Full wwPDB EM Validation Report

Sep 16, 2021 – 11:07 pm BST

PDB ID	:	7OPE
EMDB ID	:	EMD-13017
Title	:	RqcH DR variant bound to 50S-peptidyl-tRNA-RqcP RQC complex (rigid body refinement)
Authors	:	Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on	:	2021-05-31
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

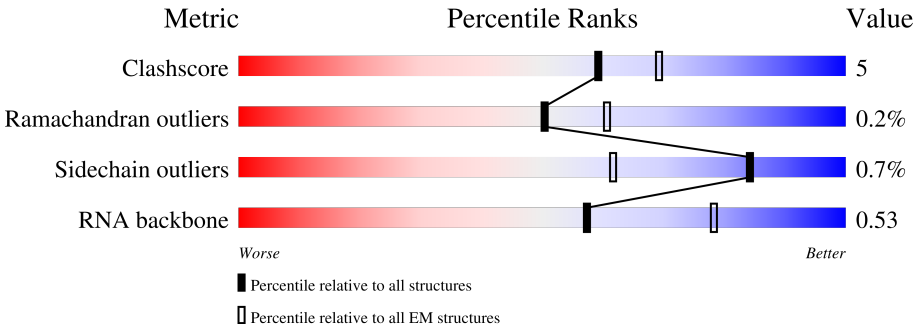
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	2926	63% 27% 6% • •
2	B	119	58% 24% 11% • 6%
3	E	277	82% 15% ••
4	F	209	86% 12% •
5	G	207	90% 9% •
6	H	179	78% 20% ••
7	I	179	83% 15% •

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Mol	Chain	Length	Quality of chain
8	K	141	82% 12% 6%
9	L	166	52% 16% 32%
10	N	145	81% 17%
11	O	122	80% 20%
12	P	146	90% 10%
13	Q	144	81% 12% 6%
14	R	120	80% 19%
15	S	120	80% 19%
16	T	115	87% 13%
17	U	119	84% 13%
18	V	102	88% 10%
19	W	113	86% 11%
20	X	95	85% 9% 5%
21	Y	103	89% 9%
22	2	76	37% 37% 14% 8%
23	a	94	85% 14%
24	b	62	94% 6%
25	c	66	98%
26	d	59	98%
27	f	59	86% 10%
28	g	49	98%
29	h	44	95% 5%
30	i	66	97%
31	j	37	100%
32	1	86	90% 7%

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Mol	Chain	Length	Quality of chain
33	0	599	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 93862 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2814	60436	26962	11170	19491	2813	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2392	1068	435	778	111	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	272	2083	1296	408	373	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	206	1569	985	289	290	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	205	1561	980	289	290	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	176	1387	883	241	256	7	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	132	Total	C	N	O	S	0	0
			974	612	172	184	6		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	113	Total	C	N	O	S	0	0
			886	559	152	174	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	142	Total	C	N	O	S	0	0
			1124	710	206	203	5		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	119	Total 954	C 583	N 186	O 181	S 4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	120	Total 913	C 564	N 176	O 172	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	115	Total 945	C 600	N 185	O 159	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	117	Total 940	C 591	N 189	O 156	S 4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	100	Total 781	C 498	N 138	O 145	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	109	Total 842	C 525	N 164	O 150	S 3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	90	Total 725	C 452	N 134	O 136	S 3	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 22 is a RNA chain called tRNA-Ala-UGC.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	70	Total	C	N	O	P	0	0
			1496	666	271	489	70		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	a	81	Total	C	N	O	0	0
			624	387	122	115		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 28 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 32 is a protein called Uncharacterized protein YabO.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	83	Total	C	N	O	S	0	0
			659	410	121	126	2		

- Molecule 33 is a protein called Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	0	532	Total	C	N	O	S	0	0
			3962	2504	705	743	10		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	97	ALA	ASP	conflict	UNP A0A6M4JI41
0	98	ALA	ARG	conflict	UNP A0A6M4JI41
0	571	GLY	-	expression tag	UNP A0A6M4JI41
0	572	SER	-	expression tag	UNP A0A6M4JI41
0	573	GLY	-	expression tag	UNP A0A6M4JI41
0	574	GLY	-	expression tag	UNP A0A6M4JI41

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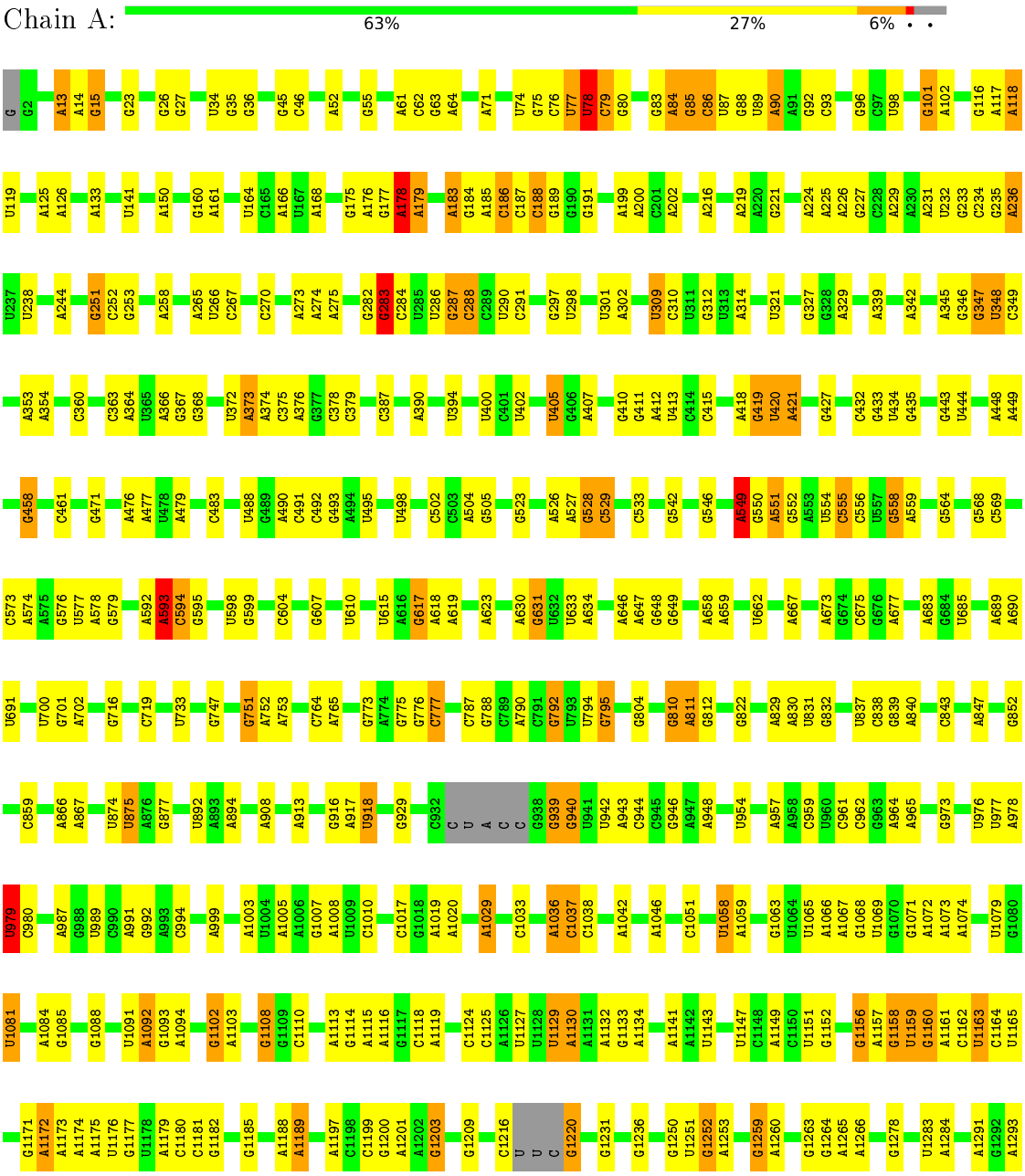
Chain	Residue	Modelled	Actual	Comment	Reference
0	575	ASP	-	expression tag	UNP A0A6M4JI41
0	576	TYR	-	expression tag	UNP A0A6M4JI41
0	577	LYS	-	expression tag	UNP A0A6M4JI41
0	578	ASP	-	expression tag	UNP A0A6M4JI41
0	579	HIS	-	expression tag	UNP A0A6M4JI41
0	580	ASP	-	expression tag	UNP A0A6M4JI41
0	581	GLY	-	expression tag	UNP A0A6M4JI41
0	582	ASP	-	expression tag	UNP A0A6M4JI41
0	583	TYR	-	expression tag	UNP A0A6M4JI41
0	584	LYS	-	expression tag	UNP A0A6M4JI41
0	585	ASP	-	expression tag	UNP A0A6M4JI41
0	586	HIS	-	expression tag	UNP A0A6M4JI41
0	587	ASP	-	expression tag	UNP A0A6M4JI41
0	588	ILE	-	expression tag	UNP A0A6M4JI41
0	589	ASP	-	expression tag	UNP A0A6M4JI41
0	590	TYR	-	expression tag	UNP A0A6M4JI41
0	591	LYS	-	expression tag	UNP A0A6M4JI41
0	592	ASP	-	expression tag	UNP A0A6M4JI41
0	593	ASP	-	expression tag	UNP A0A6M4JI41
0	594	ASP	-	expression tag	UNP A0A6M4JI41
0	595	ASP	-	expression tag	UNP A0A6M4JI41
0	596	LYS	-	expression tag	UNP A0A6M4JI41
0	597	GLY	-	expression tag	UNP A0A6M4JI41

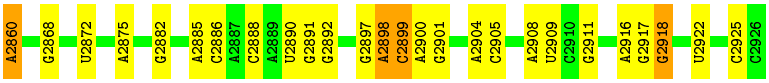
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 23S rRNA

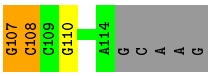
Chain A:





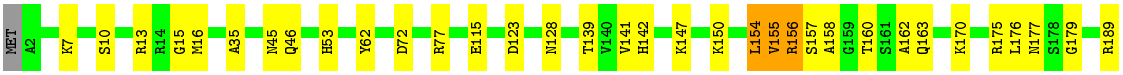
- Molecule 2: 5S rRNA

Chain B:



- Molecule 3: 50S ribosomal protein L2

Chain E:



- Molecule 4: 50S ribosomal protein L3

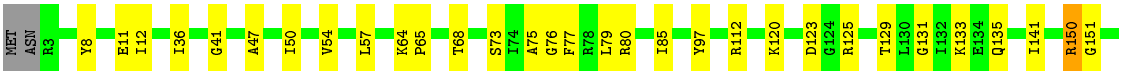
Chain F:

- Molecule 5: 50S ribosomal protein L4

Chain G:

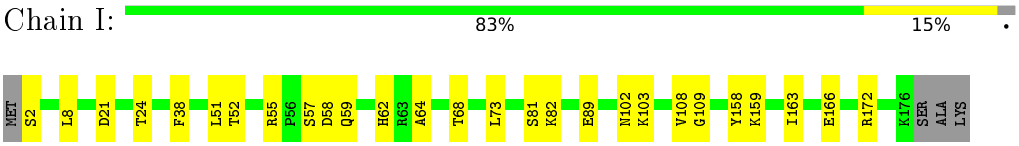
- Molecule 6: 50S ribosomal protein L5

Chain H:



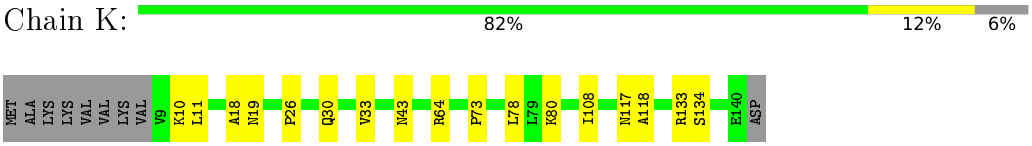
- Molecule 7: 50S ribosomal protein L6

Chain I:



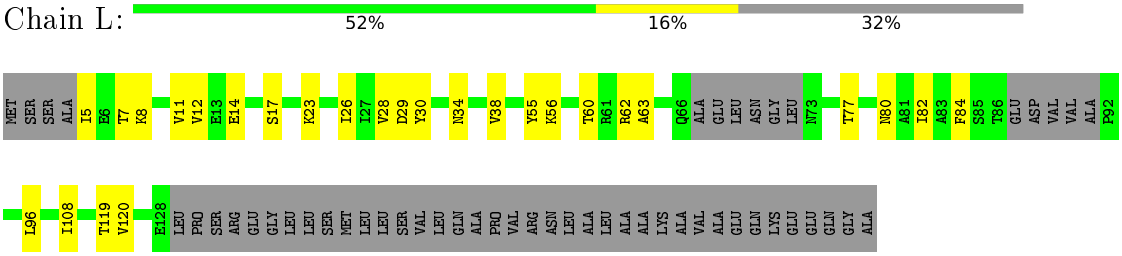
• Molecule 8: 50S ribosomal protein L11

Chain K:



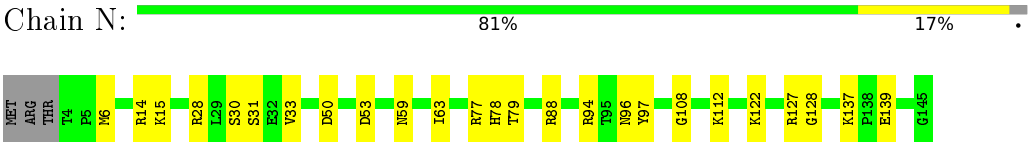
• Molecule 9: 50S ribosomal protein L10

Chain L:



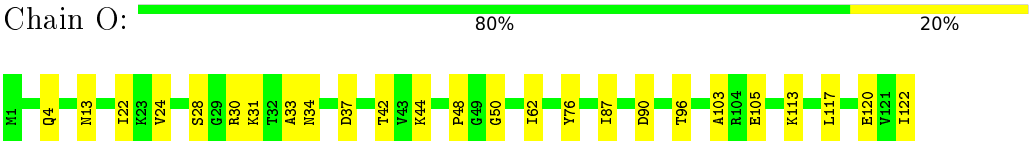
• Molecule 10: 50S ribosomal protein L13

Chain N:



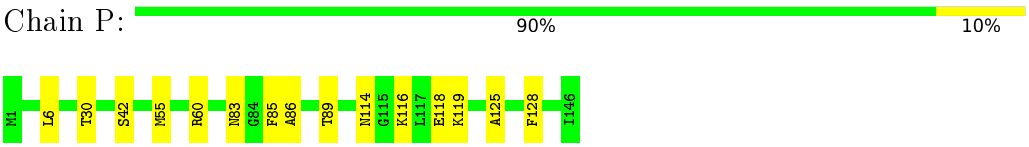
• Molecule 11: 50S ribosomal protein L14

Chain O:



