



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:37 PM UTC

PDB ID : 5NWY / pdb_00005nwy
EMDB ID : EMD-3713
Title : 2.9 Å cryo-EM structure of VemP-stalled ribosome-nascent chain complex
Authors : Su, T.; Cheng, J.; Sohmen, D.; Hedman, R.; Berninghausen, O.; von Heijne, G.; Wilson, D.N.; Beckmann, R.
Deposited on : 2017-05-08
Resolution : 2.90 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 ⓘ symbol.

The types of validation reports are described at

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

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

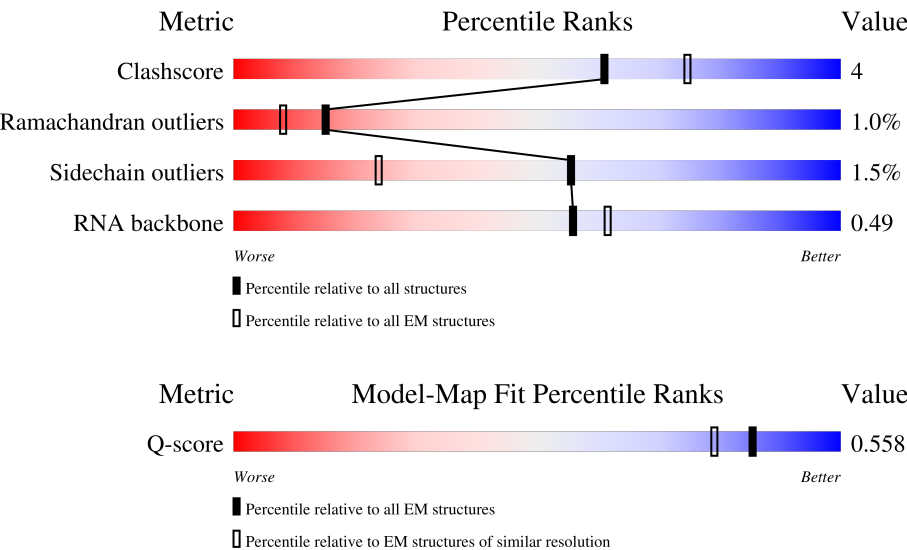
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 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.



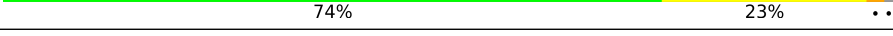
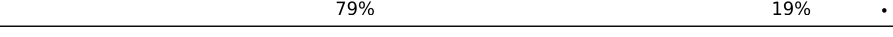
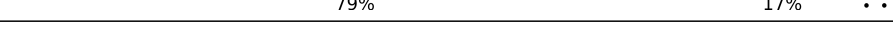
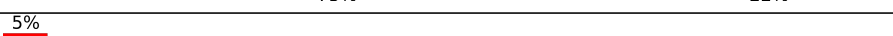
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	s	179	
2	M	75	
3	O	120	

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Mol	Chain	Length	Quality of chain
4	P	273	
5	Q	209	
6	R	201	
7	S	179	
8	T	177	
9	U	149	
10	V	142	
11	W	142	
12	X	123	
13	Y	144	
14	Z	136	
15	a	127	
16	b	117	
17	c	115	
18	d	118	
19	e	103	
20	f	110	
21	g	100	
22	h	104	
23	i	94	
24	j	85	
25	k	78	
26	l	63	
27	m	59	
28	n	57	

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Mol	Chain	Length	Quality of chain
29	o	55	
30	p	46	
31	q	65	
32	r	38	
33	N	2903	
34	L	70	
35	0	1539	
36	1	233	
37	2	233	
38	3	206	
39	4	166	
40	5	131	
41	6	156	
42	7	130	
43	8	130	
44	9	103	
45	A	129	
46	B	124	
47	C	118	
48	D	101	
49	E	89	
50	F	82	
51	G	84	
52	H	75	
53	I	92	

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Mol	Chain	Length	Quality of chain
54	J	87	5% 72% 23% ...
55	K	71	28% 54% 15% . 28%
56	t	4	75% 25%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 144142 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 protein called VemP nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	s	37	Total	C	N	O	S	0	0
			316	198	58	58	2		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	-2	MET	-	initiating methionine	UNP A0A0P7EF65
s	-1	HIS	-	expression tag	UNP A0A0P7EF65
s	0	HIS	-	expression tag	UNP A0A0P7EF65
s	1	HIS	-	expression tag	UNP A0A0P7EF65
s	2	HIS	-	expression tag	UNP A0A0P7EF65
s	3	HIS	-	expression tag	UNP A0A0P7EF65
s	4	HIS	-	expression tag	UNP A0A0P7EF65
s	5	HIS	-	expression tag	UNP A0A0P7EF65
s	6	HIS	-	expression tag	UNP A0A0P7EF65
s	7	HIS	-	expression tag	UNP A0A0P7EF65
s	8	HIS	-	expression tag	UNP A0A0P7EF65
s	9	GLY	-	expression tag	UNP A0A0P7EF65
s	10	ASP	-	expression tag	UNP A0A0P7EF65
s	11	TYR	-	expression tag	UNP A0A0P7EF65
s	12	LYS	-	expression tag	UNP A0A0P7EF65
s	13	ASP	-	expression tag	UNP A0A0P7EF65
s	14	ASP	-	expression tag	UNP A0A0P7EF65
s	15	ASP	-	expression tag	UNP A0A0P7EF65
s	16	ASP	-	expression tag	UNP A0A0P7EF65
s	17	LYS	-	expression tag	UNP A0A0P7EF65
s	18	GLU	-	expression tag	UNP A0A0P7EF65
s	19	ASN	-	expression tag	UNP A0A0P7EF65
s	20	LEU	-	expression tag	UNP A0A0P7EF65
s	21	TYR	-	expression tag	UNP A0A0P7EF65
s	22	PHE	-	expression tag	UNP A0A0P7EF65
s	23	GLN	-	expression tag	UNP A0A0P7EF65
s	24	GLY	-	expression tag	UNP A0A0P7EF65
s	25	SER	-	expression tag	UNP A0A0P7EF65

