



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:08 AM GMT

PDB ID : 3OFB  
Title : Crystal structure of the E. coli ribosome bound to chloramphenicol. This file contains the 30S subunit of the second 70S ribosome.  
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.  
Deposited on : 2010-08-14  
Resolution : 3.19 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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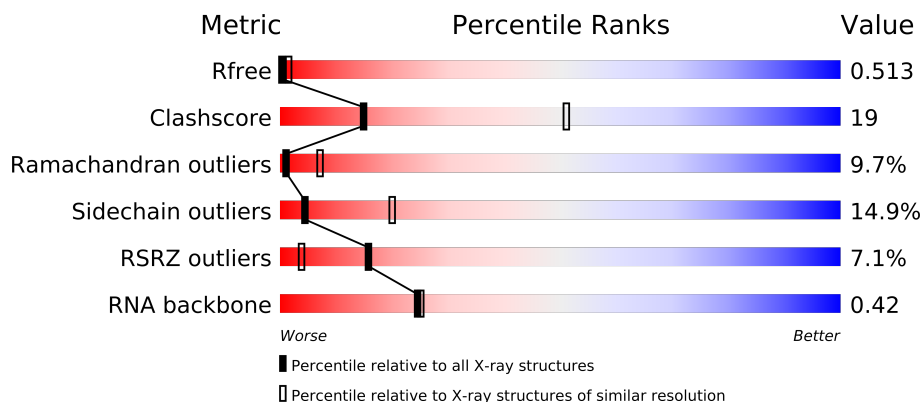
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.19 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.







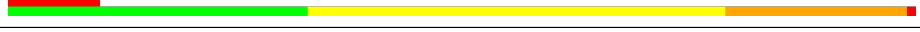




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1530	
2	B	218	
3	C	206	
4	D	205	
5	E	150	
6	F	100	
7	G	150	
8	H	129	
9	I	127	
10	J	98	
11	K	117	
12	L	123	

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Mol	Chain	Length	Quality of chain
13	M	113	
14	N	100	
15	O	88	
16	P	80	
17	Q	80	
18	R	55	
19	S	79	
20	T	85	
21	U	51	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
22	MG	A	1535	-	X
22	MG	A	1536	-	X
22	MG	A	1544	-	X
22	MG	A	1545	-	X
22	MG	A	1547	-	X
22	MG	A	1548	-	X
22	MG	A	1552	-	X
22	MG	A	1553	-	X
22	MG	A	1562	-	X
22	MG	A	1572	-	X
22	MG	A	1573	-	X

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51605 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	113	Total	C	N	O	S	0	0	0
			877	541	177	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	80	Total	C	N	O	S	0	0	0
			639	400	126	112	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	42	Total	Mg	0	0
			42	42		

- Molecule 23 is water.

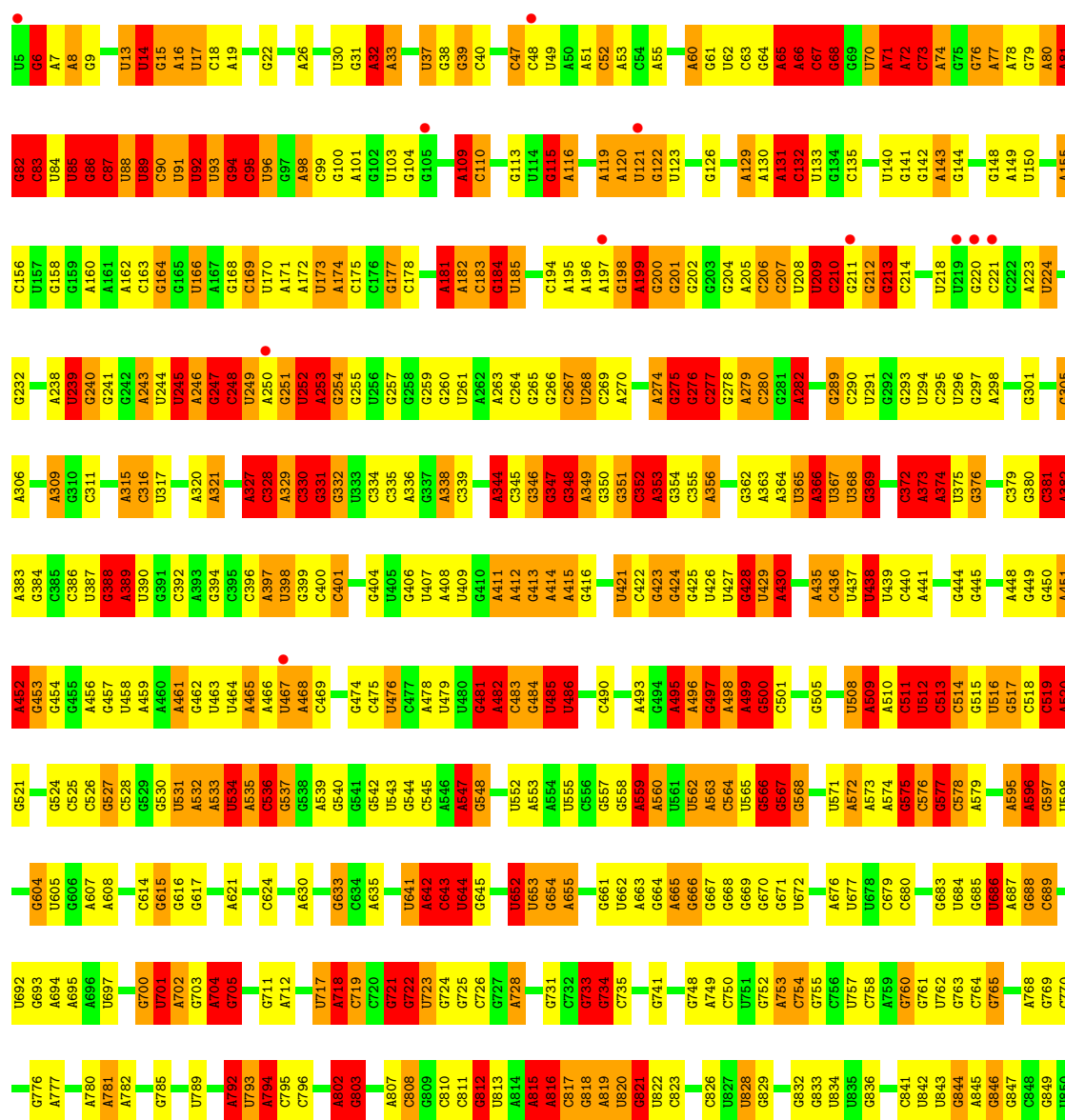
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	199	Total	O	0	0
			199	199		
23	E	1	Total	O	0	0
			1	1		
23	I	1	Total	O	0	0
			1	1		
23	N	4	Total	O	0	0
			4	4		
23	T	1	Total	O	0	0
			1	1		
23	U	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

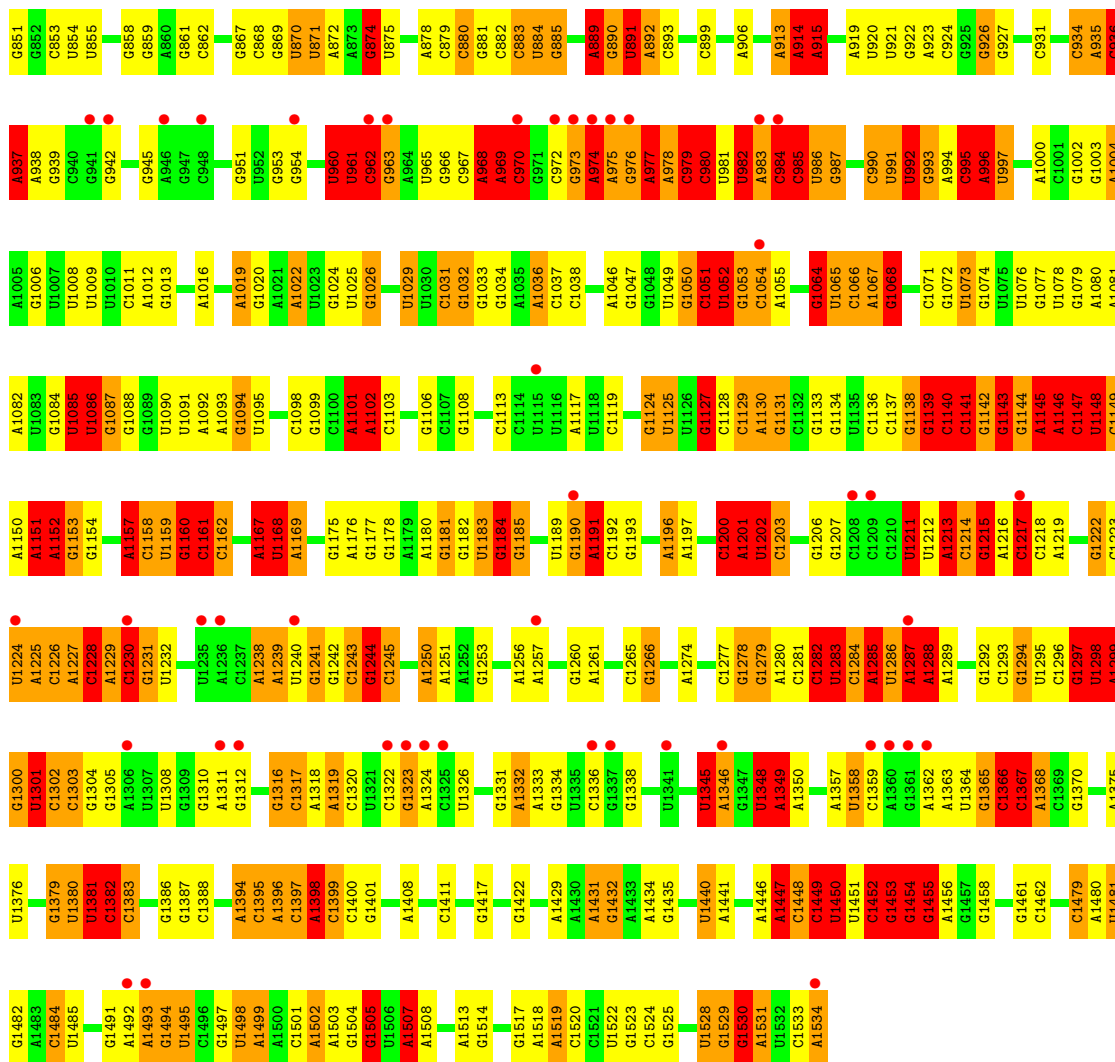
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 16S rRNA

Chain A:

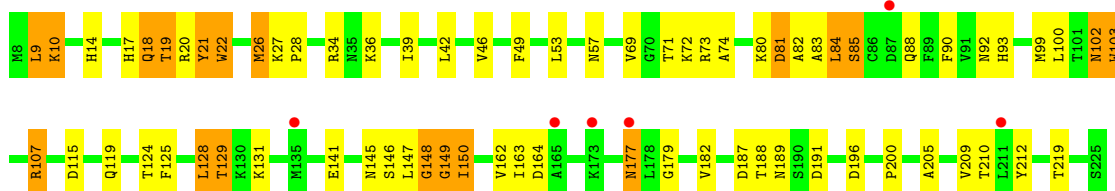






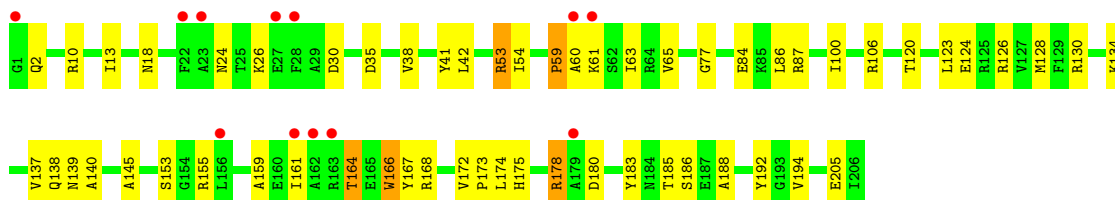
• Molecule 2: 30S ribosomal protein S2

Chain B:



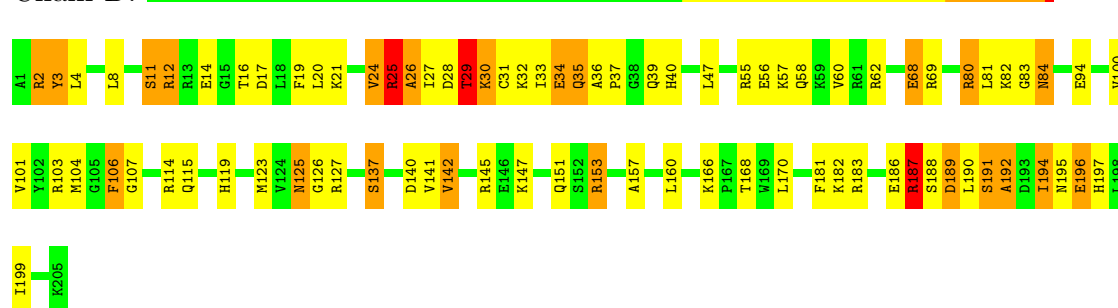
• Molecule 3: 30S ribosomal protein S3

Chain C:



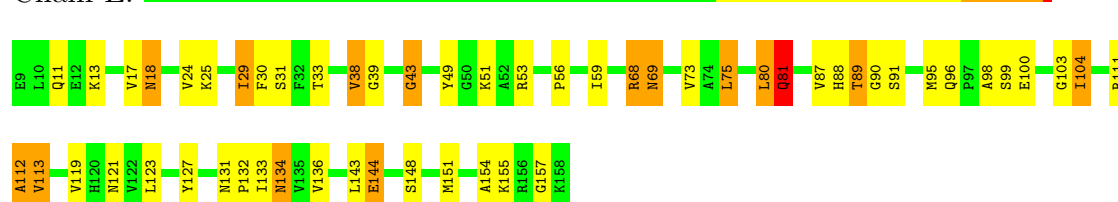
- Molecule 4: 30S ribosomal protein S4

Chain D:



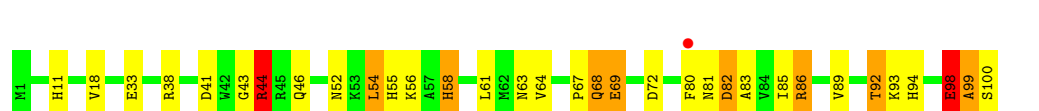
- Molecule 5: 30S ribosomal protein S5

Chain E:



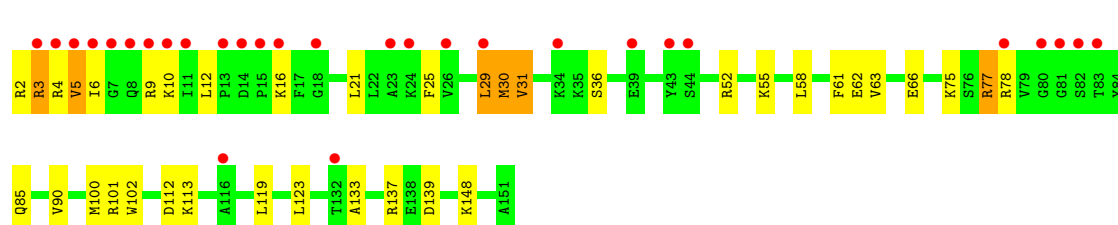
- Molecule 6: 30S ribosomal protein S6

Chain F:



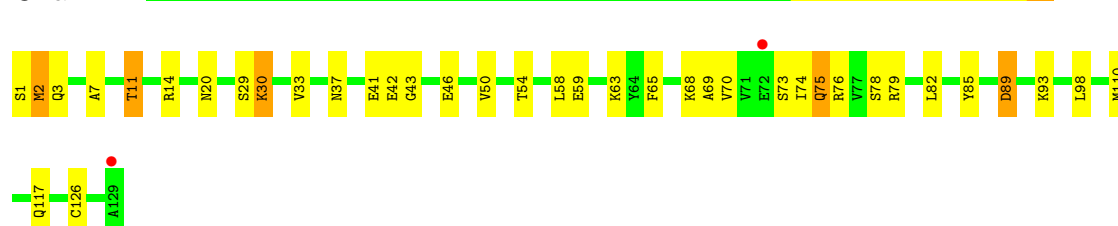
- Molecule 7: 30S ribosomal protein S7

Chain G:



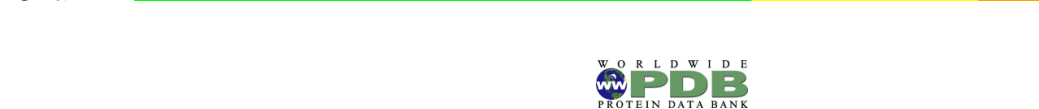
- Molecule 8: 30S ribosomal protein S8

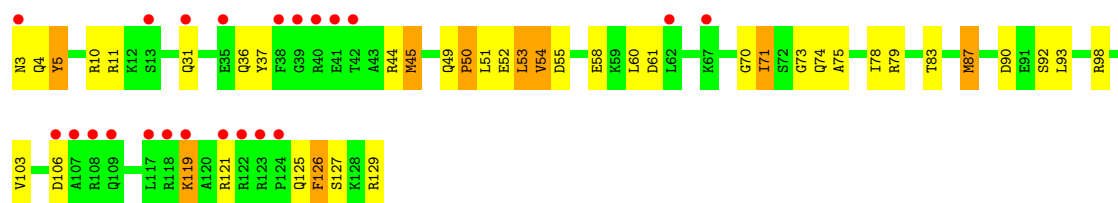
Chain H:



- Molecule 9: 30S ribosomal protein S9

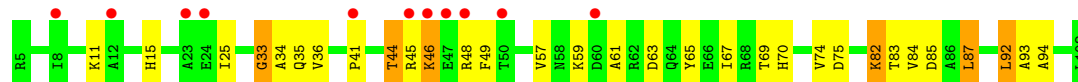
Chain I:





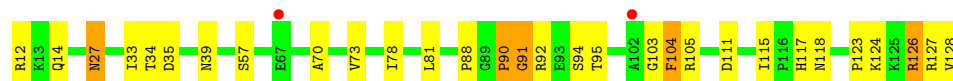
- Molecule 10: 30S ribosomal protein S10

Chain J:



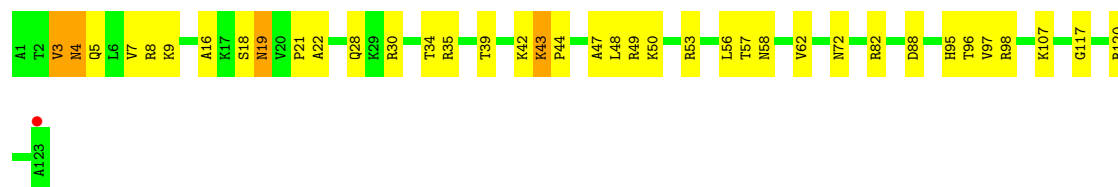
- Molecule 11: 30S ribosomal protein S11

Chain K:



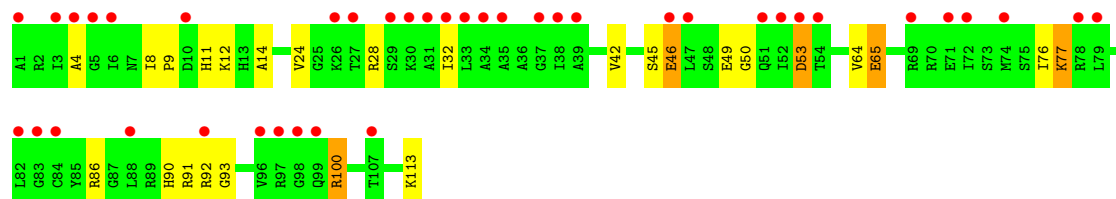
- Molecule 12: 30S ribosomal protein S12

Chain L:



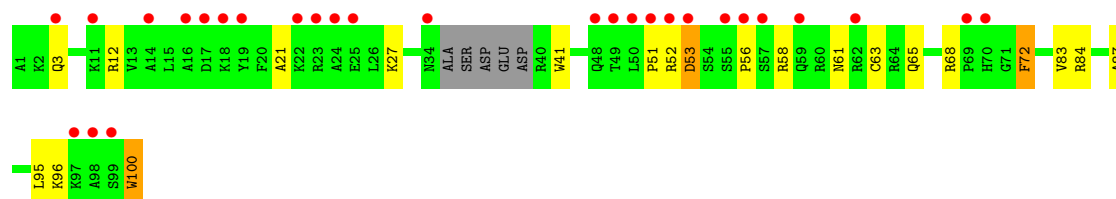
- Molecule 13: 30S ribosomal protein S13

Chain M:

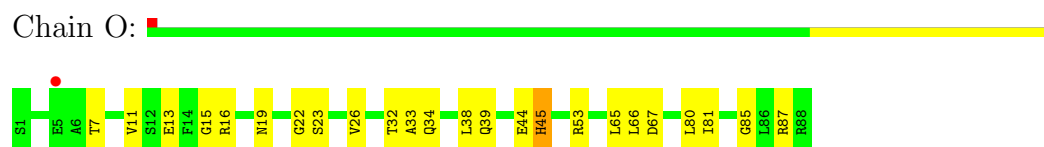


- Molecule 14: 30S ribosomal protein S14

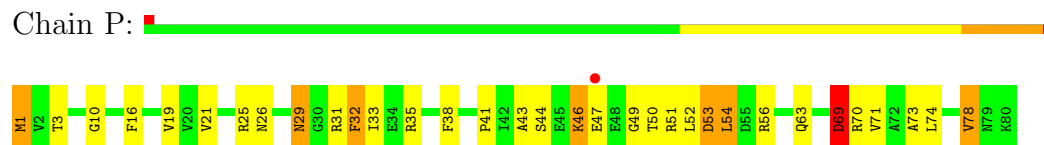
Chain N:



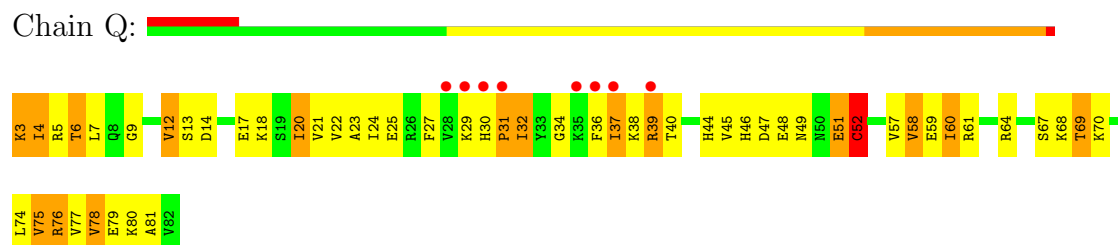
- Molecule 15: 30S ribosomal protein S15



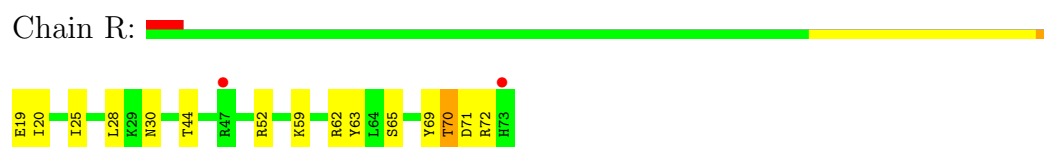
- Molecule 16: 30S ribosomal protein S16



