



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:51 AM EDT

PDB ID : 2XD0  
Title : A processed non-coding RNA regulates a bacterial antiviral system  
Authors : Blower, T.R.; Pei, X.Y.; Short, F.L.; Fineran, P.C.; Humphreys, D.P.; Luisi, B.F.; Salmond, G.P.C.  
Deposited on : 2010-04-28  
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 types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

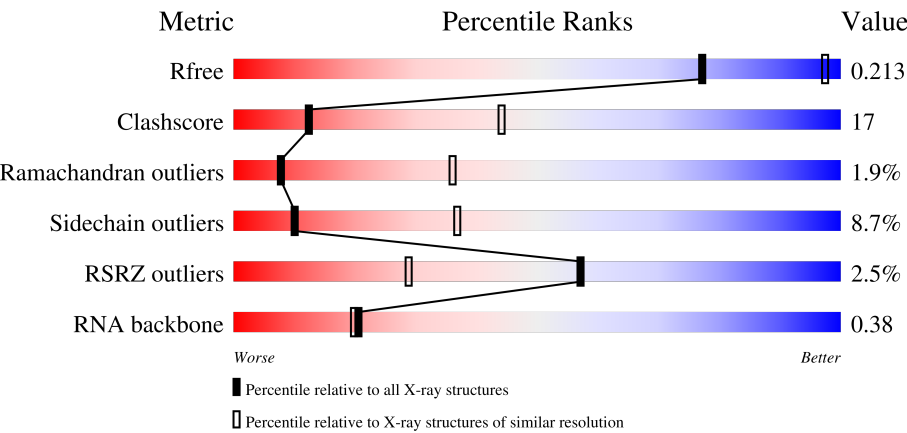
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 <sub>free</sub>	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)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	<div><div>70%</div><div>20%</div><div>• • 5%</div></div>
1	B	171	<div><div>72%</div><div>18%</div><div>5% • 5%</div></div>
1	E	171	<div><div>70%</div><div>19%</div><div>5% • 5%</div></div>
1	X	171	<div><div>67%</div><div>23%</div><div>• • 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	Y	171	
1	Z	171	
2	G	36	
2	H	36	
2	I	36	
2	U	36	
2	V	36	
2	W	36	

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
2	A23	I	32	X	-	-	-
2	A23	U	32	X	-	X	-
2	A23	V	32	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12651 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 TOXN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1316	848	218	243	7			
1	B	162	Total	C	N	O	S	0	0	0
			1316	848	218	243	7			
1	E	162	Total	C	N	O	S	0	0	0
			1316	848	218	243	7			
1	X	162	Total	C	N	O	S	0	0	0
			1316	848	218	243	7			
1	Y	162	Total	C	N	O	S	0	0	0
			1316	848	218	243	7			
1	Z	162	Total	C	N	O	S	0	0	0
			1316	848	218	243	7			

- Molecule 2 is a RNA chain called TOXI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	36	Total	C	N	O	P	0	0	0
			764	342	132	254	36			
2	H	36	Total	C	N	O	P	0	0	0
			764	342	132	254	36			
2	I	36	Total	C	N	O	P	0	0	0
			764	342	132	254	36			
2	U	36	Total	C	N	O	P	0	0	0
			764	342	132	254	36			
2	V	36	Total	C	N	O	P	0	0	0
			764	342	132	254	36			
2	W	36	Total	C	N	O	P	0	0	0
			764	342	132	254	36			

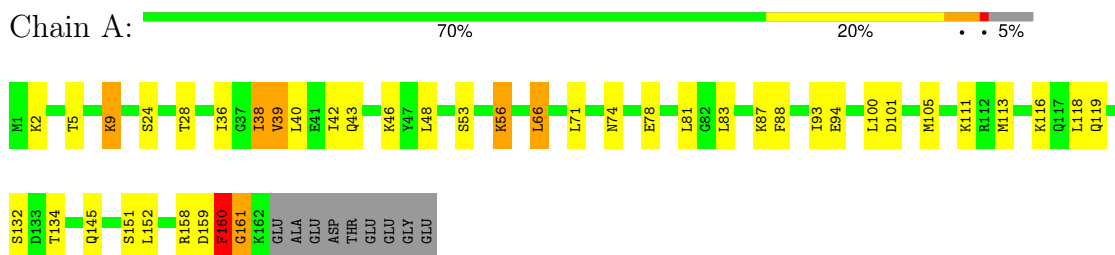
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	30	Total 30	O 30	0	0
3	E	23	Total 23	O 23	0	0
3	G	16	Total 16	O 16	0	0
3	H	20	Total 20	O 20	0	0
3	I	14	Total 14	O 14	0	0
3	U	9	Total 9	O 9	0	0
3	V	4	Total 4	O 4	0	0
3	W	6	Total 6	O 6	0	0
3	X	5	Total 5	O 5	0	0
3	Y	10	Total 10	O 10	0	0
3	Z	5	Total 5	O 5	0	0

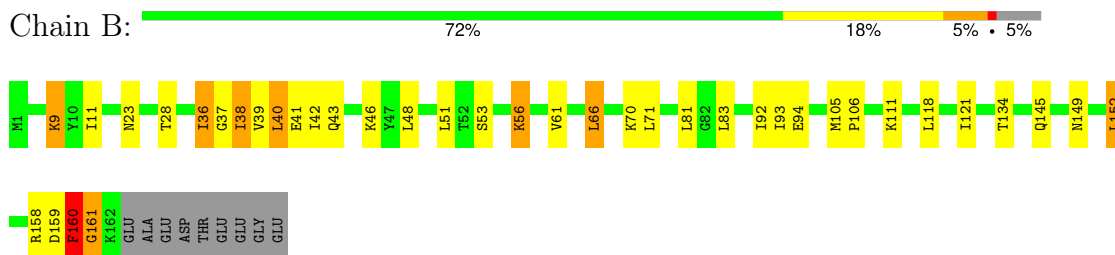
### 3 Residue-property plots

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

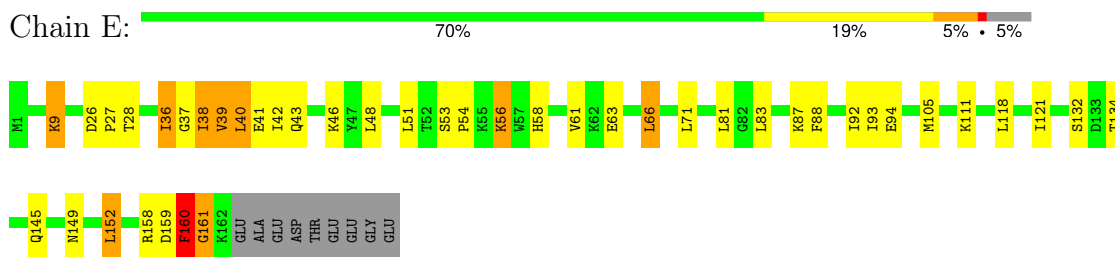
#### • Molecule 1: TOXN



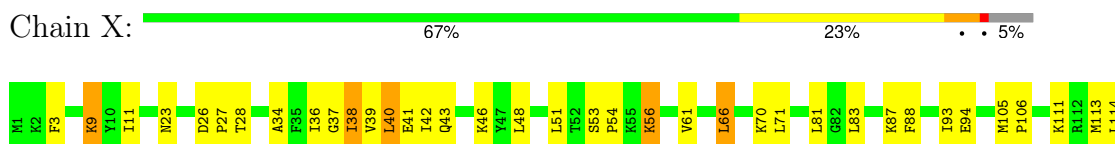
#### • Molecule 1: TOXN



#### • Molecule 1: TOXN



#### • Molecule 1: TOXN

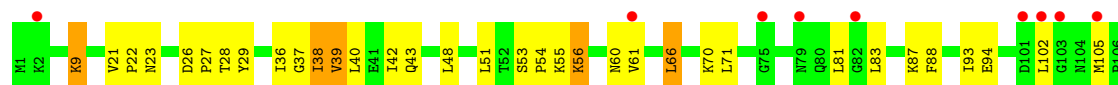




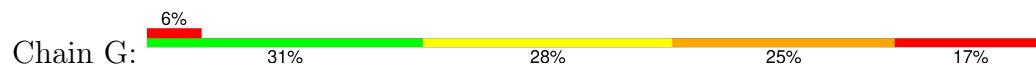
• Molecule 1: TOXN



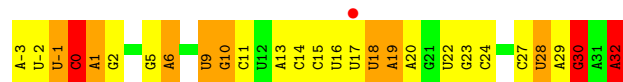
• Molecule 1: TOXN



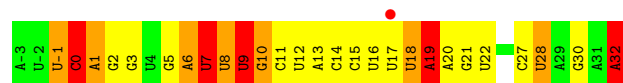
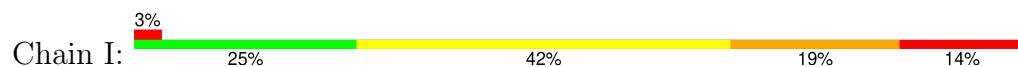
• Molecule 2: TOXI