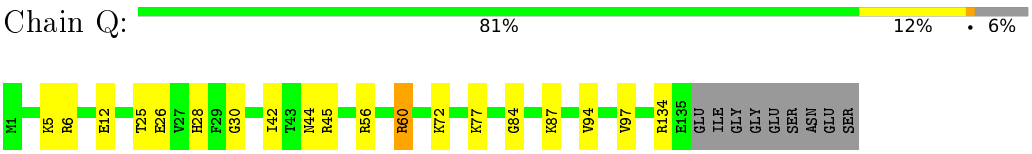
• Molecule 12: 50S ribosomal protein L15

Chain P:



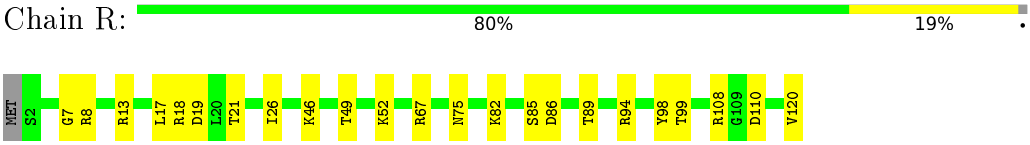
• Molecule 13: 50S ribosomal protein L16

Chain Q:



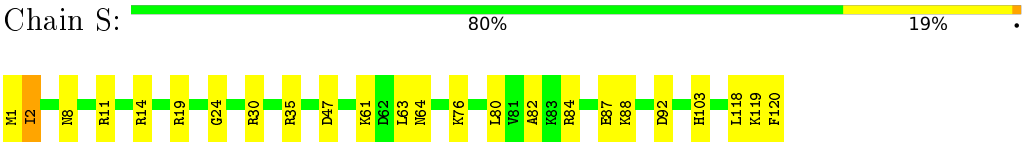
• Molecule 14: 50S ribosomal protein L17

Chain R:



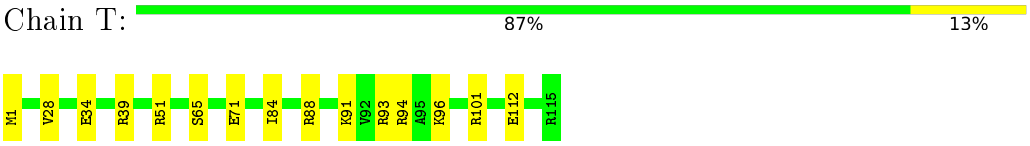
• Molecule 15: 50S ribosomal protein L18

Chain S:



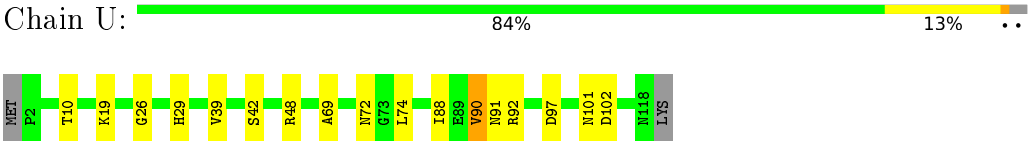
• Molecule 16: 50S ribosomal protein L19

Chain T:



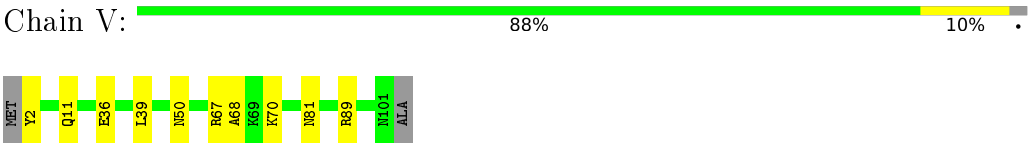
• Molecule 17: 50S ribosomal protein L20

Chain U:



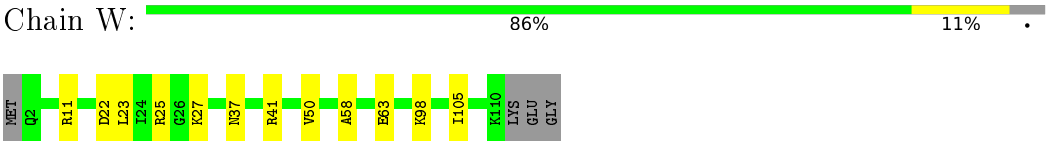
• Molecule 18: 50S ribosomal protein L21

Chain V:



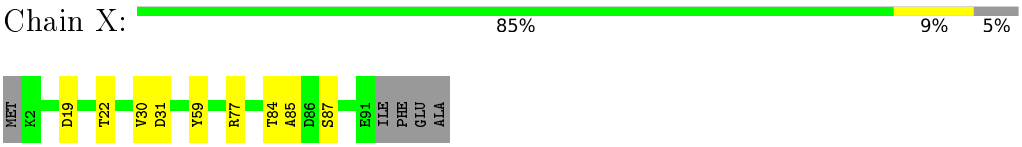
• Molecule 19: 50S ribosomal protein L22

Chain W:



• Molecule 20: 50S ribosomal protein L23

Chain X:

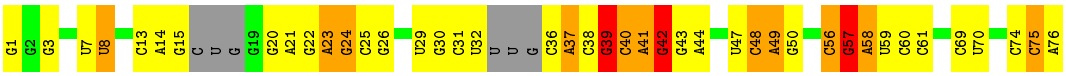


• Molecule 21: 50S ribosomal protein L24

Chain Y:

• Molecule 22: tRNA-Ala-UGC

Chain 2:

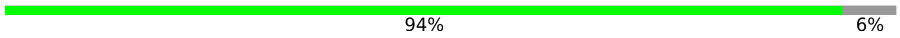


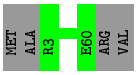
• Molecule 23: 50S ribosomal protein L27

Chain a:

• Molecule 24: 50S ribosomal protein L28

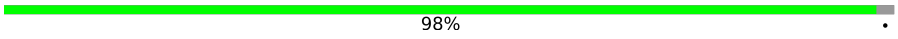
Chain b:





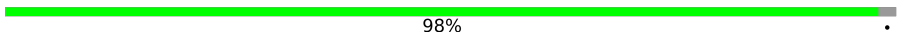
• Molecule 25: 50S ribosomal protein L29

Chain c:



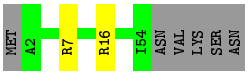
• Molecule 26: 50S ribosomal protein L30

Chain d:



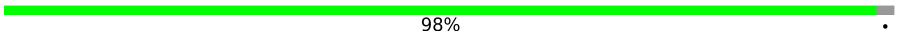
• Molecule 27: 50S ribosomal protein L32

Chain f:



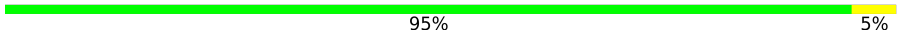
• Molecule 28: 50S ribosomal protein L33 1

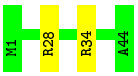
Chain g:



• Molecule 29: 50S ribosomal protein L34

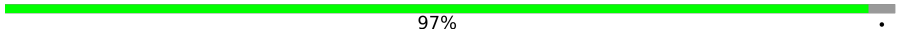
Chain h:





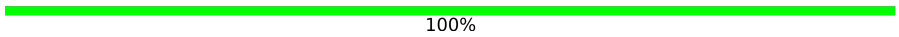
• Molecule 30: 50S ribosomal protein L35

Chain i:



• Molecule 31: 50S ribosomal protein L36

Chain j:



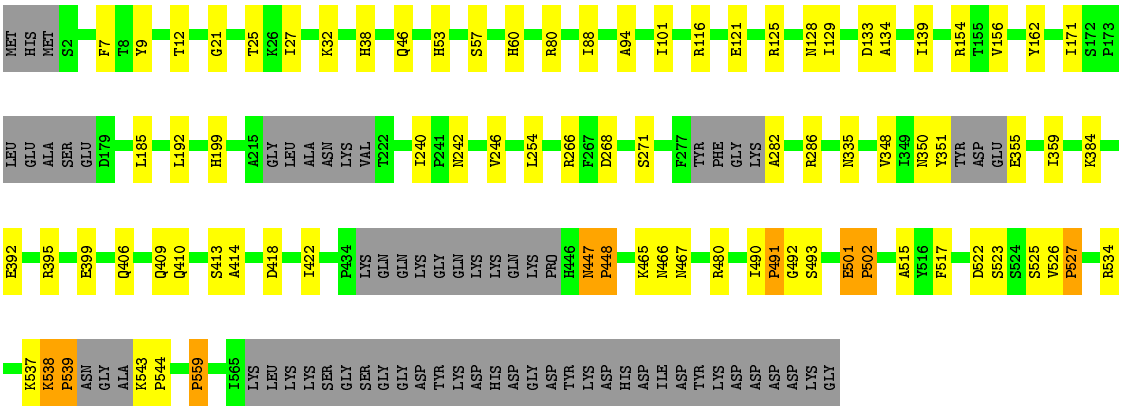
There are no outlier residues recorded for this chain.

• Molecule 32: Uncharacterized protein YabO

Chain 1:

• Molecule 33: Rqc2 homolog RqcH

Chain 0:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.20	8/67693 (0.0%)	1.15	164/105598 (0.2%)
2	B	1.03	1/2675 (0.0%)	1.31	36/4170 (0.9%)
3	E	0.70	0/2120	0.68	0/2845
4	F	0.71	0/1591	0.65	0/2132
5	G	0.68	0/1580	0.62	0/2132
6	H	0.77	0/1406	1.10	2/1888 (0.1%)
7	I	0.51	0/1360	0.63	0/1832
8	K	0.32	0/988	0.57	0/1336
9	L	0.34	0/892	0.58	0/1196
10	N	0.70	0/1147	0.62	0/1542
11	O	0.65	0/928	0.75	0/1245
12	P	0.64	0/1094	0.66	0/1457
13	Q	0.71	0/1099	0.70	0/1468
14	R	0.65	0/961	0.70	0/1284
15	S	0.56	0/922	0.71	0/1236
16	T	0.67	0/958	0.77	0/1279
17	U	0.74	0/952	0.70	0/1266
18	V	0.76	0/792	0.68	0/1063
19	W	0.64	0/851	0.72	0/1146
20	X	0.65	0/731	0.69	0/974
21	Y	0.62	0/772	0.67	1/1032 (0.1%)
22	2	0.97	1/1669 (0.1%)	1.63	37/2596 (1.4%)
23	a	0.76	0/632	0.72	0/839
24	b	0.46	0/448	0.70	0/596
25	c	0.54	0/531	0.71	0/707
26	d	0.63	0/458	0.69	0/613
27	f	0.68	0/425	0.71	1/563 (0.2%)
28	g	0.64	0/406	0.63	0/540
29	h	0.72	0/371	0.78	1/483 (0.2%)
30	i	0.66	0/519	0.68	0/680
31	j	0.75	0/300	0.63	0/393
32	1	0.68	1/662 (0.2%)	1.07	3/882 (0.3%)
33	0	0.39	4/4031 (0.1%)	0.75	18/5456 (0.3%)
All	All	1.05	15/101964 (0.0%)	1.07	263/152469 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
2	B	0	4
3	E	0	1
6	H	0	1
8	K	0	1
13	Q	0	1
18	V	0	1
22	2	0	7
All	All	0	31

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1220	G	P-OP2	7.36	1.61	1.49
1	A	1220	G	P-OP1	7.35	1.61	1.49
1	A	1939	G	O3'-P	-7.11	1.52	1.61
1	A	1940	U	C1'-N1	6.92	1.59	1.48
33	0	491	PRO	CG-CD	5.91	1.70	1.50
1	A	1867	C	C4-N4	-5.63	1.28	1.33
1	A	574	A	N9-C4	-5.63	1.34	1.37
32	1	58	VAL	C-N	5.31	1.46	1.34
22	2	25	C	C4-N4	-5.17	1.29	1.33
33	0	527	PRO	CG-CD	5.16	1.67	1.50
33	0	448	PRO	CG-CD	5.08	1.67	1.50
1	A	1467	G	C8-N7	-5.05	1.27	1.30
1	A	2333	G	C2-N2	-5.04	1.29	1.34
33	0	544	PRO	CG-CD	5.04	1.67	1.50
2	B	56	A	C5-C4	-5.04	1.35	1.38