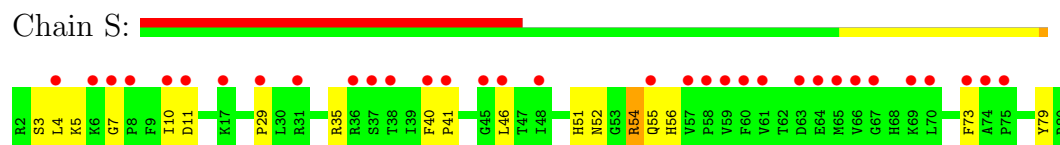
- Molecule 17: 30S ribosomal protein S17



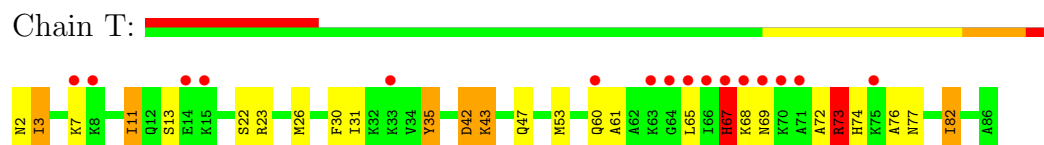
- Molecule 18: 30S ribosomal protein S18



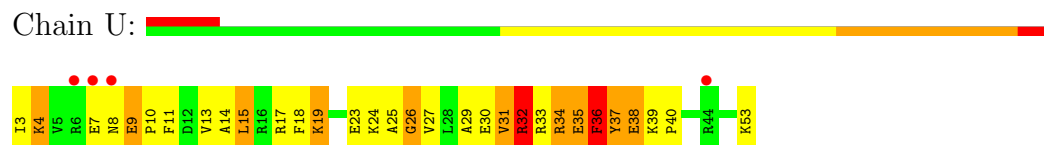
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.46Å 434.08Å 621.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.15 – 3.19 82.15 – 3.19	Depositor EDS
% Data completeness (in resolution range)	75.8 (82.15-3.19) 75.8 (82.15-3.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.191 , 0.252 0.510 , 0.513	Depositor DCC
$R_{free}$ test set	11187 reflections (1.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 60.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 759111 reflections	Xtriage
$F_o, F_c$ correlation	0.44	EDS
Total number of atoms	51605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.47	6/36762 (0.0%)	1.24	525/57350 (0.9%)
2	B	0.37	2/1736 (0.1%)	0.54	4/2338 (0.2%)
3	C	0.23	0/1652	0.44	0/2225
4	D	0.34	0/1665	0.57	0/2227
5	E	0.31	0/1119	0.55	0/1504
6	F	0.27	0/836	0.50	0/1128
7	G	0.22	0/1188	0.44	0/1591
8	H	0.26	0/989	0.49	0/1326
9	I	0.22	0/1034	0.42	0/1375
10	J	0.22	0/797	0.47	0/1077
11	K	0.25	0/893	0.51	0/1205
12	L	0.40	1/969 (0.1%)	0.56	0/1300
13	M	0.19	0/885	0.41	0/1181
14	N	0.21	0/780	0.39	0/1036
15	O	0.25	0/722	0.45	0/964
16	P	0.28	0/649	0.52	0/870
17	Q	0.27	0/658	0.51	0/881
18	R	0.28	0/463	0.46	0/621
19	S	0.21	0/653	0.42	0/877
20	T	0.25	0/671	0.50	0/888
21	U	0.31	0/431	0.60	0/570
All	All	0.41	9/55552 (0.0%)	1.07	529/82534 (0.6%)

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
2	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1396	A	O3'-P	-11.26	1.47	1.61
2	B	146	SER	C-N	10.14	1.57	1.34
1	A	562	U	O3'-P	-9.38	1.49	1.61
1	A	26	A	O3'-P	-8.83	1.50	1.61
1	A	8	A	O3'-P	-8.69	1.50	1.61
12	L	21	PRO	C-N	8.56	1.53	1.34
1	A	1047	G	O3'-P	7.32	1.70	1.61
2	B	107	ARG	C-N	6.44	1.48	1.34
1	A	1495	U	O3'-P	-5.13	1.54	1.61