• Molecule 2: TOXI

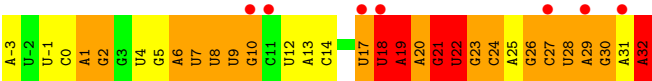


• Molecule 2: TOXI

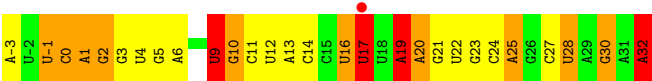
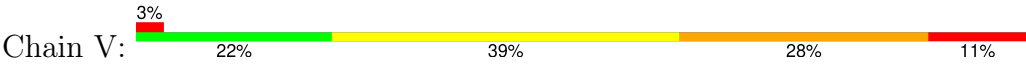


• Molecule 2: TOXI

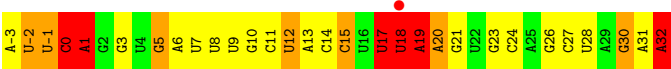
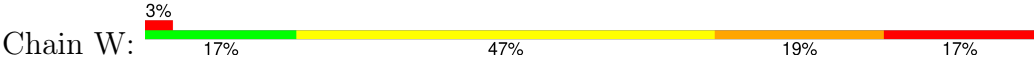




● Molecule 2: TOXI



● Molecule 2: TOXI





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.14Å 119.12Å 377.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.00 35.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.1 (35.00-3.00) 89.1 (35.00-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, $R_{free}$	0.214 , 0.258 0.216 , 0.213	Depositor DCC
$R_{free}$ test set	1762 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.76% 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: A23

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	0.63	0/1345	0.63	1/1811 (0.1%)
1	B	0.59	0/1345	0.62	1/1811 (0.1%)
1	E	0.52	0/1345	0.60	1/1811 (0.1%)
1	X	0.43	0/1345	0.56	1/1811 (0.1%)
1	Y	0.49	0/1345	0.56	1/1811 (0.1%)
1	Z	0.40	0/1345	0.53	1/1811 (0.1%)
2	G	0.98	1/825 (0.1%)	1.73	16/1283 (1.2%)
2	H	0.94	0/825	1.82	25/1283 (1.9%)
2	I	0.76	0/825	1.57	15/1283 (1.2%)
2	U	0.47	0/825	1.34	11/1283 (0.9%)
2	V	0.63	0/825	1.51	15/1283 (1.2%)
2	W	0.63	0/825	1.44	11/1283 (0.9%)
All	All	0.62	1/13020 (0.0%)	1.11	99/18564 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	E	0	2
1	X	0	1
1	Y	0	1
1	Z	0	1
2	I	2	0
2	U	3	0
2	V	2	0
All	All	7	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	18	U	N1-C2	5.92	1.43	1.38

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	21	G	P-O3'-C3'	14.45	137.04	119.70
2	H	18	U	O4'-C1'-N1	14.42	119.74	108.20
2	G	29	A	P-O3'-C3'	12.53	134.74	119.70
2	I	9	U	N1-C1'-C2'	-11.28	99.34	114.00
2	I	0	C	O4'-C1'-N1	10.98	116.98	108.20
2	V	9	U	N1-C1'-C2'	-10.75	100.02	114.00
2	I	19	A	P-O3'-C3'	-9.92	107.80	119.70
2	G	18	U	N1-C1'-C2'	9.70	126.61	114.00
2	V	1	A	P-O3'-C3'	-9.69	108.08	119.70
2	U	7	U	O4'-C1'-N1	8.68	115.14	108.20
2	U	7	U	N1-C1'-C2'	-8.61	102.53	112.00
2	W	18	U	O4'-C1'-N1	8.57	115.06	108.20
2	G	17	U	P-O3'-C3'	8.43	129.81	119.70
2	U	18	U	O4'-C1'-N1	8.42	114.94	108.20
2	V	17	U	O4'-C1'-N1	-8.42	101.47	108.20
2	V	5	G	O4'-C1'-N9	8.26	114.81	108.20
2	H	0	C	P-O3'-C3'	8.17	129.50	119.70
2	V	16	U	O4'-C1'-N1	-8.02	101.78	108.20
2	I	6	A	P-O3'-C3'	8.01	129.31	119.70
2	W	-1	U	O4'-C1'-N1	7.88	114.50	108.20
2	I	18	U	O4'-C1'-N1	7.82	114.46	108.20
2	U	22	U	N1-C1'-C2'	-7.70	103.53	112.00
2	H	18	U	C2-N1-C1'	7.45	126.64	117.70
2	H	19	A	P-O3'-C3'	7.42	128.61	119.70
2	I	17	U	O4'-C1'-N1	7.36	114.09	108.20
2	G	18	U	C2-N1-C1'	7.25	126.40	117.70
2	G	15	C	O4'-C1'-N1	-7.20	102.44	108.20
2	H	18	U	C5-C6-N1	7.19	126.29	122.70
2	I	22	U	O4'-C1'-N1	7.18	113.94	108.20
2	H	30	G	N1-C6-O6	-7.07	115.66	119.90
2	H	10	G	OP2-P-O3'	7.00	120.61	105.20
2	H	18	U	P-O3'-C3'	6.99	128.08	119.70
2	H	-1	U	O4'-C1'-N1	6.88	113.71	108.20
2	U	19	A	P-O3'-C3'	-6.84	111.49	119.70
2	W	15	C	O4'-C1'-N1	-6.84	102.73	108.20
2	H	18	U	N1-C2-O2	6.77	127.54	122.80
2	V	9	U	P-O3'-C3'	-6.74	111.61	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	18	U	N1-C2-O2	6.63	127.44	122.80
2	H	19	A	C8-N9-C4	-6.61	103.16	105.80
2	I	0	C	P-O3'-C3'	6.61	127.63	119.70
2	U	-1	U	O4'-C1'-N1	6.53	113.43	108.20
2	G	20	A	N1-C6-N6	-6.51	114.69	118.60
2	G	11	C	N1-C1'-C2'	-6.51	104.84	112.00
2	W	0	C	N1-C1'-C2'	-6.42	104.94	112.00
2	V	19	A	C3'-C2'-C1'	6.32	106.56	101.50
2	I	2	G	P-O3'-C3'	-6.25	112.19	119.70
2	H	15	C	O4'-C1'-N1	-6.25	103.20	108.20
2	H	13	A	P-O3'-C3'	6.00	126.90	119.70
2	V	9	U	C3'-C2'-C1'	5.97	106.28	101.50
2	I	19	A	C3'-C2'-C1'	5.95	106.26	101.50
2	H	28	U	O4'-C1'-N1	5.93	112.95	108.20
2	H	29	A	P-O5'-C5'	-5.90	111.46	120.90
2	U	24	C	O4'-C1'-N1	5.90	112.92	108.20
2	H	18	U	C6-N1-C1'	-5.86	113.00	121.20
2	H	5	G	O4'-C1'-N9	5.83	112.87	108.20
2	G	8	U	P-O3'-C3'	-5.77	112.78	119.70
2	I	22	U	N1-C2-O2	-5.77	118.76	122.80
2	W	19	A	P-O5'-C5'	5.69	130.01	120.90
2	G	5	G	N1-C6-O6	-5.67	116.50	119.90
2	V	3	G	P-O3'-C3'	5.64	126.47	119.70
2	I	28	U	O4'-C1'-N1	5.62	112.69	108.20
2	G	19	A	P-O3'-C3'	-5.62	112.96	119.70
2	V	1	A	N9-C1'-C2'	-5.58	105.86	112.00
2	I	7	U	P-O5'-C5'	-5.55	112.01	120.90
2	G	16	U	C3'-C2'-C1'	-5.53	97.08	101.50
2	H	16	U	P-O3'-C3'	5.49	126.29	119.70
1	B	161	GLY	N-CA-C	5.49	126.81	113.10
1	A	161	GLY	N-CA-C	5.48	126.81	113.10
1	X	161	GLY	N-CA-C	5.48	126.80	113.10
1	Y	161	GLY	N-CA-C	5.48	126.81	113.10
1	E	161	GLY	N-CA-C	5.48	126.79	113.10
1	Z	161	GLY	N-CA-C	5.48	126.80	113.10
2	W	17	U	P-O3'-C3'	5.47	126.26	119.70
2	H	30	G	N3-C2-N2	5.47	123.73	119.90
2	H	19	A	N3-C4-C5	-5.46	122.98	126.80
2	V	19	A	C8-N9-C4	-5.46	103.62	105.80
2	H	2	G	N3-C4-N9	-5.41	122.75	126.00
2	H	18	U	N1-C2-N3	-5.41	111.66	114.90
2	W	12	U	N1-C1'-C2'	-5.38	106.09	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	14	C	O4'-C1'-N1	5.35	112.48	108.20
2	U	19	A	C3'-C2'-C1'	5.34	105.78	101.50
2	G	26	G	P-O5'-C5'	-5.32	112.39	120.90
2	V	-1	U	C2-N1-C1'	5.32	124.08	117.70
2	G	8	U	N1-C2-O2	-5.32	119.08	122.80
2	U	21	G	OP2-P-O3'	5.29	116.84	105.20
2	I	9	U	O4'-C1'-N1	5.27	112.42	108.20
2	W	-2	U	O4'-C1'-N1	5.27	112.41	108.20
2	H	30	G	N3-C4-C5	-5.25	125.97	128.60
2	U	21	G	C3'-C2'-C1'	5.21	105.67	101.50
2	V	-1	U	N1-C1'-C2'	5.16	120.70	114.00
2	G	19	A	N9-C1'-C2'	-5.13	106.36	112.00
2	V	3	G	OP2-P-O3'	5.11	116.44	105.20
2	W	1	A	O4'-C1'-N9	-5.06	104.15	108.20
2	V	0	C	O4'-C1'-N1	5.05	112.24	108.20
2	H	13	A	N1-C6-N6	5.04	121.62	118.60
2	W	5	G	N1-C6-O6	-5.03	116.88	119.90
2	I	21	G	P-O3'-C3'	5.03	125.73	119.70
2	W	5	G	O4'-C1'-N9	5.02	112.22	108.20
2	H	14	C	N1-C2-O2	-5.01	115.89	118.90

