD22	1.92	0.68
1:K:22:VAL:HG21	1:K:62:VAL:HG13	1.74	0.68
1:B:6:SER:O	1:B:10:PRO:HG2	1.94	0.67
3:Y:10:DG:N2	3:Y:11:DT:C2	2.62	0.67
1:A:6:SER:O	1:A:10:PRO:CD	2.43	0.66
1:D:52:GLN:OE1	5:D:202:HOH:O	2.12	0.66
3:Y:3:DT:C2	3:Y:4:DT:C4	2.83	0.66
3:Y:3:DT:N1	3:Y:4:DT:C7	2.58	0.66
3:M:12:DT:C6	3:M:13:DT:H73	2.30	0.66
1:G:13:ASN:ND2	5:Z:101:HOH:O	2.29	0.66
1:K:17:ARG:NH1	1:K:18:GLU:OE2	2.29	0.66
3:M:12:DT:C6	3:M:13:DT:C7	2.79	0.66
1:F:7:LEU:CD2	1:F:7:LEU:O	2.39	0.66
1:B:66:ARG:HD2	1:B:67:PRO:HD3	1.76	0.65
1:J:7:LEU:HG	1:J:7:LEU:O	1.96	0.65
3:M:14:DT:C6	3:M:15:DT:C7	2.79	0.65
1:I:25:TYR:OH	1:I:31:LYS:NZ	2.29	0.65
3:Y:1:DT:C2	3:Y:2:DT:C4	2.85	0.65
3:M:14:DT:C2'	3:M:15:DT:H71	2.26	0.64
3:M:14:DT:C2	3:M:15:DT:C6	2.85	0.64
3:M:19:DC:H2''	3:M:20:DG:C8	2.32	0.64
1:B:6:SER:O	1:B:10:PRO:CD	2.46	0.64
1:H:56:LYS:NZ	5:H:201:HOH:O	2.28	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:PRO:O	1:H:68:VAL:O	2.16	0.64
1:K:3:LYS:O	1:K:6:SER:OG	2.16	0.63
3:Y:8:DC:H42	2:Z:13:DG:H1	1.45	0.63
1:J:47:LYS:O	1:J:47:LYS:CD	2.45	0.63
1:K:20:VAL:HG21	1:K:68:VAL:HG21	1.81	0.62
1:C:6:SER:O	1:C:10:PRO:HG2	1.99	0.62
1:H:4:GLY:HA3	1:H:5:GLN:HB3	1.81	0.62
1:E:48:ASN:OD1	1:E:49:THR:N	2.30	0.62
3:Y:3:DT:N1	3:Y:4:DT:C5	2.67	0.62
1:C:8:GLN:N	5:C:201:HOH:O	2.33	0.62
3:Y:1:DT:N1	3:Y:2:DT:C5	2.68	0.62
1:G:3:LYS:HG2	1:G:6:SER:HB3	1.82	0.61
1:I:45:LEU:HD21	1:I:51:SER:HB3	1.82	0.61
3:Y:1:DT:C2'	3:Y:2:DT:H71	2.30	0.61
1:J:48:ASN:OD1	1:J:50:VAL:O	2.18	0.61
3:M:7:DG:C5	3:M:8:DC:C4	2.89	0.61
3:Y:3:DT:C2	3:Y:4:DT:C6	2.88	0.61
1:C:61:THR:HG22	1:G:54:VAL:HG22	1.83	0.60
2:Z:1:DC:H2''	2:Z:2:DG:C8	2.36	0.60
2:Z:3:DG:C4	2:Z:4:DC:N4	2.69	0.60
3:Y:10:DG:N2	3:Y:11:DT:N3	2.49	0.60
3:Y:1:DT:C2	3:Y:2:DT:C7	2.84	0.60
1:B:6:SER:O	1:B:10:PRO:CG	2.48	0.60
2:Z:14:DC:H2''	2:Z:15:DA:C8	2.36	0.60
1:L:3:LYS:O	1:L:6:SER:OG	2.17	0.60
1:G:5:GLN:HE22	1:G:8:GLN:HB3	1.66	0.60
3:Y:14:DT:C6	3:Y:15:DT:H72	2.36	0.60
1:E:3:LYS:O	1:F:40:ASP:CB	2.43	0.59
3:M:15:DT:H2'	3:M:16:DT:C6	2.37	0.59
3:Y:3:DT:N3	3:Y:4:DT:C4	2.71	0.59
3:Y:17:DG:C2	3:Y:18:DC:C2	2.90	0.59
2:Z:3:DG:C2	2:Z:4:DC:N4	2.70	0.59
3:Y:1:DT:N3	3:Y:2:DT:C5	2.69	0.59
3:M:13:DT:H2''	3:M:14:DT:H71	1.84	0.59
1:A:7:LEU:HD21	1:B:45:LEU:HB2	1.85	0.58