All (529) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1396	A	P-O3'-C3'	16.36	139.33	119.70
1	A	66	A	P-O3'-C3'	-13.97	102.93	119.70
1	A	328	C	P-O3'-C3'	13.96	136.45	119.70
1	A	132	C	N1-C1'-C2'	-13.73	96.16	114.00
1	A	891	U	N1-C1'-C2'	-13.43	96.55	114.00
1	A	245	U	N1-C1'-C2'	-13.28	96.74	114.00
1	A	915	A	P-O3'-C3'	-12.76	104.39	119.70
1	A	352	C	N1-C1'-C2'	-12.55	97.69	114.00
1	A	14	U	N1-C1'-C2'	-12.15	98.21	114.00
1	A	330	C	N1-C1'-C2'	-12.07	98.31	114.00
1	A	92	U	N1-C1'-C2'	-11.80	98.66	114.00
1	A	65	A	P-O3'-C3'	11.60	133.62	119.70
1	A	1086	U	N1-C1'-C2'	-11.52	99.03	114.00
1	A	1502	A	P-O3'-C3'	11.31	133.27	119.70
1	A	643	C	N1-C1'-C2'	-11.29	99.32	114.00
1	A	1230	C	N1-C1'-C2'	-11.28	99.34	114.00
1	A	512	U	N1-C1'-C2'	-11.14	99.52	114.00
1	A	992	U	P-O3'-C3'	11.05	132.97	119.70
1	A	1148	U	N1-C1'-C2'	-10.93	99.79	114.00
1	A	1381	U	N1-C1'-C2'	-10.82	99.94	114.00
1	A	1401	G	P-O3'-C3'	-10.74	106.81	119.70
1	A	1283	U	N1-C1'-C2'	-10.73	100.06	114.00
1	A	1298	U	P-O3'-C3'	10.70	132.54	119.70
1	A	248	C	N1-C1'-C2'	-10.70	100.09	114.00
1	A	821	G	P-O3'-C3'	-10.66	106.91	119.70
1	A	513	C	N1-C1'-C2'	-10.60	100.22	114.00
1	A	116	A	P-O3'-C3'	-10.52	107.08	119.70
1	A	1068	G	P-O3'-C3'	-10.49	107.11	119.70
1	A	520	A	P-O3'-C3'	-10.42	107.20	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	A	P-O3'-C3'	10.40	132.18	119.70
1	A	1367	C	N1-C1'-C2'	-10.36	100.53	114.00
1	A	73	C	N1-C1'-C2'	-10.36	100.54	114.00
1	A	1147	C	N1-C1'-C2'	-10.30	100.61	114.00
1	A	721	G	P-O3'-C3'	10.19	131.93	119.70
1	A	1449	C	N1-C1'-C2'	-10.16	100.79	114.00
1	A	109	A	P-O3'-C3'	10.04	131.75	119.70
1	A	1052	U	N1-C1'-C2'	-10.01	100.99	114.00
1	A	1217	C	N1-C1'-C2'	-9.96	101.05	112.00
1	A	1161	C	N1-C1'-C2'	-9.88	101.14	112.00
1	A	96	U	N1-C1'-C2'	-9.83	101.19	112.00
1	A	173	U	O4'-C1'-N1	9.77	116.02	108.20
1	A	316	C	N1-C1'-C2'	-9.77	101.25	112.00
1	A	1383	C	N1-C1'-C2'	-9.70	101.33	112.00
1	A	372	C	O4'-C1'-N1	9.69	115.95	108.20
1	A	110	C	P-O3'-C3'	-9.54	108.26	119.70
1	A	1065	U	O4'-C1'-N1	9.54	115.83	108.20
1	A	979	C	N1-C1'-C2'	-9.45	101.60	112.00
1	A	566	G	P-O3'-C3'	9.44	131.02	119.70
1	A	252	U	N1-C1'-C2'	-9.42	101.63	112.00
1	A	985	C	N1-C1'-C2'	-9.42	101.63	112.00
1	A	792	A	P-O3'-C3'	9.42	131.00	119.70
1	A	73	C	O4'-C1'-N1	9.30	115.64	108.20
1	A	331	G	P-O3'-C3'	-9.26	108.59	119.70
1	A	388	G	P-O3'-C3'	9.26	130.81	119.70
1	A	936	C	O4'-C1'-N1	9.24	115.59	108.20
1	A	519	C	N1-C1'-C2'	-9.22	101.86	112.00
1	A	95	C	N1-C1'-C2'	-9.19	101.89	112.00
1	A	85	U	P-O3'-C3'	9.12	130.64	119.70
1	A	183	C	O4'-C1'-N1	9.12	115.50	108.20
1	A	1348	U	N1-C1'-C2'	-9.11	101.98	112.00
1	A	1200	C	P-O3'-C3'	9.08	130.59	119.70
1	A	1224	U	P-O3'-C3'	9.07	130.59	119.70
1	A	1202	U	N1-C1'-C2'	-9.07	102.03	112.00
1	A	428	G	P-O3'-C3'	8.97	130.46	119.70
1	A	753	A	P-O3'-C3'	8.94	130.43	119.70
1	A	1528	U	P-O3'-C3'	8.88	130.35	119.70
1	A	576	C	O4'-C1'-N1	-8.87	101.10	108.20
1	A	1051	C	N1-C1'-C2'	-8.84	102.27	112.00
1	A	564	C	N1-C1'-C2'	-8.83	102.29	112.00
1	A	577	G	P-O3'-C3'	-8.83	109.10	119.70
1	A	701	U	P-O3'-C3'	8.82	130.28	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	A	P-O3'-C3'	8.80	130.26	119.70
1	A	486	U	P-O3'-C3'	-8.79	109.15	119.70
1	A	89	U	N1-C1'-C2'	-8.78	102.34	112.00
1	A	547	A	O4'-C1'-N9	8.77	115.22	108.20
1	A	1399	C	P-O3'-C3'	8.72	130.16	119.70
2	B	146	SER	O-C-N	-8.71	108.76	122.70
1	A	643	C	O4'-C1'-N1	8.66	115.13	108.20
1	A	32	A	P-O3'-C3'	-8.62	109.35	119.70
1	A	1499	A	P-O3'-C3'	-8.60	109.38	119.70
1	A	1152	A	P-O3'-C3'	-8.54	109.45	119.70
1	A	936	C	N1-C1'-C2'	-8.53	102.62	112.00
1	A	962	C	O4'-C1'-N1	8.50	115.00	108.20
1	A	424	G	P-O3'-C3'	-8.47	109.54	119.70
1	A	962	C	N1-C1'-C2'	-8.43	102.72	112.00
1	A	1528	U	O4'-C1'-N1	8.37	114.90	108.20
1	A	717	U	N1-C1'-C2'	8.34	124.84	114.00
1	A	132	C	O4'-C1'-N1	8.33	114.86	108.20
1	A	60	A	P-O3'-C3'	8.30	129.66	119.70
1	A	1345	U	O4'-C1'-N1	8.29	114.83	108.20
1	A	495	A	P-O3'-C3'	8.28	129.63	119.70
1	A	439	U	N1-C1'-C2'	-8.24	102.94	112.00
1	A	430	A	P-O3'-C3'	-8.23	109.83	119.70
1	A	1455	G	P-O3'-C3'	-8.16	109.91	119.70
1	A	374	A	P-O3'-C3'	-8.14	109.93	119.70
1	A	253	A	P-O3'-C3'	-8.13	109.95	119.70
1	A	1447	A	P-O3'-C3'	8.10	129.42	119.70
1	A	1498	U	P-O3'-C3'	8.08	129.40	119.70
1	A	115	G	P-O3'-C3'	8.05	129.36	119.70
1	A	213	G	P-O3'-C3'	-8.01	110.09	119.70
1	A	481	G	P-O3'-C3'	7.95	129.24	119.70
1	A	961	U	N1-C1'-C2'	-7.94	103.26	112.00
1	A	277	C	P-O3'-C3'	-7.90	110.22	119.70
1	A	1301	U	P-O3'-C3'	-7.88	110.24	119.70
1	A	13	U	P-O3'-C3'	7.86	129.13	119.70
1	A	596	A	P-O3'-C3'	-7.82	110.31	119.70
1	A	889	A	P-O3'-C3'	7.82	129.09	119.70
1	A	734	G	P-O3'-C3'	-7.80	110.34	119.70
1	A	559	A	P-O3'-C3'	7.79	129.05	119.70
1	A	110	C	N1-C1'-C2'	-7.78	103.44	112.00
1	A	1141	C	N1-C1'-C2'	-7.78	103.44	112.00
1	A	348	G	P-O3'-C3'	-7.74	110.42	119.70
1	A	575	G	P-O3'-C3'	7.68	128.92	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1332	A	P-O3'-C3'	-7.68	110.48	119.70
1	A	247	G	P-O3'-C3'	-7.66	110.51	119.70
1	A	486	U	P-O5'-C5'	-7.64	108.67	120.90
1	A	381	C	P-O3'-C3'	7.64	128.87	119.70
1	A	184	G	P-O3'-C3'	-7.63	110.55	119.70
1	A	238	A	P-O3'-C3'	7.62	128.85	119.70
1	A	1282	C	P-O3'-C3'	-7.62	110.56	119.70
1	A	68	G	P-O3'-C3'	-7.61	110.56	119.70
1	A	793	U	P-O3'-C3'	-7.58	110.60	119.70
1	A	802	A	P-O3'-C3'	7.58	128.80	119.70
1	A	52	C	N1-C1'-C2'	-7.58	103.67	112.00
1	A	508	U	P-O3'-C3'	7.55	128.76	119.70
1	A	218	U	O4'-C1'-N1	7.54	114.23	108.20
1	A	641	U	P-O3'-C3'	7.52	128.72	119.70
1	A	122	G	P-O3'-C3'	-7.49	110.71	119.70
1	A	1201	A	P-O3'-C3'	7.48	128.68	119.70
1	A	248	C	O4'-C1'-N1	7.48	114.19	108.20
1	A	86	G	P-O3'-C3'	7.48	128.68	119.70
1	A	96	U	P-O3'-C3'	-7.47	110.73	119.70
1	A	70	U	O4'-C1'-N1	7.47	114.18	108.20
1	A	1227	A	P-O3'-C3'	7.45	128.64	119.70
1	A	1167	A	P-O3'-C3'	7.45	128.64	119.70
1	A	1380	U	P-O3'-C3'	7.44	128.63	119.70
1	A	1397	C	N1-C1'-C2'	-7.44	103.82	112.00
1	A	486	U	N1-C1'-C2'	-7.44	103.82	112.00
1	A	382	A	P-O3'-C3'	7.43	128.62	119.70
1	A	428	G	O4'-C1'-N9	7.40	114.12	108.20
1	A	87	C	N1-C1'-C2'	-7.36	103.91	112.00
1	A	717	U	P-O3'-C3'	7.34	128.51	119.70
1	A	1143	G	P-O3'-C3'	-7.32	110.91	119.70
1	A	979	C	P-O3'-C3'	-7.30	110.93	119.70
1	A	1142	G	P-O3'-C3'	-7.30	110.94	119.70
1	A	517	G	P-O3'-C3'	7.29	128.45	119.70
1	A	1383	C	P-O3'-C3'	-7.28	110.97	119.70
1	A	1381	U	P-O3'-C3'	-7.26	110.98	119.70
1	A	497	G	P-O3'-C3'	-7.26	110.99	119.70
1	A	209	U	P-O3'-C3'	7.26	128.41	119.70
1	A	173	U	P-O3'-C3'	7.25	128.40	119.70
1	A	453	G	P-O3'-C3'	-7.24	111.01	119.70
1	A	92	U	P-O3'-C3'	-7.24	111.01	119.70
1	A	1383	C	O4'-C1'-N1	7.23	113.99	108.20
1	A	536	C	P-O3'-C3'	-7.22	111.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1140	C	N1-C1'-C2'	-7.21	104.07	112.00
1	A	1398	A	P-O3'-C3'	-7.20	111.06	119.70
1	A	513	C	O4'-C1'-N1	7.19	113.95	108.20
1	A	132	C	P-O3'-C3'	-7.19	111.08	119.70
1	A	248	C	P-O3'-C3'	-7.16	111.11	119.70
1	A	654	G	P-O3'-C3'	-7.15	111.12	119.70
1	A	421	U	P-O3'-C3'	7.15	128.28	119.70
1	A	1064	G	P-O3'-C3'	7.08	128.20	119.70
1	A	70	U	P-O3'-C3'	7.07	128.19	119.70
1	A	174	A	P-O3'-C3'	-7.07	111.22	119.70
1	A	1230	C	P-O3'-C3'	-7.07	111.22	119.70
1	A	1053	G	P-O3'-C3'	7.04	128.15	119.70
1	A	705	G	P-O3'-C3'	-7.04	111.25	119.70
1	A	15	G	P-O3'-C3'	-7.01	111.29	119.70
1	A	240	G	P-O3'-C3'	-7.00	111.30	119.70
1	A	1367	C	O4'-C1'-N1	7.00	113.80	108.20
1	A	67	C	O4'-C1'-N1	6.98	113.79	108.20
1	A	245	U	P-O3'-C3'	-6.98	111.33	119.70
1	A	1147	C	P-O3'-C3'	-6.97	111.34	119.70
1	A	643	C	P-O3'-C3'	-6.96	111.34	119.70
1	A	686	U	O4'-C1'-N1	6.96	113.76	108.20
1	A	817	C	P-O3'-C3'	6.95	128.04	119.70
1	A	315	A	P-O3'-C3'	6.92	128.00	119.70
1	A	1282	C	N1-C1'-C2'	-6.92	104.39	112.00
1	A	792	A	O4'-C1'-N9	6.90	113.72	108.20
1	A	914	A	P-O3'-C3'	-6.88	111.45	119.70
1	A	1215	G	P-O3'-C3'	-6.87	111.46	119.70
1	A	349	A	P-O3'-C3'	-6.86	111.47	119.70
1	A	1366	C	O4'-C1'-N1	6.86	113.69	108.20
1	A	1217	C	O4'-C1'-N1	6.85	113.68	108.20
1	A	974	A	P-O3'-C3'	6.84	127.91	119.70
1	A	512	U	P-O3'-C3'	-6.81	111.53	119.70
1	A	1349	A	P-O3'-C3'	-6.78	111.56	119.70
1	A	451	A	P-O3'-C3'	6.78	127.84	119.70
1	A	534	U	N1-C1'-C2'	-6.76	104.56	112.00
1	A	116	A	N9-C1'-C2'	-6.74	104.58	112.00
1	A	1228	C	N1-C1'-C2'	-6.71	104.61	112.00
1	A	1367	C	P-O3'-C3'	-6.71	111.65	119.70
1	A	1285	A	P-O3'-C3'	6.70	127.75	119.70
1	A	331	G	N9-C1'-C2'	-6.70	104.63	112.00
1	A	794	A	P-O3'-C3'	-6.69	111.67	119.70
1	A	1211	U	P-O3'-C3'	6.68	127.72	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	996	A	P-O3'-C3'	-6.68	111.69	119.70
1	A	94	G	P-O3'-C3'	6.67	127.71	119.70
1	A	1160	G	N9-C1'-C2'	-6.64	104.69	112.00
1	A	885	G	P-O3'-C3'	-6.64	111.73	119.70
1	A	1297	G	P-O3'-C3'	6.64	127.67	119.70
1	A	1288	A	P-O3'-C3'	-6.64	111.73	119.70
1	A	931	C	O4'-C1'-N1	6.61	113.49	108.20
1	A	95	C	P-O3'-C3'	-6.60	111.78	119.70
1	A	595	A	P-O3'-C3'	6.60	127.62	119.70
1	A	14	U	P-O3'-C3'	-6.59	111.79	119.70
1	A	803	G	P-O3'-C3'	-6.58	111.80	119.70
1	A	1495	U	P-O3'-C3'	6.58	127.59	119.70
1	A	1226	C	P-O3'-C3'	6.56	127.57	119.70
1	A	251	G	P-O3'-C3'	6.55	127.56	119.70
1	A	531	U	O4'-C1'-N1	6.54	113.44	108.20
1	A	381	C	N1-C1'-C2'	6.54	122.50	114.00
1	A	486	U	O4'-C1'-N1	-6.51	102.99	108.20
1	A	72	A	P-O3'-C3'	-6.50	111.91	119.70
1	A	575	G	C4-N9-C1'	-6.49	118.07	126.50
1	A	937	A	P-O3'-C3'	-6.46	111.94	119.70
1	A	239	U	N1-C1'-C2'	-6.43	104.93	112.00
1	A	436	C	O4'-C1'-N1	-6.42	103.06	108.20
2	B	107	ARG	O-C-N	-6.42	112.43	122.70
1	A	440	C	O4'-C1'-N1	6.42	113.33	108.20
1	A	485	U	O4'-C1'-N1	-6.38	103.10	108.20
1	A	564	C	P-O3'-C3'	-6.38	112.05	119.70
1	A	995	C	N1-C1'-C2'	-6.36	105.01	112.00
1	A	328	C	O4'-C1'-N1	-6.35	103.12	108.20
1	A	68	G	N9-C1'-C2'	-6.35	105.02	112.00
1	A	247	G	N9-C1'-C2'	-6.34	105.03	112.00
1	A	697	U	O4'-C1'-N1	6.29	113.23	108.20
1	A	316	C	O4'-C1'-N1	6.28	113.23	108.20
1	A	452	A	P-O3'-C3'	-6.28	112.17	119.70
1	A	509	A	P-O3'-C3'	-6.27	112.17	119.70
1	A	421	U	O4'-C1'-N1	6.26	113.21	108.20
1	A	1151	A	P-O3'-C3'	6.25	127.20	119.70
1	A	129	A	P-O3'-C3'	6.25	127.20	119.70
1	A	1336	C	P-O3'-C3'	6.25	127.20	119.70
1	A	1161	C	P-O3'-C3'	-6.24	112.22	119.70
1	A	1449	C	O4'-C1'-N1	6.24	113.19	108.20
1	A	1196	A	P-O3'-C3'	6.23	127.18	119.70
1	A	81	A	P-O3'-C3'	6.23	127.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1127	G	P-O3'-C3'	-6.22	112.24	119.70
1	A	1160	G	P-O3'-C3'	-6.20	112.25	119.70
1	A	1530	G	P-O3'-C3'	-6.20	112.26	119.70
1	A	884	U	O4'-C1'-N1	6.20	113.16	108.20
1	A	83	C	O4'-C1'-N1	6.18	113.14	108.20
1	A	499	A	P-O3'-C3'	6.18	127.11	119.70
1	A	914	A	C3'-C2'-C1'	6.17	106.44	101.50
1	A	1308	U	O4'-C1'-N1	6.17	113.14	108.20
1	A	414	A	P-O3'-C3'	-6.16	112.31	119.70
1	A	995	C	P-O3'-C3'	-6.13	112.34	119.70
1	A	1094	G	P-O3'-C3'	6.13	127.06	119.70
1	A	356	A	O4'-C1'-N9	6.11	113.09	108.20
1	A	875	U	O4'-C1'-N1	6.11	113.09	108.20
1	A	982	U	P-O3'-C3'	6.11	127.03	119.70
1	A	765	G	P-O3'-C3'	-6.09	112.39	119.70
1	A	555	U	P-O3'-C3'	-6.09	112.39	119.70
1	A	960	U	P-O3'-C3'	6.09	127.01	119.70
1	A	1507	A	P-O3'-C3'	-6.09	112.39	119.70
1	A	1184	G	C3'-C2'-C1'	6.09	106.37	101.50
1	A	1244	G	C3'-C2'-C1'	6.08	106.36	101.50
1	A	704	A	C3'-C2'-C1'	6.07	106.36	101.50
1	A	1202	U	P-O3'-C3'	-6.07	112.42	119.70
1	A	985	C	O4'-C1'-N1	6.07	113.05	108.20
1	A	438	U	P-O3'-C3'	6.06	126.97	119.70
1	A	170	U	O4'-C1'-N1	6.05	113.04	108.20
1	A	1217	C	C3'-C2'-C1'	6.05	106.34	101.50
1	A	1319	A	P-O3'-C3'	6.05	126.97	119.70
1	A	63	C	O4'-C1'-N1	6.05	113.04	108.20
1	A	239	U	P-O3'-C3'	-6.05	112.44	119.70
1	A	71	A	C3'-C2'-C1'	6.03	106.33	101.50
1	A	428	G	C4-N9-C1'	-6.03	118.66	126.50
1	A	654	G	C3'-C2'-C1'	6.03	106.32	101.50
1	A	1345	U	P-O3'-C3'	6.03	126.93	119.70
1	A	210	C	N1-C1'-C2'	6.01	121.82	114.00
1	A	513	C	C3'-C2'-C1'	6.01	106.31	101.50
1	A	1160	G	C3'-C2'-C1'	5.99	106.29	101.50
1	A	277	C	N1-C1'-C2'	-5.99	105.42	112.00
1	A	643	C	C3'-C2'-C1'	5.99	106.29	101.50
1	A	885	G	C3'-C2'-C1'	5.98	106.29	101.50
1	A	996	A	C3'-C2'-C1'	5.98	106.28	101.50
1	A	615	G	O4'-C1'-N9	5.97	112.97	108.20
1	A	122	G	N9-C1'-C2'	-5.96	105.44	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1052	U	P-O3'-C3'	-5.96	112.55	119.70
1	A	199	A	C3'-C2'-C1'	5.94	106.25	101.50
1	A	1288	A	C3'-C2'-C1'	5.93	106.25	101.50
1	A	575	G	C8-N9-C1'	5.92	134.70	127.00
1	A	1299	A	P-O3'-C3'	-5.92	112.60	119.70
1	A	519	C	C3'-C2'-C1'	5.92	106.23	101.50
1	A	131	A	P-O3'-C3'	-5.91	112.60	119.70
1	A	291	U	O4'-C1'-N1	5.90	112.92	108.20
1	A	884	U	P-O3'-C3'	5.89	126.77	119.70
1	A	1381	U	C3'-C2'-C1'	5.89	106.21	101.50
1	A	331	G	C3'-C2'-C1'	5.89	106.21	101.50
1	A	1127	G	C3'-C2'-C1'	5.89	106.21	101.50
1	A	816	A	C3'-C2'-C1'	5.88	106.21	101.50
1	A	47	C	P-O3'-C3'	5.88	126.76	119.70
1	A	448	A	O4'-C1'-N9	5.86	112.89	108.20
1	A	247	G	C3'-C2'-C1'	5.86	106.19	101.50
1	A	253	A	C3'-C2'-C1'	5.86	106.19	101.50
1	A	1395	C	P-O3'-C3'	-5.86	112.67	119.70
1	A	1449	C	C3'-C2'-C1'	5.85	106.18	101.50
1	A	1202	U	C3'-C2'-C1'	5.85	106.18	101.50
1	A	567	G	C3'-C2'-C1'	5.85	106.18	101.50
1	A	423	G	C3'-C2'-C1'	5.84	106.17	101.50
2	B	146	SER	C-N-CA	5.84	136.29	121.70
1	A	652	U	P-O3'-C3'	5.83	126.70	119.70
1	A	885	G	N9-C1'-C2'	-5.83	105.59	112.00
1	A	733	G	P-O3'-C3'	5.83	126.69	119.70
1	A	1505	G	C3'-C2'-C1'	5.83	106.16	101.50
1	A	969	A	P-O3'-C3'	-5.82	112.71	119.70
1	A	500	G	N9-C1'-C2'	-5.82	105.60	112.00
1	A	353	A	O4'-C1'-N9	5.81	112.85	108.20
1	A	497	G	C3'-C2'-C1'	5.81	106.15	101.50
1	A	821	G	N9-C1'-C2'	-5.80	105.62	112.00
1	A	1148	U	C3'-C2'-C1'	5.80	106.14	101.50
1	A	891	U	C3'-C2'-C1'	5.80	106.14	101.50
1	A	1367	C	C3'-C2'-C1'	5.80	106.14	101.50
1	A	248	C	C3'-C2'-C1'	5.79	106.13	101.50
1	A	1244	G	P-O3'-C3'	-5.79	112.76	119.70
1	A	452	A	C3'-C2'-C1'	5.78	106.12	101.50
1	A	870	U	N1-C1'-C2'	5.78	121.51	114.00
1	A	1452	C	P-O3'-C3'	5.78	126.63	119.70
2	B	146	SER	CA-C-N	5.77	129.90	117.20
1	A	1031	C	P-O3'-C3'	5.77	126.62	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1168	U	C3'-C2'-C1'	5.77	106.12	101.50
1	A	439	U	P-O5'-C5'	-5.77	111.67	120.90
1	A	210	C	P-O3'-C3'	5.76	126.61	119.70
1	A	82	G	C3'-C2'-C1'	5.75	106.10	101.50
1	A	1366	C	N1-C1'-C2'	-5.75	105.67	112.00
1	A	686	U	P-O3'-C3'	5.75	126.60	119.70
1	A	984	C	O4'-C1'-N1	5.74	112.79	108.20
1	A	1217	C	P-O3'-C3'	-5.74	112.81	119.70
1	A	536	C	N1-C1'-C2'	-5.74	105.69	112.00
1	A	1139	G	P-O3'-C3'	5.74	126.59	119.70
1	A	224	U	O4'-C1'-N1	5.73	112.78	108.20
1	A	686	U	N1-C1'-C2'	5.73	121.45	114.00
1	A	509	A	C3'-C2'-C1'	5.73	106.08	101.50
1	A	914	A	N9-C1'-C2'	-5.72	105.71	112.00
1	A	316	C	C3'-C2'-C1'	5.71	106.07	101.50
1	A	347	G	C3'-C2'-C1'	5.70	106.06	101.50
1	A	688	G	N9-C1'-C2'	-5.70	105.72	112.00
1	A	353	A	C3'-C2'-C1'	5.70	106.06	101.50
1	A	577	G	C3'-C2'-C1'	5.69	106.05	101.50
1	A	92	U	C3'-C2'-C1'	5.68	106.05	101.50
1	A	1326	U	O4'-C1'-N1	5.68	112.74	108.20
1	A	816	A	P-O3'-C3'	-5.68	112.89	119.70
1	A	366	A	P-O3'-C3'	5.68	126.51	119.70
1	A	1146	A	C3'-C2'-C1'	5.66	106.03	101.50
1	A	1161	C	O4'-C1'-N1	5.66	112.73	108.20
1	A	642	A	P-O3'-C3'	-5.66	112.91	119.70
1	A	199	A	P-O3'-C3'	-5.66	112.91	119.70
1	A	1349	A	C3'-C2'-C1'	5.65	106.02	101.50
1	A	915	A	N9-C1'-C2'	-5.64	105.79	112.00
1	A	1332	A	N9-C1'-C2'	-5.64	105.79	112.00
1	A	965	U	P-O3'-C3'	5.64	126.47	119.70
1	A	66	A	O4'-C1'-N9	-5.64	103.69	108.20
1	A	6	G	P-O3'-C3'	-5.64	112.94	119.70
1	A	37	U	O4'-C1'-N1	5.64	112.71	108.20
1	A	87	C	O4'-C1'-N1	5.63	112.71	108.20
1	A	1145	A	P-O3'-C3'	5.63	126.46	119.70
1	A	520	A	C3'-C2'-C1'	5.63	106.00	101.50
1	A	429	U	P-O3'-C3'	5.63	126.45	119.70
1	A	184	G	C3'-C2'-C1'	5.62	106.00	101.50
1	A	1450	U	O4'-C1'-N1	5.62	112.70	108.20
1	A	414	A	C3'-C2'-C1'	5.61	105.99	101.50
1	A	821	G	C3'-C2'-C1'	5.61	105.99	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	A	P-O3'-C3'	5.61	126.43	119.70
1	A	1245	C	O4'-C1'-N1	5.60	112.68	108.20
1	A	1300	G	P-O3'-C3'	-5.59	112.99	119.70
1	A	688	G	P-O3'-C3'	-5.59	112.99	119.70
1	A	1283	U	P-O3'-C3'	-5.59	112.99	119.70
1	A	508	U	O4'-C1'-N1	5.59	112.67	108.20
1	A	132	C	C3'-C2'-C1'	5.59	105.97	101.50
1	A	511	C	N1-C1'-C2'	5.58	121.26	114.00
1	A	276	G	C3'-C2'-C1'	5.58	105.97	101.50
1	A	96	U	C3'-C2'-C1'	5.58	105.97	101.50
1	A	1499	A	N9-C1'-C2'	-5.58	105.86	112.00
1	A	14	U	C3'-C2'-C1'	5.58	105.96	101.50
1	A	1440	U	P-O3'-C3'	5.57	126.39	119.70
1	A	6	G	C3'-C2'-C1'	5.57	105.96	101.50
1	A	1484	C	O4'-C1'-N1	5.57	112.66	108.20
1	A	131	A	C3'-C2'-C1'	5.57	105.95	101.50
1	A	1284	C	P-O3'-C3'	5.56	126.38	119.70
1	A	734	G	C3'-C2'-C1'	5.56	105.95	101.50
1	A	1485	U	O4'-C1'-N1	5.56	112.65	108.20
1	A	1449	C	P-O3'-C3'	-5.55	113.03	119.70
1	A	368	U	N1-C1'-C2'	-5.55	105.89	112.00
1	A	15	G	C3'-C2'-C1'	5.54	105.94	101.50
1	A	1191	A	C3'-C2'-C1'	5.54	105.93	101.50
1	A	1051	C	O4'-C1'-N1	5.53	112.63	108.20
1	A	511	C	P-O3'-C3'	5.52	126.32	119.70
1	A	722	G	C3'-C2'-C1'	5.52	105.91	101.50
1	A	1396	A	OP2-P-O3'	5.51	117.33	105.20
1	A	1395	C	C3'-C2'-C1'	5.51	105.91	101.50
1	A	832	G	O4'-C1'-N9	5.51	112.61	108.20
1	A	1066	C	N1-C1'-C2'	-5.50	105.95	112.00
1	A	1499	A	P-O5'-C5'	-5.50	112.10	120.90
1	A	389	A	C3'-C2'-C1'	5.49	105.90	101.50
1	A	369	G	C3'-C2'-C1'	5.49	105.89	101.50
1	A	1184	G	P-O3'-C3'	-5.48	113.12	119.70
1	A	252	U	C3'-C2'-C1'	5.48	105.88	101.50
1	A	365	U	P-O3'-C3'	5.48	126.28	119.70
1	A	316	C	P-O3'-C3'	-5.48	113.13	119.70
1	A	276	G	N9-C1'-C2'	-5.48	105.98	112.00
1	A	352	C	C3'-C2'-C1'	5.47	105.88	101.50
1	A	962	C	P-O3'-C3'	-5.47	113.14	119.70
1	A	979	C	C3'-C2'-C1'	5.46	105.87	101.50
1	A	1161	C	C3'-C2'-C1'	5.45	105.86	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	828	U	O4'-C1'-N1	5.44	112.56	108.20
1	A	1157	A	P-O3'-C3'	5.44	126.23	119.70
1	A	84	U	O4'-C1'-N1	5.42	112.53	108.20
1	A	1283	U	C3'-C2'-C1'	5.42	105.83	101.50
1	A	985	C	C3'-C2'-C1'	5.40	105.82	101.50
1	A	718	A	P-O3'-C3'	-5.39	113.23	119.70
1	A	194	C	O4'-C1'-N1	-5.38	103.89	108.20
1	A	1453	G	C3'-C2'-C1'	5.38	105.81	101.50
1	A	68	G	C3'-C2'-C1'	5.38	105.80	101.50
1	A	1129	C	P-O3'-C3'	5.37	126.14	119.70
1	A	1366	C	P-O3'-C3'	-5.37	113.26	119.70
1	A	1481	U	O4'-C1'-N1	5.36	112.49	108.20
1	A	705	G	C3'-C2'-C1'	5.36	105.79	101.50
1	A	327	A	P-O3'-C3'	5.36	126.13	119.70
1	A	428	G	C8-N9-C1'	5.35	133.96	127.00
1	A	275	G	C3'-C2'-C1'	5.35	105.78	101.50
1	A	1317	C	O4'-C1'-N1	5.35	112.48	108.20
1	A	309	A	P-O3'-C3'	-5.35	113.28	119.70
1	A	939	G	O4'-C1'-N9	5.34	112.47	108.20
1	A	81	A	O4'-C1'-N9	5.33	112.46	108.20
1	A	239	U	C5-C6-N1	5.33	125.36	122.70
1	A	765	G	C4-N9-C1'	5.32	133.42	126.50
1	A	439	U	P-O3'-C3'	-5.32	113.32	119.70
1	A	26	A	P-O3'-C3'	5.31	126.07	119.70
1	A	169	C	O4'-C1'-N1	5.31	112.45	108.20
1	A	1358	U	O4'-C1'-N1	5.30	112.44	108.20
1	A	534	U	C3'-C2'-C1'	5.30	105.74	101.50
1	A	1102	A	N9-C1'-C2'	-5.30	106.17	112.00
1	A	794	A	C3'-C2'-C1'	5.30	105.74	101.50
1	A	389	A	N9-C1'-C2'	-5.29	106.18	112.00
1	A	534	U	P-O3'-C3'	-5.29	113.35	119.70
1	A	32	A	C3'-C2'-C1'	5.29	105.73	101.50
1	A	689	C	O4'-C1'-N1	-5.29	103.97	108.20
1	A	883	C	N1-C1'-C2'	5.29	120.87	114.00
1	A	282	A	C3'-C2'-C1'	5.28	105.73	101.50
1	A	1479	C	O4'-C1'-N1	5.28	112.43	108.20
1	A	1052	U	P-O5'-C5'	5.28	129.35	120.90
1	A	803	G	C3'-C2'-C1'	5.27	105.72	101.50
1	A	174	A	C3'-C2'-C1'	5.27	105.72	101.50
1	A	388	G	O3'-P-O5'	-5.27	93.98	104.00
1	A	913	A	P-O3'-C3'	5.27	126.03	119.70
1	A	960	U	O4'-C1'-N1	5.27	112.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1085	U	P-O3'-C3'	5.26	126.02	119.70
1	A	439	U	C3'-C2'-C1'	5.26	105.71	101.50
1	A	276	G	P-O3'-C3'	-5.26	113.39	119.70
1	A	1301	U	C3'-C2'-C1'	5.26	105.70	101.50
1	A	969	A	C3'-C2'-C1'	5.25	105.70	101.50
1	A	475	C	P-O3'-C3'	-5.25	113.40	119.70
1	A	1451	U	O4'-C1'-N1	5.25	112.40	108.20
1	A	32	A	N9-C1'-C2'	-5.25	106.23	112.00
1	A	213	G	C3'-C2'-C1'	5.24	105.69	101.50
1	A	277	C	O4'-C1'-N1	5.24	112.39	108.20
1	A	1086	U	C3'-C2'-C1'	5.24	105.69	101.50
1	A	110	C	O4'-C1'-N1	5.24	112.39	108.20
1	A	210	C	C2-N1-C1'	5.24	124.56	118.80
1	A	392	C	O4'-C1'-N1	5.23	112.38	108.20
1	A	874	G	C3'-C2'-C1'	5.23	105.68	101.50
1	A	1282	C	C3'-C2'-C1'	5.23	105.68	101.50
1	A	1141	C	P-O3'-C3'	-5.23	113.43	119.70
1	A	1507	A	C3'-C2'-C1'	5.22	105.68	101.50
1	A	874	G	P-O3'-C3'	-5.22	113.43	119.70
1	A	1401	G	N9-C1'-C2'	-5.22	106.26	112.00
1	A	1052	U	C3'-C2'-C1'	5.21	105.67	101.50
1	A	1066	C	P-O3'-C3'	-5.21	113.45	119.70
1	A	719	C	O4'-C1'-N1	5.21	112.36	108.20
1	A	13	U	O4'-C1'-N1	5.19	112.35	108.20
1	A	181	A	P-O3'-C3'	5.19	125.93	119.70
1	A	596	A	C3'-C2'-C1'	5.19	105.65	101.50
1	A	1191	A	P-O3'-C3'	-5.19	113.47	119.70
1	A	1184	G	N9-C1'-C2'	-5.18	106.30	112.00
1	A	374	A	C3'-C2'-C1'	5.17	105.64	101.50
1	A	937	A	N9-C1'-C2'	-5.17	106.31	112.00
1	A	500	G	P-O3'-C3'	-5.17	113.50	119.70
1	A	1453	G	P-O3'-C3'	-5.17	113.50	119.70
1	A	936	C	P-O3'-C3'	-5.17	113.50	119.70
1	A	84	U	N1-C1'-C2'	5.16	120.70	114.00
1	A	794	A	N9-C1'-C2'	-5.16	106.33	112.00
1	A	1348	U	C3'-C2'-C1'	5.16	105.62	101.50
1	A	1225	A	P-O3'-C3'	5.15	125.88	119.70
1	A	482	A	P-O3'-C3'	-5.15	113.52	119.70
1	A	980	C	O4'-C1'-N1	5.14	112.31	108.20
1	A	1283	U	O4'-C1'-N1	5.14	112.31	108.20
1	A	718	A	C3'-C2'-C1'	5.14	105.61	101.50
1	A	72	A	C3'-C2'-C1'	5.13	105.61	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1454	G	C3'-C2'-C1'	5.13	105.61	101.50
1	A	536	C	C3'-C2'-C1'	5.13	105.61	101.50
1	A	401	C	P-O5'-C5'	-5.13	112.69	120.90
1	A	373	A	N9-C1'-C2'	-5.13	106.36	112.00
1	A	96	U	O4'-C1'-N1	5.12	112.29	108.20
1	A	512	U	C3'-C2'-C1'	5.12	105.59	101.50
1	A	977	A	P-O3'-C3'	-5.12	113.56	119.70
1	A	812	G	P-O3'-C3'	5.11	125.83	119.70
1	A	1383	C	C3'-C2'-C1'	5.11	105.59	101.50
1	A	85	U	N1-C1'-C2'	5.11	120.64	114.00
1	A	644	U	O4'-C1'-N1	5.10	112.28	108.20
1	A	1398	A	N9-C1'-C2'	-5.10	106.39	112.00
1	A	73	C	C3'-C2'-C1'	5.09	105.58	101.50
1	A	968	A	O4'-C1'-N9	5.09	112.27	108.20
1	A	1213	A	P-O3'-C3'	5.09	125.81	119.70
1	A	1382	C	O4'-C1'-N1	5.09	112.27	108.20
1	A	245	U	C3'-C2'-C1'	5.09	105.57	101.50
1	A	970	C	O4'-C1'-N1	5.08	112.26	108.20
1	A	815	A	P-O3'-C3'	5.07	125.79	119.70
1	A	808	C	O4'-C1'-N1	5.07	112.25	108.20
1	A	977	A	C3'-C2'-C1'	5.06	105.55	101.50
1	A	1394	A	P-O3'-C3'	5.06	125.77	119.70
1	A	1073	U	O4'-C1'-N1	5.06	112.25	108.20
1	A	95	C	C3'-C2'-C1'	5.06	105.55	101.50
1	A	1140	C	P-O3'-C3'	-5.05	113.64	119.70
1	A	381	C	C2-N1-C1'	5.05	124.36	118.80
1	A	199	A	N9-C1'-C2'	-5.05	106.44	112.00
1	A	1101	A	P-O3'-C3'	5.05	125.76	119.70
1	A	1287	A	C3'-C2'-C1'	5.04	105.53	101.50
1	A	1399	C	O4'-C1'-N1	5.03	112.22	108.20
1	A	52	C	C3'-C2'-C1'	5.02	105.52	101.50
1	A	1066	C	C3'-C2'-C1'	5.02	105.52	101.50
1	A	1146	A	P-O3'-C3'	-5.02	113.68	119.70
1	A	87	C	C3'-C2'-C1'	5.01	105.51	101.50
1	A	973	G	P-O3'-C3'	5.01	125.72	119.70
1	A	500	G	C3'-C2'-C1'	5.00	105.50	101.50
1	A	559	A	O4'-C1'-N9	5.00	112.20	108.20
1	A	567	G	P-O3'-C3'	-5.00	113.70	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	107	ARG	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32831	0	44	671	0
2	B	1705	0	0	28	0
3	C	1625	0	0	16	0
4	D	1643	0	0	44	0
5	E	1106	0	75	28	0
6	F	818	0	0	14	0
7	G	1175	0	0	10	0
8	H	979	0	0	15	0
9	I	1022	0	0	16	0
10	J	787	0	0	8	0
11	K	877	0	0	18	0
12	L	955	0	0	11	0
13	M	877	0	0	5	0
14	N	769	0	0	7	0
15	O	714	0	0	10	0
16	P	639	0	0	13	0
17	Q	649	0	691	63	0
18	R	456	0	0	10	0
19	S	638	0	0	2	0
20	T	665	0	0	12	0
21	U	426	0	0	22	0
22	A	42	0	0	0	0
23	A	199	0	0	5	0
23	E	1	0	0	0	0
23	I	1	0	0	0	0
23	N	4	0	0	0	0
23	T	1	0	0	0	0
23	U	1	0	0	0	0
All	All	51605	0	810	959	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 19.