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Chain	Residue	Modelled	Actual	Comment	Reference
s	30	GLN	HIS	conflict	UNP A0A0P7EF65
s	59	ALA	VAL	conflict	UNP A0A0P7EF65
s	160	LEU	-	expression tag	UNP A0A0P7EF65
s	161	GLU	-	expression tag	UNP A0A0P7EF65
s	162	VAL	-	expression tag	UNP A0A0P7EF65
s	163	LEU	-	expression tag	UNP A0A0P7EF65
s	164	PHE	-	expression tag	UNP A0A0P7EF65
s	165	GLN	-	expression tag	UNP A0A0P7EF65
s	166	GLY	-	expression tag	UNP A0A0P7EF65
s	167	PRO	-	expression tag	UNP A0A0P7EF65
s	168	TYR	-	expression tag	UNP A0A0P7EF65
s	169	PRO	-	expression tag	UNP A0A0P7EF65
s	170	TYR	-	expression tag	UNP A0A0P7EF65
s	171	ASP	-	expression tag	UNP A0A0P7EF65
s	172	VAL	-	expression tag	UNP A0A0P7EF65
s	173	PRO	-	expression tag	UNP A0A0P7EF65
s	174	ASP	-	expression tag	UNP A0A0P7EF65
s	175	TYR	-	expression tag	UNP A0A0P7EF65
s	176	ALA	-	expression tag	UNP A0A0P7EF65

- Molecule 2 is a RNA chain called Gln-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	75	Total	C	N	O	P	0	0
			1594	711	281	527	75		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	176	Total	C	N	O	S	0	0
			1322	832	243	245	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	141	Total	C	N	O	S	0	0
			1031	651	179	195	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	142	Total	C	N	O	S	0	0
			1128	714	212	198	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	143	Total	C	N	O	S	0	0
			1044	649	206	188	1		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	136	Total	C	N	O	S	0	0
			1073	686	205	176	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	114	Total	C	N	O	S	0	0
			915	573	179	162	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	d	117	Total	C	N	O	0	0
			946	604	192	150		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	94	Total	C	N	O	S	0	0
			752	479	137	133	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	75	Total	C	N	O	S	0	0
			568	353	113	101	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	63	Total	C	N	O	S	0	0
			508	313	99	94	2		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	n	56	Total	C	N	O	S	0	0
			443	269	94	79	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	p	46	Total	C	N	O	S	0	0
			376	228	90	56	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	q	64	Total	C	N	O	S	0	0
			503	323	105	73	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 33 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	2897	Total	C	N	O	P	1	0
			62215	27754	11448	20115	2898		

- Molecule 34 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	0	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	3	205	Total	C	N	O	S	0	0
			1642	1026	315	297	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	7	129	Total	C	N	O	S	0	0
			978	616	173	183	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	9	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A	117	Total	C	N	O	S	0	0
			876	540	174	159	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	B	123	Total	C	N	O	S	0	0
			954	590	196	164	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	C	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	D	96	Total	C	N	O	S	0	0
			773	483	160	127	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	E	88	Total	C	N	O	S	0	0
			709	437	143	128	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	F	82	Total	C	N	O	S	0	0
			648	406	128	113	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	G	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	H	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	I	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	J	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

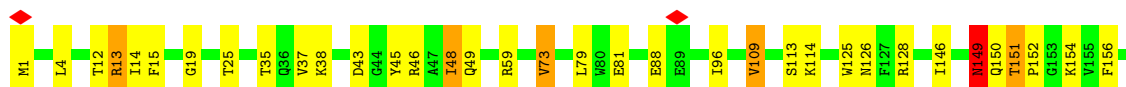
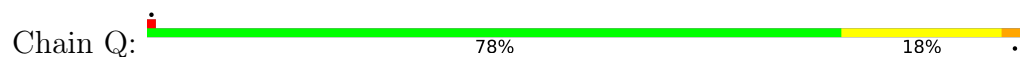
Mol	Chain	Residues	Atoms					AltConf	Trace
55	K	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 56 is a RNA chain called mRNA.

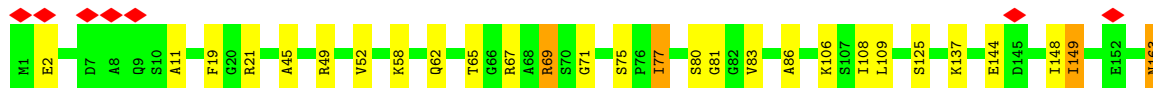
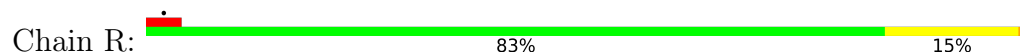
Mol	Chain	Residues	Atoms					AltConf	Trace
56	t	4	Total	C	N	O	P	0	0
			85	38	15	28	4		



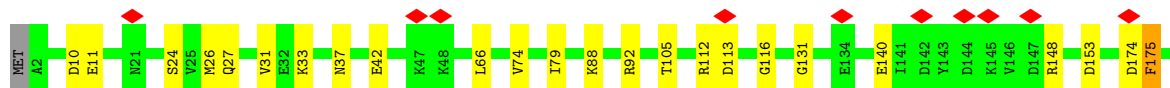
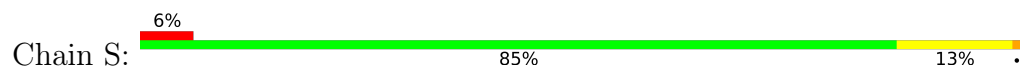
- Molecule 5: 50S ribosomal protein L3