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	32	A23	C2',C1'
2	U	32	A23	C3',C2',C1'
2	V	32	A23	C2',C1'

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	PHE	Peptide
1	A	36	ILE	Peptide
1	B	160	PHE	Peptide
1	B	36	ILE	Peptide
1	E	160	PHE	Peptide
1	E	36	ILE	Peptide
1	X	160	PHE	Peptide
1	Y	160	PHE	Peptide
1	Z	160	PHE	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	1316	0	1338	27	0
1	B	1316	0	1338	33	0
1	E	1316	0	1338	33	0
1	X	1316	0	1338	38	1
1	Y	1316	0	1338	27	1
1	Z	1316	0	1338	56	0
2	G	764	0	383	27	0
2	H	764	0	384	18	0
2	I	764	0	383	26	0
2	U	764	0	384	85	0
2	V	764	0	383	30	0
2	W	764	0	384	37	0
3	A	29	0	0	4	0
3	B	30	0	0	0	0
3	E	23	0	0	0	0
3	G	16	0	0	1	0
3	H	20	0	0	1	0
3	I	14	0	0	0	0
3	U	9	0	0	3	0
3	V	4	0	0	1	0
3	W	6	0	0	0	0
3	X	5	0	0	0	0
3	Y	10	0	0	0	0
3	Z	5	0	0	0	0
All	All	12651	0	10329	385	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 17.