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	490	ILE	C-N-CD	-29.05	56.69	120.60
22	2	49	A	O5'-P-OP2	-27.30	77.94	110.70
22	2	49	A	O5'-P-OP1	-24.78	80.96	110.70
22	2	49	A	OP1-P-OP2	18.24	146.97	119.60
1	A	2334	U	O4'-C1'-N1	15.33	120.47	108.20
22	2	48	C	OP1-P-O3'	-12.49	77.72	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2335	U	O4'-C1'-N1	11.76	117.61	108.20
2	B	43	A	N1-C6-N6	-10.44	112.33	118.60
2	B	55	A	N1-C6-N6	-10.20	112.48	118.60
1	A	1939	G	O3'-P-O5'	-10.14	84.73	104.00
22	2	48	C	OP2-P-O3'	-9.67	83.93	105.20
1	A	1757	G	O4'-C1'-N9	9.09	115.47	108.20
1	A	1956	A	N1-C6-N6	-9.04	113.18	118.60
33	0	526	VAL	C-N-CD	-8.85	101.13	120.60
32	1	16	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	1220	G	P-O5'-C5'	-8.77	106.87	120.90
1	A	2338	A	N1-C6-N6	-8.72	113.37	118.60
1	A	2343	A	C5'-C4'-O4'	8.71	119.56	109.10
6	H	150	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	2898	A	N1-C6-N6	-8.66	113.41	118.60
1	A	1957	A	N1-C6-N6	-8.61	113.43	118.60
1	A	2340	A	N1-C6-N6	-8.53	113.48	118.60
1	A	2331	U	O4'-C1'-N1	8.33	114.86	108.20
2	B	27	A	N1-C6-N6	-8.28	113.63	118.60
2	B	56	A	C5-C6-N1	8.16	121.78	117.70
1	A	593	A	N1-C6-N6	-8.07	113.76	118.60
1	A	2503	C	C6-N1-C2	-7.87	117.15	120.30
2	B	42	G	O4'-C1'-N9	7.84	114.47	108.20
22	2	1	G	OP1-P-OP2	-7.84	107.84	119.60
1	A	2340	A	O4'-C1'-N9	7.83	114.47	108.20
1	A	555	C	C6-N1-C2	-7.83	117.17	120.30
22	2	40	C	O4'-C1'-N1	7.76	114.41	108.20
2	B	39	A	C5-C6-N1	7.69	121.55	117.70
1	A	2343	A	N1-C6-N6	-7.69	113.99	118.60
1	A	2338	A	C5-C6-N1	7.68	121.54	117.70
6	H	150	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	2340	A	C5-C6-N1	7.62	121.51	117.70
2	B	39	A	N1-C6-N6	-7.62	114.03	118.60
1	A	1370	C	C6-N1-C2	-7.62	117.25	120.30
1	A	555	C	N1-C2-O2	7.62	123.47	118.90
2	B	52	G	O4'-C1'-N9	7.61	114.29	108.20
2	B	30	C	N3-C2-O2	-7.60	116.58	121.90
2	B	29	C	N3-C2-O2	-7.52	116.64	121.90
1	A	2341	U	O4'-C1'-N1	7.52	114.22	108.20
22	2	25	C	O4'-C1'-N1	7.51	114.21	108.20
1	A	2695	C	N1-C2-O2	7.36	123.31	118.90
1	A	2342	C	N3-C2-O2	-7.34	116.76	121.90
1	A	2327	A	N1-C6-N6	-7.29	114.22	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	55	A	C5-C6-N1	7.28	121.34	117.70
1	A	2503	C	N3-C2-O2	-7.16	116.89	121.90
1	A	716	G	C4-N9-C1'	7.13	135.77	126.50
1	A	2332	G	C4'-C3'-C2'	-7.12	95.48	102.60
1	A	1956	A	C5-C6-N1	7.12	121.26	117.70
22	2	23	A	N1-C6-N6	-7.12	114.33	118.60
22	2	23	A	C4-C5-C6	-7.09	113.45	117.00
2	B	43	A	C5-C6-N1	7.08	121.24	117.70
1	A	2918	G	C4-N9-C1'	7.07	135.69	126.50
2	B	39	A	O4'-C1'-N9	7.05	113.84	108.20
1	A	1947	A	C2'-C3'-O3'	7.02	124.95	109.50
1	A	1828	G	C8-N9-C4	-7.01	103.60	106.40
32	1	15	ARG	NE-CZ-NH1	6.99	123.80	120.30
2	B	56	A	N1-C6-N6	-6.94	114.44	118.60
22	2	41	A	C4-C5-C6	-6.93	113.53	117.00
1	A	1370	C	C5-C6-N1	6.92	124.46	121.00
1	A	179	A	N1-C6-N6	6.92	122.75	118.60
1	A	2343	A	C5-C6-N1	6.88	121.14	117.70
2	B	56	A	C4-C5-C6	-6.88	113.56	117.00
1	A	1866	C	N3-C2-O2	-6.86	117.10	121.90
1	A	2330	A	C5-C6-N1	6.82	121.11	117.70
1	A	1220	G	OP1-P-OP2	-6.76	109.46	119.60
1	A	1353	C	C6-N1-C2	-6.75	117.60	120.30
2	B	55	A	C4-C5-C6	-6.75	113.63	117.00
1	A	1527	C	C2-N1-C1'	6.73	126.20	118.80
22	2	23	A	C5-C6-N1	6.67	121.04	117.70
1	A	1939	G	OP2-P-O3'	6.67	119.87	105.20
2	B	30	C	N1-C2-O2	6.65	122.89	118.90
1	A	1203	G	C6-C5-N7	-6.65	126.41	130.40
1	A	1804	U	C5-C4-O4	-6.65	121.91	125.90
2	B	27	A	C5-C6-N1	6.62	121.01	117.70
1	A	555	C	N3-C2-O2	-6.56	117.31	121.90
1	A	1352	U	C2-N1-C1'	6.55	125.56	117.70
1	A	1425	C	C6-N1-C2	-6.53	117.69	120.30
1	A	1353	C	C2-N1-C1'	6.52	125.97	118.80
1	A	716	G	C8-N9-C1'	-6.51	118.54	127.00
1	A	2339	A	N1-C6-N6	-6.51	114.70	118.60
1	A	631	G	N3-C4-C5	6.48	131.84	128.60
33	0	491	PRO	N-CA-CB	6.43	111.02	103.30
1	A	2695	C	N3-C2-O2	-6.43	117.40	121.90
1	A	875	U	C2-N1-C1'	6.42	125.41	117.70
1	A	2503	C	N1-C2-O2	6.42	122.75	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1981	A	N1-C6-N6	6.42	122.45	118.60
1	A	1957	A	C4-C5-C6	-6.41	113.80	117.00
22	2	25	C	C6-N1-C2	-6.41	117.74	120.30
1	A	1370	C	C2-N1-C1'	6.39	125.83	118.80
1	A	2304	C	N1-C2-O2	6.39	122.73	118.90
22	2	14	A	N1-C6-N6	-6.38	114.77	118.60
22	2	25	C	N3-C2-O2	-6.37	117.44	121.90
1	A	2273	U	C5-C4-O4	-6.31	122.12	125.90
1	A	1957	A	C5-C6-N1	6.29	120.84	117.70
2	B	41	C	O4'-C1'-N1	6.28	113.23	108.20
22	2	57	G	N1-C6-O6	-6.28	116.13	119.90
1	A	568	G	C6-C5-N7	-6.22	126.67	130.40
29	h	34	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	B	28	C	N1-C2-O2	6.16	122.60	118.90
2	B	28	C	N3-C2-O2	-6.15	117.59	121.90
1	A	2273	U	N3-C4-O4	6.13	123.69	119.40
1	A	2343	A	C5'-C4'-C3'	-6.13	106.19	116.00
22	2	24	G	N1-C6-O6	-6.12	116.23	119.90
22	2	48	C	P-O3'-C3'	6.11	127.03	119.70
1	A	2342	C	O4'-C1'-N1	6.11	113.09	108.20
1	A	2339	A	C5-C6-N1	6.10	120.75	117.70
2	B	41	C	N3-C2-O2	-6.09	117.64	121.90
2	B	28	C	N3-C4-N4	-6.08	113.74	118.00
1	A	1952	U	O4'-C1'-N1	6.06	113.05	108.20
33	0	501	GLU	C-N-CD	-6.05	107.30	120.60
33	0	527	PRO	N-CA-CB	6.04	110.54	103.30
1	A	2918	G	C8-N9-C1'	-6.02	119.17	127.00
1	A	2327	A	C5-C6-N1	6.01	120.71	117.70
1	A	1958	G	N1-C6-O6	-6.00	116.30	119.90
1	A	2343	A	C4-C5-C6	-6.00	114.00	117.00
2	B	27	A	C4-C5-C6	-5.99	114.00	117.00
1	A	1990	C	N1-C2-O2	5.98	122.49	118.90
2	B	43	A	C4-C5-C6	-5.98	114.01	117.00
33	0	544	PRO	N-CA-CB	5.97	110.46	103.30
1	A	1804	U	N3-C4-O4	5.95	123.56	119.40
2	B	39	A	C4-C5-C6	-5.94	114.03	117.00
1	A	1370	C	N3-C4-N4	5.93	122.15	118.00
1	A	1370	C	N1-C2-O2	5.90	122.44	118.90
1	A	2330	A	O4'-C1'-N9	5.89	112.91	108.20
1	A	179	A	C5-N7-C8	-5.89	100.95	103.90
1	A	2277	C	C6-N1-C2	-5.89	117.94	120.30
2	B	28	C	N1-C1'-C2'	-5.87	105.54	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2330	A	C4-C5-C6	-5.86	114.07	117.00
1	A	2345	U	C4'-C3'-C2'	-5.86	96.74	102.60
1	A	1203	G	C4-C5-N7	5.86	113.14	110.80
1	A	186	C	C6-N1-C2	-5.85	117.96	120.30
1	A	2340	A	C4-C5-C6	-5.85	114.08	117.00
1	A	78	U	O4'-C1'-N1	5.83	112.87	108.20
1	A	1773	G	O4'-C1'-N9	5.83	112.86	108.20
33	0	448	PRO	N-CA-CB	5.83	110.30	103.30
1	A	2342	C	N1-C2-O2	5.82	122.39	118.90
22	2	13	C	N3-C2-O2	-5.81	117.83	121.90
22	2	26	G	C4'-C3'-C2'	-5.81	96.79	102.60
1	A	631	G	N3-C4-N9	-5.80	122.52	126.00
33	0	539	PRO	N-CA-CB	5.80	110.26	103.30
22	2	56	C	N3-C2-O2	-5.78	117.85	121.90
22	2	39	G	C8-N9-C4	-5.76	104.10	106.40
22	2	42	G	OP1-P-O3'	5.75	117.86	105.20
1	A	1866	C	C5'-C4'-C3'	-5.75	106.80	116.00
1	A	2330	A	N1-C6-N6	-5.75	115.15	118.60
1	A	1867	C	N3-C4-C5	5.75	124.20	121.90
1	A	1339	A	P-O3'-C3'	5.75	126.60	119.70
22	2	14	A	C5-C6-N1	5.72	120.56	117.70
1	A	179	A	N7-C8-N9	5.72	116.66	113.80
22	2	39	G	N3-C2-N2	-5.71	115.90	119.90
1	A	1953	C	N3-C2-O2	-5.70	117.91	121.90
33	0	559	PRO	N-CA-CB	5.70	110.14	103.30
1	A	86	C	C6-N1-C2	-5.69	118.02	120.30
1	A	2331	U	C5'-C4'-O4'	5.69	115.93	109.10
1	A	1467	G	C6-C5-N7	-5.68	126.99	130.40
22	2	41	A	N1-C6-N6	-5.67	115.20	118.60
1	A	1981	A	C5-C6-N6	-5.67	119.17	123.70
1	A	1828	G	N7-C8-N9	5.66	115.93	113.10
2	B	42	G	N3-C4-C5	-5.66	125.77	128.60
21	Y	50	ALA	C-N-CA	5.64	135.79	121.70
1	A	1558	G	N3-C4-N9	5.63	129.38	126.00
2	B	30	C	N3-C4-C5	5.63	124.15	121.90
1	A	1990	C	N3-C2-O2	-5.62	117.97	121.90
1	A	1957	A	O4'-C1'-N9	5.60	112.68	108.20
1	A	1370	C	C5-C4-N4	-5.59	116.28	120.20
1	A	549	A	C8-N9-C4	-5.59	103.56	105.80
1	A	1527	C	N1-C2-O2	5.59	122.26	118.90
1	A	1631	A	OP1-P-O3'	5.59	117.50	105.20
1	A	309	U	C2-N1-C1'	5.59	124.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1954	C	N3-C2-O2	-5.58	118.00	121.90
1	A	1956	A	C4-C5-C6	-5.57	114.22	117.00
1	A	179	A	C5-C6-N6	-5.56	119.25	123.70
22	2	15	G	N3-C2-N2	-5.55	116.01	119.90
33	0	502	PRO	N-CA-CB	5.54	109.95	103.30
1	A	2335	U	C5'-C4'-C3'	-5.53	107.14	116.00
2	B	42	G	N1-C6-O6	-5.52	116.59	119.90
1	A	1382	G	C4-N9-C1'	5.50	133.65	126.50
1	A	2336	G	N1-C6-O6	-5.47	116.62	119.90
32	1	50	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	979	U	O4'-C1'-N1	5.44	112.55	108.20
1	A	1558	G	N9-C4-C5	-5.43	103.23	105.40
1	A	178	A	N7-C8-N9	5.42	116.51	113.80
1	A	1527	C	C6-N1-C2	-5.42	118.13	120.30
1	A	1203	G	C4-N9-C1'	5.40	133.52	126.50
22	2	40	C	N3-C2-O2	-5.40	118.12	121.90
1	A	2338	A	C4-C5-C6	-5.40	114.30	117.00
1	A	2820	U	C5-C4-O4	-5.39	122.67	125.90
2	B	54	U	C5-C6-N1	-5.38	120.01	122.70
1	A	2695	C	C2-N1-C1'	5.37	124.71	118.80
1	A	2421	A	N1-C6-N6	5.37	121.82	118.60
2	B	43	A	C4'-C3'-C2'	-5.37	97.23	102.60
22	2	24	G	C4'-C3'-C2'	-5.37	97.23	102.60
1	A	1696	G	O4'-C1'-N9	5.35	112.48	108.20
1	A	2345	U	C5-C6-N1	-5.35	120.03	122.70
1	A	2313	C	N1-C2-O2	5.35	122.11	118.90
2	B	40	C	N3-C2-O2	-5.35	118.16	121.90
1	A	1886	G	C4-N9-C1'	5.33	133.42	126.50
1	A	1759	U	O4'-C1'-N1	5.29	112.43	108.20
1	A	1981	A	C5-N7-C8	-5.28	101.26	103.90
1	A	1467	G	N3-C4-N9	5.26	129.16	126.00
1	A	86	C	C5-C6-N1	5.26	123.63	121.00
1	A	283	G	C8-N9-C1'	5.25	133.83	127.00
2	B	42	G	C2-N3-C4	5.25	114.52	111.90
1	A	2314	C	C2-N1-C1'	5.24	124.57	118.80
1	A	2334	U	N1-C1'-C2'	-5.24	106.24	112.00
33	0	539	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	634	A	N7-C8-N9	5.22	116.41	113.80
33	0	491	PRO	CA-N-CD	-5.22	104.19	111.50
33	0	502	PRO	CA-N-CD	-5.22	104.19	111.50
33	0	448	PRO	CA-N-CD	-5.22	104.19	111.50
33	0	527	PRO	CA-N-CD	-5.21	104.20	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1448	U	C5-C4-O4	-5.21	122.77	125.90
33	0	544	PRO	CA-N-CD	-5.21	104.20	111.50
33	0	559	PRO	CA-N-CD	-5.21	104.20	111.50
1	A	1958	G	N9-C4-C5	5.20	107.48	105.40
22	2	41	A	N1-C2-N3	-5.20	126.70	129.30
1	A	2717	G	C2-N3-C4	-5.19	109.31	111.90
22	2	42	G	P-O3'-C3'	5.18	125.91	119.70
22	2	57	G	C6-C5-N7	5.17	133.50	130.40
1	A	1957	A	N9-C1'-C2'	-5.17	106.31	112.00
1	A	2536	C	N1-C2-O2	5.17	122.00	118.90
1	A	2621	G	C6-C5-N7	-5.17	127.30	130.40
1	A	1831	A	N7-C8-N9	5.17	116.38	113.80
1	A	1480	A	O4'-C1'-N9	5.16	112.33	108.20
1	A	1831	A	C5-N7-C8	-5.16	101.32	103.90
1	A	1951	G	N1-C6-O6	-5.15	116.81	119.90
22	2	57	G	C3'-C2'-C1'	-5.15	97.38	101.50
33	0	268	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	2277	C	N1-C2-O2	5.13	121.98	118.90
2	B	54	U	O4'-C1'-N1	5.13	112.30	108.20
1	A	1954	C	O4'-C1'-N1	5.13	112.30	108.20
27	f	16	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	1362	G	C6-C5-N7	-5.13	127.32	130.40
1	A	1425	C	C5-C6-N1	5.12	123.56	121.00
1	A	186	C	C2-N1-C1'	5.12	124.43	118.80
1	A	2342	C	N3-C4-N4	-5.12	114.42	118.00
1	A	1384	C	C6-N1-C2	-5.11	118.26	120.30
1	A	555	C	C5-C6-N1	5.11	123.55	121.00
1	A	1558	G	C6-C5-N7	-5.11	127.34	130.40
1	A	1671	G	P-O3'-C3'	5.10	125.82	119.70
22	2	41	A	C5-C6-N1	5.09	120.24	117.70
1	A	1203	G	C8-N9-C1'	-5.08	120.39	127.00
1	A	2340	A	C4'-C3'-C2'	-5.08	97.52	102.60
2	B	55	A	C5'-C4'-C3'	-5.08	107.88	116.00
1	A	2341	U	N1-C2-N3	5.06	117.94	114.90
1	A	1507	U	P-O3'-C3'	5.05	125.76	119.70
1	A	568	G	C4-C5-N7	5.04	112.82	110.80
1	A	1947	A	C3'-C2'-O2'	-5.04	98.69	113.30
1	A	2330	A	O3'-P-O5'	-5.03	94.45	104.00