All (959) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:3:LYS:NZ	17:Q:6:THR:HG21	1.86	0.89
1:A:366:A:O2'	1:A:394:G:N2	2.09	0.85
17:Q:30:HIS:HE1	17:Q:32:ILE:HG13	1.42	0.84
1:A:254:G:N2	17:Q:17:GLU:HG3	1.93	0.84
17:Q:3:LYS:HZ3	17:Q:6:THR:HG21	1.43	0.79
1:A:560:A:C5	5:E:127:TYR:CE2	2.71	0.78
1:A:858:G:N7	23:A:1698:HOH:O	2.18	0.77
1:A:792:A:O2'	1:A:794:A:N7	2.18	0.76
1:A:532:A:C8	3:C:192:TYR:CE2	2.75	0.75
1:A:247:G:O6	1:A:278:G:C6	2.40	0.75
1:A:513:C:O2'	1:A:514:C:O4'	2.05	0.74
11:K:27:ASN:ND2	11:K:27:ASN:N	2.36	0.74
1:A:1408:A:C2	1:A:1492:A:N6	2.55	0.74
17:Q:30:HIS:CE1	17:Q:32:ILE:HG13	2.23	0.73
5:E:29:ILE:CG2	5:E:30:PHE:N	2.51	0.72
17:Q:18:LYS:HD3	17:Q:48:GLU:OE2	1.89	0.71
1:A:198:G:O6	1:A:220:G:C4	2.43	0.71
4:D:34:GLU:O	4:D:36:ALA:N	2.22	0.71
17:Q:46:HIS:HB2	17:Q:70:LYS:HE3	1.72	0.71
1:A:1051:C:O2'	1:A:1052:U:O5'	2.07	0.71
1:A:6:G:C2'	1:A:6:G:N3	2.54	0.71
1:A:1530:G:O2'	1:A:1531:A:C8	2.44	0.70
1:A:765:G:C8	1:A:812:G:C2	2.79	0.70
1:A:1129:C:O2'	1:A:1130:A:C8	2.45	0.70
1:A:1151:A:O3'	10:J:70:HIS:CE1	2.44	0.70
21:U:24:LYS:CG	21:U:25:ALA:N	2.55	0.70
17:Q:61:ARG:HG2	17:Q:75:VAL:HG11	1.73	0.70
1:A:330:C:O2'	1:A:331:G:C8	2.45	0.69
5:E:154:ALA:HB1	8:H:65:PHE:CE2	2.27	0.69
17:Q:4:ILE:HG22	17:Q:5:ARG:H	1.58	0.69
1:A:499:A:C6	1:A:547:A:C8	2.81	0.68
1:A:495:A:C2	1:A:496:A:C6	2.81	0.68
1:A:1213:A:O2'	1:A:1214:C:C5'	2.42	0.68
1:A:1458:G:O2'	20:T:22:SER:CB	2.41	0.68
21:U:39:LYS:N	21:U:40:PRO:CD	2.57	0.67
1:A:985:C:C4	1:A:986:U:O4	2.48	0.67
12:L:43:LYS:CB	12:L:44:PRO:CD	2.73	0.67
1:A:1200:C:O2'	1:A:1201:A:OP2	2.12	0.67
1:A:986:U:C2'	1:A:987:G:C8	2.78	0.67
1:A:1217:C:O2'	1:A:1218:C:O4'	2.13	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:734:G:N2	18:R:63:TYR:CE2	2.64	0.66
1:A:277:C:OP1	17:Q:44:HIS:HE1	1.78	0.66
1:A:1533:C:H2'	1:A:1534:A:H5''	1.77	0.66
1:A:109:A:C8	1:A:327:A:O4'	2.50	0.65
1:A:1301:U:O2'	1:A:1302:C:C5	2.49	0.65
17:Q:75:VAL:O	17:Q:76:ARG:HB3	1.97	0.65
1:A:369:G:OP2	1:A:388:G:N2	2.29	0.65
1:A:1064:G:O2'	1:A:1190:G:N2	2.28	0.65
1:A:519:C:O2'	1:A:520:A:C5'	2.44	0.65
1:A:936:C:O2'	1:A:937:A:C8	2.49	0.65
20:T:73:ARG:NH1	20:T:73:ARG:CG	2.59	0.64
1:A:1160:G:C6	1:A:1181:G:O6	2.50	0.64
1:A:413:G:N2	1:A:428:G:O2'	2.31	0.64
1:A:984:C:O2'	1:A:985:C:C6	2.51	0.63
1:A:1366:C:O2'	1:A:1367:C:C6	2.52	0.63
1:A:1181:G:O2'	1:A:1182:G:O4'	2.17	0.62
1:A:515:G:N7	23:A:1731:HOH:O	2.31	0.62
17:Q:13:SER:HB3	17:Q:21:VAL:HB	1.81	0.62
1:A:718:A:C5	11:K:117:HIS:CD2	2.88	0.62
4:D:106:PHE:N	4:D:106:PHE:CD1	2.66	0.62
1:A:533:A:C2	1:A:536:C:C5	2.87	0.62
1:A:1168:U:C2'	1:A:1168:U:O2	2.46	0.62
1:A:309:A:O2'	1:A:607:A:N1	2.33	0.62
17:Q:27:PHE:CD1	17:Q:36:PHE:HB3	2.34	0.62
1:A:205:A:C6	1:A:206:C:N4	2.67	0.62
2:B:93:HIS:ND1	2:B:145:ASN:O	2.33	0.62
17:Q:59:GLU:HG2	17:Q:76:ARG:HG2	1.82	0.62
1:A:992:U:O2'	1:A:993:G:OP2	2.17	0.62
1:A:90:C:O2'	1:A:91:U:C6	2.53	0.62
5:E:157:GLY:HA3	8:H:63:LYS:NZ	2.14	0.61
1:A:372:C:O2'	1:A:373:A:P	2.58	0.61
17:Q:25:GLU:HA	17:Q:39:ARG:O	1.99	0.61
1:A:198:G:C4	1:A:199:A:C8	2.88	0.61
1:A:91:U:O2'	1:A:92:U:C6	2.52	0.61
1:A:642:A:O2'	1:A:643:C:C6	2.54	0.61
4:D:94:GLU:OE1	4:D:103:ARG:NE	2.33	0.61
1:A:1447:A:O2'	1:A:1448:C:OP1	2.18	0.61
5:E:151:MET:O	5:E:154:ALA:HB3	2.01	0.61
1:A:702:A:C8	1:A:702:A:OP1	2.54	0.61
1:A:267:C:OP2	17:Q:68:LYS:HD2	2.00	0.61
1:A:630:A:C2	23:A:1734:HOH:O	2.52	0.61
1:A:497:G:O2'	1:A:498:A:C8	2.53	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:29:LYS:HE2	17:Q:36:PHE:CZ	2.36	0.60
17:Q:29:LYS:HE2	17:Q:36:PHE:CE1	2.36	0.60
1:A:397:A:N7	1:A:547:A:O2'	2.34	0.60
1:A:496:A:O2'	1:A:497:G:C8	2.54	0.60
2:B:80:LYS:O	2:B:84:LEU:N	2.34	0.60
1:A:103:U:C2	1:A:104:G:C8	2.90	0.60
17:Q:3:LYS:HZ2	17:Q:6:THR:HG21	1.64	0.60
20:T:2:ASN:N	20:T:7:LYS:NZ	2.49	0.60
1:A:198:G:O2'	1:A:199:A:C8	2.55	0.60
17:Q:27:PHE:HD1	17:Q:36:PHE:HB3	1.66	0.60
1:A:373:A:O2'	1:A:374:A:C5'	2.50	0.60
21:U:35:GLU:O	21:U:36:PHE:CD2	2.54	0.60
1:A:158:G:C5	1:A:164:G:C6	2.90	0.60
17:Q:59:GLU:HB3	17:Q:76:ARG:O	2.01	0.60
1:A:32:A:C2'	1:A:33:A:C8	2.84	0.60
1:A:93:U:C2	1:A:95:C:N4	2.70	0.60
17:Q:25:GLU:HG2	17:Q:40:THR:HG22	1.83	0.59
1:A:608:A:OP2	23:A:1735:HOH:O	2.16	0.59
1:A:961:U:O2'	1:A:962:C:C6	2.55	0.59
1:A:265:G:O3'	17:Q:67:SER:HA	2.01	0.59
11:K:126:ARG:O	21:U:33:ARG:CZ	2.50	0.59
1:A:388:G:O2'	1:A:389:A:P	2.61	0.59
1:A:1084:G:C5	1:A:1085:U:C4	2.91	0.59
1:A:596:A:C2	1:A:597:G:C5	2.91	0.59
1:A:296:U:C2	1:A:297:G:C8	2.90	0.59
11:K:126:ARG:O	21:U:33:ARG:NH2	2.34	0.59
1:A:1124:G:O2'	1:A:1125:U:C5	2.56	0.59
1:A:1296:C:O2'	1:A:1302:C:C4	2.56	0.59
1:A:1072:G:C6	1:A:1073:U:C4	2.91	0.59
1:A:1130:A:C5	1:A:1146:A:C6	2.90	0.58
1:A:66:A:N6	1:A:67:C:N4	2.50	0.58
1:A:239:U:C5'	1:A:239:U:C6	2.85	0.58
1:A:722:G:O3'	1:A:723:U:C5	2.56	0.58
18:R:19:GLU:CD	18:R:20:ILE:N	2.57	0.58
1:A:1533:C:C2'	1:A:1534:A:H5''	2.32	0.58
1:A:1183:U:O2'	1:A:1184:G:OP1	2.20	0.58
1:A:1299:A:C2'	1:A:1299:A:N3	2.67	0.58
1:A:1381:U:C4	7:G:77:ARG:NH1	2.72	0.58
1:A:198:G:O6	1:A:220:G:C5	2.57	0.58
1:A:249:U:C2	1:A:276:G:N1	2.72	0.58
1:A:1297:G:C8	1:A:1297:G:OP2	2.57	0.58
1:A:1190:G:O2'	1:A:1191:A:P	2.61	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:577:G:C4	1:A:816:A:C2	2.93	0.57
1:A:264:C:O2'	17:Q:64:ARG:HG3	2.03	0.57
1:A:1278:G:O2'	1:A:1279:G:C2	2.57	0.57
1:A:1417:G:C6	1:A:1482:G:C6	2.92	0.57
17:Q:61:ARG:HG2	17:Q:75:VAL:CG1	2.34	0.57
1:A:130:A:O2'	1:A:131:A:O5'	2.23	0.57
1:A:246:A:C4	1:A:282:A:N6	2.73	0.57
1:A:1206:G:C6	1:A:1207:G:C5	2.93	0.57
1:A:679:C:O2	1:A:712:A:C2	2.58	0.57
1:A:476:U:C6	1:A:476:U:OP2	2.57	0.57
1:A:1084:G:OP1	1:A:1086:U:C5	2.57	0.57
1:A:1448:C:O2'	1:A:1449:C:C6	2.58	0.57
1:A:1067:A:C1'	1:A:1068:G:C8	2.87	0.57
21:U:35:GLU:OE1	21:U:37:TYR:CD1	2.58	0.57
1:A:98:A:C2	1:A:99:C:C2	2.93	0.57
1:A:764:C:N4	1:A:812:G:N1	2.52	0.56
1:A:1151:A:C6	1:A:1152:A:N6	2.73	0.56
1:A:666:G:C4	1:A:741:G:C2	2.93	0.56
1:A:764:C:N4	1:A:812:G:C6	2.73	0.56
1:A:1239:A:O2'	1:A:1241:G:C5	2.58	0.56
1:A:149:A:C2	1:A:150:U:C2	2.93	0.56
5:E:103:GLY:O	5:E:104:ILE:CG2	2.52	0.56
6:F:43:GLY:O	6:F:44:ARG:C	2.44	0.56
4:D:190:LEU:O	4:D:191:SER:O	2.23	0.56
1:A:89:U:O2'	1:A:90:C:O4'	2.23	0.56
4:D:29:THR:O	4:D:30:LYS:NZ	2.38	0.56
1:A:953:G:C6	1:A:1229:A:N6	2.73	0.56
1:A:1458:G:O3'	20:T:22:SER:CA	2.53	0.56
1:A:205:A:C5	1:A:206:C:N4	2.73	0.56
16:P:29:ASN:OD1	16:P:29:ASN:N	2.37	0.56
1:A:1147:C:O2'	1:A:1148:U:C6	2.59	0.56
21:U:31:VAL:O	21:U:33:ARG:N	2.39	0.56
1:A:71:A:O2'	1:A:72:A:O4'	2.23	0.56
1:A:449:G:N1	1:A:450:G:C6	2.74	0.56
21:U:19:LYS:NZ	21:U:19:LYS:N	2.53	0.56
1:A:858:G:O6	1:A:869:G:C8	2.59	0.56
17:Q:59:GLU:HG3	17:Q:75:VAL:HG22	1.88	0.56
1:A:1253:G:N1	1:A:1285:A:N6	2.54	0.56
1:A:330:C:O2'	1:A:331:G:O5'	2.24	0.55
4:D:81:LEU:O	4:D:83:GLY:N	2.39	0.55
1:A:861:G:C5	1:A:862:C:C5	2.94	0.55
1:A:263:A:OP1	20:T:73:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1167:A:N7	1:A:1169:A:N6	2.54	0.55
1:A:643:C:O2'	1:A:644:U:C5'	2.54	0.55
5:E:89:THR:OG1	5:E:90:GLY:N	2.39	0.55
9:I:49:GLN:N	9:I:50:PRO:CD	2.70	0.55
1:A:261:U:O2'	1:A:263:A:N7	2.39	0.55
1:A:533:A:O2'	1:A:535:A:OP2	2.25	0.55
1:A:604:G:C6	1:A:605:U:N3	2.75	0.55
17:Q:45:VAL:HG11	17:Q:60:ILE:CG2	2.36	0.55
1:A:1050:G:O2'	1:A:1051:C:C6	2.59	0.55
1:A:1191:A:OP1	3:C:2:GLN:NE2	2.40	0.55
5:E:157:GLY:HA3	8:H:63:LYS:CE	2.37	0.55
1:A:1244:G:O2'	1:A:1245:C:O4'	2.24	0.55
11:K:111:ASP:N	21:U:3:ILE:N	2.55	0.55
1:A:644:U:C2	1:A:645:G:C8	2.95	0.55
8:H:75:GLN:O	8:H:126:CYS:CB	2.55	0.55
1:A:560:A:C6	5:E:127:TYR:CE2	2.94	0.55
1:A:327:A:C2	1:A:329:A:N3	2.75	0.55
1:A:1084:G:OP1	1:A:1086:U:C6	2.60	0.55
1:A:1287:A:O2'	1:A:1288:A:C8	2.60	0.55
1:A:274:A:O2'	1:A:275:G:C8	2.59	0.55
1:A:220:G:C2	1:A:221:C:C6	2.95	0.54
17:Q:13:SER:O	17:Q:20:ILE:HB	2.07	0.54
1:A:818:G:C3'	1:A:819:A:C5'	2.85	0.54
1:A:1382:C:O2'	1:A:1383:C:C5'	2.55	0.54
1:A:1250:A:N3	1:A:1287:A:N6	2.55	0.54
1:A:202:G:O2'	1:A:468:A:C8	2.61	0.54
1:A:350:G:C6	1:A:351:G:C6	2.95	0.54
1:A:920:U:C2	1:A:921:U:C5	2.95	0.54
1:A:757:U:OP1	1:A:822:U:O2'	2.24	0.54
17:Q:12:VAL:O	17:Q:12:VAL:HG22	2.08	0.54
12:L:19:ASN:N	12:L:19:ASN:ND2	2.56	0.54
1:A:796:C:O3'	11:K:126:ARG:NH2	2.41	0.54
1:A:914:A:O2'	1:A:915:A:O4'	2.26	0.54
6:F:67:PRO:O	6:F:69:GLU:N	2.41	0.54
1:A:496:A:C2'	1:A:496:A:N3	2.70	0.54
1:A:1301:U:O2'	1:A:1302:C:C6	2.60	0.54
1:A:891:U:C5	1:A:906:A:C2	2.96	0.54
4:D:68:GLU:O	4:D:69:ARG:C	2.46	0.54
17:Q:14:ASP:OD2	17:Q:52:CYS:HB2	2.07	0.54
1:A:577:G:N9	1:A:816:A:C2	2.76	0.54
1:A:441:A:C2	1:A:497:G:C6	2.95	0.54
1:A:1167:A:O2'	1:A:1168:U:OP1	2.25	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:985:C:O2'	1:A:986:U:C5'	2.56	0.54
1:A:1461:G:C5	1:A:1462:C:C4	2.96	0.54
21:U:25:ALA:O	21:U:29:ALA:N	2.40	0.54
1:A:1494:G:N2	1:A:1495:U:C2	2.76	0.53
1:A:373:A:N3	1:A:374:A:C8	2.77	0.53
1:A:338:A:N1	1:A:351:G:N2	2.55	0.53
1:A:725:G:C5	1:A:726:C:C5	2.97	0.53
1:A:560:A:C4	5:E:127:TYR:CD2	2.97	0.53
1:A:321:A:N7	1:A:328:C:C2	2.76	0.53
1:A:140:U:O2	1:A:183:C:N4	2.42	0.53
9:I:5:TYR:CD2	9:I:5:TYR:N	2.75	0.53
1:A:367:U:C6	1:A:394:G:N2	2.77	0.53
17:Q:29:LYS:HB2	17:Q:36:PHE:CE1	2.44	0.53
1:A:1124:G:C4'	1:A:1125:U:OP1	2.56	0.53
1:A:449:G:C2	1:A:450:G:C5	2.96	0.53
5:E:68:ARG:O	5:E:69:ASN:C	2.47	0.53
10:J:45:ARG:O	10:J:46:LYS:C	2.46	0.53
2:B:19:THR:OG1	2:B:20:ARG:N	2.41	0.53
1:A:1138:G:N2	1:A:1140:C:C4	2.76	0.53
1:A:844:G:C2	1:A:846:G:O2'	2.62	0.53
1:A:1346:A:C8	1:A:1348:U:N3	2.77	0.53
6:F:18:VAL:CG2	6:F:58:HIS:CD2	2.92	0.53
1:A:1493:A:C8	1:A:1493:A:OP1	2.62	0.53
2:B:49:PHE:O	2:B:53:LEU:N	2.42	0.53
1:A:198:G:N3	1:A:199:A:C8	2.77	0.53
1:A:85:U:O2	1:A:85:U:O4'	2.27	0.53
1:A:295:C:C5	1:A:296:U:C5	2.97	0.53
1:A:552:U:C2	1:A:553:A:C8	2.97	0.53
10:J:33:GLY:O	10:J:35:GLN:N	2.42	0.53
1:A:967:C:N3	1:A:968:A:N6	2.56	0.53
1:A:560:A:C8	1:A:566:G:C4	2.98	0.52
21:U:34:ARG:O	21:U:35:GLU:O	2.26	0.52
1:A:614:C:N3	1:A:615:G:C8	2.77	0.52
14:N:100:TRP:C	14:N:100:TRP:CD1	2.83	0.52
1:A:692:U:O2'	1:A:694:A:N7	2.42	0.52
1:A:765:G:O6	1:A:811:C:C5	2.63	0.52
1:A:320:A:C2	1:A:334:C:N3	2.78	0.52
1:A:770:C:O2'	1:A:899:C:N3	2.42	0.52
1:A:1093:A:C5	1:A:1095:U:O4'	2.62	0.52
20:T:31:ILE:O	20:T:35:TYR:N	2.42	0.52
1:A:1073:U:C2	1:A:1074:G:C8	2.97	0.52
8:H:1:SER:C	8:H:3:GLN:N	2.63	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:G:C2	1:A:289:G:N7	2.77	0.52
1:A:519:C:C2'	1:A:520:A:C8	2.91	0.52
1:A:82:G:C5	1:A:89:U:C5	2.98	0.52
1:A:91:U:C4	1:A:92:U:C4	2.98	0.52
4:D:30:LYS:CD	4:D:30:LYS:N	2.72	0.52
5:E:80:LEU:O	5:E:81:GLN:CB	2.57	0.52
10:J:44:THR:OG1	10:J:70:HIS:CE1	2.63	0.52
17:Q:37:ILE:HG13	17:Q:38:LYS:O	2.10	0.52
1:A:120:A:C3'	1:A:121:U:C5'	2.88	0.52
21:U:14:ALA:O	21:U:15:LEU:O	2.28	0.52
1:A:495:A:C6	1:A:496:A:N6	2.78	0.52
1:A:722:G:O3'	1:A:723:U:C6	2.63	0.52
10:J:84:VAL:CG2	10:J:85:ASP:N	2.73	0.52
1:A:380:G:N2	1:A:383:A:OP2	2.43	0.52
1:A:1365:G:O2'	1:A:1366:C:C5'	2.58	0.52
1:A:1077:G:C2	1:A:1081:A:C2	2.98	0.52
1:A:926:G:C6	1:A:1505:G:C6	2.98	0.52
17:Q:61:ARG:CG	17:Q:75:VAL:HG11	2.40	0.51
1:A:82:G:N7	1:A:89:U:C4	2.78	0.51
1:A:1452:C:C4'	1:A:1453:G:O5'	2.58	0.51
1:A:38:G:N1	1:A:397:A:OP1	2.42	0.51
4:D:2:ARG:NH2	4:D:114:ARG:NH1	2.58	0.51
1:A:260:G:OP1	20:T:74:HIS:CE1	2.63	0.51
2:B:128:LEU:O	2:B:129:THR:C	2.49	0.51
1:A:142:G:C5	1:A:143:A:C8	2.98	0.51
6:F:41:ASP:OD2	6:F:58:HIS:CE1	2.63	0.51
1:A:995:C:N3	1:A:1046:A:O2'	2.43	0.51
1:A:129:A:O2'	1:A:130:A:C8	2.63	0.51
1:A:382:A:N7	1:A:383:A:C6	2.78	0.51
1:A:892:A:C5	1:A:893:C:C5	2.98	0.51
1:A:560:A:N7	1:A:566:G:C4	2.78	0.51
1:A:597:G:N7	1:A:598:U:C5	2.79	0.51
17:Q:47:ASP:HB3	17:Q:74:LEU:CB	2.40	0.51
1:A:568:G:N2	1:A:883:C:C2	2.79	0.51
1:A:567:G:N2	23:A:1695:HOH:O	2.43	0.51
1:A:247:G:C6	1:A:278:G:N1	2.79	0.51
1:A:1228:C:O2'	1:A:1229:A:C8	2.63	0.51
1:A:577:G:C6	1:A:812:G:N2	2.79	0.51
1:A:199:A:O2'	1:A:200:G:O4'	2.29	0.51
1:A:1124:G:O2'	1:A:1125:U:C6	2.64	0.51
1:A:183:C:O2'	1:A:184:G:C5'	2.59	0.51
1:A:1108:G:OP1	3:C:175:HIS:ND1	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:A:C2	1:A:246:A:C8	2.99	0.51
1:A:135:C:O2	16:P:1:MET:CB	2.59	0.51
1:A:1134:G:N1	1:A:1141:C:C4	2.78	0.51
1:A:985:C:O2'	1:A:986:U:O5'	2.29	0.51
1:A:64:G:C8	1:A:99:C:N4	2.78	0.51
1:A:449:G:C2	1:A:450:G:C4	2.99	0.51
1:A:1157:A:C2	1:A:1181:G:C8	2.99	0.50
1:A:295:C:C4	1:A:296:U:C4	2.99	0.50
1:A:148:G:N1	1:A:149:A:C5	2.78	0.50
1:A:990:C:C2'	1:A:991:U:O4'	2.59	0.50
1:A:961:U:O4	1:A:983:A:N6	2.44	0.50
1:A:983:A:O2'	1:A:984:C:C5'	2.59	0.50
1:A:1434:A:N6	1:A:1435:G:N1	2.59	0.50
9:I:119:LYS:O	9:I:121:ARG:N	2.44	0.50
16:P:32:PHE:CD1	16:P:32:PHE:C	2.85	0.50
17:Q:46:HIS:HB2	17:Q:70:LYS:CE	2.41	0.50
1:A:1386:G:C2	1:A:1387:G:C8	2.99	0.50
1:A:1367:C:O2'	1:A:1368:A:O4'	2.29	0.50
1:A:733:G:O2'	1:A:734:G:C5'	2.59	0.50
1:A:922:G:O2'	1:A:1398:A:N1	2.44	0.50
1:A:80:A:C6	1:A:81:A:O2'	2.65	0.50
21:U:35:GLU:CG	21:U:36:PHE:N	2.75	0.50
11:K:124:LYS:O	21:U:33:ARG:NE	2.44	0.50
1:A:268:U:C2	1:A:269:C:C5	3.00	0.50
4:D:115:GLN:NE2	4:D:153:ARG:NH2	2.59	0.50
1:A:1501:C:N4	1:A:1504:G:C2	2.79	0.50
1:A:936:C:O2'	1:A:937:A:O5'	2.30	0.50
1:A:642:A:O2'	1:A:643:C:O5'	2.30	0.50
1:A:71:A:C2	1:A:72:A:C8	3.00	0.50
1:A:1285:A:C4'	1:A:1286:U:OP1	2.60	0.50
1:A:437:U:C2'	1:A:438:U:O5'	2.59	0.50
1:A:123:U:OP1	1:A:311:C:O2'	2.28	0.50
5:E:132:PRO:O	5:E:134:ASN:N	2.45	0.50
3:C:59:PRO:O	3:C:61:LYS:N	2.45	0.50
1:A:1092:A:C6	1:A:1183:U:O2	2.64	0.50