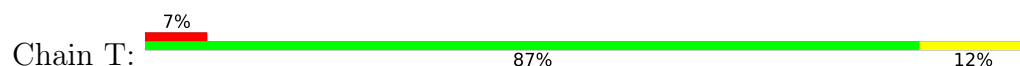
- Molecule 6: 50S ribosomal protein L4



- Molecule 7: 50S ribosomal protein L5



- Molecule 8: 50S ribosomal protein L6

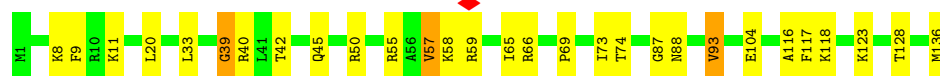
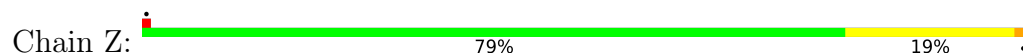


- Molecule 9: 50S ribosomal protein L9

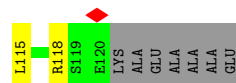




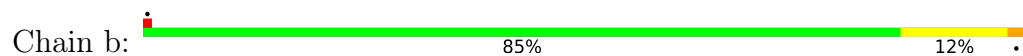
- Molecule 14: 50S ribosomal protein L16



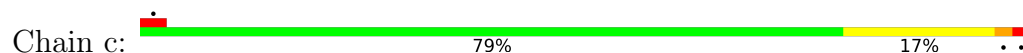
- Molecule 15: 50S ribosomal protein L17



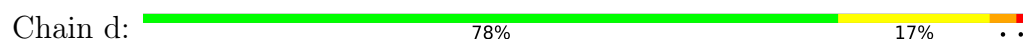
- Molecule 16: 50S ribosomal protein L18



- Molecule 17: 50S ribosomal protein L19

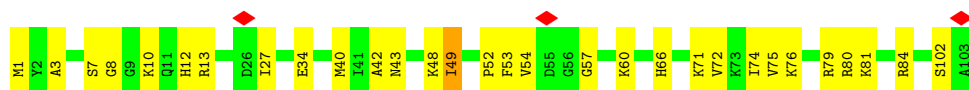


- Molecule 18: 50S ribosomal protein L20

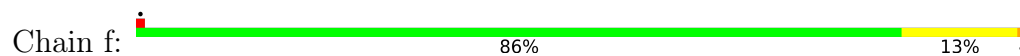


- Molecule 19: 50S ribosomal protein L21

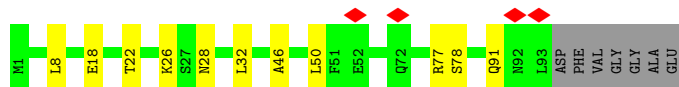
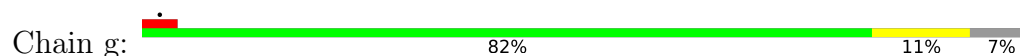




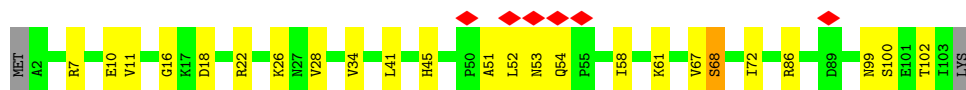
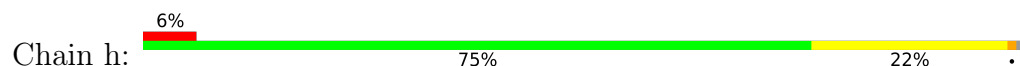
- Molecule 20: 50S ribosomal protein L22



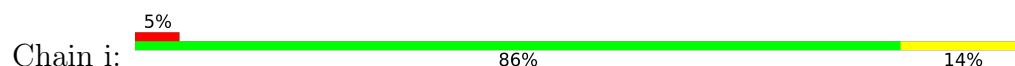
- Molecule 21: 50S ribosomal protein L23



- Molecule 22: 50S ribosomal protein L24



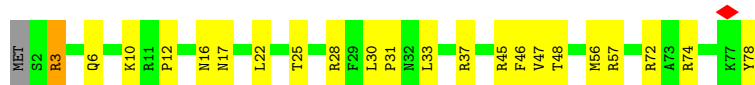
- Molecule 23: 50S ribosomal protein L25



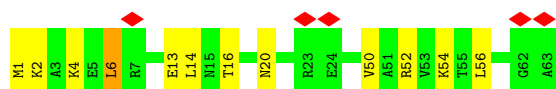
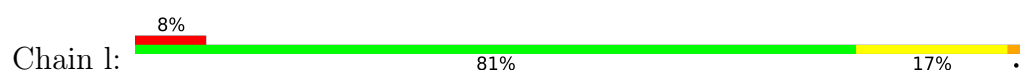
- Molecule 24: 50S ribosomal protein L27



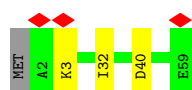
- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30



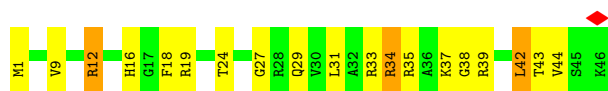
- Molecule 28: 50S ribosomal protein L32



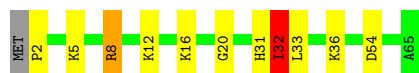
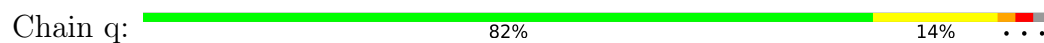
- Molecule 29: 50S ribosomal protein L33



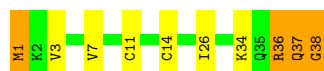
- Molecule 30: 50S ribosomal protein L34