22	2	24	G	N3-C4-C5	-5.02	126.09	128.60
1	A	1558	G	C8-N9-C1'	-5.02	120.47	127.00
1	A	2025	C	N1-C2-O2	5.01	121.91	118.90
1	A	634	A	C5-N7-C8	-5.01	101.39	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	39	G	N9-C4-C5	5.01	107.41	105.40
22	2	24	G	C5-C6-N1	5.01	114.00	111.50
1	A	2331	U	N3-C2-O2	-5.00	118.70	122.20
1	A	994	C	C5-C4-N4	-5.00	116.70	120.20
1	A	2481	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	2	23	A	Sidechain
22	2	24	G	Sidechain
22	2	39	G	Sidechain
22	2	40	C	Sidechain
22	2	41	A	Sidechain
22	2	42	G	Sidechain
22	2	57	G	Sidechain
1	A	1866	C	Sidechain
1	A	1952	U	Sidechain
1	A	1953	C	Sidechain
1	A	1955	U	Sidechain
1	A	1957	A	Sidechain
1	A	1958	G	Sidechain
1	A	2328	G	Sidechain
1	A	2331	U	Sidechain
1	A	2333	G	Sidechain
1	A	2334	U	Sidechain
1	A	2335	U	Sidechain
1	A	2336	G	Sidechain
1	A	2338	A	Sidechain
1	A	2344	U	Sidechain
1	A	2345	U	Sidechain
2	B	28	C	Sidechain
2	B	39	A	Sidechain
2	B	41	C	Sidechain
2	B	52	G	Sidechain
3	E	154	LEU	Peptide
6	H	97	TYR	Sidechain
8	K	19	ASN	Peptide
13	Q	60	ARG	Peptide
18	V	50	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60436	0	30414	330	0
2	B	2392	0	1213	7	0
3	E	2083	0	2168	29	0
4	F	1569	0	1637	19	0
5	G	1561	0	1647	13	0
6	H	1387	0	1448	74	0
7	I	1342	0	1388	19	0
8	K	974	0	1011	14	0
9	L	886	0	920	16	0
10	N	1124	0	1162	18	0
11	O	921	0	977	21	0
12	P	1082	0	1132	10	0
13	Q	1076	0	1145	13	0
14	R	954	0	983	19	0
15	S	913	0	947	26	0
16	T	945	0	1020	10	0
17	U	940	0	1005	14	0
18	V	781	0	821	9	0
19	W	842	0	899	6	0
20	X	725	0	770	7	0
21	Y	762	0	821	6	0
22	2	1496	0	759	43	0
23	a	624	0	639	0	0
24	b	444	0	487	0	0
25	c	530	0	568	0	0
26	d	456	0	491	0	0
27	f	418	0	435	0	0
28	g	401	0	413	0	0
29	h	368	0	410	0	0
30	i	512	0	564	0	0
31	j	297	0	342	0	0
32	1	659	0	705	1	0
33	0	3962	0	3687	94	0
All	All	93862	0	63028	641	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2340:A:C2	6:H:79:LEU:HD11	1.55	1.39
1:A:2334:U:O4	6:H:151:GLY:HA3	1.38	1.22
1:A:2334:U:C4	6:H:151:GLY:HA3	1.76	1.19
33:0:537:LYS:C	33:0:539:PRO:HD2	1.65	1.15
6:H:125:ARG:HG3	15:S:1:MET:HB2	1.27	1.14
1:A:2340:A:N3	6:H:79:LEU:HD11	1.64	1.10
22:2:44:A:OP1	33:0:286:ARG:NH2	1.86	1.08
1:A:2334:U:O4	6:H:151:GLY:CA	1.99	1.08
22:2:31:C:C2	33:0:125:ARG:CZ	2.36	1.08
1:A:2340:A:C2	6:H:79:LEU:CD1	2.38	1.05
33:0:414:ALA:HA	33:0:465:LYS:CB	1.87	1.05
33:0:523:SER:O	33:0:559:PRO:HD2	1.55	1.04
33:0:410:GLN:HB3	33:0:465:LYS:O	1.58	1.03
33:0:501:GLU:N	33:0:502:PRO:HD2	1.75	1.02
1:A:2340:A:N3	6:H:79:LEU:CD1	2.24	1.00
6:H:160:ALA:O	15:S:1:MET:HA	1.62	1.00
22:2:44:A:C5'	33:0:286:ARG:HH21	1.76	0.97
1:A:312:G:N2	1:A:405:U:C5	2.33	0.95
11:O:103:ALA:HA	11:O:122:ILE:OXT	1.66	0.95
6:H:125:ARG:HG3	15:S:1:MET:CB	1.95	0.95
1:A:2337:G:C2	6:H:77:PHE:CE1	2.56	0.94
33:0:501:GLU:H	33:0:502:PRO:HD2	1.31	0.93
33:0:413:SER:HB2	33:0:517:PHE:CB	1.99	0.93
22:2:31:C:O2	33:0:125:ARG:NH1	2.03	0.92
1:A:327:G:H1	1:A:400:U:H3	1.18	0.92
33:0:515:ALA:HB1	33:0:559:PRO:HD3	1.49	0.91
33:0:53:HIS:CD2	33:0:282:ALA:HA	2.04	0.91
6:H:159:THR:HG22	15:S:2:ILE:HG21	1.50	0.91
22:2:44:A:H5"	33:0:286:ARG:HH21	1.34	0.90
1:A:2340:A:H2	6:H:79:LEU:HD11	1.28	0.89
1:A:1152:G:HO2'	9:L:30:TYR:HH	1.16	0.89
22:2:36:C:OP1	22:2:37:A:N6	2.06	0.89
33:0:501:GLU:H	33:0:502:PRO:CD	1.86	0.88
1:A:1159:U:OP1	7:I:2:SER:OG	1.90	0.87
6:H:160:ALA:O	15:S:1:MET:CA	2.23	0.87
33:0:501:GLU:N	33:0:502:PRO:CD	2.36	0.87
1:A:2337:G:C5	6:H:77:PHE:CZ	2.65	0.84
1:A:810:G:O2'	1:A:811:A:O5'	1.95	0.83
1:A:2339:A:H2	6:H:76:GLY:HA3	1.43	0.83
33:0:447:ASN:H	33:0:448:PRO:HD2	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:C:O2	1:A:1220:G:N2	2.12	0.82
6:H:160:ALA:O	15:S:1:MET:N	2.12	0.82
1:A:2341:U:H5'	6:H:85:ILE:HD11	1.60	0.82
1:A:1790:U:O2'	1:A:1791:A:O4'	1.98	0.80
22:2:31:C:C2	33:0:125:ARG:NH2	2.49	0.80
6:H:73:SER:HB3	22:2:56:C:C1'	2.12	0.80
1:A:2341:U:H5'	6:H:85:ILE:CD1	2.13	0.79
33:0:409:GLN:CD	33:0:492:GLY:HA2	2.02	0.79
33:0:413:SER:CB	33:0:517:PHE:CB	2.61	0.79
6:H:73:SER:HB2	22:2:56:C:O4'	1.81	0.79
1:A:2009:G:O2'	1:A:2011:U:OP2	2.02	0.78
22:2:31:C:C2	33:0:125:ARG:NH1	2.50	0.77
1:A:1263:G:OP2	18:V:89:ARG:NH1	2.17	0.77
33:0:537:LYS:C	33:0:539:PRO:CD	2.50	0.77
6:H:125:ARG:CG	15:S:1:MET:HB2	2.12	0.77
1:A:84:A:N6	1:A:101:G:O2'	2.18	0.77
6:H:73:SER:CB	22:2:56:C:O4'	2.32	0.77
1:A:2337:G:C6	6:H:77:PHE:CZ	2.73	0.77
1:A:2806:G:OP2	1:A:2810:A:O2'	2.02	0.77
22:2:31:C:H1'	33:0:125:ARG:HD2	1.65	0.76
1:A:363:C:OP2	5:G:137:LYS:NZ	2.18	0.76
1:A:917:A:OP1	13:Q:6:ARG:NH2	2.18	0.76
22:2:44:A:P	33:0:286:ARG:NH2	2.59	0.76
6:H:125:ARG:CG	15:S:1:MET:CB	2.63	0.76
22:2:36:C:OP1	22:2:37:A:C6	2.39	0.76
18:V:68:ALA:O	18:V:89:ARG:NE	2.17	0.76
10:N:88:ARG:NH1	10:N:97:TYR:OH	2.19	0.75
14:R:94:ARG:NH1	14:R:120:VAL:O	2.19	0.75
1:A:364:A:N3	5:G:169:ASN:ND2	2.34	0.75
6:H:75:ALA:HB2	22:2:56:C:O2'	1.87	0.75
6:H:159:THR:HG22	15:S:2:ILE:CG2	2.15	0.75
1:A:840:A:OP2	1:A:2100:A:O2'	2.04	0.75
1:A:2339:A:C2	6:H:76:GLY:HA3	2.23	0.74
4:F:26:THR:OG1	4:F:190:GLY:O	2.06	0.74
22:2:44:A:C5'	33:0:286:ARG:NH2	2.50	0.74
33:0:538:LYS:N	33:0:539:PRO:CD	2.49	0.74
33:0:537:LYS:O	33:0:539:PRO:HD2	1.87	0.74
1:A:2127:U:O2'	1:A:2128:U:OP1	2.06	0.74
10:N:15:LYS:N	10:N:53:ASP:OD1	2.21	0.74
14:R:99:THR:C	14:R:120:VAL:OXT	2.26	0.74
1:A:2372:U:HO2'	1:A:2402:A:HO2'	1.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:46:LYS:O	14:R:49:THR:OG1	2.05	0.73
1:A:1114:G:N2	1:A:1141:A:O2'	2.21	0.73
33:0:523:SER:O	33:0:559:PRO:CD	2.35	0.73
1:A:2532:A:O2'	1:A:2534:G:OP2	2.06	0.73
20:X:19:ASP:O	20:X:22:THR:OG1	2.07	0.73
13:Q:25:THR:OG1	13:Q:26:GLU:OE1	2.05	0.73
33:0:53:HIS:O	33:0:57:SER:N	2.22	0.73
1:A:458:G:OP2	1:A:2435:C:O2'	2.06	0.73
1:A:2498:A:O2'	13:Q:56:ARG:NH1	2.22	0.72
1:A:2025:C:OP1	11:O:31:LYS:NZ	2.22	0.72
1:A:2339:A:H2'	6:H:77:PHE:CE2	2.25	0.72
1:A:1542:A:O2'	1:A:1544:C:N4	2.23	0.72
1:A:1694:G:O2'	14:R:110:ASP:OD1	2.07	0.72
33:0:53:HIS:NE2	33:0:282:ALA:HA	2.03	0.72
1:A:1695:A:HO2'	1:A:1696:G:P	2.12	0.71
1:A:1983:G:O2'	1:A:1985:U:O4	2.08	0.71
1:A:918:U:OP1	13:Q:5:LYS:N	2.22	0.71
1:A:1784:A:O2'	1:A:1785:G:OP1	2.06	0.71
1:A:1876:A:O2'	1:A:1877:A:N7	2.23	0.71
22:2:31:C:H1'	33:0:125:ARG:CD	2.20	0.71
4:F:95:GLN:NE2	4:F:96:GLU:O	2.23	0.71
33:0:538:LYS:N	33:0:539:PRO:HD2	2.06	0.71
1:A:79:C:O2'	1:A:390:A:N3	2.18	0.71
33:0:25:THR:OG1	33:0:38:HIS:O	2.05	0.71
14:R:19:ASP:OD1	14:R:67:ARG:NH1	2.24	0.70
1:A:282:G:O2'	1:A:283:G:O4'	2.09	0.70
1:A:1088:G:H1	1:A:1159:U:H3	1.36	0.70
22:2:31:C:N3	33:0:125:ARG:NH2	2.40	0.70
33:0:27:ILE:O	33:0:80:ARG:NH2	2.25	0.70
1:A:1259:G:OP2	17:U:19:LYS:NZ	2.18	0.70
1:A:1362:G:OP1	19:W:98:LYS:NZ	2.24	0.70
15:S:92:ASP:OD1	15:S:119:LYS:NZ	2.25	0.70
33:0:480:ARG:O	33:0:534:ARG:N	2.25	0.69
1:A:177:G:O2'	1:A:178:A:O5'	2.10	0.69
1:A:2922:U:O2'	10:N:137:LYS:NZ	2.25	0.69
1:A:419:G:N2	1:A:448:A:OP2	2.16	0.69
1:A:2595:A:N1	11:O:28:SER:OG	2.24	0.69
1:A:1036:A:O2'	1:A:1037:C:OP1	2.07	0.69
1:A:1828:G:OP1	3:E:260:ARG:NH1	2.26	0.69
1:A:2772:U:OP2	1:A:2784:C:N4	2.25	0.69
1:A:2339:A:H2'	6:H:77:PHE:HE2	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:85:PHE:O	12:P:119:LYS:NZ	2.17	0.69
1:A:1265:A:OP1	18:V:70:LYS:NZ	2.25	0.69
22:2:58:A:O2'	22:2:60:C:OP2	2.07	0.68
33:0:399:GLU:OE2	33:0:543:LYS:N	2.27	0.68
20:X:84:THR:OG1	20:X:87:SER:OG	2.05	0.68
33:0:410:GLN:HE22	33:0:467:ASN:HA	1.59	0.68
1:A:312:G:N2	1:A:405:U:C4	2.62	0.68
1:A:790:A:O2'	1:A:1704:U:OP1	2.12	0.68
1:A:1130:A:N3	1:A:1151:U:O2'	2.21	0.68
1:A:1365:U:O2'	1:A:1366:C:O4'	2.12	0.68
1:A:1315:G:OP2	1:A:1690:G:O2'	2.04	0.68
1:A:160:G:N2	1:A:168:A:OP2	2.27	0.68
1:A:2287:C:O2'	1:A:2456:C:OP2	2.11	0.67
1:A:2340:A:H2	6:H:79:LEU:CD1	1.92	0.67
7:I:57:SER:OG	7:I:59:GLN:OE1	2.04	0.67
1:A:2294:U:OP2	1:A:2295:A:O2'	2.10	0.67
14:R:52:LYS:NZ	14:R:94:ARG:O	2.27	0.67
33:0:410:GLN:CB	33:0:465:LYS:O	2.41	0.67
1:A:1403:G:N2	1:A:1406:A:OP2	2.25	0.67
1:A:1094:A:OP2	1:A:1156:G:N2	2.25	0.67
22:2:3:G:H1	22:2:70:U:H3	1.43	0.67
1:A:719:C:OP2	12:P:42:SER:OG	2.12	0.66
3:E:72:ASP:OD2	3:E:189:ARG:NH2	2.28	0.66
33:0:410:GLN:HE22	33:0:467:ASN:CA	2.08	0.66
16:T:88:ARG:NH1	16:T:112:GLU:OE1	2.29	0.66
1:A:52:A:OP2	1:A:118:A:N6	2.28	0.66
1:A:1886:G:O2'	1:A:1887:G:O4'	2.03	0.66
1:A:1530:G:O2'	1:A:1531:G:OP1	2.14	0.66
1:A:2340:A:C6	6:H:41:GLY:HA3	2.30	0.66
1:A:2513:G:OP1	13:Q:45:ARG:NH1	2.30	0.65
3:E:13:ARG:NH1	3:E:16:MET:SD	2.69	0.65
8:K:26:PRO:O	8:K:30:GLN:NE2	2.29	0.65
1:A:1991:C:O2'	1:A:1993:G:OP2	2.14	0.65
1:A:2340:A:N3	6:H:79:LEU:HD12	2.11	0.65
1:A:1216:C:N3	1:A:1220:G:N1	2.44	0.65
1:A:2121:U:N3	1:A:2255:C:OP2	2.29	0.65
1:A:161:A:OP2	1:A:166:A:N6	2.30	0.65
1:A:1364:C:OP1	1:A:1692:U:O2'	2.15	0.65
15:S:61:LYS:O	15:S:64:ASN:ND2	2.29	0.65
1:A:353:A:N3	1:A:373:A:O2'	2.31	0.64
10:N:78:HIS:ND1	10:N:79:THR:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:A:OP2	1:A:1180:C:O2'	2.14	0.64
1:A:2341:U:C5'	6:H:85:ILE:HD11	2.26	0.64
33:0:409:GLN:CG	33:0:492:GLY:HA2	2.27	0.64
14:R:99:THR:N	14:R:120:VAL:OXT	2.31	0.64
17:U:90:VAL:O	18:V:11:GLN:NE2	2.30	0.64
1:A:604:C:O2	17:U:48:ARG:NH2	2.31	0.64
1:A:2337:G:C4	6:H:77:PHE:CZ	2.86	0.64
2:B:47:C:OP2	15:S:35:ARG:NH2	2.30	0.64
1:A:312:G:C2	1:A:405:U:C4	2.85	0.64
1:A:186:C:O2'	1:A:479:A:N3	2.25	0.64
1:A:2060:A:N3	1:A:2484:G:O2'	2.28	0.64
3:E:194:GLN:NE2	3:E:198:GLU:OE1	2.31	0.64
1:A:2605:G:O2'	1:A:2608:C:OP2	2.16	0.64
1:A:867:A:N3	1:A:989:U:O2'	2.31	0.64
1:A:77:U:O2'	1:A:78:U:O5'	2.16	0.63
1:A:1291:A:OP1	17:U:10:THR:OG1	2.10	0.63
33:0:121:GLU:OE2	33:0:162:TYR:OH	2.15	0.63
6:H:54:VAL:HG13	6:H:65:PRO:HG2	1.79	0.63
10:N:59:ASN:N	10:N:128:GLY:O	2.32	0.63
1:A:2872:U:OP1	16:T:96:LYS:NZ	2.28	0.63
1:A:633:U:O3'	5:G:95:ARG:NH1	2.31	0.63
1:A:1108:G:N3	8:K:134:SER:OG	2.32	0.63
1:A:2364:A:O2'	1:A:2365:A:O5'	2.14	0.63
33:0:422:ILE:HD11	33:0:466:ASN:HA	1.80	0.63
1:A:1509:C:HO2'	1:A:2731:G:HO2'	1.47	0.62
1:A:1313:A:O2'	1:A:1314:A:OP1	2.17	0.62
1:A:1856:U:OP2	3:E:221:ARG:NH1	2.32	0.62
22:2:44:A:H5'	33:0:286:ARG:HH21	1.61	0.62
1:A:1757:G:O2'	1:A:1758:U:O3'	2.16	0.62
1:A:1843:G:OP2	1:A:1844:A:O2'	2.13	0.62
1:A:2027:A:OP2	4:F:141:ARG:NH1	2.32	0.62
1:A:2337:G:N3	6:H:77:PHE:CE1	2.66	0.62
1:A:2334:U:C6	6:H:133:LYS:HA	2.35	0.62
1:A:2548:U:O4'	1:A:2571:A:N6	2.33	0.62
1:A:2890:U:OP2	1:A:2891:G:O2'	2.13	0.62
1:A:1231:G:OP1	12:P:30:THR:OG1	2.10	0.62
12:P:55:MET:O	12:P:60:ARG:NH2	2.33	0.62
4:F:9:LYS:NZ	4:F:194:GLY:O	2.20	0.62
1:A:372:U:O2'	21:Y:67:ASN:ND2	2.33	0.62
11:O:13:ASN:ND2	11:O:96:THR:OG1	2.32	0.62
1:A:2497:A:O2'	1:A:2498:A:O4'	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:G:OP2	1:A:1172:A:O2'	2.09	0.61
33:0:409:GLN:CD	33:0:492:GLY:CA	2.68	0.61
1:A:1264:G:OP2	18:V:67:ARG:NH2	2.33	0.61
1:A:1379:U:OP2	20:X:59:TYR:OH	2.17	0.61
1:A:1124:C:OP1	8:K:133:ARG:NH2	2.33	0.61
1:A:2841:C:O2	1:A:2908:A:O2'	2.15	0.61
6:H:80:ARG:CZ	22:2:56:C:C5	2.84	0.61
1:A:1695:A:O2'	1:A:1696:G:O5'	2.13	0.61
1:A:2468:A:O2'	1:A:2629:A:OP1	2.13	0.61