11:K:90:PRO:O	11:K:91:GLY:C	2.50	0.50
1:A:396:C:O2'	1:A:398:U:OP1	2.29	0.50
6:F:81:ASN:O	6:F:83:ALA:N	2.45	0.50
1:A:407:U:C2'	1:A:408:A:C8	2.95	0.50
1:A:1363:A:C5	1:A:1365:G:C6	2.99	0.50
1:A:1101:A:C4'	1:A:1102:A:O5'	2.60	0.50
1:A:1387:G:C4	1:A:1388:C:C5	3.00	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:96:GLN:N	5:E:123:LEU:O	2.45	0.50
8:H:89:ASP:N	8:H:89:ASP:OD1	2.45	0.50
1:A:986:U:C2'	1:A:987:G:O5'	2.60	0.49
18:R:59:LYS:O	18:R:63:TYR:CD1	2.65	0.49
1:A:1381:U:O2'	1:A:1382:C:O5'	2.30	0.49
4:D:191:SER:O	4:D:192:ALA:CB	2.60	0.49
1:A:996:A:O2'	1:A:997:U:O4'	2.29	0.49
1:A:160:A:O2'	1:A:344:A:N6	2.44	0.49
16:P:69:ASP:O	16:P:73:ALA:N	2.45	0.49
1:A:14:U:O2	1:A:16:A:C8	2.65	0.49
1:A:1319:A:N6	1:A:1323:G:C2	2.80	0.49
4:D:25:ARG:O	4:D:26:ALA:C	2.50	0.49
1:A:461:A:P	1:A:462:G:OP2	2.70	0.49
1:A:1004:A:C4	1:A:1026:G:N7	2.80	0.49
1:A:495:A:N1	1:A:496:A:N6	2.61	0.49
1:A:937:A:C2	1:A:1379:G:C6	3.00	0.49
1:A:82:G:C6	1:A:89:U:C5	3.00	0.49
1:A:373:A:C2	1:A:374:A:C8	3.00	0.49
1:A:374:A:C5'	1:A:452:A:N1	2.75	0.49
1:A:131:A:C2	1:A:132:C:N3	2.81	0.49
2:B:27:LYS:N	2:B:28:PRO:CD	2.74	0.49
5:E:18:ASN:N	5:E:18:ASN:OD1	2.46	0.49
1:A:1159:U:O4'	1:A:1182:G:N2	2.44	0.49
17:Q:25:GLU:CG	17:Q:40:THR:HG22	2.42	0.49
4:D:28:ASP:O	4:D:29:THR:O	2.29	0.49
1:A:686:U:O2'	1:A:687:A:C8	2.65	0.49
1:A:687:A:N3	1:A:700:G:N2	2.60	0.49
1:A:212:G:O2'	1:A:213:G:O5'	2.30	0.49
1:A:1052:U:O2'	1:A:1055:A:OP2	2.30	0.49
1:A:1365:G:C2	1:A:1366:C:C2	3.01	0.49
1:A:142:G:C6	1:A:143:A:C8	3.00	0.49
1:A:335:C:C2'	1:A:336:A:C8	2.95	0.49
1:A:765:G:O6	1:A:811:C:C4	2.65	0.49
1:A:38:G:C2	1:A:397:A:C2	3.00	0.49
1:A:973:G:O2'	14:N:68:ARG:NH2	2.46	0.49
17:Q:29:LYS:HD2	17:Q:34:GLY:HA2	1.95	0.49
4:D:3:TYR:O	4:D:4:LEU:CB	2.60	0.49
3:C:155:ARG:NE	3:C:159:ALA:O	2.45	0.49
1:A:680:C:C2	1:A:711:G:N2	2.80	0.49
1:A:812:G:O2'	1:A:813:U:C6	2.65	0.49
1:A:382:A:C8	1:A:383:A:C5	3.00	0.49
1:A:754:C:C2'	1:A:754:C:O2	2.61	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:247:G:C6	1:A:278:G:C2	3.01	0.49
1:A:975:A:O2'	1:A:976:G:OP2	2.30	0.49
1:A:982:U:C4'	1:A:983:A:O5'	2.61	0.49
1:A:1117:A:C6	1:A:1184:G:O6	2.65	0.49
2:B:80:LYS:O	2:B:81:ASP:C	2.51	0.49
1:A:1073:U:C4	1:A:1074:G:N7	2.81	0.49
1:A:1239:A:N6	1:A:1299:A:N6	2.60	0.49
1:A:926:G:C6	1:A:1505:G:C5	3.01	0.49
1:A:276:G:O2'	1:A:277:C:C6	2.66	0.49
1:A:1160:G:O6	1:A:1181:G:O6	2.30	0.49
1:A:1449:C:O2'	1:A:1450:U:O4'	2.30	0.49
1:A:94:G:C4'	1:A:95:C:OP1	2.61	0.49
1:A:1417:G:N2	1:A:1484:C:C4	2.81	0.49
1:A:979:C:OP2	1:A:981:U:O4	2.31	0.49
5:E:33:THR:OG1	5:E:49:TYR:CZ	2.66	0.49
5:E:38:VAL:CG1	5:E:39:GLY:N	2.76	0.49
4:D:104:MET:CG	4:D:104:MET:O	2.61	0.49
1:A:248:C:O2'	1:A:249:U:O4'	2.31	0.49
1:A:994:A:N3	1:A:995:C:C6	2.81	0.49
16:P:52:LEU:O	16:P:53:ASP:CB	2.61	0.49
1:A:542:G:N3	1:A:543:U:C6	2.81	0.48
5:E:112:ALA:O	5:E:113:VAL:C	2.52	0.48
1:A:86:G:O2'	1:A:87:C:OP2	2.30	0.48
1:A:223:A:C6	1:A:224:U:C4	3.01	0.48
5:E:148:SER:O	5:E:151:MET:N	2.42	0.48
1:A:935:A:O2'	1:A:936:C:C6	2.66	0.48
17:Q:17:GLU:O	17:Q:18:LYS:HB2	2.13	0.48
1:A:962:C:C4	1:A:974:A:N6	2.82	0.48
1:A:66:A:C6	1:A:67:C:C4	3.01	0.48
3:C:120:THR:CG2	3:C:120:THR:O	2.60	0.48
3:C:124:GLU:N	3:C:124:GLU:CD	2.67	0.48
17:Q:59:GLU:HG3	17:Q:59:GLU:O	2.12	0.48
1:A:1160:G:O2'	1:A:1161:C:C5'	2.62	0.48
1:A:1181:G:C2'	1:A:1182:G:C8	2.95	0.48
1:A:82:G:O2'	1:A:83:C:C4'	2.62	0.48
1:A:486:U:C2'	1:A:486:U:O2	2.62	0.48
10:J:63:ASP:OD2	14:N:84:ARG:NH1	2.45	0.48
1:A:961:U:C4	1:A:983:A:C6	3.02	0.48
1:A:914:A:O2'	1:A:915:A:O5'	2.31	0.48
1:A:1431:A:C6	1:A:1432:G:N1	2.82	0.48
2:B:9:LEU:O	2:B:10:LYS:CB	2.62	0.48
1:A:1033:G:O2'	1:A:1034:G:O5'	2.32	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:22:VAL:HG21	17:Q:58:VAL:HG21	1.96	0.48
1:A:1146:A:O2'	1:A:1147:C:C5'	2.61	0.48
1:A:1296:C:C4	1:A:1297:G:N2	2.82	0.48
1:A:1524:C:OP2	11:K:124:LYS:NZ	2.47	0.48
1:A:1277:C:O2'	1:A:1279:G:C8	2.66	0.48
4:D:187:ARG:C	4:D:189:ASP:N	2.67	0.48
4:D:2:ARG:NH2	4:D:114:ARG:CD	2.77	0.48
1:A:922:G:C2	1:A:923:A:C4	3.02	0.48
12:L:56:LEU:CB	12:L:58:ASN:OD1	2.62	0.48
3:C:172:VAL:O	3:C:174:LEU:N	2.47	0.48
1:A:327:A:N1	1:A:329:A:C2	2.82	0.48
1:A:542:G:C4	1:A:543:U:C5	3.02	0.48
1:A:1265:C:C4	1:A:1266:G:N7	2.82	0.48
1:A:364:A:C2	1:A:365:U:O4	2.67	0.48
1:A:1003:G:N2	1:A:1038:C:C2	2.81	0.48
17:Q:23:ALA:C	17:Q:24:ILE:HD12	2.33	0.48
1:A:148:G:C2	1:A:149:A:C4	3.01	0.48
1:A:274:A:O2'	1:A:275:G:O5'	2.32	0.48
1:A:687:A:C2	1:A:704:A:C5	3.02	0.48
1:A:355:C:C4	1:A:356:A:N7	2.82	0.48
5:E:98:ALA:N	5:E:121:ASN:O	2.46	0.48
12:L:82:ARG:N	12:L:95:HIS:O	2.47	0.48
1:A:62:U:O2'	1:A:379:C:O2	2.31	0.48
1:A:1130:A:N7	1:A:1146:A:C6	2.82	0.48
1:A:320:A:C2	1:A:334:C:C2	3.01	0.48
1:A:223:A:C5	1:A:224:U:C5	3.02	0.48
1:A:1008:U:C4	1:A:1022:A:C2	3.02	0.48
17:Q:4:ILE:HG22	17:Q:5:ARG:N	2.27	0.47
1:A:1449:C:O2'	1:A:1450:U:C5'	2.62	0.47
1:A:962:C:O2'	1:A:963:G:C8	2.67	0.47
1:A:295:C:C6	1:A:296:U:C5	3.02	0.47
2:B:102:ASN:CG	2:B:102:ASN:O	2.52	0.47
7:G:21:LEU:O	7:G:25:PHE:N	2.47	0.47
1:A:969:A:O2'	1:A:970:C:C5'	2.62	0.47
1:A:255:G:O3'	17:Q:18:LYS:HD2	2.14	0.47
1:A:974:A:O2'	1:A:975:A:P	2.72	0.47
1:A:177:G:O2'	1:A:1448:C:C5'	2.62	0.47
1:A:701:U:O2'	1:A:702:A:OP2	2.32	0.47
1:A:815:A:C2	1:A:1529:G:C4	3.03	0.47
17:Q:9:GLY:O	17:Q:57:VAL:HG13	2.14	0.47
1:A:375:U:C4	1:A:376:G:N7	2.83	0.47
7:G:4:ARG:CG	7:G:5:VAL:N	2.77	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1151:A:N6	1:A:1152:A:N6	2.63	0.47
1:A:1525:G:OP1	21:U:37:TYR:CD1	2.67	0.47
4:D:187:ARG:NH1	4:D:196:GLU:OE2	2.47	0.47
1:A:37:U:O2	1:A:548:G:C2	2.67	0.47
1:A:579:A:C2	1:A:763:G:C4	3.03	0.47
1:A:1151:A:C4	1:A:1152:A:N7	2.82	0.47
6:F:81:ASN:O	6:F:82:ASP:C	2.53	0.47
1:A:17:U:C2	1:A:18:C:C5	3.03	0.47
1:A:55:A:OP2	1:A:352:C:N4	2.47	0.47
17:Q:46:HIS:NE2	17:Q:48:GLU:HG2	2.28	0.47
1:A:89:U:O2'	1:A:90:C:O5'	2.32	0.47
1:A:32:A:C2	1:A:33:A:C5	3.03	0.47
1:A:184:G:N2	1:A:185:U:C2	2.83	0.47
1:A:1090:U:C2	1:A:1091:U:C5	3.03	0.47
16:P:69:ASP:O	16:P:70:ARG:C	2.53	0.47
4:D:25:ARG:O	4:D:26:ALA:O	2.33	0.47
1:A:981:U:O4	1:A:1222:G:O6	2.33	0.47
1:A:509:A:N3	1:A:543:U:O2'	2.47	0.47
3:C:84:GLU:C	3:C:86:LEU:N	2.68	0.47
1:A:386:C:C4	1:A:387:U:C5	3.03	0.47
1:A:1480:A:C5	1:A:1481:U:C5	3.03	0.47
1:A:1150:A:N6	1:A:1151:A:N6	2.62	0.47
1:A:575:G:C6	1:A:821:G:C5	3.02	0.47
1:A:1513:A:C6	1:A:1514:G:C6	3.03	0.47
1:A:1303:C:N4	1:A:1304:G:C2	2.83	0.47
1:A:171:A:C6	1:A:172:A:N1	2.83	0.47
9:I:106:ASP:OD1	9:I:106:ASP:N	2.48	0.47
1:A:248:C:O2'	1:A:249:U:O5'	2.32	0.47
1:A:309:A:O2'	1:A:607:A:C2	2.68	0.47
1:A:295:C:C4	1:A:296:U:C5	3.03	0.47
9:I:45:MET:O	9:I:49:GLN:N	2.48	0.47
6:F:67:PRO:O	6:F:68:GLN:C	2.52	0.47
1:A:382:A:N7	1:A:383:A:N6	2.63	0.47
1:A:375:U:C2	1:A:376:G:C8	3.03	0.47
4:D:125:ASN:N	4:D:141:VAL:O	2.48	0.47
1:A:666:G:C5	1:A:741:G:N1	2.83	0.47
1:A:836:G:C6	1:A:851:G:C5	3.03	0.47
1:A:481:G:O2'	1:A:483:C:N4	2.48	0.47
1:A:671:G:N1	1:A:672:U:C2	2.83	0.47
1:A:1146:A:C6	1:A:1147:C:C4	3.03	0.46
3:C:137:VAL:O	3:C:138:GLN:C	2.53	0.46
1:A:974:A:OP1	14:N:68:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:704:A:C2'	1:A:705:G:C8	2.97	0.46
1:A:1215:G:C4	1:A:1216:A:N7	2.83	0.46
18:R:63:TYR:CE2	18:R:69:TYR:OH	2.69	0.46
1:A:1161:C:O2	1:A:1176:A:C2	2.68	0.46
18:R:70:THR:OG1	18:R:71:ASP:N	2.48	0.46
1:A:789:U:N3	1:A:792:A:OP2	2.48	0.46
1:A:701:U:O2'	1:A:702:A:P	2.73	0.46
1:A:1178:G:OP2	9:I:98:ARG:NH2	2.49	0.46
3:C:10:ARG:O	3:C:13:ILE:O	2.32	0.46
1:A:254:G:OP1	17:Q:69:THR:OG1	2.33	0.46
17:Q:68:LYS:HG2	17:Q:69:THR:HG23	1.96	0.46
1:A:511:C:O2'	1:A:512:U:C5'	2.63	0.46
1:A:67:C:O2'	1:A:68:G:OP2	2.33	0.46
1:A:761:G:C2	1:A:762:U:C2	3.04	0.46
1:A:669:G:C2	1:A:670:G:C4	3.03	0.46
1:A:668:G:O2'	15:O:45:HIS:CB	2.64	0.46
1:A:198:G:O2'	1:A:199:A:P	2.74	0.46
1:A:1184:G:C2	1:A:1185:G:C8	3.04	0.46
12:L:22:ALA:O	12:L:58:ASN:ND2	2.48	0.46
1:A:252:U:O4	1:A:253:A:N6	2.49	0.46
1:A:1092:A:C2	1:A:1183:U:N3	2.84	0.46
2:B:92:ASN:OD1	2:B:93:HIS:ND1	2.49	0.46
21:U:35:GLU:OE2	21:U:35:GLU:CA	2.64	0.46
1:A:687:A:C2	1:A:700:G:N2	2.84	0.46
1:A:363:A:OP1	12:L:30:ARG:N	2.49	0.46
1:A:1282:C:O2'	1:A:1283:U:C6	2.69	0.46
7:G:2:ARG:CG	7:G:3:ARG:N	2.77	0.46
4:D:11:SER:O	4:D:12:ARG:C	2.53	0.46
1:A:577:G:O2'	1:A:578:C:C5'	2.64	0.46
1:A:1072:G:C2	1:A:1073:U:C2	3.04	0.46
1:A:666:G:C6	1:A:741:G:C6	3.04	0.46
11:K:104:PHE:N	11:K:104:PHE:CD1	2.84	0.46
1:A:557:G:C6	1:A:558:G:N1	2.84	0.46
1:A:1202:U:O2'	1:A:1203:C:C5'	2.64	0.46
1:A:245:U:C6	1:A:245:U:C5'	2.99	0.46
1:A:560:A:N7	1:A:566:G:C5	2.84	0.46
1:A:505:G:C6	1:A:535:A:C2	3.04	0.46
8:H:30:LYS:O	8:H:33:VAL:N	2.49	0.46
1:A:765:G:C8	1:A:812:G:N3	2.84	0.46
1:A:1064:G:N2	1:A:1190:G:O2'	2.49	0.46
20:T:2:ASN:O	20:T:3:ILE:C	2.54	0.46
1:A:1243:C:C2	1:A:1244:G:N7	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1480:A:C4	1:A:1481:U:C6	3.04	0.46
1:A:655:A:N6	1:A:752:G:N2	2.63	0.46
1:A:1375:A:O2'	7:G:101:ARG:NH2	2.48	0.46
1:A:663:A:O3'	18:R:52:ARG:NH2	2.49	0.46
20:T:23:ARG:CB	20:T:60:GLN:NE2	2.79	0.46
1:A:879:C:C2'	1:A:880:C:O5'	2.64	0.45
1:A:328:C:O2	1:A:328:C:C2'	2.63	0.45
1:A:822:U:C2	1:A:823:C:C5	3.05	0.45
15:O:81:ILE:O	15:O:85:GLY:N	2.49	0.45
1:A:181:A:N6	1:A:195:A:OP2	2.50	0.45
1:A:577:G:C8	1:A:816:A:N1	2.85	0.45
1:A:1067:A:C4'	1:A:1068:G:O5'	2.63	0.45
1:A:604:G:C2	1:A:635:A:C2	3.05	0.45
1:A:1461:G:C6	1:A:1462:C:C4	3.04	0.45
1:A:1004:A:N3	1:A:1026:G:C5	2.84	0.45
1:A:1231:G:C5	1:A:1232:U:C5	3.05	0.45
1:A:198:G:O2'	1:A:199:A:O5'	2.35	0.45
1:A:276:G:OP1	17:Q:13:SER:OG	2.24	0.45
4:D:186:GLU:O	4:D:187:ARG:CB	2.65	0.45
1:A:552:U:C4	1:A:553:A:N7	2.85	0.45
1:A:995:C:O2'	1:A:996:A:O5'	2.33	0.45
18:R:28:LEU:C	18:R:30:ASN:N	2.69	0.45
20:T:42:ASP:O	20:T:43:LYS:C	2.55	0.45
17:Q:30:HIS:CG	17:Q:31:PRO:HD2	2.51	0.45
6:F:86:ARG:NH1	18:R:63:TYR:CB	2.79	0.45
1:A:289:G:C6	1:A:290:C:N4	2.85	0.45
13:M:64:VAL:O	13:M:65:GLU:C	2.55	0.45
1:A:1084:G:C6	1:A:1085:U:O4	2.70	0.45
1:A:321:A:O2'	1:A:1435:G:O2'	2.34	0.45
1:A:994:A:O2'	1:A:995:C:C6	2.70	0.45
1:A:579:A:C6	1:A:763:G:C6	3.04	0.45
19:S:35:ARG:NH2	19:S:51:HIS:CD2	2.84	0.45
11:K:35:ASP:OD2	11:K:39:ASN:N	2.49	0.45
8:H:20:ASN:O	8:H:20:ASN:ND2	2.49	0.45
2:B:115:ASP:O	2:B:119:GLN:CB	2.65	0.45
2:B:71:THR:O	2:B:72:LYS:C	2.55	0.45
1:A:76:G:N2	1:A:95:C:C2	2.85	0.45
1:A:449:G:N1	1:A:450:G:C5	2.85	0.45
1:A:386:C:C5	1:A:387:U:C5	3.05	0.45
17:Q:49:ASN:HB3	17:Q:51:GLU:HG2	1.99	0.45
1:A:1078:U:C5	1:A:1079:G:C5	3.04	0.45
1:A:1261:A:N7	1:A:1274:A:C2	2.85	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:126:PHE:CG	9:I:126:PHE:O	2.69	0.45
1:A:986:U:O2'	1:A:987:G:O5'	2.35	0.45
1:A:693:G:OP1	11:K:126:ARG:NH1	2.50	0.45
8:H:1:SER:O	8:H:3:GLN:N	2.49	0.45
1:A:435:A:C5	1:A:436:C:C5	3.05	0.45
4:D:25:ARG:CG	4:D:25:ARG:NH1	2.79	0.45
1:A:293:G:C2	1:A:305:G:N3	2.85	0.45
1:A:1229:A:O2'	1:A:1230:C:O4'	2.35	0.45
1:A:1346:A:N1	7:G:9:ARG:NH2	2.65	0.45
1:A:1133:G:C6	1:A:1134:G:N7	2.85	0.45
1:A:1292:G:C6	1:A:1293:C:C4	3.05	0.45
12:L:97:VAL:O	12:L:97:VAL:CG2	2.64	0.45
7:G:61:PHE:O	7:G:63:VAL:N	2.48	0.45
1:A:960:U:O2'	1:A:1223:C:C5'	2.65	0.45
1:A:71:A:C2	1:A:72:A:C5	3.05	0.45
4:D:29:THR:C	4:D:31:CYS:N	2.71	0.45
1:A:919:A:C2	1:A:920:U:C5	3.05	0.45
17:Q:47:ASP:HB3	17:Q:74:LEU:HB3	1.99	0.45
17:Q:47:ASP:OD1	17:Q:74:LEU:HD23	2.17	0.45
1:A:1215:G:N3	1:A:1216:A:C8	2.85	0.45
1:A:980:C:O3'	14:N:12:ARG:NH2	2.50	0.45
1:A:1080:A:OP1	5:E:51:LYS:NZ	2.50	0.45
1:A:1071:C:C5'	5:E:53:ARG:NH1	2.80	0.45
2:B:17:HIS:CG	2:B:18:GLN:N	2.84	0.45
1:A:166:U:OP2	1:A:166:U:C6	2.70	0.45
1:A:781:A:O2'	1:A:1522:U:O2	2.35	0.44
15:O:44:GLU:O	15:O:45:HIS:C	2.55	0.44
12:L:97:VAL:O	12:L:98:ARG:C	2.56	0.44
15:O:22:GLY:O	15:O:23:SER:C	2.56	0.44
1:A:1106:G:O2'	3:C:168:ARG:NH1	2.50	0.44
1:A:131:A:C6	1:A:232:G:C6	3.06	0.44
1:A:624:C:O2'	16:P:10:GLY:CA	2.64	0.44
1:A:1119:C:OP1	9:I:10:ARG:NH2	2.51	0.44
1:A:665:A:C2'	1:A:725:G:N2	2.80	0.44
1:A:461:A:O5'	1:A:462:G:OP2	2.36	0.44
2:B:83:ALA:O	2:B:85:SER:N	2.51	0.44
1:A:39:G:C4	1:A:404:G:N2	2.86	0.44
1:A:976:G:O5'	1:A:1358:U:O2'	2.34	0.44
1:A:1153:G:C6	1:A:1154:G:N7	2.85	0.44
8:H:11:THR:CG2	8:H:14:ARG:NH1	2.80	0.44
18:R:19:GLU:CG	18:R:20:ILE:N	2.80	0.44
1:A:765:G:C5	1:A:812:G:C5	3.06	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:25:ALA:O	21:U:26:GLY:C	2.55	0.44
1:A:1160:G:O6	1:A:1181:G:C6	2.70	0.44
1:A:889:A:O2'	1:A:890:G:O5'	2.35	0.44
1:A:86:G:O2'	1:A:87:C:P	2.76	0.44
11:K:103:GLY:O	11:K:104:PHE:C	2.56	0.44
1:A:1507:A:C6	1:A:1530:G:C5	3.05	0.44
1:A:71:A:N3	1:A:72:A:C8	2.86	0.44
1:A:922:G:O2'	1:A:1398:A:C2	2.71	0.44
1:A:652:U:O2'	1:A:653:U:P	2.76	0.44
10:J:49:PHE:O	10:J:65:TYR:N	2.50	0.44
2:B:148:GLY:O	2:B:150:ILE:N	2.50	0.44
1:A:484:G:C4'	1:A:485:U:O5'	2.66	0.44
1:A:1054:C:O2'	1:A:1055:A:C5'	2.66	0.44
1:A:327:A:C2	1:A:329:A:C4	3.06	0.44
6:F:11:HIS:CD2	6:F:54:LEU:CD2	3.01	0.44
1:A:1130:A:C6	1:A:1131:G:N7	2.86	0.44
11:K:92:ARG:NH2	11:K:111:ASP:OD1	2.51	0.44
1:A:1346:A:C8	1:A:1348:U:C2	3.06	0.44
1:A:481:G:C4'	1:A:482:A:OP1	2.65	0.44
4:D:11:SER:O	4:D:14:GLU:N	2.51	0.44
9:I:75:ALA:O	9:I:79:ARG:N	2.51	0.44
1:A:728:A:C8	15:O:53:ARG:NH2	2.86	0.44
1:A:279:A:OP1	1:A:280:C:O2'	2.35	0.44
1:A:1098:C:C4	1:A:1099:G:N7	2.86	0.44
15:O:7:THR:O	15:O:11:VAL:N	2.51	0.44
1:A:867:G:C4	1:A:868:C:C5	3.06	0.44
1:A:768:A:C4	1:A:769:G:C8	3.06	0.44
1:A:363:A:N6	1:A:364:A:C6	2.86	0.43
1:A:1310:G:C6	1:A:1311:A:C6	3.06	0.43