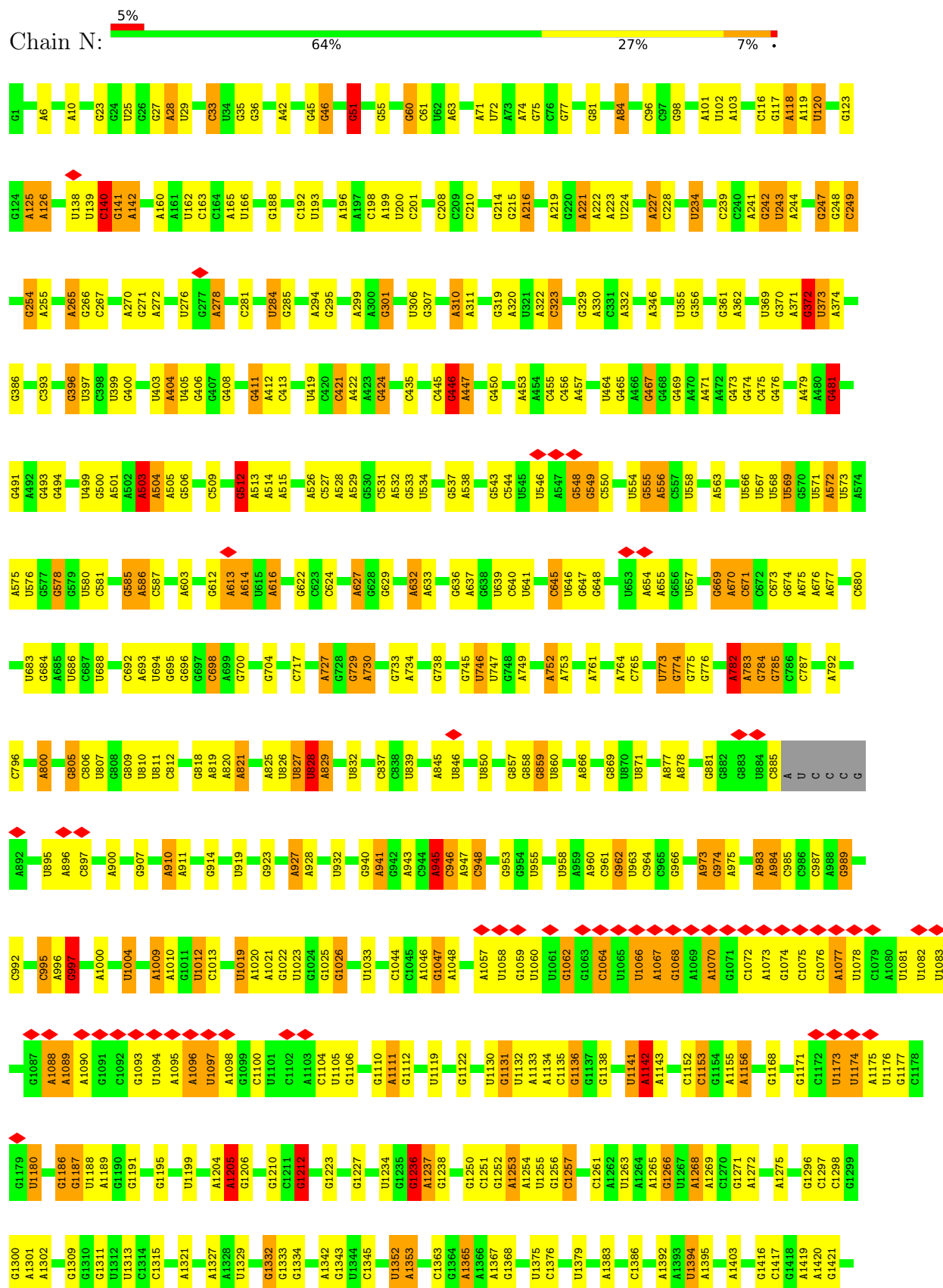
- Molecule 31: 50S ribosomal protein L35



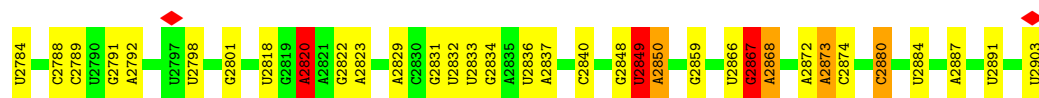
- Molecule 32: 50S ribosomal protein L36