All (385) 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)
2:U:32:A23:H2	1:Z:53:SER:CA	1.53	1.38
2:U:32:A23:H2	1:Z:53:SER:CB	1.65	1.24
2:U:32:A23:H2	1:Z:53:SER:HB3	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:32:A23:C2	1:Z:53:SER:HB3	1.86	1.05
2:U:32:A23:C2	1:Z:53:SER:N	2.21	1.04
2:U:32:A23:H2	1:Z:53:SER:N	1.75	1.02
1:B:158:ARG:HG2	1:B:158:ARG:HH11	1.26	1.00
2:V:16:U:H5'	2:V:17:U:H5'	1.45	0.98
2:U:12:U:H3'	3:U:2006:HOH:O	1.63	0.98
1:X:9:LYS:HD2	1:X:9:LYS:H	1.28	0.98
1:Z:9:LYS:H	1:Z:9:LYS:HD2	1.29	0.96
1:E:9:LYS:H	1:E:9:LYS:HD2	1.29	0.96
2:U:32:A23:C2	1:Z:53:SER:CA	2.44	0.95
1:B:9:LYS:H	1:B:9:LYS:HD2	1.31	0.94
2:W:32:A23:H2'	2:W:32:A23:N3	1.80	0.94
1:A:9:LYS:H	1:A:9:LYS:HD2	1.30	0.94
1:E:158:ARG:HG2	1:E:158:ARG:HH11	1.31	0.94
1:Y:158:ARG:HG2	1:Y:158:ARG:HH11	1.34	0.92
1:Y:9:LYS:H	1:Y:9:LYS:HD2	1.33	0.91
1:X:158:ARG:HG2	1:X:158:ARG:HH11	1.34	0.91
1:Z:158:ARG:HG2	1:Z:158:ARG:HH11	1.33	0.90
2:G:18:U:H4'	2:G:19:A:H5''	1.54	0.88
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.40	0.87
2:U:32:A23:H2	1:Z:53:SER:HA	1.57	0.86
2:G:18:U:C4'	2:G:19:A:H5''	2.06	0.85
2:W:32:A23:N3	2:W:32:A23:C2'	2.29	0.85
2:V:16:U:C5'	2:V:17:U:H5'	2.07	0.84
2:U:27:C:H41	1:Z:116:LYS:NZ	1.75	0.83
2:U:5:G:O2'	1:Z:122:ARG:NH2	2.13	0.82
2:U:6:A:HO2'	1:Z:115:TYR:HH	1.20	0.82
2:U:9:U:O2'	2:U:10:G:H5''	1.80	0.81
2:U:7:U:O4	1:Z:119:GLN:HB2	1.82	0.80
1:B:158:ARG:HG2	1:B:158:ARG:NH1	1.99	0.78
2:G:0:C:C2'	2:G:1:A:H5'	2.14	0.77
2:W:19:A:O2'	2:W:20:A:C8	2.36	0.77
2:U:6:A:C4	1:Z:102:LEU:HD12	2.21	0.76
1:A:101:ASP:HA	3:A:2017:HOH:O	1.85	0.75
1:B:53:SER:N	2:I:32:A23:H2	2.03	0.74
1:E:158:ARG:HG2	1:E:158:ARG:NH1	2.03	0.73
2:H:32:A23:C2'	2:H:32:A23:N3	2.39	0.72
1:X:158:ARG:HG2	1:X:158:ARG:NH1	2.04	0.71
2:U:6:A:C8	1:Z:102:LEU:HB2	2.25	0.71
2:W:18:U:H4'	2:W:19:A:O5'	1.91	0.71
2:I:19:A:H8	2:I:19:A:H5''	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:13:A:H2'	2:U:14:C:O4'	1.88	0.70
2:G:20:A:H5'	3:G:2009:HOH:O	1.91	0.70
1:Y:158:ARG:HG2	1:Y:158:ARG:NH1	2.05	0.69
1:Z:158:ARG:HG2	1:Z:158:ARG:NH1	2.04	0.69
2:U:30:G:H4'	2:U:30:G:OP1	1.92	0.69
2:V:17:U:H2'	2:V:17:U:O2	1.92	0.68
1:A:158:ARG:HG2	1:A:158:ARG:NH1	2.07	0.67
2:U:-3:A:C8	1:X:23:ASN:ND2	2.63	0.67
2:U:17:U:H4'	2:U:18:U:OP2	1.93	0.66
2:U:25:A:C8	2:U:26:G:N2	2.64	0.66
2:W:0:C:C2	1:Z:60:ASN:HB3	2.30	0.66
2:V:32:A23:H2	1:X:53:SER:HB3	1.77	0.65
2:G:18:U:H4'	2:G:19:A:C5'	2.25	0.65
1:Y:159:ASP:O	1:Y:160:PHE:CB	2.45	0.65
1:E:9:LYS:H	1:E:9:LYS:CD	2.05	0.64
2:U:30:G:C8	1:Z:113:MET:HB2	2.33	0.64
1:E:159:ASP:O	1:E:160:PHE:CB	2.46	0.64
2:U:32:A23:N3	2:U:32:A23:O2'	2.30	0.64
1:Z:159:ASP:O	1:Z:160:PHE:CB	2.46	0.64
1:X:66:LEU:HD21	1:X:134:THR:HG22	1.80	0.63
1:Z:9:LYS:H	1:Z:9:LYS:CD	2.05	0.63
2:V:32:A23:H2	1:X:53:SER:CA	2.28	0.63
1:X:159:ASP:O	1:X:160:PHE:CB	2.46	0.63
2:G:-1:U:H2'	2:G:-1:U:O2	1.99	0.62
2:G:0:C:C3'	2:G:1:A:H5'	2.29	0.62
2:V:16:U:H5'	2:V:17:U:C5'	2.23	0.62
2:I:7:U:C5'	2:I:7:U:H6	2.12	0.62
1:B:159:ASP:O	1:B:160:PHE:CB	2.47	0.62
2:W:10:G:H2'	2:W:11:C:O4'	2.00	0.62
1:E:66:LEU:HD21	1:E:134:THR:HG22	1.82	0.62
2:U:32:A23:N3	1:Z:53:SER:HB3	2.14	0.62
2:W:32:A23:H2	1:Y:53:SER:N	2.15	0.61
2:W:-3:A:O2'	2:W:-2:U:H5'	2.00	0.61
2:U:32:A23:C2	1:Z:53:SER:CB	2.47	0.61
1:B:9:LYS:H	1:B:9:LYS:CD	2.09	0.61
2:V:32:A23:H2	1:X:53:SER:CB	2.30	0.61
2:U:19:A:H2'	2:U:20:A:C8	2.36	0.61
2:I:-1:U:H5''	2:I:0:C:OP1	2.01	0.61
2:U:1:A:HO2'	2:U:2:G:H8	1.47	0.60
2:W:27:C:C4	2:W:28:U:C4	2.89	0.60
1:B:53:SER:CA	2:I:32:A23:H2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:32:A23:C2	1:Z:53:SER:H	2.10	0.60
2:V:23:G:O2'	2:V:24:C:H5'	2.01	0.60
1:X:9:LYS:H	1:X:9:LYS:CD	2.05	0.60
1:Y:9:LYS:H	1:Y:9:LYS:CD	2.09	0.60
1:A:159:ASP:O	1:A:160:PHE:CB	2.49	0.60
2:V:4:U:C4	2:V:21:G:C6	2.90	0.60
2:V:19:A:O2'	2:V:20:A:C8	2.45	0.59
2:W:17:U:H4'	2:W:18:U:OP1	2.03	0.59
2:U:25:A:H5'	2:U:26:G:OP2	2.02	0.59
2:I:5:G:C5	2:I:8:U:C5	2.90	0.59
2:V:9:U:C5'	2:V:9:U:H6	2.16	0.59
2:U:22:U:O2'	2:U:23:G:H8	1.86	0.58
2:I:9:U:HO2'	2:I:10:G:H8	1.48	0.58
2:U:7:U:O2'	2:U:8:U:H5'	2.02	0.58
2:U:27:C:H5'	2:U:28:U:H5''	1.84	0.58
2:G:0:C:H2'	2:G:1:A:H5'	1.84	0.58
2:H:32:A23:N3	2:H:32:A23:H2'	2.16	0.58
2:U:1:A:C2	2:U:2:G:C5	2.92	0.58
2:I:5:G:C4	2:I:8:U:C5	2.92	0.57
1:Y:66:LEU:HD21	1:Y:134:THR:HG22	1.86	0.57
2:U:19:A:O2'	2:U:20:A:O4'	2.22	0.57
1:Z:66:LEU:HD21	1:Z:134:THR:HG22	1.84	0.57
1:A:83:LEU:HD12	1:A:83:LEU:C	2.25	0.57
2:G:16:U:H3'	2:G:16:U:C6	2.40	0.57
2:U:12:U:H2'	2:U:13:A:H8	1.68	0.57
2:V:9:U:C6	2:V:9:U:H5'	2.40	0.56
2:U:10:G:O6	2:U:25:A:C4	2.58	0.56
2:U:28:U:C5	2:U:29:A:C8	2.93	0.56
1:Z:83:LEU:HD12	1:Z:83:LEU:C	2.25	0.56
2:U:27:C:N4	1:Z:116:LYS:NZ	2.51	0.56
1:A:9:LYS:H	1:A:9:LYS:CD	2.04	0.56
2:U:32:A23:H4'	1:Z:29:TYR:CD1	2.40	0.56
2:U:22:U:HO2'	2:U:23:G:H8	1.47	0.56
1:X:9:LYS:HD2	1:X:9:LYS:N	2.11	0.56
2:I:9:U:O2'	2:I:10:G:H8	1.89	0.56
2:U:5:G:H2'	2:U:6:A:H5'	1.88	0.55
2:U:1:A:O2'	2:U:2:G:H8	1.90	0.55
2:I:14:C:O2'	2:I:15:C:H5'	2.06	0.55
1:A:53:SER:N	2:H:32:A23:H2	2.22	0.55
2:W:-3:A:N6	1:Z:21:VAL:O	2.40	0.54
1:B:83:LEU:C	1:B:83:LEU:HD12	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:22:U:O2'	2:U:23:G:C8	2.60	0.54
2:U:5:G:N2	2:U:21:G:C4	2.75	0.54
2:U:24:C:C4	2:U:25:A:N7	2.76	0.54
2:W:10:G:C5	2:W:11:C:C4	2.96	0.54
1:A:87:LYS:HD3	1:A:88:PHE:CZ	2.42	0.53
1:B:23:ASN:ND2	2:H:-3:A:C8	2.76	0.53
2:V:9:U:H6	2:V:9:U:H5'	1.72	0.53
1:X:83:LEU:C	1:X:83:LEU:HD12	2.28	0.53
2:G:19:A:O2'	2:G:20:A:C8	2.58	0.53
2:V:12:U:H2'	2:V:13:A:H8	1.74	0.53
1:E:9:LYS:HD2	1:E:9:LYS:N	2.12	0.53
2:U:23:G:C6	2:U:24:C:N4	2.76	0.53
1:A:66:LEU:HD21	1:A:134:THR:HG22	1.90	0.53
1:Z:38:ILE:H	1:Z:48:LEU:HD23	1.75	0.52
2:U:4:U:H1'	2:U:20:A:C4	2.45	0.51
1:B:36:ILE:HB	1:B:51:LEU:HD11	1.92	0.51
1:B:66:LEU:HD21	1:B:134:THR:HG22	1.91	0.51
2:U:26:G:N7	2:U:27:C:C4	2.79	0.51
1:E:83:LEU:C	1:E:83:LEU:HD12	2.31	0.51
2:G:10:G:H2'	2:G:11:C:C6	2.45	0.51
1:B:158:ARG:NH1	1:B:158:ARG:CG	2.71	0.51
1:Y:83:LEU:C	1:Y:83:LEU:HD12	2.30	0.51
2:U:6:A:C5	1:Z:102:LEU:HD12	2.46	0.50
2:W:23:G:H2'	2:W:24:C:H6	1.76	0.50
2:W:10:G:C6	2:W:11:C:N3	2.79	0.50
2:U:1:A:C2	2:U:2:G:C4	3.00	0.50
2:H:0:C:H1'	2:H:1:A:OP1	2.12	0.50
2:W:23:G:H2'	2:W:24:C:C6	2.47	0.50
2:U:9:U:H5	3:U:2008:HOH:O	1.95	0.50
1:E:66:LEU:HD21	1:E:134:THR:CG2	2.42	0.49
2:U:32:A23:H3'	1:Z:29:TYR:CE1	2.46	0.49
2:G:1:A:O5'	2:G:1:A:H8	1.95	0.49
2:U:25:A:H5''	2:U:26:G:N2	2.26	0.49
2:I:9:U:O2'	2:I:10:G:O5'	2.30	0.49
2:U:27:C:H5	1:Z:116:LYS:HZ1	1.61	0.49
1:B:9:LYS:HD2	1:B:9:LYS:N	2.14	0.49
2:V:4:U:H1'	2:V:20:A:C4	2.48	0.49
2:U:9:U:OP2	2:U:9:U:H3'	2.13	0.48
1:X:105:MET:HE2	1:X:111:LYS:HB2	1.95	0.48
2:U:19:A:HO2'	2:U:20:A:C1'	2.25	0.48
2:G:-1:U:O2	2:G:-1:U:C2'	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:9:U:H2'	2:W:9:U:O2	2.12	0.48
1:Y:66:LEU:HA	1:Y:66:LEU:HD12	1.64	0.48
1:E:26:ASP:HA	1:E:27:PRO:HD3	1.72	0.48
2:U:23:G:O2'	2:U:24:C:H5'	2.14	0.48
1:X:38:ILE:H	1:X:48:LEU:HD23	1.78	0.48
1:X:66:LEU:HD21	1:X:134:THR:CG2	2.43	0.48
1:X:42:ILE:HG12	1:X:43:GLN:HG3	1.96	0.48
2:V:9:U:C5'	2:V:9:U:C6	2.97	0.48
1:A:74:ASN:OD1	1:A:119:GLN:HG2	2.14	0.48
2:W:18:U:H4'	2:W:19:A:C5'	2.44	0.47
2:U:27:C:H3'	2:U:28:U:H4'	1.96	0.47
2:V:-3:A:C8	1:Y:23:ASN:ND2	2.83	0.47
1:E:42:ILE:HG12	1:E:43:GLN:HG3	1.97	0.47
2:U:12:U:H1'	2:U:23:G:N2	2.29	0.47
2:U:30:G:OP1	2:U:30:G:C4'	2.62	0.47
2:U:32:A23:O1C	1:Z:55:LYS:HE2	2.14	0.47
1:Y:87:LYS:HD3	1:Y:88:PHE:CZ	2.50	0.47
2:V:32:A23:H8	1:X:34:ALA:H	1.80	0.47
1:B:42:ILE:HG12	1:B:43:GLN:HG3	1.97	0.47
1:Z:158:ARG:NH1	1:Z:158:ARG:CG	2.75	0.47
2:U:26:G:C8	2:U:27:C:C2	3.03	0.46
2:I:27:C:H2'	2:I:28:U:O4'	2.14	0.46
2:U:24:C:C2'	2:U:25:A:O5'	2.63	0.46
1:B:38:ILE:H	1:B:48:LEU:HD23	1.80	0.46
1:B:105:MET:HE2	1:B:111:LYS:HB2	1.98	0.46
2:H:22:U:C2	2:H:23:G:C8	3.03	0.46
2:G:1:A:H2'	2:G:2:G:O4'	2.16	0.46
1:E:36:ILE:HB	1:E:51:LEU:HD11	1.97	0.46
2:I:13:A:C6	2:I:14:C:C4	3.04	0.46
2:U:5:G:N2	2:U:8:U:C4	2.84	0.46
2:U:12:U:H2'	2:U:13:A:C8	2.49	0.46
1:X:53:SER:HB2	1:X:54:PRO:HD2	1.98	0.46
1:Y:38:ILE:H	1:Y:48:LEU:HD23	1.79	0.46
2:G:29:A:O4'	2:G:30:G:C2	2.69	0.46
2:U:4:U:O2	2:U:21:G:H5'	2.16	0.46
1:X:36:ILE:HB	1:X:51:LEU:HD11	1.98	0.46
2:U:7:U:O2'	2:U:8:U:C5'	2.63	0.46
2:W:-3:A:H2'	2:W:-2:U:O4'	2.16	0.46
1:B:38:ILE:CD1	1:B:46:LYS:HB3	2.46	0.46
2:W:7:U:H2'	2:W:8:U:H5'	1.98	0.46
2:H:27:C:N4	2:H:28:U:C4	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:32:A23:N3	2:I:32:A23:C2'	2.71	0.46
2:U:19:A:C2'	2:U:20:A:C8	2.98	0.46
2:W:-2:U:O4	1:Z:22:PRO:HA	2.17	0.46
2:W:0:C:H3'	2:W:1:A:H5'	1.97	0.46
1:A:151:SER:HB2	3:A:2026:HOH:O	2.15	0.45
1:Y:53:SER:HB2	1:Y:54:PRO:HD2	1.98	0.45
1:Y:56:LYS:H	1:Y:56:LYS:HD2	1.81	0.45
1:Z:66:LEU:HD21	1:Z:134:THR:CG2	2.46	0.45
1:Z:42:ILE:HG12	1:Z:43:GLN:HG3	1.98	0.45
2:V:30:G:C8	1:X:113:MET:HB2	2.51	0.45
1:Z:36:ILE:HB	1:Z:51:LEU:HD11	1.99	0.45
1:Z:105:MET:HE2	1:Z:111:LYS:HB2	1.98	0.45
2:H:0:C:O2'	2:H:1:A:P	2.74	0.45
1:X:56:LYS:H	1:X:56:LYS:HD2	1.81	0.45
1:Z:53:SER:HB2	1:Z:54:PRO:HD2	1.97	0.45
2:G:0:C:O4'	2:G:0:C:P	2.74	0.45
2:G:16:U:C6	2:G:16:U:C3'	2.99	0.45
2:G:26:G:H2'	2:G:27:C:C6	2.52	0.45
1:X:3:PHE:CE2	1:X:114:LEU:HD22	2.52	0.45
1:Y:159:ASP:O	1:Y:160:PHE:HB2	2.17	0.45
2:G:15:C:O2'	2:G:16:U:H5'	2.16	0.45
2:H:1:A:OP2	2:H:1:A:H8	2.00	0.45
1:A:105:MET:HE2	1:A:111:LYS:HB2	1.99	0.45
2:G:19:A:C2	2:G:20:A:C2	3.05	0.45
2:H:27:C:H2'	2:H:28:U:O4'	2.17	0.45
1:X:66:LEU:HD12	1:X:66:LEU:HA	1.64	0.45
2:U:27:C:H3'	2:U:28:U:C5'	2.47	0.44
1:Y:42:ILE:HG12	1:Y:43:GLN:HG3	1.99	0.44
2:V:32:A23:H2	1:X:53:SER:N	2.33	0.44
1:Z:87:LYS:HD3	1:Z:88:PHE:CZ	2.52	0.44
1:B:105:MET:HE2	1:B:105:MET:HB3	1.90	0.44
2:W:26:G:H2'	2:W:27:C:O4'	2.18	0.44
1:Z:56:LYS:H	1:Z:56:LYS:HD2	1.83	0.44
2:G:18:U:O4'	2:G:19:A:H5''	2.16	0.44
2:W:23:G:O2'	2:W:24:C:H5'	2.16	0.44
2:U:4:U:H4'	3:U:2004:HOH:O	2.18	0.44
1:Z:26:ASP:HA	1:Z:27:PRO:HD3	1.75	0.44
1:Z:56:LYS:H	1:Z:56:LYS:CD	2.30	0.44
1:E:105:MET:HE2	1:E:105:MET:HB3	1.90	0.44
2:H:0:C:O2	2:H:0:C:O5'	2.35	0.44
2:W:17:U:O2	2:W:17:U:O4'	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:87:LYS:HD3	1:X:88:PHE:CZ	2.53	0.44
1:B:92:ILE:C	1:B:92:ILE:HD12	2.38	0.44
1:E:38:ILE:CD1	1:E:46:LYS:HB3	2.48	0.44
1:Y:56:LYS:H	1:Y:56:LYS:CD	2.30	0.44
1:E:53:SER:HB2	1:E:54:PRO:HD2	1.99	0.43
2:V:9:U:H2'	2:V:10:G:C8	2.52	0.43
1:A:56:LYS:CD	1:A:56:LYS:H	2.31	0.43
1:B:66:LEU:HA	1:B:66:LEU:HD12	1.68	0.43
1:E:37:GLY:HA2	1:E:48:LEU:HD22	1.99	0.43
1:A:24:SER:HB2	3:A:2005:HOH:O	2.18	0.43
2:U:27:C:H3'	2:U:28:U:C4'	2.47	0.43
2:V:27:C:H2'	2:V:28:U:O4'	2.18	0.43
1:Y:61:VAL:HG13	1:Y:70:LYS:HD2	2.00	0.43
1:B:56:LYS:CD	1:B:56:LYS:H	2.31	0.43
1:Y:66:LEU:HD21	1:Y:134:THR:CG2	2.48	0.43
1:Z:9:LYS:HD2	1:Z:9:LYS:N	2.12	0.43
1:E:87:LYS:HD3	1:E:88:PHE:CZ	2.54	0.43
2:I:8:U:H6	2:I:8:U:H2'	1.66	0.43
2:U:-3:A:N7	1:X:23:ASN:CG	2.72	0.43
1:Z:36:ILE:HG12	1:Z:121:ILE:HD13	2.01	0.43
1:A:9:LYS:HD2	1:A:9:LYS:N	2.12	0.43
1:A:42:ILE:HG12	1:A:43:GLN:HG3	2.01	0.43
2:I:13:A:C5	2:I:14:C:C5	3.06	0.43
2:V:22:U:C2	2:V:23:G:C8	3.07	0.43
2:W:14:C:H2'	2:W:15:C:C6	2.53	0.43
1:Z:38:ILE:H	1:Z:48:LEU:CD2	2.30	0.43
2:V:23:G:P	3:V:2002:HOH:O	2.76	0.43
2:U:32:A23:H5''	2:U:32:A23:H1'	1.12	0.43
2:W:10:G:C6	2:W:11:C:C4	3.07	0.43
1:Z:66:LEU:HA	1:Z:66:LEU:HD12	1.73	0.43
1:A:38:ILE:H	1:A:48:LEU:HD23	1.84	0.42
1:E:36:ILE:HD12	1:E:36:ILE:HA	1.84	0.42
2:I:7:U:H6	2:I:7:U:H5'	1.80	0.42
2:U:5:G:C2	2:U:21:G:C4	3.07	0.42
2:V:2:G:O5'	2:V:2:G:H8	2.02	0.42
2:V:13:A:C5	2:V:14:C:C5	3.08	0.42
2:W:5:G:O2'	2:W:7:U:C5	2.72	0.42
2:W:13:A:O2'	2:W:14:C:H5'	2.19	0.42
1:Y:149:ASN:ND2	1:Y:152:LEU:HB2	2.34	0.42
1:Z:61:VAL:CG1	1:Z:70:LYS:HD2	2.49	0.42
1:A:38:ILE:CD1	1:A:46:LYS:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASN:ND2	1:B:152:LEU:HB2	2.34	0.42
2:U:9:U:H2'	2:U:9:U:P	2.59	0.42
2:W:27:C:N4	2:W:28:U:C4	2.86	0.42
1:E:38:ILE:H	1:E:48:LEU:CD2	2.32	0.42
1:E:39:VAL:HG13	1:E:132:SER:OG	2.19	0.42
1:E:105:MET:HE2	1:E:111:LYS:HB2	2.01	0.42
2:G:21:G:O2'	2:G:22:U:P	2.77	0.42
1:Y:36:ILE:HB	1:Y:51:LEU:HD11	2.00	0.42
1:B:61:VAL:CG1	1:B:70:LYS:HD2	2.50	0.42
1:E:38:ILE:H	1:E:48:LEU:HD23	1.84	0.42
2:G:15:C:H2'	2:G:16:U:C6	2.54	0.42
2:H:-3:A:H2'	2:H:-2:U:O4'	2.19	0.42
2:I:9:U:O2'	2:I:10:G:P	2.76	0.42
2:U:29:A:O2'	2:U:30:G:P	2.78	0.42
1:X:37:GLY:HA2	1:X:48:LEU:HD22	2.01	0.42
1:A:113:MET:HB2	2:H:30:G:C8	2.55	0.42
1:X:26:ASP:HA	1:X:27:PRO:HD3	1.73	0.42
1:X:38:ILE:H	1:X:48:LEU:CD2	2.32	0.42
2:H:9:U:O2'	2:H:10:G:H5'	2.19	0.42
2:U:24:C:C4	2:U:25:A:C8	3.08	0.42
2:V:10:G:C2	2:V:25:A:C2	3.08	0.42
1:X:159:ASP:O	1:X:160:PHE:HB2	2.20	0.42
1:Y:3:PHE:CE2	1:Y:114:LEU:HD22	2.55	0.42
1:B:36:ILE:HG12	1:B:121:ILE:HD13	2.01	0.42
1:E:56:LYS:CD	1:E:56:LYS:H	2.31	0.42
2:G:4:U:C4	2:G:21:G:C6	3.08	0.42
2:W:31:A:C2	1:Y:54:PRO:HD3	2.54	0.42
1:A:78:GLU:HG3	3:A:2014:HOH:O	2.18	0.42
1:A:83:LEU:HD12	1:A:83:LEU:O	2.19	0.42
1:E:48:LEU:HG	1:E:92:ILE:HG12	2.02	0.42
1:E:159:ASP:O	1:E:160:PHE:HB2	2.18	0.42
2:W:14:C:H2'	2:W:15:C:H6	1.85	0.42
1:A:2:LYS:HG2	2:H:6:A:C2	2.55	0.41
1:A:5:THR:HG23	1:A:100:LEU:CD2	2.50	0.41
1:B:56:LYS:H	1:B:56:LYS:HD2	1.84	0.41
2:I:7:U:H6	2:I:7:U:H5''	1.85	0.41
2:U:12:U:H6	2:U:12:U:O5'	2.02	0.41
2:U:22:U:O2'	2:U:23:G:O5'	2.38	0.41
2:V:16:U:C4'	2:V:17:U:H5'	2.48	0.41
1:A:116:LYS:HE3	2:H:28:U:O2	2.21	0.41
1:E:63:GLU:HB2	2:I:12:U:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:U:OP2	2:I:9:U:H3'	2.20	0.41
1:X:36:ILE:HG12	1:X:121:ILE:HD13	2.03	0.41
1:X:40:LEU:HD23	1:X:41:GLU:N	2.36	0.41
1:X:56:LYS:H	1:X:56:LYS:CD	2.28	0.41
1:Z:37:GLY:HA2	1:Z:48:LEU:HD22	2.01	0.41
1:A:56:LYS:H	1:A:56:LYS:HD2	1.86	0.41
2:I:10:G:H2'	2:I:11:C:C6	2.55	0.41
1:A:39:VAL:HG13	1:A:132:SER:OG	2.21	0.41
1:E:56:LYS:H	1:E:56:LYS:HD2	1.85	0.41
2:W:30:G:C8	1:Y:113:MET:HB2	2.56	0.41
1:Y:58:HIS:O	1:Y:61:VAL:HG12	2.20	0.41
1:Z:114:LEU:HD23	1:Z:114:LEU:HA	1.93	0.41
1:B:40:LEU:HD23	1:B:41:GLU:N	2.35	0.41
1:E:9:LYS:CD	1:E:9:LYS:N	2.80	0.41
2:W:12:U:H6	2:W:12:U:O5'	2.03	0.41
1:X:61:VAL:CG1	1:X:70:LYS:HD2	2.51	0.41
1:X:149:ASN:ND2	1:X:152:LEU:HB2	2.36	0.41
1:B:53:SER:N	2:I:32:A23:C2	2.79	0.41
1:E:58:HIS:O	1:E:61:VAL:HG12	2.21	0.41
2:I:0:C:O2'	2:I:1:A:H5'	2.21	0.41
2:U:27:C:H41	1:Z:116:LYS:HZ2	1.63	0.41
2:U:27:C:H5'	2:U:28:U:OP2	2.21	0.41
1:B:36:ILE:HD12	1:B:36:ILE:HA	1.81	0.41
1:B:53:SER:HA	2:I:32:A23:H2	1.99	0.41
1:E:149:ASN:ND2	1:E:152:LEU:HB2	2.36	0.41
2:G:8:U:H4'	2:G:9:U:OP1	2.21	0.41
2:G:17:U:O2	2:G:17:U:H2'	2.20	0.41
2:H:20:A:H5'	3:H:2008:HOH:O	2.21	0.41
2:H:23:G:H2'	2:H:24:C:C6	2.56	0.41
2:I:19:A:H5''	2:I:19:A:C8	2.45	0.41
2:W:-3:A:C8	1:Z:23:ASN:ND2	2.89	0.41
1:X:38:ILE:CD1	1:X:46:LYS:HB3	2.50	0.41
1:Z:159:ASP:O	1:Z:160:PHE:HB2	2.19	0.41
1:B:11:ILE:HD13	1:B:11:ILE:HA	1.94	0.41
2:U:5:G:C2'	2:U:6:A:H5'	2.50	0.41
2:V:-1:U:O2	2:V:-1:U:H2'	2.20	0.41
2:W:-1:U:O2	2:W:-1:U:H2'	2.21	0.41
2:W:5:G:N2	2:W:21:G:H1'	2.37	0.40
1:E:36:ILE:HG12	1:E:121:ILE:HD13	2.03	0.40
1:E:40:LEU:HD23	1:E:41:GLU:N	2.37	0.40
1:E:158:ARG:NH1	1:E:158:ARG:CG	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:32:A23:C2'	2:G:32:A23:N3	2.83	0.40
2:U:18:U:H4'	2:U:19:A:O4'	2.21	0.40
1:X:83:LEU:HD12	1:X:83:LEU:O	2.22	0.40
2:U:29:A:O2'	2:U:30:G:OP2	2.36	0.40
1:X:11:ILE:HD13	1:X:11:ILE:HA	1.96	0.40
1:B:105:MET:HA	1:B:106:PRO:HD3	1.96	0.40
1:B:159:ASP:O	1:B:160:PHE:HB3	2.21	0.40
2:U:9:U:H1'	2:U:10:G:O4'	2.20	0.40
2:W:32:A23:H2	1:Y:52:THR:C	2.41	0.40
1:Z:39:VAL:HG13	1:Z:132:SER:OG	2.22	0.40
1:B:37:GLY:HA2	1:B:48:LEU:HD22	2.04	0.40
2:V:10:G:H2'	2:V:11:C:C6	2.57	0.40
1:Y:105:MET:HE2	1:Y:111:LYS:HB2	2.02	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:X:106:PRO:CG	1:Y:155:GLU:OE1[4_455]	2.06	0.14