1:A:401:C:O2'	1:A:621:A:O2'	2.36	0.43
1:A:881:G:C6	1:A:882:C:C4	3.06	0.43
1:A:1051:C:O2'	1:A:1052:U:O4'	2.36	0.43
1:A:1381:U:N3	7:G:77:ARG:CZ	2.81	0.43
1:A:375:U:N3	1:A:376:G:N7	2.66	0.43
1:A:760:G:C6	1:A:761:G:C4	3.06	0.43
1:A:768:A:C5	1:A:769:G:N7	2.86	0.43
4:D:123:MET:CE	4:D:126:GLY:O	2.67	0.43
1:A:465:A:C8	1:A:467:U:OP1	2.71	0.43
1:A:614:C:C4	1:A:615:G:N7	2.87	0.43
21:U:14:ALA:O	21:U:15:LEU:C	2.57	0.43
6:F:98:GLU:O	6:F:99:ALA:CB	2.66	0.43
3:C:18:ASN:ND2	3:C:53:ARG:NH1	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:32:THR:O	15:O:33:ALA:C	2.57	0.43
1:A:559:A:C4'	1:A:560:A:O5'	2.66	0.43
1:A:65:A:C4	1:A:200:G:O2'	2.72	0.43
1:A:1145:A:O2'	1:A:1146:A:C5'	2.66	0.43
1:A:373:A:C5'	1:A:373:A:C8	3.01	0.43
11:K:123:PRO:O	21:U:34:ARG:N	2.51	0.43
1:A:155:A:C6	1:A:156:C:C4	3.06	0.43
2:B:187:ASP:O	2:B:189:ASN:N	2.51	0.43
9:I:51:LEU:C	9:I:53:LEU:N	2.71	0.43
1:A:499:A:O2'	1:A:500:G:C8	2.71	0.43
1:A:1319:A:C6	1:A:1323:G:C4	3.06	0.43
1:A:182:A:C4	1:A:184:G:N7	2.87	0.43
1:A:780:A:C2	1:A:803:G:C6	3.07	0.43
1:A:1012:A:C5	1:A:1013:G:N7	2.86	0.43
1:A:982:U:C1'	1:A:983:A:N7	2.82	0.43
1:A:276:G:O2'	1:A:277:C:C5'	2.67	0.43
1:A:78:A:C6	1:A:79:G:C6	3.07	0.43
1:A:953:G:C6	1:A:954:G:C6	3.06	0.43
5:E:33:THR:OG1	5:E:49:TYR:OH	2.36	0.43
9:I:90:ASP:OD1	9:I:92:SER:N	2.52	0.43
1:A:661:G:C2	1:A:662:U:C6	3.07	0.43
1:A:1408:A:N1	1:A:1494:G:C5	2.87	0.43
1:A:1217:C:O2'	1:A:1218:C:C5'	2.67	0.43
1:A:861:G:C6	1:A:862:C:C4	3.06	0.43
1:A:1008:U:C4	1:A:1009:U:C4	3.07	0.43
1:A:652:U:O2'	1:A:653:U:O5'	2.37	0.43
1:A:168:G:C6	1:A:169:C:C5	3.07	0.43
1:A:257:G:C2	1:A:270:A:N1	2.87	0.43
1:A:247:G:C6	1:A:278:G:C6	3.06	0.43
1:A:1494:G:C6	1:A:1495:U:C4	3.07	0.43
1:A:1130:A:N7	1:A:1146:A:N6	2.67	0.43
1:A:1366:C:O2'	1:A:1367:C:C5'	2.67	0.43
1:A:71:A:C2	1:A:72:A:N7	2.87	0.43
1:A:64:G:N7	1:A:99:C:C4	2.86	0.43
1:A:604:G:C5	1:A:605:U:C4	3.07	0.43
1:A:1138:G:C2'	1:A:1139:G:OP1	2.66	0.43
9:I:87:MET:N	9:I:87:MET:SD	2.91	0.43
1:A:505:G:OP2	1:A:534:U:O2'	2.36	0.43
1:A:386:C:C4	1:A:387:U:C4	3.07	0.43
1:A:1333:A:N6	1:A:1334:G:C2	2.87	0.43
2:B:99:MET:O	2:B:103:TRP:CB	2.67	0.43
1:A:399:G:C6	1:A:400:C:C4	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1494:G:N1	1:A:1495:U:C4	2.87	0.43
1:A:71:A:C6	1:A:100:G:C5	3.06	0.43
1:A:666:G:C2	1:A:667:G:C8	3.07	0.43
4:D:141:VAL:CG1	4:D:142:VAL:N	2.82	0.43
4:D:58:GLN:OE1	4:D:58:GLN:CA	2.67	0.43
1:A:515:G:N2	1:A:537:G:C4	2.87	0.42
1:A:1157:A:C6	1:A:1180:A:C6	3.07	0.42
1:A:1159:U:C5	1:A:1182:G:O2'	2.72	0.42
1:A:1278:G:C4'	1:A:1279:G:O5'	2.67	0.42
5:E:88:HIS:ND1	5:E:134:ASN:OD1	2.51	0.42
9:I:71:ILE:O	9:I:75:ALA:N	2.52	0.42
1:A:444:G:C2	1:A:445:G:C8	3.07	0.42
17:Q:46:HIS:CE1	17:Q:48:GLU:HG2	2.54	0.42
1:A:516:U:O2'	1:A:519:C:N3	2.52	0.42
1:A:77:A:C2	1:A:93:U:C2	3.07	0.42
1:A:1523:G:P	11:K:124:LYS:NZ	2.92	0.42
1:A:664:G:N2	1:A:666:G:C8	2.87	0.42
4:D:29:THR:O	4:D:31:CYS:N	2.52	0.42
1:A:575:G:C6	1:A:821:G:N7	2.87	0.42
1:A:1091:U:O2	1:A:1093:A:C8	2.72	0.42
17:Q:47:ASP:HB3	17:Q:74:LEU:HB2	2.01	0.42
1:A:683:G:C2	1:A:684:U:C2	3.08	0.42
6:F:46:GLN:OE1	6:F:55:HIS:O	2.37	0.42
1:A:490:C:OP1	4:D:145:ARG:NH2	2.52	0.42
13:M:53:ASP:N	13:M:53:ASP:OD2	2.53	0.42
20:T:61:ALA:O	20:T:67:HIS:CG	2.72	0.42
5:E:155:LYS:HB3	8:H:70:VAL:CG2	2.48	0.42
4:D:60:VAL:CG2	4:D:194:ILE:CG2	2.97	0.42
1:A:276:G:O2'	1:A:277:C:O5'	2.37	0.42
1:A:1157:A:C5	1:A:1180:A:C6	3.07	0.42
1:A:1157:A:C6	1:A:1180:A:C5	3.07	0.42
1:A:652:U:O4	1:A:752:G:C2'	2.67	0.42
1:A:525:C:N4	1:A:526:C:N4	2.68	0.42
1:A:1162:C:C2	1:A:1175:G:N2	2.88	0.42
1:A:853:C:C4	1:A:854:U:C5	3.08	0.42
1:A:495:A:C2	1:A:496:A:N6	2.88	0.42
1:A:519:C:O2'	1:A:520:A:O4'	2.37	0.42
1:A:1182:G:C4'	1:A:1183:U:C5'	2.97	0.42
1:A:666:G:C5	1:A:741:G:C6	3.07	0.42
4:D:20:LEU:O	4:D:21:LYS:C	2.56	0.42
19:S:40:PHE:CB	19:S:41:PRO:CD	2.96	0.42
3:C:166:TRP:O	3:C:167:TYR:CB	2.66	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:17:ASP:OD1	4:D:19:PHE:N	2.52	0.42
1:A:411:A:O2'	1:A:412:A:O4'	2.36	0.42
2:B:93:HIS:CG	2:B:145:ASN:O	2.72	0.42
1:A:721:G:C4'	1:A:722:G:O5'	2.67	0.42
1:A:120:A:O5'	1:A:120:A:C8	2.72	0.42
1:A:579:A:N1	1:A:763:G:C5	2.87	0.42
1:A:386:C:N4	1:A:387:U:O4	2.52	0.42
1:A:1231:G:C4	1:A:1232:U:C6	3.07	0.42
9:I:70:GLY:O	9:I:73:GLY:N	2.52	0.42
1:A:209:U:C5'	1:A:210:C:OP2	2.68	0.42
1:A:254:G:O2'	17:Q:17:GLU:O	2.36	0.42
1:A:858:G:N7	1:A:869:G:C5	2.88	0.42
1:A:512:U:O2'	1:A:513:C:C5'	2.68	0.42
1:A:765:G:O6	1:A:811:C:N4	2.52	0.42
1:A:1296:C:C5	1:A:1297:G:N2	2.87	0.42
1:A:878:A:C5	1:A:879:C:C5	3.08	0.42
1:A:1316:G:N1	1:A:1319:A:OP2	2.53	0.42
1:A:87:C:O2'	1:A:88:U:C4'	2.67	0.42
9:I:51:LEU:O	9:I:53:LEU:N	2.52	0.42
4:D:100:VAL:O	4:D:101:VAL:C	2.57	0.42
1:A:544:G:C5	1:A:545:C:C5	3.08	0.42
1:A:951:G:OP2	13:M:100:ARG:NH2	2.52	0.42
1:A:962:C:O2'	1:A:963:G:O4'	2.37	0.42
1:A:277:C:OP1	17:Q:44:HIS:CE1	2.66	0.42
1:A:1011:C:N3	1:A:1019:A:C2	2.88	0.42
1:A:1148:U:O2'	1:A:1149:C:C5'	2.68	0.42
1:A:1177:G:N7	1:A:1178:G:C5	2.88	0.42
16:P:38:PHE:CE2	16:P:51:ARG:CB	3.03	0.42
1:A:1518:A:C2	1:A:1519:A:C2	3.07	0.42
1:A:1454:G:O2'	1:A:1455:G:C5'	2.68	0.42
3:C:38:VAL:O	3:C:42:LEU:N	2.53	0.42
1:A:1143:G:C2'	1:A:1144:G:C8	3.03	0.42
17:Q:68:LYS:O	17:Q:69:THR:OG1	2.37	0.42
1:A:566:G:C4'	1:A:567:G:OP1	2.67	0.42
1:A:764:C:C4	1:A:812:G:O6	2.73	0.42
1:A:206:C:O5'	1:A:207:C:OP2	2.38	0.42
21:U:37:TYR:O	21:U:38:GLU:CG	2.68	0.42
1:A:844:G:N3	1:A:846:G:O2'	2.53	0.42
1:A:685:G:N2	1:A:704:A:OP2	2.53	0.42
1:A:979:C:C5	1:A:1318:A:N1	2.88	0.42
6:F:99:ALA:O	6:F:100:SER:CB	2.68	0.42
1:A:539:A:N6	1:A:540:G:O6	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:137:SER:O	4:D:181:PHE:CD2	2.72	0.42
1:A:1146:A:C2	1:A:1147:C:C2	3.08	0.42
1:A:1200:C:O2'	1:A:1201:A:P	2.78	0.42
1:A:1242:G:N2	1:A:1302:C:O2	2.53	0.42
1:A:1157:A:C4'	1:A:1158:C:O5'	2.67	0.42
2:B:81:ASP:CG	2:B:82:ALA:N	2.73	0.42
21:U:31:VAL:O	21:U:32:ARG:C	2.58	0.42
1:A:1072:G:C5	1:A:1073:U:C5	3.08	0.42
17:Q:45:VAL:HG21	17:Q:60:ILE:HG21	2.02	0.42
2:B:72:LYS:O	2:B:74:ALA:N	2.53	0.42
1:A:960:U:O2'	1:A:1223:C:C4'	2.68	0.42
16:P:74:LEU:O	16:P:78:VAL:CG2	2.68	0.42
20:T:11:ILE:C	20:T:13:SER:N	2.74	0.42
1:A:563:A:N3	1:A:563:A:C2'	2.82	0.42
1:A:428:G:C2	1:A:430:A:N6	2.88	0.41
8:H:7:ALA:O	8:H:11:THR:OG1	2.38	0.41
16:P:21:VAL:O	16:P:33:ILE:N	2.52	0.41
1:A:126:G:OP1	1:A:633:G:N2	2.53	0.41
4:D:32:LYS:CB	4:D:35:GLN:OE1	2.68	0.41
6:F:80:PHE:CD1	6:F:80:PHE:N	2.88	0.41
1:A:427:U:C4	1:A:428:G:C6	3.08	0.41
8:H:85:TYR:CE1	17:Q:36:PHE:HE2	2.38	0.41
1:A:79:G:N2	1:A:91:U:C2	2.88	0.41
1:A:83:C:C4	1:A:85:U:N3	2.88	0.41
11:K:124:LYS:O	21:U:33:ARG:CZ	2.69	0.41
1:A:1386:G:N2	1:A:1387:G:C4	2.89	0.41
1:A:1002:G:C6	1:A:1003:G:C6	3.08	0.41
1:A:836:G:C5	1:A:851:G:C6	3.08	0.41
1:A:749:A:C2	1:A:750:C:C2	3.08	0.41
1:A:1440:U:OP2	1:A:1440:U:C6	2.73	0.41
1:A:1294:G:C8	1:A:1294:G:OP2	2.74	0.41
1:A:855:U:C5	1:A:871:U:O4	2.73	0.41
1:A:66:A:C6	1:A:67:C:N4	2.88	0.41
1:A:1250:A:C2	1:A:1287:A:C6	3.08	0.41
1:A:408:A:C2	1:A:435:A:C2	3.08	0.41
1:A:1479:C:C2	1:A:1480:A:C8	3.09	0.41
4:D:21:LYS:CG	4:D:21:LYS:O	2.68	0.41
4:D:107:GLY:N	4:D:157:ALA:CB	2.83	0.41
2:B:90:PHE:N	2:B:149:GLY:O	2.54	0.41
12:L:50:LYS:N	12:L:50:LYS:CD	2.84	0.41
2:B:209:VAL:CG2	2:B:210:THR:N	2.83	0.41
5:E:157:GLY:CA	8:H:63:LYS:NZ	2.81	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:821:G:O2'	1:A:822:U:C5'	2.68	0.41
1:A:977:A:O2'	1:A:978:A:C5'	2.68	0.41
1:A:1453:G:C2'	1:A:1453:G:N3	2.82	0.41
1:A:16:A:O2'	1:A:17:U:C5'	2.69	0.41
1:A:1026:G:N1	1:A:1036:A:N6	2.69	0.41
1:A:171:A:C6	1:A:172:A:C6	3.09	0.41
1:A:776:G:N1	1:A:802:A:OP1	2.53	0.41
1:A:934:C:N3	1:A:1345:U:C5	2.88	0.41
1:A:577:G:C8	1:A:816:A:C2	3.08	0.41
18:R:62:ARG:CB	18:R:69:TYR:CE1	3.04	0.41
1:A:83:C:N4	1:A:85:U:C4	2.88	0.41
1:A:1124:G:O2'	1:A:1127:G:O6	2.39	0.41
4:D:187:ARG:O	4:D:189:ASP:N	2.54	0.41
1:A:978:A:C8	1:A:1319:A:C2	3.08	0.41
1:A:552:U:N3	1:A:553:A:N7	2.69	0.41
1:A:568:G:O2'	1:A:574:A:N1	2.54	0.41
1:A:1386:G:N3	1:A:1387:G:C8	2.88	0.41
1:A:923:A:C6	1:A:924:C:C4	3.09	0.41
1:A:195:A:C5	1:A:196:A:C6	3.08	0.41
15:O:11:VAL:O	15:O:15:GLY:CA	2.69	0.41
16:P:50:THR:O	16:P:51:ARG:CZ	2.69	0.41
9:I:74:GLN:O	9:I:78:ILE:N	2.53	0.41
17:Q:68:LYS:O	17:Q:69:THR:HG23	2.20	0.41
1:A:200:G:N1	1:A:201:G:C5	2.88	0.41
1:A:1151:A:C2'	1:A:1152:A:O5'	2.69	0.41
1:A:79:G:N1	1:A:80:A:N6	2.68	0.41
1:A:374:A:OP1	1:A:452:A:N1	2.53	0.41
1:A:642:A:O2'	1:A:643:C:C5'	2.68	0.41
1:A:704:A:O2'	1:A:705:G:C5'	2.68	0.41
15:O:23:SER:O	15:O:26:VAL:CB	2.69	0.41
4:D:84:ASN:C	4:D:84:ASN:ND2	2.74	0.41
1:A:1211:U:O2'	1:A:1213:A:C2	2.74	0.41
1:A:976:G:C2	1:A:1363:A:C2	3.08	0.41
1:A:415:A:N1	1:A:428:G:O6	2.54	0.41
1:A:890:G:O2'	1:A:906:A:N6	2.54	0.41
1:A:1348:U:O2'	1:A:1349:A:C8	2.73	0.41
1:A:204:G:C6	1:A:465:A:C2	3.08	0.41
17:Q:77:VAL:HG12	17:Q:78:VAL:N	2.35	0.41
1:A:1218:C:C2'	1:A:1219:A:C8	3.04	0.41
1:A:1184:G:N3	1:A:1185:G:C8	2.89	0.41
1:A:1279:G:OP2	1:A:1279:G:N2	2.54	0.41
4:D:187:ARG:CZ	4:D:191:SER:OG	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:978:A:C6	1:A:1319:A:C5	3.08	0.41
2:B:49:PHE:CG	2:B:212:TYR:OH	2.74	0.41
1:A:115:G:C2	1:A:289:G:C5	3.09	0.41
1:A:386:C:N4	1:A:387:U:C4	2.89	0.41
1:A:195:A:C6	1:A:196:A:N1	2.89	0.41
1:A:168:G:C6	1:A:169:C:C4	3.09	0.41
2:B:57:ASN:OD1	2:B:219:THR:O	2.39	0.41
1:A:73:C:O2'	1:A:74:A:C8	2.73	0.41
12:L:35:ARG:O	12:L:53:ARG:N	2.54	0.41
7:G:29:LEU:O	7:G:30:MET:O	2.39	0.41
1:A:938:A:O2'	1:A:1376:U:O2'	2.39	0.41
16:P:25:ARG:O	16:P:26:ASN:ND2	2.54	0.41
1:A:872:A:C4	1:A:874:G:N7	2.89	0.41
1:A:1238:A:N6	1:A:1302:C:N4	2.69	0.41
17:Q:37:ILE:HD11	17:Q:39:ARG:CZ	2.51	0.41
1:A:163:C:C2'	1:A:164:G:O5'	2.69	0.41
1:A:66:A:N3	1:A:66:A:C2'	2.83	0.41
1:A:66:A:C6	1:A:67:C:C5	3.09	0.41
1:A:669:G:N1	1:A:670:G:C5	2.89	0.41
10:J:92:LEU:O	10:J:94:ALA:N	2.54	0.41
1:A:113:G:N2	1:A:353:A:C8	2.89	0.41
4:D:56:GLU:OE1	4:D:56:GLU:CA	2.68	0.41
1:A:65:A:N1	1:A:381:C:C5	2.90	0.40
1:A:331:G:O2'	1:A:332:G:P	2.79	0.40
1:A:1357:A:C5	1:A:1358:U:C4	3.09	0.40
1:A:1363:A:C6	1:A:1365:G:O6	2.73	0.40
1:A:71:A:C2'	1:A:72:A:O5'	2.69	0.40
4:D:187:ARG:O	4:D:191:SER:OG	2.39	0.40
1:A:818:G:O2'	1:A:820:U:C5	2.73	0.40
1:A:821:G:C4	1:A:822:U:C5	3.09	0.40
1:A:1348:U:O2'	1:A:1349:A:C5'	2.70	0.40
1:A:1189:U:O2'	3:C:175:HIS:CD2	2.74	0.40
1:A:922:G:C6	1:A:923:A:C6	3.09	0.40
1:A:687:A:C2	1:A:704:A:C6	3.09	0.40
1:A:1215:G:C2	1:A:1216:A:C5	3.08	0.40
1:A:684:U:O2'	11:K:39:ASN:OD1	2.39	0.40
7:G:30:MET:O	7:G:31:VAL:CB	2.68	0.40
1:A:571:U:C5'	1:A:572:A:OP2	2.69	0.40
2:B:21:TYR:CD1	2:B:21:TYR:N	2.89	0.40
1:A:253:A:O2'	1:A:254:G:O5'	2.38	0.40
2:B:141:GLU:O	2:B:145:ASN:N	2.53	0.40
1:A:259:G:C4	1:A:260:G:C8	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:100:LEU:O	2:B:102:ASN:N	2.54	0.40
2:B:162:VAL:CG2	2:B:163:ILE:N	2.85	0.40
12:L:3:VAL:CG2	12:L:4:ASN:N	2.84	0.40
13:M:8:ILE:N	13:M:9:PRO:CD	2.84	0.40
1:A:1029:U:O2'	1:A:1032:G:N2	2.54	0.40
1:A:346:G:C2'	1:A:346:G:N3	2.85	0.40
13:M:86:ARG:NH1	13:M:90:HIS:CD2	2.89	0.40
15:O:66:LEU:O	15:O:67:ASP:C	2.59	0.40
4:D:195:ASN:O	4:D:197:HIS:N	2.55	0.40
6:F:92:THR:O	6:F:93:LYS:CG	2.70	0.40
1:A:1297:G:O2'	1:A:1298:U:OP2	2.39	0.40
1:A:158:G:N2	1:A:162:A:N6	2.69	0.40
1:A:76:G:N2	1:A:95:C:N3	2.69	0.40
1:A:1125:U:C2	1:A:1127:G:N7	2.89	0.40
5:E:132:PRO:C	5:E:134:ASN:N	2.74	0.40
1:A:1004:A:C8	1:A:1025:U:O2'	2.75	0.40
1:A:1215:G:O2'	1:A:1216:A:C5'	2.69	0.40
1:A:807:A:C5	1:A:808:C:C4	3.09	0.40
1:A:49:U:O4	1:A:362:G:N2	2.54	0.40
5:E:43:GLY:O	5:E:73:VAL:N	2.55	0.40
1:A:676:A:C4	1:A:677:U:C5	3.09	0.40
1:A:91:U:O2'	1:A:92:U:C5'	2.69	0.40
1:A:1243:C:N4	1:A:1244:G:O6	2.54	0.40
1:A:408:A:C5	1:A:409:U:C5	3.09	0.40
1:A:527:G:C2	1:A:528:C:C6	3.09	0.40
1:A:347:G:O2'	1:A:348:G:O5'	2.39	0.40
1:A:1087:G:C2	1:A:1088:G:C5	3.10	0.40
1:A:1408:A:C2	1:A:1494:G:C4	3.09	0.40
1:A:198:G:C4	1:A:199:A:N7	2.89	0.40
17:Q:13:SER:CB	17:Q:21:VAL:HB	2.50	0.40
1:A:704:A:O2'	1:A:705:G:O5'	2.39	0.40
1:A:833:G:C5	1:A:834:U:C5	3.10	0.40
16:P:16:PHE:CZ	16:P:38:PHE:CD1	3.10	0.40
1:A:1076:U:N3	1:A:1082:A:C2	2.89	0.40
8:H:68:LYS:CD	8:H:69:ALA:N	2.84	0.40
14:N:72:PHE:CD1	14:N:72:PHE:C	2.94	0.40
14:N:83:VAL:O	14:N:87:ALA:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	216/218 (99%)	149 (69%)	49 (23%)	18 (8%)	1	9
3	C	204/206 (99%)	145 (71%)	39 (19%)	20 (10%)	1	7
4	D	203/205 (99%)	138 (68%)	42 (21%)	23 (11%)	1	4
5	E	148/150 (99%)	106 (72%)	24 (16%)	18 (12%)	1	3
6	F	98/100 (98%)	68 (69%)	19 (19%)	11 (11%)	1	4
7	G	148/150 (99%)	98 (66%)	42 (28%)	8 (5%)	3	24
8	H	127/129 (98%)	89 (70%)	29 (23%)	9 (7%)	2	13
9	I	125/127 (98%)	90 (72%)	23 (18%)	12 (10%)	1	7
10	J	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	1
11	K	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
12	L	121/123 (98%)	83 (69%)	30 (25%)	8 (7%)	2	16
13	M	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	1	5
14	N	91/100 (91%)	60 (66%)	26 (29%)	5 (6%)	3	23
15	O	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	6	37
16	P	78/80 (98%)	49 (63%)	19 (24%)	10 (13%)	0	3
17	Q	78/80 (98%)	61 (78%)	8 (10%)	9 (12%)	1	4
18	R	53/55 (96%)	42 (79%)	10 (19%)	1 (2%)	12	59
19	S	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	8
20	T	83/85 (98%)	61 (74%)	13 (16%)	9 (11%)	1	5
21	U	49/51 (96%)	21 (43%)	12 (24%)	16 (33%)	0	0
All	All	2307/2354 (98%)	1575 (68%)	509 (22%)	223 (10%)	1	7