1:A:2080:A:O2'	1:A:2643:A:N6	2.34	0.60
1:A:1065:U:OP1	1:A:1081:U:O2'	2.17	0.60
1:A:2665:U:O2'	4:F:46:TYR:OH	2.19	0.60
1:A:2337:G:C5	6:H:77:PHE:HZ	2.19	0.60
1:A:2856:G:N2	1:A:2909:U:OP2	2.34	0.60
14:R:52:LYS:NZ	14:R:98:TYR:OH	2.25	0.60
6:H:73:SER:HB3	22:2:56:C:H1'	1.83	0.60
1:A:2054:C:OP1	4:F:153:ARG:NH2	2.35	0.60
1:A:1036:A:O2'	1:A:1038:C:OP2	2.20	0.60
1:A:2026:A:O5'	4:F:130:ARG:NH1	2.33	0.60
6:H:80:ARG:CZ	22:2:56:C:C4	2.85	0.60
33:0:410:GLN:HE22	33:0:467:ASN:CB	2.15	0.60
1:A:1199:C:OP1	17:U:92:ARG:NH2	2.35	0.60
2:B:26:C:O2	2:B:57:G:N2	2.33	0.60
17:U:39:VAL:O	17:U:42:SER:OG	2.11	0.60
22:2:31:C:C4	33:0:125:ARG:NH2	2.69	0.60
33:0:60:HIS:NE2	33:0:271:SER:O	2.34	0.59
1:A:2341:U:C5'	6:H:85:ILE:CD1	2.79	0.59
11:O:13:ASN:OD1	11:O:96:THR:N	2.35	0.59
1:A:1811:C:O2	1:A:2637:G:O2'	2.04	0.59
1:A:2130:G:N2	1:A:2218:U:O2	2.30	0.59
1:A:2688:G:N2	1:A:2691:A:OP2	2.35	0.59
5:G:101:LEU:O	5:G:106:ARG:NH2	2.35	0.59
14:R:99:THR:CA	14:R:120:VAL:OXT	2.50	0.59
1:A:347:G:O2'	1:A:348:U:OP1	2.19	0.59
33:0:409:GLN:HG3	33:0:492:GLY:HA2	1.83	0.59
1:A:2333:G:O2'	6:H:129:THR:HG21	2.03	0.59
1:A:2882:G:N2	1:A:2885:A:OP2	2.29	0.59
7:I:8:LEU:HD22	7:I:52:THR:HG22	1.83	0.59
1:A:546:G:N1	1:A:549:A:OP2	2.35	0.59
1:A:2333:G:O2'	6:H:129:THR:CG2	2.51	0.59
1:A:753:A:OP1	3:E:7:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:G:O2'	1:A:1149:A:N6	2.36	0.58
33:0:525:SER:O	33:0:527:PRO:HD2	2.03	0.58
1:A:1820:A:N6	1:A:1857:G:O2'	2.35	0.58
33:0:418:ASP:HB3	33:0:466:ASN:CB	2.33	0.58
1:A:251:G:O2'	1:A:2461:A:OP1	2.11	0.58
11:O:87:ILE:HD13	11:O:90:ASP:O	2.04	0.58
1:A:1125:C:O4'	8:K:133:ARG:NH1	2.36	0.58
10:N:14:ARG:NH2	10:N:50:ASP:O	2.36	0.58
33:0:392:GLU:OE1	33:0:395:ARG:NH2	2.37	0.58
1:A:420:U:O2'	1:A:421:A:O5'	2.22	0.57
1:A:843:C:O3'	5:G:62:ARG:NH2	2.37	0.57
5:G:109:ALA:O	5:G:112:SER:OG	2.17	0.57
13:Q:77:LYS:NZ	13:Q:84:GLY:O	2.32	0.57
1:A:2334:U:C5	6:H:133:LYS:HA	2.39	0.57
1:A:1501:U:O2'	1:A:1502:G:N7	2.37	0.57
1:A:2665:U:HO2'	4:F:46:TYR:HH	1.52	0.57
1:A:448:A:O2'	1:A:449:A:O4'	2.11	0.57
3:E:77:ARG:NH2	3:E:115:GLU:OE2	2.38	0.57
1:A:2106:A:OP1	1:A:2267:G:N2	2.33	0.57
1:A:1830:G:OP2	3:E:150:LYS:NZ	2.38	0.57
9:L:29:ASP:OD1	9:L:30:TYR:N	2.38	0.57
1:A:2830:A:O2'	1:A:2831:A:OP2	2.22	0.57
1:A:1757:G:O2'	1:A:1758:U:O5'	2.23	0.56
16:T:28:VAL:HG12	16:T:84:ILE:HG22	1.87	0.56
1:A:2054:C:OP2	4:F:153:ARG:NE	2.38	0.56
1:A:83:G:N2	1:A:102:A:OP2	2.22	0.56
1:A:1010:C:O2'	1:A:2302:A:N3	2.37	0.56
3:E:45:ASN:OD1	3:E:46:GLN:N	2.38	0.56
1:A:2332:G:H4'	6:H:123:ASP:HA	1.87	0.56
1:A:1127:U:O2	8:K:117:ASN:ND2	2.37	0.56
1:A:1782:G:OP1	16:T:93:ARG:NH1	2.38	0.56
1:A:2324:C:OP2	15:S:14:ARG:NE	2.37	0.55
14:R:99:THR:O	14:R:120:VAL:OXT	2.23	0.55
11:O:33:ALA:HB1	11:O:37:ASP:CB	2.36	0.55
33:0:410:GLN:NE2	33:0:467:ASN:HA	2.20	0.55
1:A:2038:G:OP1	19:W:41:ARG:NH1	2.40	0.55
1:A:675:C:O2	1:A:685:U:O2'	2.24	0.55
1:A:623:A:O2'	1:A:2048:U:OP1	2.24	0.55
1:A:2712:C:O2	11:O:76:TYR:OH	2.24	0.55
1:A:1883:A:O2'	1:A:1884:G:OP1	2.23	0.55
1:A:2684:G:O2'	1:A:2693:G:O6	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:83:ASN:O	12:P:119:LYS:NZ	2.24	0.55
33:0:409:GLN:NE2	33:0:492:GLY:HA2	2.21	0.55
1:A:777:C:OP1	1:A:1804:U:O2'	2.20	0.55
1:A:2406:A:O2'	15:S:120:PHE:OXT	2.24	0.55
12:P:116:LYS:NZ	12:P:118:GLU:OE2	2.41	0.54
1:A:1972:U:O2'	1:A:1973:U:OP2	2.26	0.54
7:I:89:GLU:OE1	7:I:89:GLU:N	2.40	0.54
33:0:410:GLN:OE1	33:0:467:ASN:N	2.40	0.54
1:A:339:A:O3'	21:Y:90:LYS:NZ	2.41	0.54
9:L:5:ILE:N	9:L:8:LYS:HZ3	2.05	0.54
1:A:593:A:O2'	1:A:594:C:O5'	2.26	0.54
1:A:2859:G:O2'	1:A:2860:A:O5'	2.24	0.54
1:A:1058:U:O4	10:N:31:SER:OG	2.24	0.54
3:E:142:HIS:ND1	3:E:193:GLY:O	2.40	0.54
6:H:158:THR:HG22	6:H:160:ALA:H	1.73	0.54
33:0:522:ASP:C	33:0:559:PRO:HG2	2.28	0.54
1:A:116:G:OP2	1:A:118:A:O2'	2.26	0.54
1:A:1110:C:OP1	8:K:80:LYS:NZ	2.41	0.54
3:E:154:LEU:O	3:E:156:ARG:N	2.41	0.54
22:2:44:A:H5'	33:0:286:ARG:NH2	2.20	0.54
1:A:373:A:N1	21:Y:15:LYS:NZ	2.56	0.53
1:A:2334:U:O4	6:H:151:GLY:C	2.46	0.53
33:0:185:LEU:HD11	33:0:192:LEU:HD13	1.91	0.53
6:H:75:ALA:CB	22:2:56:C:O2'	2.57	0.53
11:O:22:ILE:HD11	11:O:42:THR:HG23	1.89	0.53
11:O:120:GLU:OE1	16:T:65:SER:OG	2.25	0.53
4:F:43:ASN:OD1	4:F:44:ASP:N	2.41	0.53
1:A:490:A:OP1	5:G:46:GLN:N	2.42	0.53
7:I:158:TYR:O	7:I:172:ARG:NH1	2.39	0.53
10:N:30:SER:HA	10:N:33:VAL:HG22	1.91	0.53
15:S:24:GLY:O	15:S:47:ASP:N	2.42	0.53
1:A:1498:U:O2'	1:A:1499:A:N7	2.42	0.53
1:A:1981:A:OP1	11:O:44:LYS:NZ	2.31	0.53
13:Q:30:GLY:O	13:Q:134:ARG:NH2	2.41	0.53
10:N:50:ASP:OD1	10:N:122:LYS:NZ	2.42	0.53
13:Q:42:ILE:HD12	13:Q:97:VAL:HG21	1.92	0.52
1:A:287:G:N3	1:A:288:C:N4	2.58	0.52
1:A:488:U:O2	5:G:46:GLN:NE2	2.41	0.52
1:A:2233:C:OP1	3:E:147:LYS:NZ	2.42	0.52
1:A:236:A:H61	1:A:476:A:H61	1.57	0.52
1:A:1033:C:O2'	1:A:1046:A:N3	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2364:A:HO2'	1:A:2365:A:P	2.33	0.52
8:K:117:ASN:OD1	8:K:118:ALA:N	2.42	0.52
1:A:1113:A:OP1	33:0:384:LYS:NZ	2.43	0.52
1:A:1462:G:HO2'	1:A:1633:G:HO2'	1.58	0.52
15:S:30:ARG:NH2	15:S:47:ASP:OD1	2.43	0.52
22:2:31:C:H1'	33:0:125:ARG:NE	2.25	0.52
3:E:155:VAL:O	3:E:160:THR:OG1	2.19	0.52
1:A:2344:U:O2'	6:H:125:ARG:HG2	2.10	0.52
1:A:792:G:O2'	1:A:795:G:O2'	2.16	0.51
2:B:21:G:O2'	2:B:22:G:O5'	2.15	0.51
6:H:159:THR:HA	15:S:2:ILE:HG22	1.91	0.51
7:I:108:VAL:HG13	7:I:109:GLY:H	1.76	0.51
33:0:409:GLN:CD	33:0:492:GLY:C	2.69	0.51
1:A:2104:U:OP2	1:A:2267:G:O2'	2.16	0.51
1:A:2404:G:N2	1:A:2407:A:OP2	2.31	0.51
11:O:48:PRO:O	11:O:50:GLY:N	2.43	0.51
15:S:87:GLU:OE2	15:S:88:LYS:NZ	2.43	0.51
1:A:1759:U:HO2'	1:A:1760:A:P	2.34	0.51
14:R:8:ARG:O	14:R:13:ARG:NH2	2.43	0.51
1:A:274:A:HO2'	1:A:415:C:HO2'	1.41	0.51
1:A:2334:U:O4	6:H:151:GLY:N	2.44	0.51
1:A:2850:G:O6	4:F:163:ARG:NH1	2.44	0.51
33:0:447:ASN:H	33:0:448:PRO:CD	2.19	0.51
1:A:52:A:OP2	1:A:116:G:N1	2.43	0.51
1:A:1008:A:HO2'	1:A:2525:C:HO2'	1.59	0.51
33:0:523:SER:N	33:0:559:PRO:HG2	2.26	0.51
1:A:1452:C:H2'	1:A:1453:A:C8	2.46	0.51
1:A:1129:U:N3	1:A:1132:A:OP2	2.41	0.50
1:A:1993:G:O2'	1:A:1996:C:OP2	2.18	0.50
1:A:2337:G:C4	6:H:77:PHE:CE1	2.99	0.50
15:S:19:ARG:NH1	15:S:47:ASP:OD2	2.43	0.50
1:A:1460:G:O2'	1:A:1631:A:N6	2.44	0.50
1:A:1970:C:N4	1:A:1994:C:O4'	2.45	0.50
22:2:31:C:N1	33:0:125:ARG:CZ	2.73	0.50
7:I:59:GLN:OE1	7:I:62:HIS:ND1	2.44	0.50
1:A:2278:U:N3	1:A:2282:G:OP2	2.41	0.50
1:A:2279:G:N2	1:A:2305:G:OP1	2.45	0.50
33:0:128:ASN:OD1	33:0:129:ILE:N	2.45	0.50
9:L:7:THR:O	9:L:11:VAL:HG23	2.12	0.50
9:L:77:THR:O	9:L:80:ASN:ND2	2.44	0.50
1:A:1956:A:H2'	1:A:1957:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:8:LEU:CD2	7:I:52:THR:HG22	2.42	0.50
9:L:56:LYS:O	9:L:60:THR:OG1	2.18	0.50
33:0:94:ALA:HB2	33:0:101:ILE:HD11	1.94	0.49
1:A:274:A:O2'	1:A:415:C:O2'	2.15	0.49
1:A:420:U:HO2'	1:A:421:A:P	2.34	0.49
15:S:8:ASN:OD1	15:S:11:ARG:NH2	2.45	0.49
3:E:53:HIS:CE1	3:E:219:THR:HG23	2.48	0.49
33:0:409:GLN:NE2	33:0:493:SER:N	2.59	0.49
33:0:409:GLN:OE1	33:0:492:GLY:C	2.50	0.49
1:A:347:G:HO2'	1:A:348:U:P	2.35	0.49
1:A:1831:A:H2	1:A:1844:A:H62	1.61	0.49
1:A:2420:G:O2'	1:A:2421:A:O5'	2.30	0.49
3:E:176:LEU:O	3:E:179:GLY:N	2.40	0.49
17:U:90:VAL:HG12	18:V:39:LEU:HD13	1.94	0.49
33:0:9:TYR:O	33:0:12:THR:OG1	2.27	0.49
1:A:528:G:HO2'	1:A:529:C:P	2.36	0.49
1:A:2922:U:O3'	10:N:137:LYS:NZ	2.46	0.49
1:A:1189:A:OP1	10:N:28:ARG:NH1	2.43	0.49
8:K:33:VAL:HG12	8:K:64:ARG:HG2	1.94	0.49
1:A:13:A:O2'	1:A:15:G:N7	2.45	0.49
1:A:265:A:N3	1:A:477:A:O2'	2.39	0.49
1:A:1263:G:N2	1:A:1266:A:OP2	2.38	0.49
1:A:1462:G:O2'	1:A:1633:G:O2'	2.28	0.49
33:0:53:HIS:CD2	33:0:282:ALA:CA	2.89	0.49
1:A:1158:G:O2'	1:A:1159:U:O5'	2.31	0.49
1:A:630:A:H5'	5:G:89:VAL:HG21	1.93	0.48
1:A:1734:A:OP2	1:A:1743:A:N6	2.32	0.48
10:N:63:ILE:O	10:N:94:ARG:NH2	2.46	0.48
3:E:123:ASP:OD1	3:E:128:ASN:ND2	2.45	0.48
1:A:45:G:H21	1:A:183:A:H61	1.61	0.48
1:A:85:G:N1	1:A:98:U:C2	2.82	0.48
1:A:776:G:OP1	3:E:10:SER:OG	2.32	0.48
1:A:1339:A:H4'	1:A:1340:A:H5'	1.95	0.48
33:0:410:GLN:NE2	33:0:467:ASN:CA	2.74	0.48
1:A:2320:U:O2'	1:A:2403:C:O2	2.30	0.48
1:A:2333:G:HO2'	6:H:129:THR:CG2	2.27	0.48
1:A:2340:A:H2	6:H:79:LEU:CG	2.25	0.48
8:K:10:LYS:C	8:K:11:LEU:HD12	2.34	0.48
1:A:1759:U:H3	1:A:1774:A:H62	1.61	0.48
33:0:406:GLN:NE2	33:0:492:GLY:O	2.32	0.48
33:0:522:ASP:CA	33:0:559:PRO:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:A:N3	1:A:2515:G:O2'	2.42	0.48
12:P:125:ALA:HB3	12:P:128:PHE:HE1	1.79	0.48
1:A:1853:G:OP2	3:E:53:HIS:ND1	2.46	0.48
3:E:141:VAL:CG1	3:E:190:ALA:HB1	2.44	0.48
1:A:527:A:O2'	21:Y:42:LYS:O	2.32	0.48
1:A:2688:G:O2'	1:A:2690:G:N7	2.35	0.48
5:G:112:SER:O	5:G:115:SER:OG	2.23	0.48
8:K:18:ALA:HB3	8:K:43:ASN:ND2	2.28	0.48
1:A:965:A:N3	2:B:78:U:O2'	2.46	0.47
3:E:15:GLY:O	3:E:204:ASN:ND2	2.46	0.47
33:0:133:ASP:OD1	33:0:134:ALA:N	2.47	0.47
1:A:1516:A:N7	1:A:1569:A:N1	2.62	0.47
1:A:64:A:H61	1:A:90:A:H61	1.62	0.47
1:A:1475:G:HO2'	1:A:1476:C:H6	1.60	0.47
1:A:27:G:N2	1:A:558:G:O2'	2.47	0.47
1:A:2898:A:O2'	1:A:2899:C:OP1	2.28	0.47
15:S:63:LEU:O	15:S:76:LYS:NZ	2.37	0.47
17:U:90:VAL:HG23	17:U:91:ASN:H	1.79	0.47
7:I:64:ALA:O	7:I:68:THR:HG23	2.15	0.47
1:A:461:C:O2	1:A:1893:U:O2'	2.30	0.47
1:A:1417:A:O2'	1:A:1418:U:OP2	2.25	0.47
1:A:1574:G:N1	1:A:1592:A:OP2	2.43	0.47
1:A:2333:G:HO2'	6:H:129:THR:HG22	1.80	0.47
1:A:2335:U:H2'	1:A:2336:G:C4	2.49	0.47
6:H:135:GLN:HG2	6:H:141:ILE:HG21	1.96	0.47
10:N:108:GLY:O	10:N:112:LYS:NZ	2.48	0.47
16:T:34:GLU:OE2	16:T:39:ARG:NH2	2.48	0.47
1:A:177:G:HO2'	1:A:178:A:P	2.36	0.47
1:A:1846:G:OP2	3:E:156:ARG:NH2	2.44	0.47
1:A:2593:A:OP1	1:A:2677:G:O2'	2.29	0.47
9:L:14:GLU:O	9:L:17:SER:OG	2.21	0.47
1:A:1092:A:N3	9:L:62:ARG:NH1	2.63	0.47
1:A:1252:G:O2'	1:A:1253:A:OP2	2.33	0.47
14:R:18:ARG:O	14:R:21:THR:OG1	2.30	0.47
1:A:1645:C:OP1	20:X:77:ARG:NH1	2.48	0.46
32:1:67:THR:O	32:1:67:THR:HG23	2.16	0.46
1:A:2340:A:C2	6:H:77:PHE:HB3	2.51	0.46
1:A:2823:C:O2'	1:A:2824:G:O4'	2.25	0.46
17:U:97:ASP:OD1	17:U:101:ASN:ND2	2.49	0.46
1:A:312:G:C2	1:A:405:U:O4	2.68	0.46
19:W:58:ALA:O	19:W:63:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2063:U:HO2'	1:A:2064:G:P	2.39	0.46
1:A:2334:U:C4	6:H:151:GLY:CA	2.66	0.46
11:O:113:LYS:O	11:O:117:LEU:HD23	2.16	0.46
17:U:102:ASP:OD2	18:V:2:TYR:OH	2.28	0.46
22:2:44:A:H5"	33:0:286:ARG:NH2	2.17	0.46
1:A:1698:G:O6	14:R:7:GLY:N	2.44	0.46
11:O:87:ILE:HD13	11:O:90:ASP:H	1.81	0.46
21:Y:85:VAL:HG13	21:Y:88:GLY:O	2.15	0.46
33:0:240:ILE:HG23	33:0:240:ILE:O	2.16	0.46
1:A:523:G:N1	1:A:526:A:OP2	2.45	0.46
1:A:2334:U:OP2	6:H:131:GLY:N	2.49	0.46
4:F:15:VAL:O	4:F:23:ILE:N	2.49	0.46
14:R:17:LEU:O	14:R:21:THR:HG23	2.15	0.46
33:0:21:GLY:N	33:0:88:ILE:O	2.44	0.46
8:K:78:LEU:HD13	8:K:108:ILE:HG23	1.98	0.46
1:A:1036:A:HO2'	1:A:1037:C:P	2.33	0.46
17:U:88:ILE:HG22	17:U:88:ILE:O	2.15	0.46
1:A:273:A:OP2	1:A:297:G:N2	2.42	0.45
1:A:2080:A:N6	1:A:2643:A:O2'	2.45	0.45
4:F:111:THR:OG1	4:F:170:THR:HG22	2.16	0.45
6:H:80:ARG:NE	22:2:56:C:C4	2.84	0.45
9:L:34:ASN:O	9:L:38:VAL:HG23	2.16	0.45