## 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	160/171 (94%)	155 (97%)	2 (1%)	3 (2%)	8	36
1	B	160/171 (94%)	154 (96%)	3 (2%)	3 (2%)	8	36
1	E	160/171 (94%)	154 (96%)	3 (2%)	3 (2%)	8	36
1	X	160/171 (94%)	152 (95%)	5 (3%)	3 (2%)	8	36
1	Y	160/171 (94%)	154 (96%)	3 (2%)	3 (2%)	8	36
1	Z	160/171 (94%)	154 (96%)	3 (2%)	3 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	960/1026 (94%)	923 (96%)	19 (2%)	18 (2%)	8	36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	PHE
1	B	160	PHE
1	E	160	PHE
1	X	160	PHE
1	Y	160	PHE
1	Z	160	PHE
1	A	161	GLY
1	B	161	GLY
1	E	161	GLY
1	X	161	GLY
1	Y	161	GLY
1	Z	161	GLY
1	A	38	ILE
1	B	38	ILE
1	E	38	ILE
1	X	38	ILE
1	Y	38	ILE
1	Z	38	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	149/156 (96%)	136 (91%)	13 (9%)	10	37
1	B	149/156 (96%)	136 (91%)	13 (9%)	10	37
1	E	149/156 (96%)	136 (91%)	13 (9%)	10	37
1	X	149/156 (96%)	136 (91%)	13 (9%)	10	37
1	Y	149/156 (96%)	136 (91%)	13 (9%)	10	37
1	Z	149/156 (96%)	136 (91%)	13 (9%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	894/936 (96%)	816 (91%)	78 (9%)	10	37