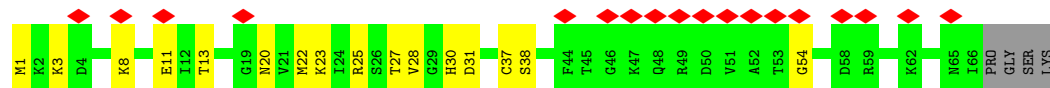
• Molecule 33: 23S rRNA



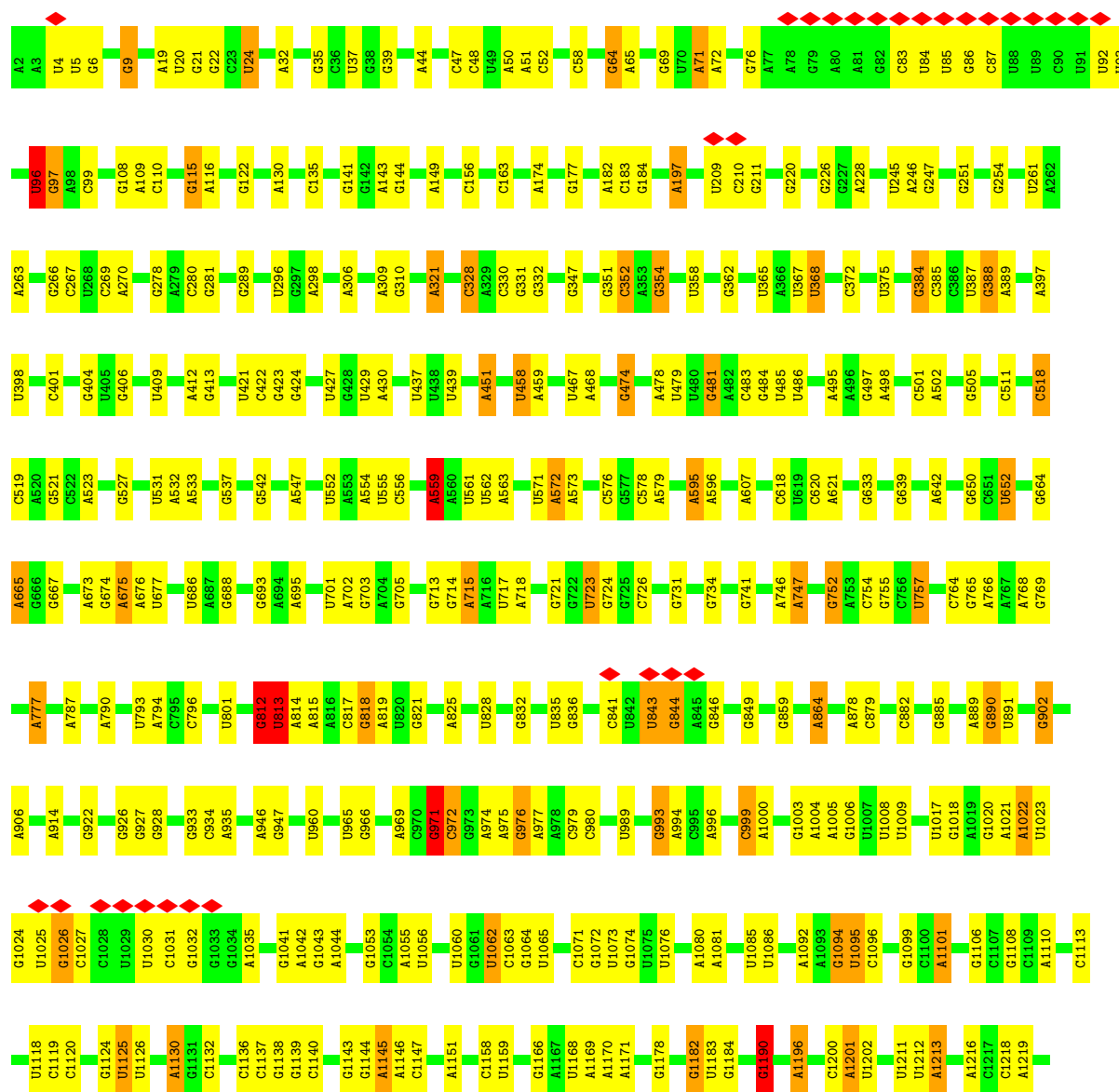


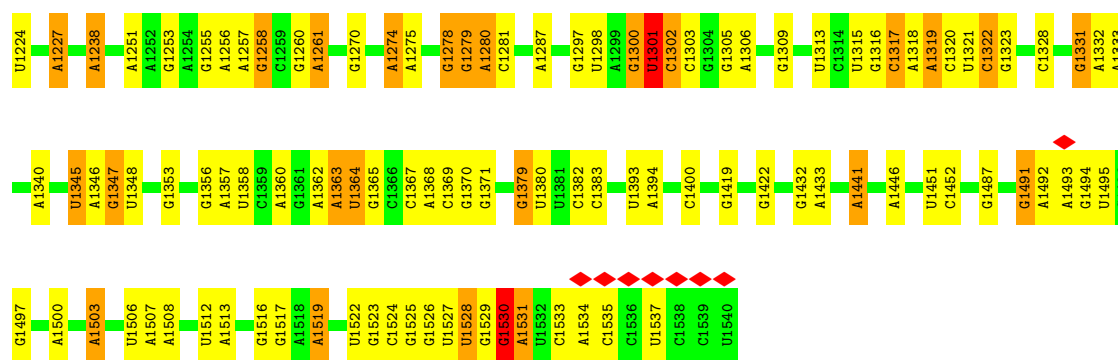


• Molecule 34: 50S ribosomal protein L31

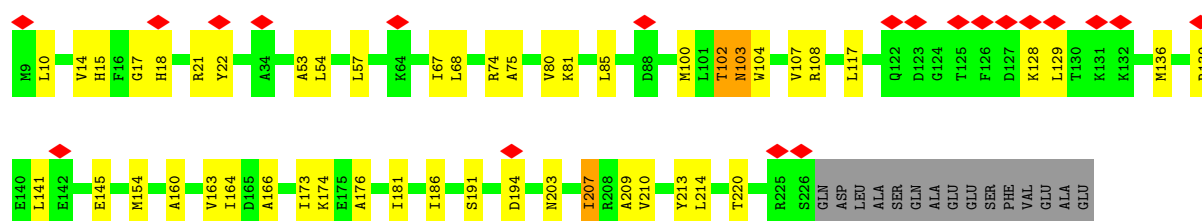
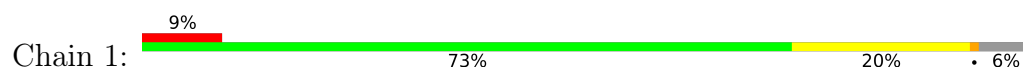


• Molecule 35: 16S rRNA

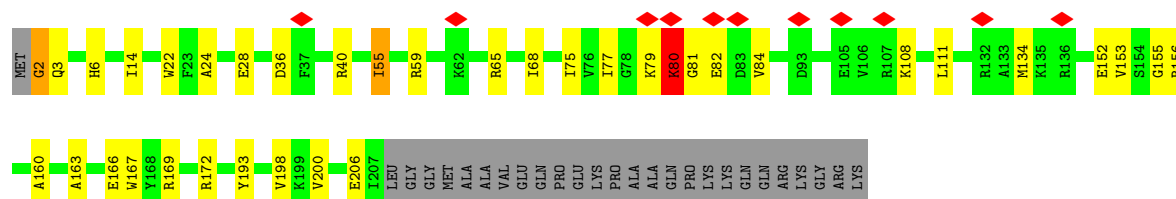
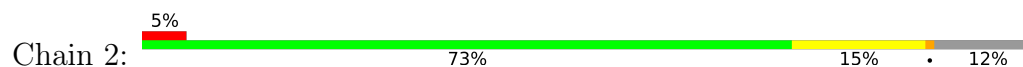