33:0:246:VAL:O	33:0:246:VAL:HG13	2.16	0.45
9:L:82:ILE:HD12	9:L:84:PHE:CE2	2.51	0.45
12:P:86:ALA:O	12:P:89:THR:HG22	2.16	0.45
22:2:56:C:H2'	22:2:57:G:O4'	2.17	0.45
1:A:610:U:OP1	18:V:81:ASN:ND2	2.47	0.45
8:K:73:PRO:CG	8:K:78:LEU:HD21	2.46	0.45
22:2:7:U:H3'	22:2:8:U:H5'	1.98	0.45
22:2:42:G:O3'	33:0:32:LYS:NZ	2.50	0.45
1:A:287:G:H21	1:A:288:C:H42	1.63	0.45
1:A:1542:A:N3	1:A:1625:C:O2'	2.49	0.45
4:F:28:ILE:HD12	4:F:188:ILE:HD12	1.99	0.45
1:A:187:C:HO2'	1:A:188:C:H6	1.64	0.45
1:A:1485:A:H2	1:A:1600:G:H21	1.65	0.45
1:A:2703:G:H4'	11:O:30:ARG:HE	1.81	0.45
4:F:40:THR:OG1	4:F:43:ASN:OD1	2.31	0.45
6:H:12:ILE:HD11	6:H:173:VAL:HG12	1.98	0.45
19:W:50:VAL:HG13	19:W:105:ILE:HD12	1.98	0.45
33:0:348:VAL:O	33:0:359:ILE:N	2.41	0.45
1:A:747:G:O2'	1:A:1677:A:N3	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1895:A:N6	1:A:1904:G:O2'	2.49	0.45
3:E:162:ALA:HB1	3:E:175:ARG:O	2.17	0.45
19:W:22:ASP:OD1	19:W:25:ARG:NH1	2.46	0.45
1:A:64:A:H61	1:A:90:A:N6	2.14	0.45
1:A:2341:U:H5'	6:H:85:ILE:HD12	1.94	0.45
6:H:125:ARG:HG3	15:S:1:MET:CG	2.44	0.45
1:A:2053:C:O2'	1:A:2054:C:O5'	2.34	0.45
4:F:48:ALA:HB1	4:F:83:LEU:O	2.17	0.45
8:K:73:PRO:HG2	8:K:78:LEU:HD21	1.99	0.45
1:A:569:C:O2	1:A:598:U:O2'	2.34	0.44
4:F:206:VAL:O	4:F:206:VAL:HG13	2.16	0.44
9:L:28:VAL:HG12	9:L:108:ILE:HA	1.98	0.44
11:O:24:VAL:HG11	11:O:33:ALA:HB2	1.99	0.44
33:0:171:ILE:N	33:0:199:HIS:O	2.50	0.44
1:A:2063:U:O2'	1:A:2064:G:O5'	2.33	0.44
1:A:2252:A:OP1	3:E:170:LYS:NZ	2.45	0.44
1:A:2344:U:H4'	1:A:2345:U:OP1	2.17	0.44
13:Q:44:ASN:OD1	13:Q:45:ARG:N	2.50	0.44
33:0:525:SER:O	33:0:527:PRO:CD	2.64	0.44
1:A:1968:U:OP1	1:A:2633:U:O2'	2.33	0.44
3:E:35:ALA:O	3:E:62:TYR:N	2.51	0.44
4:F:134:SER:OG	4:F:135:HIS:N	2.50	0.44
7:I:166:GLU:OE1	7:I:166:GLU:N	2.42	0.44
22:2:47:U:O2'	22:2:50:G:OP1	2.33	0.44
1:A:1849:U:OP1	3:E:177:ASN:ND2	2.50	0.44
1:A:2344:U:H2'	1:A:2345:U:C6	2.52	0.44
22:2:38:C:H2'	22:2:39:G:C8	2.52	0.44
1:A:1699:A:N6	1:A:2035:C:O4'	2.48	0.44
9:L:108:ILE:HG22	9:L:108:ILE:O	2.18	0.44
33:0:7:PHE:HA	33:0:254:LEU:HD11	1.99	0.44
7:I:108:VAL:HG13	7:I:109:GLY:N	2.32	0.44
13:Q:72:LYS:O	13:Q:94:VAL:N	2.48	0.44
1:A:492:C:H2'	1:A:493:G:O4'	2.18	0.43
1:A:617:G:N2	1:A:2060:A:OP1	2.48	0.43
1:A:751:G:H2'	1:A:773:G:H22	1.82	0.43
1:A:2817:C:O2'	1:A:2834:A:N3	2.45	0.43
18:V:36:GLU:OE1	18:V:36:GLU:N	2.51	0.43
19:W:23:LEU:O	19:W:27:LYS:NZ	2.45	0.43
1:A:1163:U:H2'	1:A:1164:C:C6	2.53	0.43
1:A:2630:C:H5"	22:2:75:C:OP1	2.17	0.43
17:U:88:ILE:O	17:U:90:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:A:H62	1:A:979:U:H3	1.67	0.43
1:A:1783:C:OP1	16:T:94:ARG:NE	2.51	0.43
2:B:107:G:HO2'	2:B:108:C:H6	1.65	0.43
22:2:31:C:O2	33:0:125:ARG:CZ	2.50	0.43
1:A:1158:G:HO2'	1:A:1159:U:P	2.40	0.43
1:A:85:G:C6	1:A:98:U:N3	2.86	0.43
1:A:2688:G:OP2	7:I:159:LYS:NZ	2.47	0.43
16:T:71:GLU:OE1	16:T:101:ARG:NH1	2.51	0.43
14:R:26:ILE:O	14:R:82:LYS:NZ	2.51	0.43
12:P:125:ALA:HB3	12:P:128:PHE:CE1	2.54	0.43
14:R:85:SER:OG	14:R:86:ASP:N	2.52	0.43
22:2:57:G:C2'	22:2:58:A:H5'	2.48	0.43
3:E:157:SER:OG	3:E:158:ALA:N	2.52	0.43
10:N:96:ASN:O	10:N:127:ARG:NH2	2.47	0.43
33:0:242:ASN:HB3	33:0:266:ARG:HG2	2.00	0.43
1:A:2670:A:OP1	10:N:77:ARG:NH1	2.48	0.43
7:I:21:ASP:OD1	7:I:24:THR:OG1	2.31	0.43
22:2:69:C:H2'	22:2:70:U:C6	2.54	0.42
1:A:273:A:OP2	1:A:297:G:N1	2.49	0.42
1:A:1464:A:H2	1:A:1627:A:H62	1.67	0.42
1:A:2316:A:O2'	1:A:2317:A:O5'	2.34	0.42
3:E:264:ASN:OD1	3:E:265:LYS:N	2.51	0.42
1:A:354:A:OP1	21:Y:14:GLY:N	2.52	0.42
1:A:1058:U:O2	10:N:28:ARG:NH1	2.52	0.42
7:I:55:ARG:NH2	7:I:58:ASP:OD1	2.51	0.42
1:A:2337:G:C6	6:H:77:PHE:CE2	3.07	0.42
6:H:125:ARG:O	15:S:1:MET:HB2	2.20	0.42
33:0:409:GLN:HE22	33:0:493:SER:N	2.18	0.42
1:A:342:A:N1	1:A:366:A:O2'	2.47	0.42
1:A:2337:G:N3	6:H:77:PHE:HE1	2.14	0.42
7:I:38:PHE:CE2	7:I:73:LEU:HD21	2.55	0.42
10:N:6:MET:SD	10:N:6:MET:N	2.93	0.42
15:S:82:ALA:HA	15:S:118:LEU:HD11	2.02	0.42
1:A:1159:U:O2'	1:A:1160:G:OP2	2.30	0.42
1:A:2089:A:O2'	1:A:2090:G:OP2	2.37	0.42
11:O:24:VAL:CG1	11:O:33:ALA:HB2	2.49	0.42
1:A:1283:U:O2'	12:P:6:LEU:O	2.35	0.42
6:H:73:SER:CB	22:2:56:C:C1'	2.87	0.42
13:Q:28:HIS:O	13:Q:134:ARG:NH2	2.53	0.42
20:X:30:VAL:HG12	20:X:31:ASP:N	2.35	0.42
1:A:1046:A:OP2	1:A:1200:G:N1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1765:G:N2	1:A:1768:A:OP2	2.52	0.41
9:L:55:TYR:CE2	9:L:82:ILE:HD11	2.55	0.41
11:O:34:ASN:O	11:O:62:ILE:HG21	2.20	0.41
11:O:105:GLU:OE1	11:O:105:GLU:N	2.52	0.41
33:0:335:ASN:ND2	33:0:348:VAL:HG13	2.35	0.41
1:A:2888:C:P	16:T:91:LYS:HZ1	2.43	0.41
6:H:36:ILE:CG2	6:H:57:LEU:HD11	2.50	0.41
1:A:2343:A:H2'	1:A:2344:U:C6	2.55	0.41
5:G:167:ALA:HA	5:G:170:ILE:HD13	2.02	0.41
1:A:376:A:O2'	1:A:378:C:OP2	2.29	0.41
1:A:1452:C:H2'	1:A:1453:A:H8	1.84	0.41
1:A:2577:G:O2'	11:O:4:GLN:NE2	2.50	0.41
2:B:48:G:HO2'	2:B:49:G:P	2.42	0.41
17:U:26:GLY:O	17:U:29:HIS:ND1	2.53	0.41
20:X:84:THR:OG1	20:X:85:ALA:O	2.38	0.41
22:2:37:A:H2'	22:2:38:C:C6	2.56	0.41
1:A:1017:C:O2'	1:A:1029:A:N3	2.49	0.41
1:A:2341:U:H4'	6:H:68:THR:OG1	2.21	0.41
1:A:2466:C:HO2'	1:A:2628:G:HO2'	1.65	0.41
22:2:43:G:P	33:0:32:LYS:HZ2	2.43	0.41
1:A:939:G:O2'	1:A:940:G:O5'	2.38	0.41
1:A:1322:G:N1	1:A:1325:A:OP2	2.54	0.41
6:H:47:ALA:O	6:H:50:ILE:HG22	2.20	0.41
13:Q:12:GLU:O	13:Q:87:LYS:NZ	2.54	0.41
17:U:69:ALA:O	17:U:74:LEU:N	2.48	0.41
33:0:515:ALA:HB1	33:0:559:PRO:CD	2.35	0.41
1:A:221:G:H22	1:A:238:U:H4'	1.86	0.41
1:A:1681:U:O2'	1:A:1789:A:N3	2.48	0.41
1:A:2233:C:OP2	3:E:150:LYS:NZ	2.53	0.41
33:0:350:ASN:OD1	33:0:351:TYR:N	2.54	0.41
1:A:1366:C:O2'	14:R:108:ARG:NH1	2.45	0.41
1:A:1965:A:OP2	1:A:1991:C:N4	2.47	0.41
6:H:12:ILE:HG12	6:H:172:GLN:HB3	2.03	0.41
1:A:551:A:O2'	1:A:552:G:O5'	2.38	0.41
1:A:2875:A:OP2	1:A:2891:G:N1	2.49	0.41
2:B:35:C:O2	15:S:103:HIS:NE2	2.44	0.41
7:I:163:ILE:HD12	7:I:163:ILE:H	1.86	0.41
9:L:12:VAL:HG23	9:L:63:ALA:HB2	2.03	0.41
14:R:86:ASP:O	14:R:89:THR:OG1	2.34	0.41
33:0:46:GLN:N	33:0:46:GLN:OE1	2.53	0.41
33:0:139:ILE:HD13	33:0:156:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:0:522:ASP:HA	33:0:559:PRO:HG2	2.03	0.41
1:A:283:G:O6	1:A:287:G:N2	2.53	0.41
1:A:775:G:H3'	1:A:776:G:H5'	2.03	0.41
1:A:2774:C:H42	1:A:2788:G:H1	1.69	0.41
5:G:53:ASN:OD1	5:G:54:ARG:N	2.52	0.41
1:A:2667:G:HO2'	1:A:2668:A:H8	1.69	0.40
3:E:139:THR:N	3:E:163:GLN:OE1	2.54	0.40
7:I:81:SER:OG	7:I:82:LYS:N	2.54	0.40
1:A:1773:G:HO2'	1:A:1774:A:P	2.44	0.40
5:G:146:LEU:O	5:G:147:SER:OG	2.33	0.40
10:N:139:GLU:OE1	10:N:139:GLU:N	2.55	0.40
33:0:350:ASN:ND2	33:0:355:GLU:OE2	2.54	0.40
1:A:1164:C:H2'	1:A:1165:U:O4'	2.21	0.40
1:A:1691:A:O2'	1:A:1692:U:OP2	2.24	0.40
1:A:2713:U:OP2	16:T:51:ARG:NH1	2.54	0.40
7:I:51:LEU:HD13	7:I:52:THR:N	2.36	0.40
7:I:102:ASN:OD1	7:I:103:LYS:N	2.55	0.40
8:K:33:VAL:HG12	8:K:64:ARG:CG	2.52	0.40
9:L:26:ILE:HG21	9:L:96:LEU:HD13	2.03	0.40
11:O:103:ALA:HB1	11:O:105:GLU:OE1	2.20	0.40
13:Q:26:GLU:OE1	13:Q:26:GLU:N	2.55	0.40
14:R:85:SER:O	14:R:89:THR:HG23	2.22	0.40
15:S:80:LEU:HD21	15:S:84:ARG:CZ	2.51	0.40
9:L:119:THR:HG22	9:L:120:VAL:N	2.36	0.40
20:X:30:VAL:HG12	20:X:31:ASP:OD1	2.22	0.40
1:A:2855:G:OP1	4:F:78:ARG:NH2	2.55	0.40
6:H:8:TYR:HA	6:H:12:ILE:HD12	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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
3	E	270/277 (98%)	256 (95%)	12 (4%)	2 (1%)	22 61
4	F	204/209 (98%)	187 (92%)	17 (8%)	0	100 100
5	G	203/207 (98%)	184 (91%)	19 (9%)	0	100 100
6	H	174/179 (97%)	166 (95%)	8 (5%)	0	100 100
7	I	173/179 (97%)	153 (88%)	20 (12%)	0	100 100
8	K	130/141 (92%)	115 (88%)	15 (12%)	0	100 100
9	L	107/166 (64%)	106 (99%)	1 (1%)	0	100 100
10	N	140/145 (97%)	127 (91%)	13 (9%)	0	100 100
11	O	120/122 (98%)	105 (88%)	15 (12%)	0	100 100
12	P	144/146 (99%)	136 (94%)	8 (6%)	0	100 100
13	Q	133/144 (92%)	117 (88%)	16 (12%)	0	100 100
14	R	117/120 (98%)	106 (91%)	11 (9%)	0	100 100
15	S	118/120 (98%)	105 (89%)	12 (10%)	1 (1%)	19 58
16	T	113/115 (98%)	105 (93%)	8 (7%)	0	100 100
17	U	115/119 (97%)	106 (92%)	8 (7%)	1 (1%)	17 56
18	V	98/102 (96%)	80 (82%)	18 (18%)	0	100 100
19	W	107/113 (95%)	94 (88%)	13 (12%)	0	100 100
20	X	88/95 (93%)	83 (94%)	5 (6%)	0	100 100
21	Y	99/103 (96%)	84 (85%)	15 (15%)	0	100 100
23	a	79/94 (84%)	71 (90%)	8 (10%)	0	100 100
24	b	56/62 (90%)	50 (89%)	6 (11%)	0	100 100
25	c	63/66 (96%)	61 (97%)	2 (3%)	0	100 100
26	d	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
27	f	51/59 (86%)	47 (92%)	4 (8%)	0	100 100
28	g	46/49 (94%)	41 (89%)	5 (11%)	0	100 100
29	h	42/44 (96%)	41 (98%)	1 (2%)	0	100 100
30	i	62/66 (94%)	59 (95%)	3 (5%)	0	100 100
31	j	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
32	1	81/86 (94%)	79 (98%)	2 (2%)	0	100 100
33	0	518/599 (86%)	476 (92%)	39 (8%)	3 (1%)	25 64
All	All	3742/4023 (93%)	3428 (92%)	307 (8%)	7 (0%)	50 79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	156	ARG
15	S	2	ILE
33	0	491	PRO
3	E	155	VAL
33	0	447	ASN
33	0	538	LYS
17	U	90	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
3	E	220/225 (98%)	220 (100%)	0	100	100
4	F	167/170 (98%)	167 (100%)	0	100	100
5	G	169/170 (99%)	168 (99%)	1 (1%)	86	94
6	H	151/154 (98%)	145 (96%)	6 (4%)	31	66
7	I	148/151 (98%)	148 (100%)	0	100	100
8	K	102/110 (93%)	102 (100%)	0	100	100
9	L	98/138 (71%)	97 (99%)	1 (1%)	76	90
10	N	120/123 (98%)	120 (100%)	0	100	100
11	O	101/101 (100%)	101 (100%)	0	100	100
12	P	110/110 (100%)	109 (99%)	1 (1%)	78	91
13	Q	109/116 (94%)	108 (99%)	1 (1%)	78	91
14	R	99/100 (99%)	98 (99%)	1 (1%)	76	90
15	S	93/93 (100%)	93 (100%)	0	100	100
16	T	100/100 (100%)	99 (99%)	1 (1%)	76	90
17	U	96/98 (98%)	95 (99%)	1 (1%)	76	90
18	V	83/84 (99%)	83 (100%)	0	100	100
19	W	90/93 (97%)	88 (98%)	2 (2%)	52	79
20	X	81/85 (95%)	81 (100%)	0	100	100
21	Y	85/87 (98%)	84 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	a	63/74 (85%)	62 (98%)	1 (2%)	62 84
24	b	47/50 (94%)	47 (100%)	0	100 100
25	c	56/57 (98%)	56 (100%)	0	100 100
26	d	52/53 (98%)	52 (100%)	0	100 100
27	f	47/53 (89%)	46 (98%)	1 (2%)	53 79
28	g	46/47 (98%)	46 (100%)	0	100 100
29	h	39/39 (100%)	38 (97%)	1 (3%)	46 76
30	i	54/56 (96%)	54 (100%)	0	100 100
31	j	35/35 (100%)	35 (100%)	0	100 100
32	1	73/75 (97%)	72 (99%)	1 (1%)	67 86
33	0	374/527 (71%)	372 (100%)	2 (0%)	88 95
All	All	3108/3374 (92%)	3086 (99%)	22 (1%)	84 94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	G	10	ASN
6	H	11	GLU
6	H	64	LYS
6	H	112	ARG
6	H	120	LYS
6	H	150	ARG
6	H	165	GLU
9	L	23	LYS
12	P	114	ASN
13	Q	60	ARG
14	R	75	ASN
16	T	1	MET
17	U	72	ASN
19	W	11	ARG
19	W	37	ASN
21	Y	89	LYS
23	a	22	ARG
27	f	7	ARG
29	h	28	ARG
32	1	63	LEU
33	0	116	ARG
33	0	154	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
17	U	101	ASN
21	Y	67	ASN
30	i	60	GLN
32	1	61	ASN
33	0	326	GLN
33	0	335	ASN
33	0	385	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2808/2926 (95%)	667 (23%)	61 (2%)
2	B	111/119 (93%)	30 (27%)	3 (2%)
22	2	67/76 (88%)	15 (22%)	3 (4%)
All	All	2986/3121 (95%)	712 (23%)	67 (2%)