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	28	THR
1	A	39	VAL
1	A	40	LEU
1	A	56	LYS
1	A	66	LEU
1	A	71	LEU
1	A	81	LEU
1	A	93	ILE
1	A	94	GLU
1	A	118	LEU
1	A	145	GLN
1	A	152	LEU
1	B	9	LYS
1	B	28	THR
1	B	39	VAL
1	B	40	LEU
1	B	56	LYS
1	B	66	LEU
1	B	71	LEU
1	B	81	LEU
1	B	93	ILE
1	B	94	GLU
1	B	118	LEU
1	B	145	GLN
1	B	152	LEU
1	E	9	LYS
1	E	28	THR
1	E	39	VAL
1	E	40	LEU
1	E	56	LYS
1	E	66	LEU
1	E	71	LEU
1	E	81	LEU
1	E	93	ILE
1	E	94	GLU
1	E	118	LEU

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Mol	Chain	Res	Type
1	E	145	GLN
1	E	152	LEU
1	X	9	LYS
1	X	28	THR
1	X	39	VAL
1	X	40	LEU
1	X	56	LYS
1	X	66	LEU
1	X	71	LEU
1	X	81	LEU
1	X	93	ILE
1	X	94	GLU
1	X	118	LEU
1	X	145	GLN
1	X	152	LEU
1	Y	9	LYS
1	Y	28	THR
1	Y	39	VAL
1	Y	40	LEU
1	Y	56	LYS
1	Y	66	LEU
1	Y	71	LEU
1	Y	81	LEU
1	Y	93	ILE
1	Y	94	GLU
1	Y	118	LEU
1	Y	145	GLN
1	Y	152	LEU
1	Z	9	LYS
1	Z	28	THR
1	Z	39	VAL
1	Z	40	LEU
1	Z	56	LYS
1	Z	66	LEU
1	Z	71	LEU
1	Z	81	LEU
1	Z	93	ILE
1	Z	94	GLU
1	Z	118	LEU
1	Z	145	GLN
1	Z	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	60	ASN
1	B	43	GLN
1	B	60	ASN
1	E	43	GLN
1	E	60	ASN
1	X	43	GLN
1	X	60	ASN
1	Y	43	GLN
1	Y	60	ASN
1	Z	43	GLN
1	Z	60	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	35/36 (97%)	11 (31%)	1 (2%)
2	H	35/36 (97%)	11 (31%)	1 (2%)
2	I	35/36 (97%)	15 (42%)	3 (8%)
2	U	35/36 (97%)	21 (60%)	2 (5%)
2	V	35/36 (97%)	13 (37%)	3 (8%)
2	W	35/36 (97%)	10 (28%)	2 (5%)
All	All	210/216 (97%)	81 (38%)	12 (5%)