3:Y:4:DT:H2'	3:Y:5:DT:H72	1.84	0.58
1:C:32:LEU:HD22	1:C:52:GLN:HE22	1.68	0.58
3:M:7:DG:C4	3:M:8:DC:C4	2.91	0.58
1:K:63:VAL:HG12	1:L:52:GLN:HB3	1.86	0.58
3:M:7:DG:N9	3:M:8:DC:C5	2.72	0.58
2:Z:3:DG:N1	2:Z:4:DC:N4	2.52	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:19:DC:H2''	3:M:20:DG:H8	1.67	0.57
1:E:4:GLY:HA2	1:F:41:GLN:HB3	1.86	0.57
1:B:3:LYS:O	1:B:6:SER:OG	2.21	0.57
2:N:3:DG:C6	2:N:4:DC:N4	2.73	0.57
1:F:3:LYS:O	1:F:6:SER:OG	2.24	0.56
3:M:7:DG:C2	3:M:8:DC:C2	2.94	0.56
1:K:4:GLY:O	1:L:40:ASP:HB2	2.07	0.55
3:Y:6:DT:C2	3:Y:7:DG:C5	2.94	0.55
1:A:6:SER:O	1:A:10:PRO:HD2	2.07	0.55
2:Z:14:DC:H2''	2:Z:15:DA:H8	1.72	0.55
1:D:45:LEU:HD11	1:D:51:SER:HB3	1.89	0.54
1:I:15:LEU:HD21	1:I:64:PRO:HG3	1.90	0.54
3:Y:1:DT:H2'	3:Y:2:DT:H71	1.88	0.54
3:M:12:DT:C2'	3:M:13:DT:H71	2.37	0.54
3:M:15:DT:H2''	3:M:16:DT:H5'	1.88	0.54
1:J:48:ASN:CG	1:J:49:THR:H	2.11	0.54
1:J:7:LEU:CG	1:J:7:LEU:O	2.55	0.54
3:Y:10:DG:C2	3:Y:11:DT:N3	2.76	0.54
2:N:2:DG:C2	3:M:20:DG:N2	2.75	0.54
3:Y:1:DT:C1'	3:Y:2:DT:H71	2.39	0.53
2:Z:4:DC:H2''	2:Z:5:DA:C8	2.43	0.53
3:Y:10:DG:N3	3:Y:11:DT:C5	2.77	0.53
1:F:56:LYS:NZ	5:F:202:HOH:O	2.41	0.53
1:B:5:GLN:HE22	1:C:42:PHE:HE1	1.57	0.53
1:K:2:ALA:HA	1:L:39:PHE:O	2.08	0.53
3:M:12:DT:C5	3:M:13:DT:H73	2.44	0.53
1:F:18:GLU:HB3	1:F:20:VAL:HG12	1.89	0.53
3:M:14:DT:C6	3:M:15:DT:H71	2.44	0.53
3:Y:7:DG:H4'	3:Y:8:DC:OP1	2.09	0.53
1:E:15:LEU:HD13	1:E:22:VAL:HG11	1.91	0.52
3:Y:1:DT:O2	3:Y:2:DT:N1	2.42	0.52
3:Y:4:DT:H2''	3:Y:5:DT:O5'	2.08	0.52
3:M:9:DC:H1'	3:M:10:DG:C8	2.43	0.52
2:Z:4:DC:H2''	2:Z:5:DA:H8	1.75	0.52
1:E:16:ARG:NE	1:E:37:GLU:O	2.39	0.52
1:A:54:VAL:HG22	1:I:61:THR:HG22	1.92	0.51
1:K:18:GLU:HB3	1:K:20:VAL:HG23	1.91	0.51
1:L:40:ASP:C	1:L:40:ASP:OD1	2.49	0.51
1:E:20:VAL:HG22	1:E:66:ARG:HD3	1.93	0.51
3:M:14:DT:C6	3:M:15:DT:H73	2.45	0.51
3:M:15:DT:H2'	3:M:16:DT:H6	1.76	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:10:DA:C2	2:Z:11:DC:C2	2.99	0.51
1:E:48:ASN:CG	1:E:49:THR:H	2.14	0.50
1:E:7:LEU:HD21	1:F:45:LEU:HD12	1.93	0.50
3:Y:6:DT:C1'	3:Y:7:DG:C8	2.94	0.50
1:A:2:ALA:N	1:B:39:PHE:O	2.44	0.50
1:G:5:GLN:OE1	1:G:8:GLN:NE2	2.45	0.50
3:M:9:DC:C2	3:M:10:DG:C5	3.00	0.50
2:N:3:DG:C6	2:N:4:DC:C4	3.00	0.50
1:E:37:GLU:CD	1:E:45:LEU:HB3	2.32	0.49