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	81	ASP
2	B	84	LEU

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Mol	Chain	Res	Type
2	B	102	ASN
2	B	129	THR
2	B	150	ILE
3	C	59	PRO
3	C	63	ILE
4	D	24	VAL
4	D	25	ARG
4	D	26	ALA
4	D	35	GLN
4	D	80	ARG
4	D	82	LYS
4	D	191	SER
4	D	192	ALA
5	E	31	SER
5	E	100	GLU
5	E	144	GLU
6	F	44	ARG
6	F	68	GLN
6	F	82	ASP
6	F	99	ALA
7	G	29	LEU
7	G	30	MET
7	G	31	VAL
7	G	52	ARG
9	I	71	ILE
11	K	70	ALA
11	K	118	ASN
11	K	126	ARG
11	K	127	ARG
13	M	4	ALA
13	M	65	GLU
14	N	95	LEU
16	P	63	GLN
17	Q	52	CYS
19	S	46	LEU
20	T	3	ILE
20	T	43	LYS
20	T	65	LEU
21	U	4	LYS
21	U	8	ASN
21	U	9	GLU
21	U	15	LEU

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Mol	Chain	Res	Type
21	U	23	GLU
21	U	32	ARG
21	U	35	GLU
21	U	36	PHE
21	U	38	GLU
2	B	26	MET
2	B	85	SER
2	B	128	LEU
2	B	148	GLY
2	B	149	GLY
2	B	205	ALA
3	C	60	ALA
3	C	77	GLY
3	C	87	ARG
3	C	100	ILE
3	C	140	ALA
3	C	178	ARG
3	C	205	GLU
4	D	12	ARG
4	D	27	ILE
4	D	29	THR
4	D	39	GLN
4	D	47	LEU
4	D	187	ARG
4	D	188	SER
5	E	29	ILE
5	E	68	ARG
5	E	69	ASN
5	E	81	GLN
5	E	104	ILE
5	E	111	ARG
5	E	143	LEU
6	F	85	ILE
6	F	94	HIS
6	F	98	GLU
7	G	36	SER
7	G	62	GLU
7	G	113	LYS
7	G	133	ALA
8	H	2	MET
8	H	30	LYS
8	H	43	GLY

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Mol	Chain	Res	Type
8	H	117	GLN
9	I	44	ARG
9	I	54	VAL
9	I	58	GLU
10	J	34	ALA
10	J	44	THR
10	J	46	LYS
10	J	57	VAL
10	J	74	VAL
10	J	83	THR
10	J	93	ALA
11	K	14	GLN
11	K	90	PRO
11	K	91	GLY
11	K	104	PHE
12	L	8	ARG
12	L	16	ALA
12	L	34	THR
12	L	43	LYS
12	L	117	GLY
13	M	11	HIS
13	M	14	ALA
13	M	49	GLU
13	M	76	ILE
14	N	21	ALA
14	N	53	ASP
15	O	13	GLU
16	P	31	ARG
16	P	78	VAL
17	Q	69	THR
17	Q	76	ARG
18	R	70	THR
19	S	4	LEU
19	S	7	GLY
20	T	82	ILE
21	U	30	GLU
21	U	31	VAL
21	U	34	ARG
2	B	73	ARG
3	C	130	ARG
3	C	145	ALA
3	C	164	THR

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Mol	Chain	Res	Type
3	C	173	PRO
3	C	186	SER
3	C	188	ALA
4	D	3	TYR
4	D	33	ILE
4	D	40	HIS
5	E	38	VAL
5	E	43	GLY
5	E	75	LEU
5	E	112	ALA
6	F	92	THR
8	H	29	SER
8	H	41	GLU
9	I	11	ARG
9	I	52	GLU
9	I	55	ASP
10	J	87	LEU
11	K	88	PRO
12	L	42	LYS
12	L	47	ALA
13	M	45	SER
13	M	46	GLU
13	M	77	LYS
16	P	47	GLU
16	P	53	ASP
17	Q	12	VAL
17	Q	31	PRO
17	Q	79	GLU
20	T	72	ALA
20	T	77	ASN
21	U	7	GLU
21	U	11	PHE
2	B	18	GLN
2	B	22	TRP
3	C	180	ASP
4	D	11	SER
5	E	56	PRO
8	H	98	LEU
10	J	61	ALA
10	J	82	LYS
13	M	42	VAL
13	M	93	GLY

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Mol	Chain	Res	Type
15	O	19	ASN
16	P	54	LEU
16	P	69	ASP
17	Q	78	VAL
19	S	3	SER
20	T	67	HIS
20	T	76	ALA
21	U	10	PRO
21	U	26	GLY
2	B	177	ASN
2	B	179	GLY
2	B	188	THR
2	B	200	PRO
3	C	24	ASN
3	C	65	VAL
3	C	128	MET
4	D	68	GLU
4	D	196	GLU
5	E	113	VAL
8	H	74	ILE
9	I	103	VAL
9	I	119	LYS
10	J	36	VAL
10	J	75	ASP
15	O	87	ARG
16	P	43	ALA
16	P	46	LYS
17	Q	81	ALA
19	S	54	ARG
19	S	79	TYR
20	T	73	ARG
4	D	166	LYS
5	E	89	THR
6	F	63	ASN
6	F	69	GLU
8	H	58	LEU
9	I	31	GLN
9	I	127	SER
10	J	41	PRO
17	Q	4	ILE
13	M	50	GLY
4	D	37	PRO

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Mol	Chain	Res	Type
5	E	17	VAL
10	J	33	GLY
14	N	56	PRO
16	P	49	GLY
6	F	64	VAL
12	L	7	VAL
19	S	29	PRO
3	C	54	ILE
14	N	51	PRO
9	I	50	PRO
10	J	25	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	
2	B	180/180 (100%)	156 (87%)	24 (13%)	6	27
3	C	170/170 (100%)	152 (89%)	18 (11%)	10	38
4	D	172/172 (100%)	140 (81%)	32 (19%)	2	11
5	E	113/113 (100%)	94 (83%)	19 (17%)	3	14
6	F	87/87 (100%)	75 (86%)	12 (14%)	5	24
7	G	123/123 (100%)	101 (82%)	22 (18%)	2	12
8	H	104/104 (100%)	87 (84%)	17 (16%)	3	15
9	I	105/105 (100%)	89 (85%)	16 (15%)	4	19
10	J	86/86 (100%)	77 (90%)	9 (10%)	10	39
11	K	90/90 (100%)	77 (86%)	13 (14%)	5	22
12	L	103/103 (100%)	86 (84%)	17 (16%)	3	14
13	M	91/91 (100%)	80 (88%)	11 (12%)	7	32
14	N	79/83 (95%)	67 (85%)	12 (15%)	4	19
15	O	76/76 (100%)	69 (91%)	7 (9%)	13	47
16	P	65/65 (100%)	52 (80%)	13 (20%)	2	9
17	Q	74/74 (100%)	61 (82%)	13 (18%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	R	48/48 (100%)	44 (92%)	4 (8%)	16 55
19	S	70/70 (100%)	62 (89%)	8 (11%)	8 35
20	T	65/65 (100%)	53 (82%)	12 (18%)	2 11
21	U	44/44 (100%)	33 (75%)	11 (25%)	1 3
All	All	1945/1949 (100%)	1655 (85%)	290 (15%)	4 20

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9	LEU
2	B	10	LYS
2	B	14	HIS
2	B	19	THR
2	B	21	TYR
2	B	22	TRP
2	B	26	MET
2	B	34	ARG
2	B	36	LYS
2	B	39	ILE
2	B	42	LEU
2	B	46	VAL
2	B	69	VAL
2	B	88	GLN
2	B	103	TRP
2	B	124	THR
2	B	125	PHE
2	B	131	LYS
2	B	147	LEU
2	B	164	ASP
2	B	177	ASN
2	B	182	VAL
2	B	191	ASP
2	B	196	ASP
3	C	26	LYS
3	C	30	ASP
3	C	35	ASP
3	C	41	TYR
3	C	53	ARG
3	C	106	ARG
3	C	123	LEU
3	C	126	ARG

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Mol	Chain	Res	Type
3	C	134	LYS
3	C	139	ASN
3	C	153	SER
3	C	161	ILE
3	C	164	THR
3	C	166	TRP
3	C	178	ARG
3	C	183	TYR
3	C	185	THR
3	C	194	VAL
4	D	2	ARG
4	D	8	LEU
4	D	16	THR
4	D	24	VAL
4	D	25	ARG
4	D	29	THR
4	D	30	LYS
4	D	34	GLU
4	D	55	ARG
4	D	57	LYS
4	D	62	ARG
4	D	80	ARG
4	D	84	ASN
4	D	106	PHE
4	D	119	HIS
4	D	125	ASN
4	D	127	ARG
4	D	137	SER
4	D	140	ASP
4	D	142	VAL
4	D	147	LYS
4	D	151	GLN
4	D	153	ARG
4	D	160	LEU
4	D	168	THR
4	D	170	LEU
4	D	182	LYS
4	D	183	ARG
4	D	187	ARG
4	D	189	ASP
4	D	194	ILE
4	D	199	ILE

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Mol	Chain	Res	Type
5	E	11	GLN
5	E	13	LYS
5	E	18	ASN
5	E	24	VAL
5	E	25	LYS
5	E	59	ILE
5	E	75	LEU
5	E	80	LEU
5	E	81	GLN
5	E	87	VAL
5	E	91	SER
5	E	95	MET
5	E	99	SER
5	E	119	VAL
5	E	131	ASN
5	E	133	ILE
5	E	134	ASN
5	E	136	VAL
5	E	144	GLU
6	F	33	GLU
6	F	38	ARG
6	F	44	ARG
6	F	52	ASN
6	F	54	LEU
6	F	56	LYS
6	F	58	HIS
6	F	61	LEU
6	F	72	ASP
6	F	86	ARG
6	F	89	VAL
6	F	98	GLU
7	G	3	ARG
7	G	5	VAL
7	G	6	ILE
7	G	10	LYS
7	G	12	LEU
7	G	16	LYS
7	G	55	LYS
7	G	58	LEU
7	G	66	GLU
7	G	75	LYS
7	G	77	ARG

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Mol	Chain	Res	Type
7	G	78	ARG
7	G	85	GLN
7	G	90	VAL
7	G	100	MET
7	G	102	TRP
7	G	112	ASP
7	G	119	LEU
7	G	123	LEU
7	G	137	ARG
7	G	139	ASP
7	G	148	LYS
8	H	2	MET
8	H	11	THR
8	H	37	ASN
8	H	42	GLU
8	H	46	GLU
8	H	50	VAL
8	H	54	THR
8	H	59	GLU
8	H	73	SER
8	H	75	GLN
8	H	76	ARG
8	H	78	SER
8	H	79	ARG
8	H	82	LEU
8	H	89	ASP
8	H	93	LYS
8	H	110	MET
9	I	3	ASN
9	I	4	GLN
9	I	5	TYR
9	I	36	GLN
9	I	37	TYR
9	I	45	MET
9	I	53	LEU
9	I	54	VAL
9	I	60	LEU
9	I	61	ASP
9	I	83	THR
9	I	87	MET
9	I	93	LEU
9	I	125	GLN

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Mol	Chain	Res	Type
9	I	126	PHE
9	I	129	ARG
10	J	11	LYS
10	J	15	HIS
10	J	48	ARG
10	J	59	LYS
10	J	67	ILE
10	J	69	THR
10	J	82	LYS
10	J	87	LEU
10	J	92	LEU
11	K	12	ARG
11	K	27	ASN
11	K	33	ILE
11	K	34	THR
11	K	57	SER
11	K	73	VAL
11	K	78	ILE
11	K	81	LEU
11	K	94	SER
11	K	95	THR
11	K	105	ARG
11	K	115	ILE
11	K	128	VAL
12	L	3	VAL
12	L	4	ASN
12	L	5	GLN
12	L	9	LYS
12	L	18	SER
12	L	19	ASN
12	L	28	GLN
12	L	39	THR
12	L	48	LEU
12	L	49	ARG
12	L	57	THR
12	L	62	VAL
12	L	72	ASN
12	L	88	ASP
12	L	96	THR
12	L	107	LYS
12	L	120	ARG
13	M	12	LYS

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Mol	Chain	Res	Type
13	M	24	VAL
13	M	28	ARG
13	M	32	ILE
13	M	46	GLU
13	M	53	ASP
13	M	77	LYS
13	M	91	ARG
13	M	92	ARG
13	M	100	ARG
13	M	113	LYS
14	N	3	GLN
14	N	27	LYS
14	N	41	TRP
14	N	52	ARG
14	N	53	ASP
14	N	58	ARG
14	N	61	ASN
14	N	63	CYS
14	N	65	GLN
14	N	72	PHE
14	N	96	LYS
14	N	100	TRP
15	O	16	ARG
15	O	34	GLN
15	O	38	LEU
15	O	39	GLN
15	O	45	HIS
15	O	65	LEU
15	O	80	LEU
16	P	1	MET
16	P	3	THR
16	P	19	VAL
16	P	29	ASN
16	P	32	PHE
16	P	35	ARG
16	P	41	PRO
16	P	44	SER
16	P	46	LYS
16	P	54	LEU
16	P	56	ARG
16	P	69	ASP
16	P	71	VAL

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Mol	Chain	Res	Type
17	Q	3	LYS
17	Q	6	THR
17	Q	7	LEU
17	Q	20	ILE
17	Q	32	ILE
17	Q	37	ILE
17	Q	39	ARG
17	Q	51	GLU
17	Q	52	CYS
17	Q	58	VAL
17	Q	60	ILE
17	Q	75	VAL
17	Q	80	LYS
18	R	25	ILE
18	R	44	THR
18	R	65	SER
18	R	72	ARG
19	S	5	LYS
19	S	10	ILE
19	S	11	ASP
19	S	52	ASN
19	S	54	ARG
19	S	55	GLN
19	S	56	HIS
19	S	73	PHE
20	T	11	ILE
20	T	26	MET
20	T	30	PHE
20	T	35	TYR
20	T	42	ASP
20	T	47	GLN
20	T	53	MET
20	T	67	HIS
20	T	68	LYS
20	T	69	ASN
20	T	73	ARG
20	T	82	ILE
21	U	4	LYS
21	U	9	GLU
21	U	13	VAL
21	U	17	ARG
21	U	18	PHE

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Mol	Chain	Res	Type
21	U	19	LYS
21	U	27	VAL
21	U	32	ARG
21	U	36	PHE
21	U	37	TYR
21	U	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
17	Q	44	HIS
17	Q	49	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1529/1530 (99%)	540 (35%)	242 (15%)

All (540) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	A
1	A	8	A
1	A	9	G
1	A	13	U
1	A	14	U
1	A	15	G
1	A	16	A
1	A	17	U
1	A	19	A
1	A	22	G
1	A	31	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	40	C
1	A	47	C
1	A	48	C
1	A	51	A

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Mol	Chain	Res	Type
1	A	52	C
1	A	53	A
1	A	61	G
1	A	65	A
1	A	66	A
1	A	67	C
1	A	68	G
1	A	70	U
1	A	71	A
1	A	72	A
1	A	73	C
1	A	74	A
1	A	76	G
1	A	77	A
1	A	80	A
1	A	81	A
1	A	82	G
1	A	83	C
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	89	U
1	A	90	C
1	A	91	U
1	A	92	U
1	A	93	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	98	A
1	A	101	A
1	A	110	C
1	A	115	G
1	A	116	A
1	A	119	A
1	A	120	A
1	A	121	U
1	A	122	G
1	A	131	A
1	A	132	C
1	A	133	U

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Mol	Chain	Res	Type
1	A	141	G
1	A	143	A
1	A	144	G
1	A	155	A
1	A	164	G
1	A	166	U
1	A	174	A
1	A	175	C
1	A	177	G
1	A	178	C
1	A	181	A
1	A	182	A
1	A	184	G
1	A	185	U
1	A	198	G
1	A	199	A
1	A	200	G
1	A	201	G
1	A	206	C
1	A	207	C
1	A	208	U
1	A	209	U
1	A	210	C
1	A	211	G
1	A	212	G
1	A	213	G
1	A	214	C
1	A	239	U
1	A	240	G
1	A	241	G
1	A	243	A
1	A	244	U
1	A	245	U
1	A	246	A
1	A	247	G
1	A	248	C
1	A	249	U
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	A
1	A	254	G

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Mol	Chain	Res	Type
1	A	266	G
1	A	267	C
1	A	268	U
1	A	275	G
1	A	276	G
1	A	277	C
1	A	280	C
1	A	289	G
1	A	294	U
1	A	298	A
1	A	301	G
1	A	305	G
1	A	306	A
1	A	315	A
1	A	316	C
1	A	317	U
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	332	G
1	A	338	A
1	A	339	C
1	A	344	A
1	A	345	C
1	A	346	G
1	A	347	G
1	A	348	G
1	A	349	A
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	368	U
1	A	369	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	376	G
1	A	381	C
1	A	382	A

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Mol	Chain	Res	Type
1	A	384	G
1	A	389	A
1	A	390	U
1	A	397	A
1	A	398	U
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	416	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	425	G
1	A	426	U
1	A	428	G
1	A	429	U
1	A	430	A
1	A	435	A
1	A	438	U
1	A	452	A
1	A	453	G
1	A	454	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	459	A
1	A	461	A
1	A	463	U
1	A	464	U
1	A	465	A
1	A	466	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	474	G
1	A	476	U
1	A	478	A
1	A	479	U
1	A	481	G

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Mol	Chain	Res	Type
1	A	482	A
1	A	483	C
1	A	484	G
1	A	485	U
1	A	486	U
1	A	493	A
1	A	496	A
1	A	497	G
1	A	498	A
1	A	500	G
1	A	501	C
1	A	508	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	512	U
1	A	513	C
1	A	514	C
1	A	516	U
1	A	517	G
1	A	518	C
1	A	519	C
1	A	520	A
1	A	521	G
1	A	524	G
1	A	527	G
1	A	530	G
1	A	532	A
1	A	533	A
1	A	534	U
1	A	535	A
1	A	536	C
1	A	537	G
1	A	548	G
1	A	559	A
1	A	560	A
1	A	562	U
1	A	563	A
1	A	564	C
1	A	565	U
1	A	566	G
1	A	567	G

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Mol	Chain	Res	Type
1	A	568	G
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	C
1	A	577	G
1	A	578	C
1	A	596	A
1	A	597	G
1	A	604	G
1	A	616	G
1	A	617	G
1	A	633	G
1	A	642	A
1	A	643	C
1	A	644	U
1	A	653	U
1	A	654	G
1	A	655	A
1	A	665	A
1	A	666	G
1	A	688	G
1	A	689	C
1	A	695	A
1	A	700	G
1	A	701	U
1	A	702	A
1	A	703	G
1	A	704	A
1	A	705	G
1	A	718	A
1	A	719	C
1	A	721	G
1	A	722	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	733	G
1	A	734	G
1	A	735	C
1	A	748	G