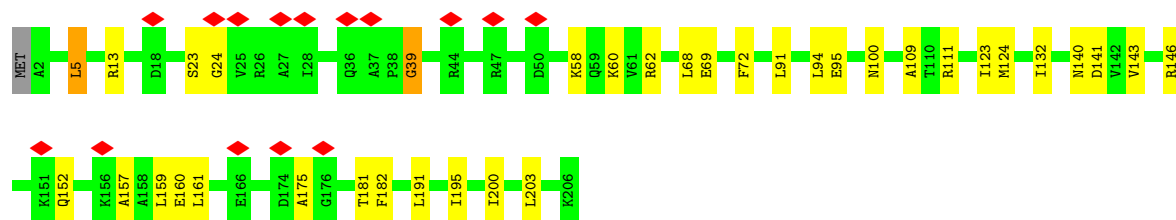
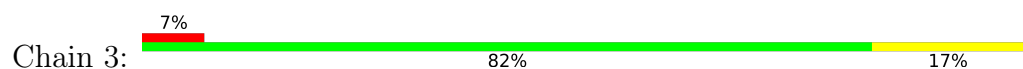
• Molecule 36: 30S ribosomal protein S2



• Molecule 37: 30S ribosomal protein S3

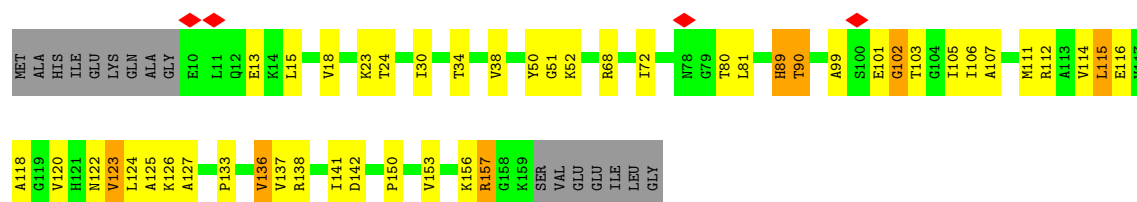


• Molecule 38: 30S ribosomal protein S4

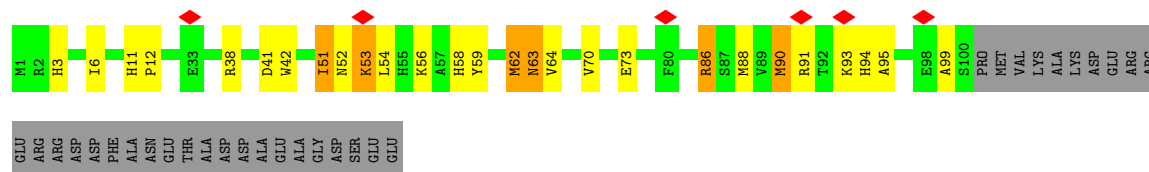


• Molecule 39: 30S ribosomal protein S5

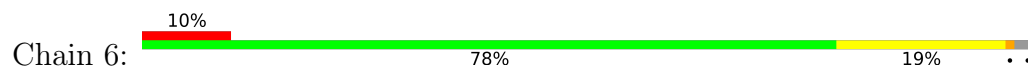




• Molecule 40: 30S ribosomal protein S6



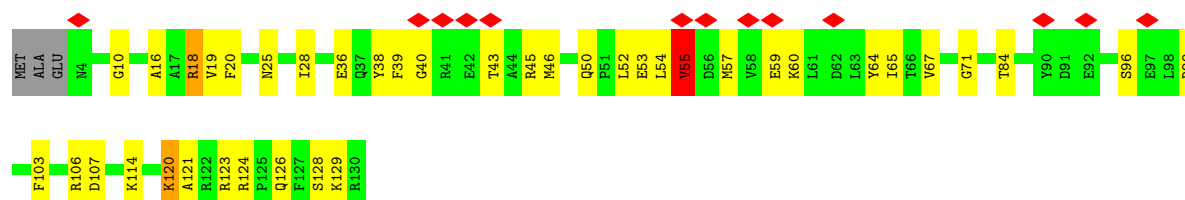
• Molecule 41: 30S ribosomal protein S7



• Molecule 42: 30S ribosomal protein S8

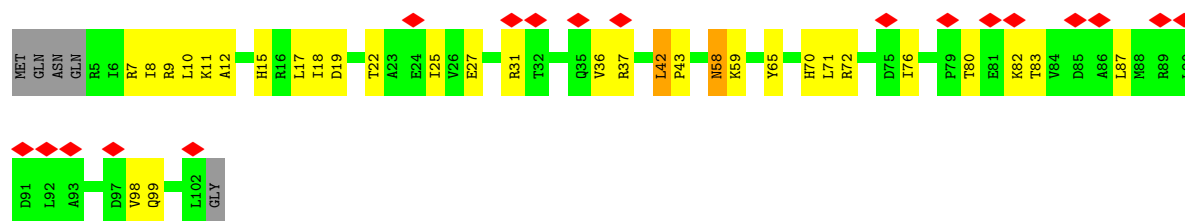


• Molecule 43: 30S ribosomal protein S9



• Molecule 44: 30S ribosomal protein S10

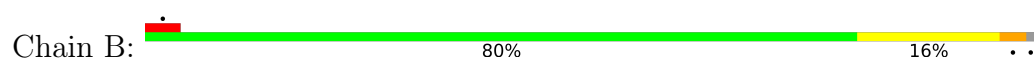




- Molecule 45: 30S ribosomal protein S11



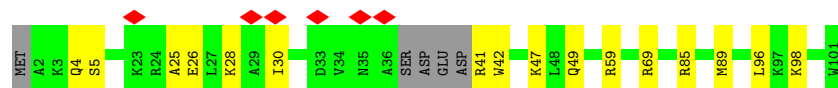
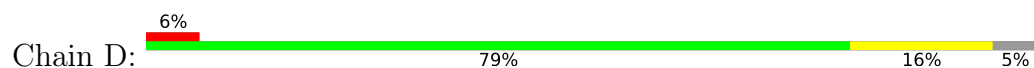
- Molecule 46: 30S ribosomal protein S12