All (712) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	46	C
1	A	55	G
1	A	61	A
1	A	62	C
1	A	63	G
1	A	71	A
1	A	74	U
1	A	75	G
1	A	76	C
1	A	77	U
1	A	78	U
1	A	79	C
1	A	80	G

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Mol	Chain	Res	Type
1	A	84	A
1	A	85	G
1	A	86	C
1	A	87	U
1	A	89	U
1	A	90	A
1	A	92	G
1	A	93	C
1	A	96	G
1	A	101	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	125	A
1	A	126	A
1	A	133	A
1	A	141	U
1	A	150	A
1	A	164	U
1	A	175	G
1	A	176	A
1	A	178	A
1	A	179	A
1	A	183	A
1	A	184	G
1	A	185	A
1	A	188	C
1	A	189	G
1	A	191	G
1	A	199	A
1	A	200	A
1	A	202	A
1	A	216	A
1	A	219	A
1	A	224	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	229	A
1	A	231	A
1	A	232	U
1	A	233	G

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Mol	Chain	Res	Type
1	A	234	C
1	A	235	G
1	A	236	A
1	A	244	A
1	A	251	G
1	A	252	C
1	A	253	G
1	A	258	A
1	A	266	U
1	A	267	C
1	A	270	C
1	A	275	A
1	A	283	G
1	A	284	C
1	A	286	U
1	A	287	G
1	A	288	C
1	A	290	U
1	A	291	C
1	A	298	U
1	A	301	U
1	A	302	A
1	A	309	U
1	A	310	C
1	A	314	A
1	A	321	U
1	A	329	A
1	A	345	A
1	A	346	G
1	A	348	U
1	A	349	C
1	A	360	C
1	A	367	G
1	A	368	G
1	A	373	A
1	A	374	A
1	A	375	C
1	A	379	C
1	A	387	C
1	A	394	U
1	A	402	U
1	A	405	U