1:K:40:ASP:C	1:K:40:ASP:OD1	2.51	0.49
5:D:201:HOH:O	1:L:12:LEU:HD11	2.12	0.49
3:M:1:DT:H2'	3:M:2:DT:C5	2.47	0.49
3:Y:4:DT:H2'	3:Y:5:DT:C7	2.43	0.49
1:B:8:GLN:HG2	1:B:8:GLN:O	2.14	0.48
1:D:39:PHE:O	1:L:2:ALA:N	2.46	0.48
1:E:37:GLU:OE2	1:E:45:LEU:HB3	2.13	0.48
1:K:6:SER:O	1:K:10:PRO:CG	2.60	0.48
3:M:12:DT:H2'	3:M:13:DT:H71	1.93	0.48
3:Y:5:DT:C2'	3:Y:6:DT:H71	2.43	0.48
1:J:23:SER:HB3	1:J:31:LYS:HE3	1.95	0.48
1:B:35:GLN:HB3	1:B:47:LYS:HG2	1.96	0.48
1:D:43:VAL:HG23	1:L:7:LEU:HD23	1.96	0.48
2:N:6:DA:H2''	2:N:7:DA:O5'	2.14	0.48
1:A:48:ASN:CG	1:A:49:THR:H	2.16	0.48
2:Z:3:DG:N1	2:Z:4:DC:C4	2.81	0.47
1:C:15:LEU:HD13	1:C:22:VAL:HG11	1.97	0.47
1:H:48:ASN:OD1	1:H:48:ASN:N	2.47	0.47
3:Y:8:DC:H1'	3:Y:9:DC:H5'	1.95	0.47
1:C:16:ARG:O	1:C:19:ARG:HG3	2.15	0.47
3:M:14:DT:H2'	3:M:15:DT:H71	1.94	0.47
3:M:2:DT:H2''	3:M:3:DT:O5'	2.13	0.47
2:N:6:DA:C2	2:N:7:DA:C4	3.03	0.47
1:E:8:GLN:NE2	5:E:204:HOH:O	2.46	0.47
1:G:61:THR:HG22	1:H:54:VAL:HG22	1.95	0.47
1:F:48:ASN:CG	1:F:49:THR:H	2.18	0.47
1:K:5:GLN:NE2	5:K:201:HOH:O	2.25	0.47
3:M:15:DT:C2'	3:M:16:DT:H71	2.40	0.47
1:B:28:ASN:OD1	1:B:30:ILE:HG22	2.15	0.46
1:H:7:LEU:HD11	1:I:45:LEU:HD12	1.97	0.46
1:A:49:THR:HG22	1:A:49:THR:O	2.15	0.46
3:M:6:DT:H2''	3:M:7:DG:C8	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:ASP:C	1:F:40:ASP:OD1	2.54	0.46
1:G:15:LEU:HD13	1:G:22:VAL:HG11	1.97	0.46
1:K:63:VAL:HG12	1:L:52:GLN:CB	2.46	0.46
1:E:21:PRO:HG2	1:E:65:SER:HB2	1.98	0.46
1:F:66:ARG:HH21	1:J:49:THR:C	2.19	0.46
1:E:64:PRO:HD2	1:F:51:SER:O	2.15	0.46
3:M:16:DT:H2"	3:M:17:DG:N7	2.30	0.46
3:M:7:DG:N3	3:M:8:DC:C6	2.84	0.46
1:J:15:LEU:HD13	1:J:22:VAL:HG11	1.98	0.45
2:N:1:DC:H2"	2:N:2:DG:C8	2.51	0.45
1:J:18:GLU:HB2	1:J:20:VAL:HG23	1.98	0.45
1:K:48:ASN:O	1:K:49:THR:C	2.54	0.45
3:M:15:DT:C6	3:M:16:DT:H73	2.51	0.45
3:Y:3:DT:O2	3:Y:4:DT:C6	2.70	0.45
2:Z:12:DG:H2"	2:Z:13:DG:C8	2.52	0.45
2:N:3:DG:C5	2:N:4:DC:C4	3.05	0.45
2:N:2:DG:H1	3:M:19:DC:H42	1.64	0.45
1:A:17:ARG:O	1:A:19:ARG:NH1	2.50	0.45
1:E:4:GLY:CA	1:F:41:GLN:HB3	2.46	0.45
1:G:18:GLU:HB2	1:G:20:VAL:HG23	1.99	0.45
1:L:25:TYR:HB2	1:L:61:THR:HG23	1.98	0.45
3:Y:17:DG:C2	3:Y:18:DC:N3	2.85	0.45
1:G:40:ASP:OD1	1:G:40:ASP:C	2.55	0.45
1:B:17:ARG:HD2	1:B:17:ARG:HA	1.73	0.45