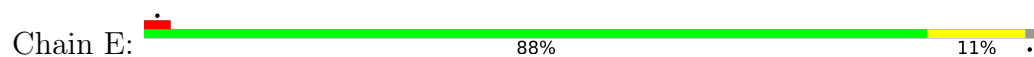
- Molecule 47: 30S ribosomal protein S13



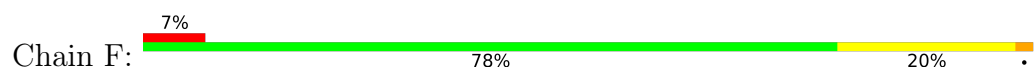
- Molecule 48: 30S ribosomal protein S14

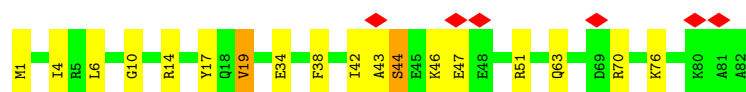


- Molecule 49: 30S ribosomal protein S15

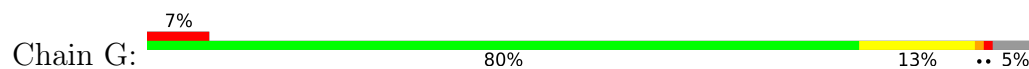


- Molecule 50: 30S ribosomal protein S16





- Molecule 51: 30S ribosomal protein S17



- Molecule 52: 30S ribosomal protein S18



- Molecule 53: 30S ribosomal protein S19



- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S21



- Molecule 56: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	400024	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	398.912, 398.912, 398.912	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	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	s	0.95	1/326 (0.3%)	0.92	0/441
2	M	0.51	0/1779	0.77	3/2768 (0.1%)
3	O	0.65	1/2828 (0.0%)	0.83	7/4410 (0.2%)
4	P	1.72	39/2121 (1.8%)	1.42	17/2852 (0.6%)
5	Q	1.54	13/1585 (0.8%)	1.29	10/2134 (0.5%)
6	R	1.20	8/1571 (0.5%)	1.09	5/2113 (0.2%)
7	S	0.84	0/1434	0.89	0/1926
8	T	0.83	0/1342	0.87	0/1816
9	U	0.96	1/364 (0.3%)	1.14	1/490 (0.2%)
10	V	0.76	0/1045	0.73	0/1410
11	W	1.42	10/1151 (0.9%)	1.10	0/1551
12	X	1.53	8/947 (0.8%)	1.27	4/1268 (0.3%)
13	Y	1.65	14/1053 (1.3%)	1.44	7/1403 (0.5%)
14	Z	1.42	4/1092 (0.4%)	1.20	2/1460 (0.1%)
15	a	1.65	10/973 (1.0%)	1.35	5/1301 (0.4%)
16	b	1.05	2/901 (0.2%)	1.04	5/1209 (0.4%)
17	c	1.38	4/927 (0.4%)	1.21	4/1240 (0.3%)
18	d	1.57	7/959 (0.7%)	1.32	9/1278 (0.7%)
19	e	1.39	6/828 (0.7%)	1.21	1/1107 (0.1%)
20	f	1.33	2/864 (0.2%)	1.14	1/1156 (0.1%)
21	g	1.21	0/744	1.11	0/994
22	h	1.00	1/787 (0.1%)	1.06	0/1051
23	i	0.96	0/765	0.90	0/1025
24	j	1.50	5/575 (0.9%)	1.37	6/762 (0.8%)
25	k	1.35	1/634 (0.2%)	1.16	2/848 (0.2%)
26	l	0.89	0/509	1.00	1/677 (0.1%)
27	m	1.18	0/452	1.14	1/605 (0.2%)
28	n	1.48	2/449 (0.4%)	1.40	6/599 (1.0%)
29	o	1.44	5/416 (1.2%)	1.01	0/554
30	p	1.73	5/379 (1.3%)	1.60	5/498 (1.0%)
31	q	1.50	0/512	1.35	2/676 (0.3%)
32	r	1.42	3/302 (1.0%)	1.34	3/397 (0.8%)
33	N	0.95	273/69681 (0.4%)	0.95	169/108706 (0.2%)
34	L	0.77	0/531	0.90	1/709 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	0	0.76	29/36966 (0.1%)	0.84	48/57666 (0.1%)
36	1	1.02	1/1735 (0.1%)	0.99	2/2338 (0.1%)
37	2	1.08	4/1651 (0.2%)	0.97	3/2225 (0.1%)
38	3	0.95	2/1664 (0.1%)	1.02	2/2227 (0.1%)
39	4	1.52	6/1118 (0.5%)	1.35	7/1504 (0.5%)
40	5	1.16	5/835 (0.6%)	1.14	3/1128 (0.3%)
41	6	0.83	0/1195	0.86	1/1602 (0.1%)
42	7	1.15	1/988 (0.1%)	1.04	0/1326
43	8	1.08	1/1033 (0.1%)	1.13	2/1375 (0.1%)
44	9	0.94	1/796 (0.1%)	1.02	2/1077 (0.2%)
45	A	1.10	0/892	1.12	3/1205 (0.2%)
46	B	1.37	5/968 (0.5%)	1.24	3/1300 (0.2%)
47	C	1.09	1/892 (0.1%)	1.07	0/1193
48	D	1.09	0/784	1.14	0/1043
49	E	1.21	2/717 (0.3%)	1.03	1/959 (0.1%)
50	F	1.18	3/658 (0.5%)	1.19	5/884 (0.6%)
51	G	1.08	1/657 (0.2%)	1.06	1/881 (0.1%)
52	H	1.20	0/462	1.15	1/621 (0.2%)
53	I	1.01	1/652 (0.2%)	1.00	1/877 (0.1%)
54	J	1.19	2/670 (0.3%)	1.20	2/888 (0.2%)
55	K	1.32	5/430 (1.2%)	1.22	1/570 (0.2%)
56	t	0.64	0/94	0.88	0/144
All	All	1.00	495/156683 (0.3%)	0.98	365/234467 (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
4	P	0	3
5	Q	0	1
7	S	0	2
9	U	0	1
10	V	0	1
13	Y	0	2
14	Z	0	2
22	h	0	1
31	q	0	1
33	N	0	7
35	0	0	5
36	1	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	2	0	2
39	4	0	5
40	5	0	2
43	8	0	4
45	A	0	1
46	B	0	2
51	G	0	2
53	I	0	1
54	J	0	1
55	K	0	1
All	All	0	50