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Mol	Chain	Res	Type
1	A	407	A
1	A	410	G
1	A	411	G
1	A	412	A
1	A	413	U
1	A	418	A
1	A	419	G
1	A	420	U
1	A	421	A
1	A	427	G
1	A	432	C
1	A	433	G
1	A	434	U
1	A	435	G
1	A	444	U
1	A	458	G
1	A	471	G
1	A	483	C
1	A	491	C
1	A	495	U
1	A	498	U
1	A	502	C
1	A	504	A
1	A	505	G
1	A	528	G
1	A	529	C
1	A	533	C
1	A	542	G
1	A	550	G
1	A	551	A
1	A	554	U
1	A	555	C
1	A	556	C
1	A	559	A
1	A	564	G
1	A	573	C
1	A	576	G
1	A	577	U
1	A	578	A
1	A	579	G
1	A	592	A
1	A	593	A

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Mol	Chain	Res	Type
1	A	594	C
1	A	595	G
1	A	599	G
1	A	607	G
1	A	615	U
1	A	617	G
1	A	618	A
1	A	619	A
1	A	631	G
1	A	646	A
1	A	647	A
1	A	648	G
1	A	649	G
1	A	658	A
1	A	659	A
1	A	662	U
1	A	667	A
1	A	673	A
1	A	677	A
1	A	683	A
1	A	690	A
1	A	691	U
1	A	700	U
1	A	701	G
1	A	702	A
1	A	733	U
1	A	752	A
1	A	764	C
1	A	765	A
1	A	777	C
1	A	787	C
1	A	788	G
1	A	792	G
1	A	794	U
1	A	795	G
1	A	804	G
1	A	810	G
1	A	811	A
1	A	812	G
1	A	822	G
1	A	829	A
1	A	830	A

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Mol	Chain	Res	Type
1	A	831	U
1	A	832	G
1	A	837	U
1	A	838	C
1	A	839	G
1	A	847	A
1	A	852	G
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	877	G
1	A	892	U
1	A	908	A
1	A	913	A
1	A	916	G
1	A	918	U
1	A	929	G
1	A	939	G
1	A	940	G
1	A	942	U
1	A	943	A
1	A	944	C
1	A	946	G
1	A	948	A
1	A	954	U
1	A	957	A
1	A	959	C
1	A	961	C
1	A	962	C
1	A	964	A
1	A	973	G
1	A	977	U
1	A	978	A
1	A	979	U
1	A	980	C
1	A	987	A
1	A	991	A
1	A	992	G
1	A	999	A
1	A	1003	A
1	A	1005	A

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Mol	Chain	Res	Type
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1029	A
1	A	1036	A
1	A	1037	C
1	A	1042	A
1	A	1051	C
1	A	1058	U
1	A	1059	A
1	A	1063	G
1	A	1067	A
1	A	1068	G
1	A	1069	U
1	A	1071	G
1	A	1073	A
1	A	1079	U
1	A	1081	U
1	A	1084	A
1	A	1085	G
1	A	1091	U
1	A	1092	A
1	A	1093	G
1	A	1102	G
1	A	1103	A
1	A	1108	G
1	A	1115	A
1	A	1116	A
1	A	1118	C
1	A	1119	A
1	A	1129	U
1	A	1130	A
1	A	1133	G
1	A	1134	A
1	A	1143	U
1	A	1147	U
1	A	1156	G
1	A	1157	A
1	A	1158	G
1	A	1159	U
1	A	1160	G
1	A	1161	A

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Mol	Chain	Res	Type
1	A	1162	C
1	A	1163	U
1	A	1173	A
1	A	1174	A
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1179	A
1	A	1181	C
1	A	1182	G
1	A	1185	G
1	A	1188	A
1	A	1189	A
1	A	1197	A
1	A	1201	A
1	A	1203	G
1	A	1209	G
1	A	1236	G
1	A	1251	U
1	A	1252	G
1	A	1259	G
1	A	1260	A
1	A	1278	G
1	A	1284	A
1	A	1293	A
1	A	1295	U
1	A	1296	G
1	A	1305	A
1	A	1306	G
1	A	1307	U
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1319	G
1	A	1323	A
1	A	1333	C
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1343	C

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Mol	Chain	Res	Type
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1363	G
1	A	1364	C
1	A	1365	U
1	A	1366	C
1	A	1368	U
1	A	1370	C
1	A	1371	G
1	A	1372	C
1	A	1375	A
1	A	1376	G
1	A	1380	U
1	A	1384	C
1	A	1385	G
1	A	1388	A
1	A	1389	C
1	A	1391	U
1	A	1404	A
1	A	1417	A
1	A	1418	U
1	A	1424	A
1	A	1425	C
1	A	1426	A
1	A	1427	G
1	A	1428	G
1	A	1431	G
1	A	1434	A
1	A	1435	U
1	A	1436	U
1	A	1442	A
1	A	1448	U
1	A	1449	C
1	A	1451	U
1	A	1459	U
1	A	1460	G
1	A	1465	A
1	A	1466	U
1	A	1472	G
1	A	1473	A
1	A	1474	C

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Mol	Chain	Res	Type
1	A	1476	C
1	A	1481	G
1	A	1489	U
1	A	1490	A
1	A	1499	A
1	A	1500	U
1	A	1501	U
1	A	1502	G
1	A	1506	A
1	A	1507	U
1	A	1508	C
1	A	1516	A
1	A	1525	G
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	G
1	A	1532	A
1	A	1533	A
1	A	1536	A
1	A	1539	C
1	A	1540	A
1	A	1542	A
1	A	1543	U
1	A	1545	C
1	A	1550	C
1	A	1551	C
1	A	1553	A
1	A	1556	A
1	A	1558	G
1	A	1559	C
1	A	1560	U
1	A	1561	G
1	A	1566	G
1	A	1568	G
1	A	1569	A
1	A	1570	U
1	A	1571	G
1	A	1576	G
1	A	1577	C

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Mol	Chain	Res	Type
1	A	1595	U
1	A	1602	U
1	A	1608	A
1	A	1614	A
1	A	1615	A
1	A	1617	A
1	A	1626	U
1	A	1632	G
1	A	1652	C
1	A	1653	A
1	A	1655	A
1	A	1661	A
1	A	1672	A
1	A	1684	U
1	A	1685	A
1	A	1692	U
1	A	1693	C
1	A	1696	G
1	A	1697	A
1	A	1699	A
1	A	1700	A
1	A	1705	C
1	A	1708	U
1	A	1710	A
1	A	1712	G
1	A	1713	A
1	A	1719	G
1	A	1738	U
1	A	1743	A
1	A	1745	A
1	A	1748	G
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1761	G
1	A	1762	G
1	A	1766	C
1	A	1767	A
1	A	1768	A
1	A	1771	C
1	A	1776	A

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Mol	Chain	Res	Type
1	A	1778	A
1	A	1779	G
1	A	1782	G
1	A	1785	G
1	A	1793	G
1	A	1802	A
1	A	1811	C
1	A	1812	A
1	A	1814	A
1	A	1820	A
1	A	1829	C
1	A	1830	G
1	A	1839	A
1	A	1841	G
1	A	1845	A
1	A	1846	G
1	A	1864	G
1	A	1865	C
1	A	1867	C
1	A	1872	C
1	A	1877	A
1	A	1882	A
1	A	1883	A
1	A	1884	G
1	A	1885	A
1	A	1887	G
1	A	1891	G
1	A	1898	G
1	A	1899	U
1	A	1904	G
1	A	1935	G
1	A	1948	A
1	A	1958	G
1	A	1959	G
1	A	1960	U
1	A	1967	A
1	A	1968	U
1	A	1969	U
1	A	1972	U
1	A	1973	U
1	A	1984	U
1	A	1989	A

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Mol	Chain	Res	Type
1	A	1993	G
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2020	U
1	A	2022	U
1	A	2025	C
1	A	2026	A
1	A	2049	A
1	A	2051	U
1	A	2052	A
1	A	2054	C
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2064	G
1	A	2072	C
1	A	2078	A
1	A	2081	G
1	A	2084	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2098	G
1	A	2109	G
1	A	2121	U
1	A	2123	A
1	A	2125	U
1	A	2128	U
1	A	2129	G
1	A	2219	G
1	A	2227	A
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2240	U
1	A	2245	G
1	A	2246	G
1	A	2249	G
1	A	2252	A
1	A	2254	A

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Mol	Chain	Res	Type
1	A	2255	C
1	A	2267	G
1	A	2268	G
1	A	2280	G
1	A	2296	A
1	A	2308	G
1	A	2312	C
1	A	2315	A
1	A	2316	A
1	A	2317	A
1	A	2323	C
1	A	2325	U
1	A	2331	U
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2339	A
1	A	2340	A
1	A	2341	U
1	A	2343	A
1	A	2345	U
1	A	2347	G
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2351	A
1	A	2354	G
1	A	2356	A
1	A	2363	C
1	A	2364	A
1	A	2374	G
1	A	2376	C
1	A	2379	C
1	A	2390	A
1	A	2401	G
1	A	2412	G
1	A	2414	C
1	A	2415	U
1	A	2417	A
1	A	2420	G

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Mol	Chain	Res	Type
1	A	2421	A
1	A	2425	G
1	A	2430	U
1	A	2431	U
1	A	2435	C
1	A	2451	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2474	G
1	A	2476	G
1	A	2477	A
1	A	2488	A
1	A	2505	A
1	A	2507	A
1	A	2509	C
1	A	2511	A
1	A	2520	U
1	A	2523	G
1	A	2527	C
1	A	2531	G
1	A	2532	A
1	A	2533	U
1	A	2534	G
1	A	2542	A
1	A	2547	A
1	A	2548	U
1	A	2549	C
1	A	2564	G
1	A	2583	U
1	A	2591	U
1	A	2595	A
1	A	2596	G
1	A	2598	G

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Mol	Chain	Res	Type
1	A	2601	A
1	A	2602	C
1	A	2607	G
1	A	2611	G
1	A	2613	U
1	A	2631	A
1	A	2632	G
1	A	2638	U
1	A	2639	C
1	A	2642	U
1	A	2644	U
1	A	2652	G
1	A	2659	G
1	A	2665	U
1	A	2674	G
1	A	2689	A
1	A	2690	G
1	A	2696	C
1	A	2711	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2743	G
1	A	2755	U
1	A	2762	A
1	A	2764	G
1	A	2765	G
1	A	2773	G
1	A	2779	A
1	A	2785	U
1	A	2789	C
1	A	2794	A
1	A	2798	C
1	A	2806	G
1	A	2807	A
1	A	2808	U
1	A	2818	C
1	A	2820	U
1	A	2823	C
1	A	2824	G
1	A	2826	A
1	A	2831	A

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Mol	Chain	Res	Type
1	A	2843	G
1	A	2859	G
1	A	2860	A
1	A	2868	G
1	A	2886	C
1	A	2892	G
1	A	2897	G
1	A	2899	C
1	A	2900	A
1	A	2901	G
1	A	2905	C
1	A	2911	G
1	A	2916	A
1	A	2917	G
1	A	2918	G
1	A	2925	C
2	B	10	G
2	B	13	A
2	B	15	C
2	B	19	G
2	B	22	G
2	B	23	U
2	B	24	C
2	B	32	U
2	B	33	U
2	B	35	C
2	B	38	U
2	B	39	A
2	B	40	C
2	B	48	G
2	B	49	G
2	B	50	A
2	B	53	U
2	B	54	U
2	B	55	A
2	B	56	A
2	B	62	U
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	97	A

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Mol	Chain	Res	Type
2	B	101	U
2	B	107	G
2	B	108	C
2	B	110	G
22	2	8	U
22	2	20	G
22	2	21	A
22	2	22	G
22	2	29	U
22	2	30	G
22	2	32	U
22	2	37	A
22	2	48	C
22	2	49	A
22	2	58	A
22	2	59	U
22	2	61	C
22	2	75	C
22	2	76	A

All (67) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	88	G
1	A	92	G
1	A	175	G
1	A	224	A
1	A	252	C
1	A	347	G
1	A	411	G
1	A	443	G
1	A	528	G
1	A	549	A
1	A	554	U
1	A	558	G
1	A	631	G
1	A	689	A
1	A	751	G
1	A	831	U
1	A	976	U
1	A	1036	A
1	A	1066	A

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Mol	Chain	Res	Type
1	A	1172	A
1	A	1250	G
1	A	1294	A
1	A	1305	A
1	A	1313	A
1	A	1339	A
1	A	1351	U
1	A	1435	U
1	A	1448	U
1	A	1507	U
1	A	1525	G
1	A	1530	G
1	A	1565	U
1	A	1567	U
1	A	1570	U
1	A	1631	A
1	A	1671	G
1	A	1691	A
1	A	1758	U
1	A	1784	A
1	A	1813	A
1	A	1828	G
1	A	1882	A
1	A	1883	A
1	A	1886	G
1	A	1947	A
1	A	2127	U
1	A	2254	A
1	A	2295	A
1	A	2316	A
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2344	U
1	A	2420	G
1	A	2452	U
1	A	2454	A
1	A	2468	A
1	A	2510	G
1	A	2631	A
1	A	2805	A
1	A	2904	A

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Mol	Chain	Res	Type
2	B	48	G
2	B	49	G
2	B	55	A
22	2	48	C
22	2	58	A
22	2	74	C

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.