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Mol	Chain	Res	Type
1	A	754	C
1	A	755	G
1	A	758	C
1	A	760	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	803	G
1	A	810	C
1	A	812	G
1	A	815	A
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	820	U
1	A	821	G
1	A	826	C
1	A	828	U
1	A	829	G
1	A	841	C
1	A	842	U
1	A	843	U
1	A	844	G
1	A	845	A
1	A	846	G
1	A	847	G
1	A	849	G
1	A	859	G
1	A	870	U
1	A	871	U
1	A	874	G
1	A	880	C
1	A	885	G
1	A	889	A
1	A	890	G
1	A	891	U

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Mol	Chain	Res	Type
1	A	892	A
1	A	914	A
1	A	915	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	937	A
1	A	942	G
1	A	945	G
1	A	960	U
1	A	961	U
1	A	962	C
1	A	963	G
1	A	966	G
1	A	968	A
1	A	969	A
1	A	970	C
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	979	C
1	A	980	C
1	A	982	U
1	A	983	A
1	A	984	C
1	A	985	C
1	A	986	U
1	A	987	G
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	995	C
1	A	996	A
1	A	997	U
1	A	1000	A
1	A	1004	A

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Mol	Chain	Res	Type
1	A	1006	G
1	A	1016	A
1	A	1019	A
1	A	1020	G
1	A	1022	A
1	A	1024	G
1	A	1026	G
1	A	1029	U
1	A	1031	C
1	A	1032	G
1	A	1036	A
1	A	1037	C
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1052	U
1	A	1053	G
1	A	1054	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1087	G
1	A	1094	G
1	A	1101	A
1	A	1102	A
1	A	1103	C
1	A	1113	C
1	A	1124	G
1	A	1125	U
1	A	1127	G
1	A	1128	C
1	A	1130	A
1	A	1131	G
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C

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Mol	Chain	Res	Type
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1144	G
1	A	1145	A
1	A	1146	A
1	A	1147	C
1	A	1148	U
1	A	1149	C
1	A	1151	A
1	A	1152	A
1	A	1153	G
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1162	C
1	A	1168	U
1	A	1169	A
1	A	1181	G
1	A	1183	U
1	A	1184	G
1	A	1185	G
1	A	1190	G
1	A	1191	A
1	A	1192	C
1	A	1193	G
1	A	1196	A
1	A	1197	A
1	A	1200	C
1	A	1201	A
1	A	1202	U
1	A	1203	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1217	C
1	A	1222	G
1	A	1224	U
1	A	1225	A

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Mol	Chain	Res	Type
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1229	A
1	A	1230	C
1	A	1231	G
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1241	G
1	A	1243	C
1	A	1244	G
1	A	1250	A
1	A	1251	A
1	A	1256	A
1	A	1257	A
1	A	1260	G
1	A	1266	G
1	A	1278	G
1	A	1279	G
1	A	1280	A
1	A	1281	C
1	A	1282	C
1	A	1283	U
1	A	1284	C
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1294	G
1	A	1295	U
1	A	1297	G
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	C
1	A	1303	C
1	A	1305	G
1	A	1312	G
1	A	1316	G
1	A	1317	C

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Mol	Chain	Res	Type
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1324	A
1	A	1332	A
1	A	1338	G
1	A	1346	A
1	A	1348	U
1	A	1349	A
1	A	1350	A
1	A	1359	C
1	A	1362	A
1	A	1364	U
1	A	1365	G
1	A	1367	C
1	A	1368	A
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1382	C
1	A	1394	A
1	A	1395	C
1	A	1396	A
1	A	1397	C
1	A	1398	A
1	A	1400	C
1	A	1411	C
1	A	1422	G
1	A	1429	A
1	A	1431	A
1	A	1432	G
1	A	1441	A
1	A	1446	A
1	A	1447	A
1	A	1448	C
1	A	1449	C
1	A	1450	U
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1455	G
1	A	1456	A

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Mol	Chain	Res	Type
1	A	1491	G
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1505	G
1	A	1507	A
1	A	1508	A
1	A	1517	G
1	A	1519	A
1	A	1520	C
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1534	A

All (242) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	13	U
1	A	14	U
1	A	15	G
1	A	30	U
1	A	32	A
1	A	47	C
1	A	52	C
1	A	60	A
1	A	65	A
1	A	66	A
1	A	70	U
1	A	71	A
1	A	72	A
1	A	73	C
1	A	81	A
1	A	82	G
1	A	85	U
1	A	86	G
1	A	87	C

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Mol	Chain	Res	Type
1	A	89	U
1	A	90	C
1	A	92	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	109	A
1	A	115	G
1	A	116	A
1	A	119	A
1	A	131	A
1	A	132	C
1	A	173	U
1	A	174	A
1	A	181	A
1	A	184	G
1	A	197	A
1	A	199	A
1	A	213	G
1	A	239	U
1	A	240	G
1	A	243	A
1	A	245	U
1	A	247	G
1	A	248	C
1	A	251	G
1	A	252	U
1	A	253	A
1	A	274	A
1	A	275	G
1	A	276	G
1	A	279	A
1	A	282	A
1	A	305	G
1	A	315	A
1	A	316	C
1	A	327	A
1	A	328	C
1	A	330	C
1	A	331	G
1	A	347	G
1	A	348	G

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Mol	Chain	Res	Type
1	A	351	G
1	A	352	C
1	A	353	A
1	A	366	A
1	A	368	U
1	A	369	G
1	A	372	C
1	A	373	A
1	A	388	G
1	A	389	A
1	A	411	A
1	A	414	A
1	A	421	U
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	438	U
1	A	451	A
1	A	452	A
1	A	453	G
1	A	481	G
1	A	482	A
1	A	484	G
1	A	486	U
1	A	495	A
1	A	497	G
1	A	499	A
1	A	500	G
1	A	508	U
1	A	509	A
1	A	511	C
1	A	512	U
1	A	513	C
1	A	517	G
1	A	519	C
1	A	520	A
1	A	531	U
1	A	534	U
1	A	535	A
1	A	536	C

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Mol	Chain	Res	Type
1	A	547	A
1	A	548	G
1	A	559	A
1	A	563	A
1	A	564	C
1	A	566	G
1	A	575	G
1	A	577	G
1	A	595	A
1	A	596	A
1	A	641	U
1	A	643	C
1	A	652	U
1	A	654	G
1	A	686	U
1	A	688	G
1	A	701	U
1	A	704	A
1	A	717	U
1	A	718	A
1	A	721	G
1	A	722	G
1	A	733	G
1	A	734	G
1	A	753	A
1	A	792	A
1	A	794	A
1	A	802	A
1	A	815	A
1	A	816	A
1	A	817	C
1	A	821	G
1	A	870	U
1	A	874	G
1	A	884	U
1	A	885	G
1	A	889	A
1	A	891	U
1	A	913	A
1	A	914	A
1	A	934	C
1	A	935	A

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Mol	Chain	Res	Type
1	A	936	C
1	A	960	U
1	A	961	U
1	A	962	C
1	A	969	A
1	A	974	A
1	A	975	A
1	A	977	A
1	A	978	A
1	A	979	C
1	A	982	U
1	A	983	A
1	A	984	C
1	A	985	C
1	A	992	U
1	A	995	C
1	A	996	A
1	A	1049	U
1	A	1051	C
1	A	1052	U
1	A	1064	G
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1101	A
1	A	1102	A
1	A	1124	G
1	A	1127	G
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1145	A
1	A	1146	A
1	A	1147	C
1	A	1148	U
1	A	1151	A
1	A	1152	A

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Mol	Chain	Res	Type
1	A	1157	A
1	A	1158	C
1	A	1160	G
1	A	1161	C
1	A	1167	A
1	A	1168	U
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1200	C
1	A	1201	A
1	A	1202	U
1	A	1215	G
1	A	1217	C
1	A	1227	A
1	A	1229	A
1	A	1244	G
1	A	1278	G
1	A	1282	C
1	A	1283	U
1	A	1285	A
1	A	1287	A
1	A	1288	A
1	A	1298	U
1	A	1299	A
1	A	1301	U
1	A	1331	G
1	A	1345	U
1	A	1348	U
1	A	1349	A
1	A	1366	C
1	A	1367	C
1	A	1380	U
1	A	1381	U
1	A	1394	A
1	A	1395	C
1	A	1396	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1447	A
1	A	1449	C

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Mol	Chain	Res	Type
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1455	G
1	A	1498	U
1	A	1499	A
1	A	1502	A
1	A	1505	G
1	A	1507	A
1	A	1528	U
1	A	1530	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 42 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.

## 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	1530/1530 (100%)	0.18	57 (3%) 39 8	43, 110, 301, 420	0
2	B	218/218 (100%)	0.10	6 (2%) 50 11	121, 173, 237, 292	0
3	C	206/206 (100%)	0.33	12 (5%) 22 5	79, 158, 229, 303	0
4	D	205/205 (100%)	-0.11	0 100 100	39, 61, 122, 254	0
5	E	150/150 (100%)	-0.01	0 100 100	67, 99, 157, 252	0
6	F	100/100 (100%)	-0.18	1 (1%) 79 29	72, 116, 176, 217	0
7	G	150/150 (100%)	0.77	29 (19%) 2 1	101, 233, 303, 344	0
8	H	129/129 (100%)	0.06	2 (1%) 68 20	68, 113, 170, 246	0
9	I	127/127 (100%)	0.87	22 (17%) 2 1	116, 201, 289, 319	0
10	J	98/98 (100%)	0.78	11 (11%) 6 2	114, 204, 278, 301	0
11	K	117/117 (100%)	0.09	2 (1%) 67 19	68, 117, 175, 239	0
12	L	123/123 (100%)	-0.00	1 (0%) 83 35	44, 89, 144, 226	0
13	M	113/113 (100%)	1.84	40 (35%) 1 0	226, 447, 522, 562	0
14	N	95/100 (95%)	1.67	28 (29%) 1 1	123, 239, 369, 399	0
15	O	88/88 (100%)	0.00	1 (1%) 77 27	76, 122, 190, 265	0
16	P	80/80 (100%)	0.11	1 (1%) 74 24	49, 105, 165, 226	0
17	Q	80/80 (100%)	0.33	8 (10%) 8 2	61, 112, 163, 194	0
18	R	55/55 (100%)	0.13	2 (3%) 41 8	48, 91, 159, 236	0
19	S	79/79 (100%)	2.12	33 (41%) 1 0	206, 416, 490, 515	0
20	T	85/85 (100%)	0.70	16 (18%) 2 1	76, 142, 200, 234	0
21	U	51/51 (100%)	0.47	4 (7%) 13 3	82, 115, 208, 290	0
All	All	3879/3884 (99%)	0.34	276 (7%) 16 4	39, 130, 351, 562	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	8	PRO	9.3
14	N	57	SER	8.6
14	N	18	LYS	8.2
1	A	984	C	7.5
14	N	56	PRO	7.5
19	S	70	LEU	7.3
19	S	64	GLU	6.9
19	S	41	PRO	6.9
13	M	83	GLY	6.7
1	A	219	U	6.5
14	N	19	TYR	6.4
7	G	8	GLN	6.4
1	A	1346	A	6.2
14	N	17	ASP	6.2
7	G	7	GLY	6.2
14	N	52	ARG	6.2
1	A	1257	A	5.9
19	S	17	LYS	5.9
7	G	10	LYS	5.8
3	C	61	LYS	5.8
13	M	29	SER	5.7
20	T	67	HIS	5.6
1	A	983	A	5.5
13	M	4	ALA	5.5
12	L	123	ALA	5.5
13	M	30	LYS	5.4
1	A	121	U	5.4
1	A	946	A	5.3
7	G	9	ARG	5.3
14	N	14	ALA	5.2
13	M	99	GLN	5.2
7	G	16	LYS	5.1
13	M	38	ILE	5.1
1	A	1362	A	5.0
3	C	60	ALA	5.0
7	G	80	GLY	5.0
13	M	51	GLN	5.0
14	N	98	ALA	4.9
20	T	64	GLY	4.8
1	A	1240	U	4.8
14	N	16	ALA	4.8
19	S	65	MET	4.8
19	S	63	ASP	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	M	84	CYS	4.7
13	M	26	LYS	4.7
1	A	962	C	4.7
19	S	38	THR	4.6
13	M	107	THR	4.6
13	M	32	ILE	4.6
13	M	82	LEU	4.5
1	A	972	C	4.5
19	S	60	PHE	4.5
14	N	55	SER	4.5
1	A	1235	U	4.5
9	I	42	THR	4.5
1	A	1236	A	4.5
14	N	51	PRO	4.5
1	A	1311	A	4.4
1	A	1361	G	4.4
13	M	5	GLY	4.4
7	G	23	ALA	4.4
1	A	1493	A	4.3
13	M	31	ALA	4.3
9	I	31	GLN	4.3
19	S	29	PRO	4.2
13	M	35	ALA	4.1
9	I	38	PHE	4.1
1	A	1217	C	4.1
9	I	119	LYS	4.1
9	I	123	ARG	4.0
7	G	81	GLY	4.0
9	I	107	ALA	4.0
14	N	23	ARG	4.0
10	J	60	ASP	4.0
13	M	3	ILE	4.0
7	G	4	ARG	4.0
1	A	1492	A	3.9
1	A	1359	C	3.9
7	G	24	LYS	3.9
1	A	1312	G	3.9
9	I	40	ARG	3.9
19	S	48	ILE	3.8
13	M	39	ALA	3.8
10	J	48	ARG	3.8
3	C	163	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
7	G	43	TYR	3.8
13	M	52	ILE	3.8
7	G	83	THR	3.7
19	S	75	PRO	3.7
21	U	8	ASN	3.7
3	C	27	GLU	3.7
14	N	3	GLN	3.7
14	N	59	GLN	3.7
7	G	116	ALA	3.7
19	S	7	GLY	3.7
13	M	97	ARG	3.7
9	I	39	GLY	3.7
20	T	68	LYS	3.6
13	M	10	ASP	3.6
14	N	49	THR	3.6
13	M	88	LEU	3.6
13	M	92	ARG	3.6
9	I	122	ARG	3.5
13	M	96	VAL	3.5
3	C	161	ILE	3.5
7	G	14	ASP	3.4
9	I	106	ASP	3.4
19	S	45	GLY	3.4
1	A	1115	U	3.4
1	A	976	G	3.4
9	I	108	ARG	3.4
1	A	942	G	3.4
19	S	46	LEU	3.4
13	M	79	LEU	3.4
21	U	6	ARG	3.4
7	G	18	GLY	3.3
14	N	25	GLU	3.3
7	G	29	LEU	3.3
10	J	41	PRO	3.3
13	M	98	GLY	3.3
21	U	7	GLU	3.3
1	A	1324	A	3.3
3	C	28	PHE	3.3
1	A	1224	U	3.3
1	A	1054	C	3.2
14	N	34	ASN	3.2
19	S	61	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
14	N	53	ASP	3.2
9	I	124	PRO	3.2
3	C	162	ALA	3.2
3	C	22	PHE	3.2
13	M	74	MET	3.2
20	T	65	LEU	3.2
3	C	23	ALA	3.1
2	B	165	ALA	3.1
19	S	4	LEU	3.1
19	S	67	GLY	3.1
1	A	974	A	3.1
7	G	44	SER	3.1
19	S	69	LYS	3.1
1	A	1190	G	3.1
2	B	87	ASP	3.1
19	S	10	ILE	3.1
7	G	132	THR	3.1
15	O	5	GLU	3.0
9	I	117	LEU	3.0
13	M	34	ALA	3.0
20	T	33	LYS	3.0
10	J	8	ILE	3.0
17	Q	35	LYS	3.0
14	N	48	GLN	3.0
20	T	15	LYS	3.0
9	I	109	GLN	2.9
1	A	1323	G	2.9
13	M	54	THR	2.9
10	J	45	ARG	2.9
1	A	941	G	2.9
7	G	11	ILE	2.9
19	S	36	ARG	2.9
10	J	47	GLU	2.9
7	G	26	VAL	2.8
14	N	11	LYS	2.8
1	A	220	G	2.8
1	A	1230	C	2.8
9	I	118	ARG	2.8
9	I	62	LEU	2.8
7	G	3	ARG	2.8
2	B	135	MET	2.7
18	R	47	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
7	G	34	LYS	2.7
13	M	37	GLY	2.7
1	A	1325	C	2.7
17	Q	30	HIS	2.7
19	S	73	PHE	2.7
11	K	67	GLU	2.7
17	Q	31	PRO	2.7
2	B	173	LYS	2.7
17	Q	36	PHE	2.7
2	B	211	LEU	2.7
13	M	6	ILE	2.7
20	T	66	ILE	2.7
7	G	13	PRO	2.6
1	A	973	G	2.6
14	N	97	LYS	2.6
7	G	5	VAL	2.6
7	G	39	GLU	2.6
19	S	74	ALA	2.6
9	I	121	ARG	2.6
10	J	12	ALA	2.6
7	G	78	ARG	2.6
13	M	72	ILE	2.6
1	A	975	A	2.6
8	H	72	GLU	2.6
19	S	59	VAL	2.6
10	J	24	GLU	2.6
1	A	1306	A	2.6
20	T	8	LYS	2.6
19	S	66	VAL	2.5
9	I	67	LYS	2.5
13	M	33	LEU	2.5
10	J	50	THR	2.5
14	N	50	LEU	2.5
13	M	46	GLU	2.5
19	S	6	LYS	2.5
20	T	60	GLN	2.5
1	A	963	G	2.5
13	M	71	GLU	2.5
9	I	13	SER	2.5
19	S	11	ASP	2.4
1	A	48	C	2.4
3	C	1	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
7	G	15	PRO	2.4
10	J	23	ALA	2.4
20	T	63	LYS	2.4
14	N	69	PRO	2.4
1	A	5	U	2.4
11	K	102	ALA	2.4
20	T	71	ALA	2.4
13	M	47	LEU	2.4
1	A	970	C	2.4
13	M	1	ALA	2.4
17	Q	29	LYS	2.4
1	A	211	G	2.3
20	T	69	ASN	2.3
6	F	80	PHE	2.3
20	T	70	LYS	2.3
1	A	1322	C	2.3
1	A	197	A	2.3
1	A	1336	C	2.3
13	M	27	THR	2.3
18	R	73	HIS	2.3
1	A	1341	U	2.3
1	A	1534	A	2.3
17	Q	28	VAL	2.3
13	M	53	ASP	2.2
19	S	55	GLN	2.2
1	A	105	G	2.2
1	A	1337	G	2.2
16	P	47	GLU	2.2
2	B	177	ASN	2.2
19	S	31	ARG	2.2
17	Q	39	ARG	2.2
1	A	954	G	2.2
1	A	250	A	2.2
14	N	62	ARG	2.2
1	A	1209	C	2.2
13	M	69	ARG	2.2
10	J	46	LYS	2.2
21	U	44	ARG	2.2
20	T	75	LYS	2.2
20	T	14	GLU	2.2
1	A	948	C	2.1
7	G	82	SER	2.1

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Mol	Chain	Res	Type	RSRZ
19	S	58	PRO	2.1
9	I	41	GLU	2.1
1	A	1360	A	2.1
9	I	35	GLU	2.1
9	I	3	ASN	2.1
20	T	7	LYS	2.1
1	A	467	U	2.1
13	M	78	ARG	2.1
3	C	179	ALA	2.1
14	N	99	SER	2.1
3	C	156	LEU	2.1
1	A	1287	A	2.1
8	H	129	ALA	2.1
19	S	40	PHE	2.1
14	N	24	ALA	2.1
14	N	70	HIS	2.1
1	A	221	C	2.1
1	A	1208	C	2.1
7	G	6	ILE	2.1
19	S	37	SER	2.0
14	N	22	LYS	2.0
17	Q	37	ILE	2.0
19	S	57	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1573	1/1	1.03	36.07	171,171,171,171	0
22	MG	A	1552	1/1	0.69	24.65	243,243,243,243	0
22	MG	A	1548	1/1	0.34	15.49	243,243,243,243	0
22	MG	A	1547	1/1	1.11	12.26	271,271,271,271	0
22	MG	A	1553	1/1	0.22	11.10	209,209,209,209	0
22	MG	A	1545	1/1	0.29	7.36	133,133,133,133	0
22	MG	A	1535	1/1	0.40	6.41	131,131,131,131	0
22	MG	A	1562	1/1	0.69	4.79	214,214,214,214	0
22	MG	A	1536	1/1	0.19	3.77	140,140,140,140	0
22	MG	A	1544	1/1	0.28	2.33	116,116,116,116	0
22	MG	A	1572	1/1	0.21	2.30	148,148,148,148	0
22	MG	A	1540	1/1	0.26	1.57	222,222,222,222	0
22	MG	A	1556	1/1	0.16	1.48	79,79,79,79	0
22	MG	A	1560	1/1	0.21	1.44	220,220,220,220	0
22	MG	A	1570	1/1	0.21	1.43	140,140,140,140	0
22	MG	A	1567	1/1	0.26	0.77	200,200,200,200	0
22	MG	A	1558	1/1	0.23	0.60	160,160,160,160	0
22	MG	A	1569	1/1	0.26	0.41	130,130,130,130	0
22	MG	A	1565	1/1	0.43	0.23	143,143,143,143	0
22	MG	A	1557	1/1	0.21	-0.34	123,123,123,123	0
22	MG	A	1543	1/1	0.18	-0.39	220,220,220,220	0
22	MG	A	1549	1/1	0.50	-0.44	279,279,279,279	0
22	MG	A	1550	1/1	0.19	-0.80	205,205,205,205	0
22	MG	A	1574	1/1	0.19	-0.81	73,73,73,73	0
22	MG	A	1546	1/1	0.15	-0.85	116,116,116,116	0
22	MG	A	1539	1/1	0.15	-0.89	77,77,77,77	0
22	MG	A	1561	1/1	0.20	-1.06	259,259,259,259	0
22	MG	A	1554	1/1	0.15	-1.24	60,60,60,60	0
22	MG	A	1551	1/1	0.17	-1.29	141,141,141,141	0
22	MG	A	1	1/1	0.11	-1.67	123,123,123,123	0
22	MG	A	1538	1/1	0.14	-1.75	47,47,47,47	0
22	MG	A	1568	1/1	0.17	-2.09	85,85,85,85	0
22	MG	A	1571	1/1	0.19	-2.43	106,106,106,106	0
22	MG	A	1559	1/1	0.18	-2.47	27,27,27,27	0
22	MG	A	1555	1/1	0.13	-2.61	196,196,196,196	0
22	MG	A	1541	1/1	0.11	-2.83	82,82,82,82	0
22	MG	A	1566	1/1	0.08	-3.07	82,82,82,82	0
22	MG	A	1564	1/1	0.12	-3.12	111,111,111,111	0
22	MG	A	1542	1/1	0.07	-3.52	71,71,71,71	0
22	MG	A	1537	1/1	0.08	-3.80	65,65,65,65	0
22	MG	A	1575	1/1	0.07	-6.82	121,121,121,121	0
22	MG	A	1563	1/1	0.08	-6.92	176,176,176,176	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.