All (81) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	0	C
2	G	1	A
2	G	6	A
2	G	17	U
2	G	18	U
2	G	19	A
2	G	20	A
2	G	27	C
2	G	29	A
2	G	30	G
2	G	32	A23
2	H	-1	U
2	H	0	C
2	H	1	A

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Mol	Chain	Res	Type
2	H	6	A
2	H	9	U
2	H	11	C
2	H	17	U
2	H	18	U
2	H	19	A
2	H	30	G
2	H	32	A23
2	I	-1	U
2	I	0	C
2	I	1	A
2	I	3	G
2	I	6	A
2	I	7	U
2	I	8	U
2	I	9	U
2	I	10	G
2	I	16	U
2	I	18	U
2	I	19	A
2	I	20	A
2	I	30	G
2	I	32	A23
2	U	0	C
2	U	1	A
2	U	2	G
2	U	6	A
2	U	8	U
2	U	9	U
2	U	10	G
2	U	17	U
2	U	18	U
2	U	19	A
2	U	20	A
2	U	21	G
2	U	22	U
2	U	23	G
2	U	26	G
2	U	27	C
2	U	28	U
2	U	29	A
2	U	30	G

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Mol	Chain	Res	Type
2	U	31	A
2	U	32	A23
2	V	0	C
2	V	1	A
2	V	2	G
2	V	6	A
2	V	9	U
2	V	10	G
2	V	17	U
2	V	19	A
2	V	20	A
2	V	25	A
2	V	28	U
2	V	30	G
2	V	32	A23
2	W	0	C
2	W	1	A
2	W	3	G
2	W	6	A
2	W	17	U
2	W	18	U
2	W	19	A
2	W	20	A
2	W	30	G
2	W	32	A23

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	29	A
2	H	0	C
2	I	7	U
2	I	9	U
2	I	19	A
2	U	19	A
2	U	21	G
2	V	1	A
2	V	9	U
2	V	19	A
2	W	18	U
2	W	19	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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
2	A23	G	32	-	19,28,29	3.72	13 (68%)	21,43,46	4.65	13 (61%)
2	A23	U	32	2	19,28,29	2.79	12 (63%)	21,43,46	6.21	12 (57%)
2	A23	W	32	2	19,28,29	3.04	11 (57%)	21,43,46	4.36	10 (47%)
2	A23	H	32	2	19,28,29	3.29	13 (68%)	21,43,46	4.27	10 (47%)
2	A23	I	32	-	19,28,29	3.15	12 (63%)	21,43,46	5.24	18 (85%)
2	A23	V	32	2	19,28,29	2.96	12 (63%)	21,43,46	5.69	13 (61%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A23	G	32	-	-	2/3/35/36	0/4/4/4
2	A23	U	32	2	3/3/6/6	3/3/35/36	0/4/4/4
2	A23	W	32	2	-	0/3/35/36	0/4/4/4
2	A23	H	32	2	-	2/3/35/36	0/4/4/4
2	A23	I	32	-	2/2/6/6	2/3/35/36	0/4/4/4
2	A23	V	32	2	2/2/6/6	2/3/35/36	0/4/4/4

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	32	A23	C4-N3	-10.46	1.21	1.35
2	H	32	A23	C4-N3	-8.45	1.24	1.35
2	W	32	A23	C4-N3	-8.07	1.24	1.35
2	I	32	A23	C4-N3	-8.01	1.24	1.35
2	V	32	A23	C4-N3	-6.02	1.27	1.35
2	U	32	A23	C4-N3	-5.87	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	32	A23	C2-N3	4.96	1.39	1.32
2	V	32	A23	C2-N3	4.80	1.39	1.32
2	G	32	A23	C3'-C4'	-4.74	1.40	1.52
2	I	32	A23	C2'-C3'	-4.59	1.43	1.53
2	V	32	A23	C2'-C3'	-4.42	1.43	1.53
2	G	32	A23	C2-N3	4.37	1.38	1.32
2	U	32	A23	C2-N3	4.29	1.38	1.32
2	W	32	A23	C2-N3	4.23	1.38	1.32
2	I	32	A23	C2-N3	4.23	1.38	1.32
2	G	32	A23	O4'-C1'	4.11	1.46	1.40
2	H	32	A23	C2'-C3'	-3.95	1.44	1.53
2	I	32	A23	C5-N7	-3.87	1.25	1.39
2	W	32	A23	C6-C5	-3.81	1.29	1.43
2	I	32	A23	C6-C5	-3.81	1.29	1.43
2	G	32	A23	C6-C5	-3.71	1.29	1.43
2	G	32	A23	O4'-C4'	-3.71	1.36	1.45
2	U	32	A23	C2-N1	3.67	1.40	1.33
2	V	32	A23	C2-N1	3.61	1.40	1.33
2	W	32	A23	C5-N7	-3.58	1.27	1.39
2	U	32	A23	C1'-N9	-3.56	1.41	1.49
2	H	32	A23	C5-N7	-3.56	1.27	1.39
2	H	32	A23	C3'-C4'	-3.48	1.43	1.52
2	W	32	A23	C2'-C3'	-3.46	1.45	1.53
2	H	32	A23	C5'-C4'	-3.38	1.41	1.51
2	G	32	A23	C2-N1	3.31	1.39	1.33
2	V	32	A23	C5-N7	-3.29	1.28	1.39
2	U	32	A23	C2'-C3'	-3.28	1.46	1.53
2	G	32	A23	C5'-C4'	-3.27	1.41	1.51
2	U	32	A23	C6-C5	-3.26	1.31	1.43
2	V	32	A23	C6-C5	-3.24	1.31	1.43
2	G	32	A23	C5-N7	-3.19	1.28	1.39
2	G	32	A23	C2'-C3'	-3.17	1.46	1.53
2	H	32	A23	C6-C5	-3.09	1.31	1.43
2	H	32	A23	O5'-C5'	-3.07	1.35	1.44
2	W	32	A23	C2-N1	3.03	1.39	1.33
2	U	32	A23	C5-N7	-2.95	1.29	1.39
2	I	32	A23	C5'-C4'	-2.93	1.42	1.51
2	W	32	A23	C3'-C4'	-2.90	1.45	1.52
2	V	32	A23	C1'-N9	-2.88	1.42	1.49
2	U	32	A23	C8-N7	2.84	1.39	1.34
2	I	32	A23	C3'-C4'	-2.84	1.45	1.52
2	I	32	A23	C2-N1	2.82	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	32	A23	C3'-C4'	-2.80	1.45	1.52
2	H	32	A23	C2-N1	2.77	1.38	1.33
2	W	32	A23	C8-N7	2.76	1.39	1.34
2	G	32	A23	C6-N6	2.74	1.43	1.34
2	V	32	A23	C5'-C4'	-2.69	1.43	1.51
2	V	32	A23	O2'-C2'	-2.66	1.26	1.46
2	V	32	A23	C8-N7	2.63	1.39	1.34
2	I	32	A23	O2'-C2'	-2.62	1.26	1.46
2	U	32	A23	O2'-C2'	-2.61	1.26	1.46
2	I	32	A23	C1'-N9	-2.59	1.43	1.49
2	V	32	A23	O5'-C5'	-2.56	1.36	1.44
2	W	32	A23	O2'-C2'	-2.56	1.27	1.46
2	W	32	A23	C5'-C4'	-2.55	1.43	1.51
2	H	32	A23	O2'-C2'	-2.48	1.27	1.46
2	G	32	A23	C8-N7	2.48	1.39	1.34
2	G	32	A23	O5'-C5'	-2.43	1.37	1.44
2	H	32	A23	C8-N7	2.37	1.39	1.34
2	H	32	A23	O4'-C4'	-2.30	1.39	1.45
2	U	32	A23	C3'-C4'	-2.28	1.47	1.52
2	U	32	A23	C5'-C4'	-2.26	1.44	1.51
2	I	32	A23	O4'-C4'	-2.08	1.40	1.45
2	W	32	A23	O5'-C5'	-2.07	1.38	1.44
2	H	32	A23	C1'-N9	-2.07	1.44	1.49
2	U	32	A23	PC-O1C	2.05	1.57	1.50
2	I	32	A23	O5'-C5'	-2.02	1.38	1.44