3:Y:10:DG:C4	3:Y:11:DT:C5	3.05	0.44
2:N:11:DC:H42	3:M:10:DG:H1	1.66	0.44
1:C:8:GLN:O	1:C:12:LEU:HG	2.18	0.44
1:L:15:LEU:HD13	1:L:22:VAL:HG11	1.98	0.44
1:C:21:PRO:HD2	1:C:66:ARG:HB3	2.00	0.44
1:C:23:SER:HB3	1:C:31:LYS:NZ	2.33	0.44
1:L:46:LEU:HD23	1:L:52:GLN:HE21	1.82	0.44
1:C:67:PRO:O	1:C:68:VAL:HB	2.18	0.44
1:F:15:LEU:HD13	1:F:22:VAL:HG11	1.98	0.44
2:Z:1:DC:H2"	2:Z:2:DG:H8	1.79	0.44
1:D:40:ASP:OD1	1:D:40:ASP:C	2.56	0.44
1:E:7:LEU:HD11	1:F:45:LEU:HB2	2.00	0.43
3:M:12:DT:C2	3:M:13:DT:C5	3.06	0.43
3:Y:1:DT:C4	2:Z:20:DA:N1	2.84	0.43
1:C:8:GLN:O	1:C:8:GLN:HG2	2.17	0.43
1:H:61:THR:HG21	1:I:52:GLN:OE1	2.18	0.43
1:B:61:THR:HG22	1:C:54:VAL:HG22	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:14:DT:N1	3:M:15:DT:C5	2.86	0.43
2:N:3:DG:C4	2:N:4:DC:C5	3.06	0.43
3:Y:7:DG:H2''	3:Y:8:DC:H6	1.84	0.43
1:D:61:THR:HG22	1:E:54:VAL:HG22	1.99	0.43
1:G:48:ASN:OD1	1:G:49:THR:N	2.51	0.43
3:M:14:DT:C5	3:M:15:DT:H73	2.53	0.43
3:Y:10:DG:C4	3:Y:11:DT:C7	3.01	0.43
1:H:25:TYR:O	1:H:60:SER:N	2.44	0.43
1:L:23:SER:HB3	1:L:31:LYS:HE3	2.01	0.43
1:D:7:LEU:HD11	1:E:45:LEU:HD13	1.99	0.43
1:G:5:GLN:NE2	1:G:8:GLN:HB3	2.30	0.43
3:M:7:DG:C4	3:M:8:DC:C6	3.06	0.43
1:E:46:LEU:HA	1:E:46:LEU:HD23	1.75	0.42
1:F:9:ASP:O	1:F:13:ASN:HB2	2.19	0.42
1:G:6:SER:O	1:G:10:PRO:HG2	2.18	0.42
1:F:61:THR:HG22	1:J:54:VAL:HG22	2.00	0.42
1:E:61:THR:HG23	1:F:54:VAL:HG22	2.01	0.42
1:G:45:LEU:HD11	1:G:51:SER:HB3	2.01	0.42
1:K:16:ARG:HG3	1:K:36:ILE:O	2.20	0.42
1:L:16:ARG:O	1:L:19:ARG:HD2	2.20	0.42
3:Y:14:DT:C2	3:Y:15:DT:C4	3.08	0.42
1:C:67:PRO:O	1:C:68:VAL:CB	2.67	0.41
1:H:5:GLN:N	1:H:5:GLN:OE1	2.53	0.41
1:D:6:SER:OG	1:D:7:LEU:N	2.53	0.41
1:J:16:ARG:O	1:J:16:ARG:HG2	2.19	0.41
1:L:66:ARG:O	1:L:67:PRO:C	2.57	0.41
3:M:15:DT:H2'	3:M:16:DT:C7	2.42	0.41
1:I:11:PHE:CE1	1:I:15:LEU:HD11	2.54	0.41
3:Y:3:DT:C1'	3:Y:4:DT:H72	2.51	0.41
1:C:3:LYS:O	1:C:6:SER:OG	2.31	0.41
1:F:22:VAL:HG21	1:F:36:ILE:HD11	2.03	0.41
1:D:45:LEU:HB2	1:L:7:LEU:HD21	2.03	0.41
3:Y:10:DG:H1	2:Z:11:DC:H42	1.69	0.41
1:J:7:LEU:HD21	1:K:45:LEU:HB2	2.03	0.41
1:E:2:ALA:N	1:E:6:SER:HG	2.19	0.41
3:M:14:DT:N3	3:M:15:DT:C4	2.88	0.41
1:G:13:ASN:OD1	1:G:16:ARG:NH2	2.30	0.41
2:Z:7:DA:C6	2:Z:8:DA:C6	3.09	0.41
1:G:3:LYS:HG3	1:G:4:GLY:N	2.35	0.41