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	32	A23	C4'-O4'-C1'	-17.99	93.45	109.92
2	V	32	A23	C4'-O4'-C1'	-13.75	97.33	109.92
2	G	32	A23	C5-C6-N1	-10.94	94.14	120.23
2	U	32	A23	C1'-N9-C4	-10.92	107.45	126.64
2	V	32	A23	C1'-N9-C4	-10.42	108.33	126.64
2	G	32	A23	C2'-C1'-N9	10.22	135.25	112.56
2	W	32	A23	C5-C6-N1	-10.10	96.14	120.23
2	U	32	A23	C5-C6-N1	-9.97	96.47	120.23
2	H	32	A23	C5-C6-N6	9.80	135.24	120.31
2	H	32	A23	C5-C6-N1	-9.53	97.50	120.23
2	U	32	A23	C4-C5-N7	9.44	119.31	109.34
2	I	32	A23	C5-C6-N1	-9.39	97.84	120.23
2	I	32	A23	C4'-O4'-C1'	-9.38	101.33	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	32	A23	C5-C6-N1	-9.32	98.00	120.23
2	I	32	A23	C4-C5-N7	8.64	118.47	109.34
2	W	32	A23	C4-C5-N7	8.37	118.18	109.34
2	V	32	A23	C4-C5-N7	8.04	117.83	109.34
2	I	32	A23	C1'-N9-C4	-7.92	112.72	126.64
2	G	32	A23	C5-C6-N6	7.81	132.21	120.31
2	I	32	A23	C5-C6-N6	7.38	131.55	120.31
2	W	32	A23	C5-C6-N6	7.33	131.48	120.31
2	W	32	A23	C1'-N9-C4	-7.06	114.24	126.64
2	U	32	A23	C5-C6-N6	7.01	130.99	120.31
2	V	32	A23	C2'-C1'-N9	6.87	127.80	112.56
2	G	32	A23	O4'-C1'-N9	6.78	117.74	108.75
2	H	32	A23	C2'-C1'-N9	6.66	127.34	112.56
2	I	32	A23	C2'-C1'-N9	6.57	127.15	112.56
2	V	32	A23	C5-C6-N6	6.40	130.06	120.31
2	W	32	A23	C2'-C1'-N9	6.26	126.47	112.56
2	H	32	A23	C4-C5-N7	6.19	115.88	109.34
2	H	32	A23	C1'-N9-C4	-6.10	115.92	126.64
2	I	32	A23	O4'-C1'-C2'	-5.92	96.51	106.61
2	U	32	A23	C6-C5-C4	5.69	128.97	117.90
2	U	32	A23	N6-C6-N1	5.53	130.15	118.33
2	G	32	A23	N6-C6-N1	5.48	130.05	118.33
2	V	32	A23	C6-C5-C4	5.46	128.51	117.90
2	V	32	A23	N6-C6-N1	5.34	129.75	118.33
2	W	32	A23	N6-C6-N1	5.06	129.14	118.33
2	V	32	A23	C3'-C2'-C1'	-4.90	91.83	103.55
2	V	32	A23	O4'-C1'-C2'	-4.61	98.74	106.61
2	U	32	A23	O4'-C1'-C2'	-4.60	98.75	106.61
2	H	32	A23	C6-C5-C4	4.54	126.73	117.90
2	H	32	A23	O4'-C1'-N9	-4.45	102.84	108.75
2	I	32	A23	N6-C6-N1	4.39	127.72	118.33
2	I	32	A23	C3'-C2'-C1'	-4.34	93.17	103.55
2	I	32	A23	C6-C5-C4	3.93	125.54	117.90
2	G	32	A23	O4'-C4'-C5'	3.84	121.65	109.33
2	W	32	A23	C6-C5-C4	3.82	125.32	117.90
2	W	32	A23	C4'-O4'-C1'	-3.77	106.48	109.92
2	G	32	A23	C6-C5-C4	3.76	125.22	117.90
2	G	32	A23	C4-C5-N7	3.75	113.30	109.34
2	I	32	A23	O4'-C1'-N9	-3.64	103.91	108.75
2	G	32	A23	O2'-PC-O1C	-3.57	106.33	115.76
2	W	32	A23	O4'-C1'-N9	3.42	113.28	108.75
2	I	32	A23	O2'-PC-O1C	-3.35	106.91	115.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	32	A23	O2'-C2'-C3'	-3.33	90.32	104.34
2	U	32	A23	C2'-C1'-N9	3.31	119.91	112.56
2	W	32	A23	N3-C2-N1	-3.27	124.23	128.67
2	I	32	A23	N3-C2-N1	-3.20	124.33	128.67
2	I	32	A23	C5'-C4'-C3'	-3.19	103.75	114.38
2	G	32	A23	N3-C2-N1	-3.18	124.36	128.67
2	H	32	A23	N6-C6-N1	3.10	124.95	118.33
2	V	32	A23	C5'-C4'-C3'	-3.02	104.31	114.38
2	U	32	A23	O4'-C4'-C3'	-3.02	98.54	104.92
2	I	32	A23	O2'-C2'-C3'	-2.98	91.80	104.34
2	I	32	A23	O2C-PC-O1C	-2.80	100.85	109.89
2	I	32	A23	O4'-C4'-C5'	-2.71	100.66	109.33
2	U	32	A23	C3'-C2'-C1'	-2.68	97.14	103.55
2	H	32	A23	O2C-PC-O1C	-2.63	101.40	109.89
2	G	32	A23	O4'-C4'-C3'	2.44	110.06	104.92
2	G	32	A23	C5'-C4'-C3'	-2.32	106.67	114.38
2	G	32	A23	O4'-C1'-C2'	-2.19	102.86	106.61
2	U	32	A23	N3-C2-N1	-2.18	125.71	128.67
2	H	32	A23	N3-C2-N1	-2.15	125.76	128.67
2	I	32	A23	O4'-C4'-C3'	-2.01	100.67	104.92
2	V	32	A23	N3-C2-N1	-2.00	125.96	128.67

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	32	A23	C2'
2	I	32	A23	C1'
2	U	32	A23	C3'
2	U	32	A23	C2'
2	U	32	A23	C1'
2	V	32	A23	C2'
2	V	32	A23	C1'

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	32	A23	O4'-C4'-C5'-O5'
2	G	32	A23	O4'-C4'-C5'-O5'
2	I	32	A23	O4'-C4'-C5'-O5'
2	I	32	A23	C3'-C4'-C5'-O5'
2	V	32	A23	C3'-C4'-C5'-O5'
2	G	32	A23	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	H	32	A23	C3'-C4'-C5'-O5'
2	U	32	A23	O4'-C4'-C5'-O5'
2	U	32	A23	C3'-C4'-C5'-O5'
2	V	32	A23	O4'-C4'-C5'-O5'
2	U	32	A23	C4'-C5'-O5'-P

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	32	A23	1	0
2	U	32	A23	16	0
2	W	32	A23	4	0
2	H	32	A23	3	0
2	I	32	A23	5	0
2	V	32	A23	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	1
2	G	1
2	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	31:A	O3'	32:A23	P	1.36
1	G	31:A	O3'	32:A23	P	1.30
1	W	31:A	O3'	32:A23	P	1.23

## 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	162/171 (94%)	-0.66	0 100 100	11, 24, 65, 90	0
1	B	162/171 (94%)	-0.64	0 100 100	14, 32, 76, 105	0
1	E	162/171 (94%)	-0.54	0 100 100	10, 44, 88, 127	0
1	X	162/171 (94%)	-0.26	0 100 100	49, 69, 111, 144	0
1	Y	162/171 (94%)	-0.42	0 100 100	37, 54, 90, 124	0
1	Z	162/171 (94%)	0.37	16 (9%) 7 2	45, 99, 216, 288	0
2	G	35/36 (97%)	-0.01	2 (5%) 23 8	34, 47, 94, 154	0
2	H	35/36 (97%)	-0.33	1 (2%) 51 23	27, 37, 88, 115	0
2	I	35/36 (97%)	-0.12	1 (2%) 51 23	34, 60, 91, 151	0
2	U	35/36 (97%)	1.12	7 (20%) 1 0	107, 144, 217, 235	0
2	V	35/36 (97%)	-0.12	1 (2%) 51 23	63, 76, 100, 134	0
2	W	35/36 (97%)	-0.06	1 (2%) 51 23	41, 72, 131, 159	0
All	All	1182/1242 (95%)	-0.28	29 (2%) 57 29	10, 57, 144, 288	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	17	U	5.3
2	W	18	U	4.3
2	G	17	U	3.6
2	V	17	U	3.6
1	Z	107	ASN	3.3
1	Z	105	MET	3.1
1	Z	110	TYR	3.1
1	Z	102	LEU	3.1
2	H	17	U	3.1
1	Z	101	ASP	3.0
1	Z	61	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	Z	117	GLN	2.8
2	U	18	U	2.7
1	Z	108	THR	2.7
2	U	11	C	2.6
2	G	18	U	2.6
2	U	29	A	2.4
1	Z	75	GLY	2.3
2	U	17	U	2.3
1	Z	82	GLY	2.3
2	U	31	A	2.3
2	U	10	G	2.3
1	Z	103	GLY	2.3
1	Z	2	LYS	2.2
2	U	27	C	2.2
1	Z	112	ARG	2.2
1	Z	162	LYS	2.2
1	Z	114	LEU	2.0
1	Z	79	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A23	U	32	25/26	0.82	0.24	151,166,177,199	0
2	A23	V	32	25/26	0.92	0.16	59,63,69,71	0
2	A23	W	32	25/26	0.93	0.14	42,51,55,59	0
2	A23	I	32	25/26	0.95	0.14	20,23,43,52	0
2	A23	G	32	25/26	0.96	0.12	24,31,39,44	0
2	A23	H	32	25/26	0.96	0.12	22,23,31,35	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.