3:Y:11:DT:C6	3:Y:12:DT:H72	2.55	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.73	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ASN:HB3	1:C:17:ARG:NH1	2.36	0.41
1:B:7:LEU:HD11	1:C:45:LEU:HD13	2.04	0.40
1:E:7:LEU:HD12	1:F:39:PHE:HA	2.03	0.40
3:Y:2:DT:C4	2:Z:19:DA:N1	2.90	0.40
1:F:20:VAL:HA	1:F:21:PRO:HD3	1.92	0.40
1:C:19:ARG:HG2	1:C:35:GLN:NE2	2.36	0.40
3:M:13:DT:C2'	3:M:14:DT:H71	2.49	0.40
1:L:20:VAL:HA	1:L:21:PRO:HD3	1.92	0.40
3:Y:7:DG:H2''	3:Y:8:DC:C6	2.56	0.40
1:K:50:VAL:O	1:K:50:VAL:HG23	2.20	0.40
3:Y:17:DG:C4	3:Y:18:DC:C4	3.10	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	62/68 (91%)	60 (97%)	2 (3%)	0	100	100
1	B	65/68 (96%)	62 (95%)	3 (5%)	0	100	100
1	C	65/68 (96%)	59 (91%)	6 (9%)	0	100	100
1	D	65/68 (96%)	61 (94%)	4 (6%)	0	100	100
1	E	64/68 (94%)	63 (98%)	1 (2%)	0	100	100
1	F	63/68 (93%)	61 (97%)	2 (3%)	0	100	100
1	G	65/68 (96%)	60 (92%)	5 (8%)	0	100	100
1	H	63/68 (93%)	57 (90%)	6 (10%)	0	100	100
1	I	63/68 (93%)	61 (97%)	2 (3%)	0	100	100
1	J	63/68 (93%)	63 (100%)	0	0	100	100
1	K	66/68 (97%)	60 (91%)	6 (9%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	64/68 (94%)	61 (95%)	3 (5%)	0	100	100
All	All	768/816 (94%)	728 (95%)	40 (5%)	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	58/62 (94%)	58 (100%)	0	100	100
1	B	61/62 (98%)	57 (93%)	4 (7%)	16	49
1	C	61/62 (98%)	53 (87%)	8 (13%)	4	18
1	D	61/62 (98%)	58 (95%)	3 (5%)	25	61
1	E	60/62 (97%)	52 (87%)	8 (13%)	4	17
1	F	59/62 (95%)	54 (92%)	5 (8%)	10	38
1	G	61/62 (98%)	58 (95%)	3 (5%)	25	61
1	H	60/62 (97%)	58 (97%)	2 (3%)	38	73
1	I	60/62 (97%)	52 (87%)	8 (13%)	4	17
1	J	58/62 (94%)	57 (98%)	1 (2%)	60	85
1	K	62/62 (100%)	59 (95%)	3 (5%)	25	62
1	L	59/62 (95%)	52 (88%)	7 (12%)	5	22
All	All	720/744 (97%)	668 (93%)	52 (7%)	14	45

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	SER
1	B	7	LEU
1	B	45	LEU
1	B	66	ARG
1	C	5	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	6	SER
1	C	19	ARG
1	C	20	VAL
1	C	49	THR
1	C	50	VAL
1	C	63	VAL
1	C	66	ARG
1	D	3	LYS
1	D	6	SER
1	D	9	ASP
1	E	5	GLN
1	E	7	LEU
1	E	31	LYS
1	E	45	LEU
1	E	47	LYS
1	E	49	THR
1	E	50	VAL
1	E	61	THR
1	F	3	LYS
1	F	6	SER
1	F	20	VAL
1	F	45	LEU
1	F	50	VAL
1	G	3	LYS
1	G	19	ARG
1	G	66	ARG
1	H	66	ARG
1	H	68	VAL
1	I	18	GLU
1	I	20	VAL
1	I	31	LYS
1	I	37	GLU
1	I	38	SER
1	I	49	THR
1	I	66	ARG
1	I	68	VAL
1	J	65	SER
1	K	7	LEU
1	K	45	LEU
1	K	68	VAL
1	L	3	LYS
1	L	6	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	20	VAL
1	L	37	GLU
1	L	48	ASN
1	L	49	THR
1	L	66	ARG

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	52	GLN
1	C	5	GLN
1	C	35	GLN
1	C	52	GLN
1	E	5	GLN
1	L	8	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 12 ligands modelled in this entry, 12 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	64/68 (94%)	-0.26	2 (3%) 49 21	27, 55, 75, 82	0
1	B	67/68 (98%)	-0.39	0 100 100	26, 49, 72, 90	0
1	C	67/68 (98%)	-0.43	0 100 100	22, 48, 69, 85	0
1	D	67/68 (98%)	-0.42	0 100 100	26, 42, 67, 83	0
1	E	66/68 (97%)	-0.32	0 100 100	26, 45, 72, 92	0
1	F	65/68 (95%)	-0.48	2 (3%) 49 21	27, 46, 72, 91	0
1	G	67/68 (98%)	-0.43	1 (1%) 73 46	25, 45, 71, 89	0
1	H	65/68 (95%)	-0.42	1 (1%) 73 46	27, 43, 74, 97	0
1	I	65/68 (95%)	-0.44	2 (3%) 49 21	26, 51, 77, 93	0
1	J	65/68 (95%)	-0.59	0 100 100	28, 45, 66, 73	0
1	K	68/68 (100%)	-0.36	0 100 100	28, 49, 75, 88	0
1	L	66/68 (97%)	-0.51	0 100 100	26, 44, 69, 88	0
2	N	20/20 (100%)	-0.23	0 100 100	61, 69, 77, 78	0
2	Z	20/20 (100%)	-0.07	0 100 100	82, 92, 106, 110	0
3	M	20/20 (100%)	-0.12	0 100 100	53, 66, 77, 79	0
3	Y	20/20 (100%)	-0.09	0 100 100	76, 95, 106, 107	0
All	All	872/896 (97%)	-0.39	8 (0%) 84 63	22, 49, 87, 110	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	4	GLY	4.6
1	I	66	ARG	3.3
1	F	66	ARG	2.9
1	A	4	GLY	2.7
1	A	3	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	68	VAL	2.3
1	F	2	ALA	2.3
1	G	66	ARG	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	ZN	D	101	1/1	0.90	0.25	33,33,33,33	1
4	ZN	J	101	1/1	0.91	0.11	34,34,34,34	1
4	ZN	A	101	1/1	0.92	0.12	24,24,24,24	1
4	ZN	E	101	1/1	0.93	0.12	33,33,33,33	1
4	ZN	F	101	1/1	0.95	0.25	48,48,48,48	1
4	ZN	H	101	1/1	0.96	0.28	32,32,32,32	1
4	ZN	K	101	1/1	0.96	0.22	30,30,30,30	1
4	ZN	B	101	1/1	0.96	0.13	34,34,34,34	1
4	ZN	G	101	1/1	0.97	0.12	35,35,35,35	1
4	ZN	I	101	1/1	0.98	0.18	45,45,45,45	1
4	ZN	L	101	1/1	0.99	0.16	26,26,26,26	1
4	ZN	C	101	1/1	0.99	0.23	29,29,29,29	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.