All (495) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	2502	G	P-OP2	14.19	1.77	1.49
33	N	1156	A	P-OP2	12.94	1.74	1.49
33	N	1333	G	P-OP2	10.93	1.70	1.49
33	N	783	A	P-OP2	10.79	1.70	1.49
39	4	127	ALA	C-O	-10.56	1.10	1.23
33	N	945	A	P-OP2	10.45	1.69	1.49
4	P	221	ARG	CA-C	-10.45	1.38	1.53
33	N	1639	C	P-OP1	10.32	1.69	1.49
13	Y	51	GLU	C-O	10.20	1.37	1.23
33	N	945	A	P-OP1	10.08	1.69	1.49
33	N	1664	A	P-OP2	10.07	1.69	1.49
4	P	219	THR	C-O	9.96	1.35	1.24
33	N	1670	C	P-OP1	9.80	1.68	1.49
46	B	23	ALA	N-CA	9.71	1.58	1.46
15	a	2	ARG	C-O	-9.71	1.11	1.24
33	N	2074	U	P-OP1	9.70	1.68	1.49
4	P	213	TRP	CD2-CE2	9.69	1.57	1.41
40	5	63	ASN	C-O	-9.42	1.09	1.23
33	N	2588	G	P-OP1	9.40	1.67	1.49
33	N	2005	A	P-OP1	9.15	1.67	1.49
33	N	827	U	P-OP1	9.03	1.67	1.49
33	N	450	G	P-OP2	9.03	1.67	1.49
29	o	50	LYS	C-O	-8.73	1.15	1.24
33	N	828	U	O3'-P	-8.73	1.48	1.61
33	N	943	A	P-OP2	8.71	1.66	1.49
54	J	5	LYS	C-O	-8.70	1.17	1.24
33	N	2025	C	P-OP2	8.63	1.66	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	2349	G	O3'-P	-8.60	1.48	1.61
33	N	2445	G	O3'-P	-8.58	1.48	1.61
33	N	567	U	P-OP1	8.54	1.66	1.49
35	0	578	C	P-OP1	8.49	1.66	1.49
33	N	800	A	P-OP1	8.48	1.66	1.49
4	P	213	TRP	CA-C	-8.47	1.39	1.52
33	N	963	U	O3'-P	-8.38	1.48	1.61
5	Q	162	ALA	CA-C	-8.29	1.41	1.52
4	P	48	ARG	C-O	-8.29	1.13	1.23
33	N	1604	C	P-OP1	8.26	1.65	1.49
33	N	1777	U	O3'-P	-8.26	1.48	1.61
32	r	38	GLY	N-CA	8.22	1.58	1.45
33	N	2615	U	P-OP1	8.21	1.65	1.49
35	0	21	G	P-OP1	8.21	1.65	1.49
33	N	2589	A	O3'-P	-8.20	1.48	1.61
33	N	1774	C	P-OP1	8.19	1.65	1.49
33	N	2502	G	O5'-C5'	-8.17	1.30	1.42
4	P	238	ARG	C-O	8.07	1.34	1.24
35	0	757	U	O3'-P	-8.04	1.49	1.61
6	R	80	SER	C-O	-8.03	1.12	1.23
33	N	2060	A	O3'-P	-8.03	1.49	1.61
13	Y	22	GLY	C-O	-7.99	1.11	1.23
33	N	963	U	P-OP1	7.94	1.64	1.49
33	N	787	C	O3'-P	-7.91	1.49	1.61
33	N	1828	G	P-OP2	7.90	1.64	1.49
4	P	204	VAL	CA-C	-7.87	1.42	1.52
33	N	782	A	O3'-P	-7.86	1.49	1.61
33	N	1968	G	O3'-P	-7.86	1.49	1.61
33	N	692	C	O3'-P	-7.83	1.49	1.61
35	0	20	U	O3'-P	-7.83	1.49	1.61
13	Y	18	ARG	CZ-NH1	7.79	1.43	1.32
33	N	576	U	P-OP1	7.78	1.64	1.49
13	Y	62	PRO	C-O	7.78	1.33	1.23
4	P	230	HIS	CA-C	-7.75	1.43	1.52
33	N	2687	U	O3'-P	-7.75	1.49	1.61
33	N	585	G	O3'-P	-7.75	1.49	1.61
33	N	825	A	O3'-P	-7.75	1.49	1.61
33	N	1009	A	O3'-P	-7.74	1.49	1.61
33	N	948	C	P-OP1	7.70	1.64	1.49
39	4	30	ILE	C-O	-7.70	1.16	1.24
33	N	1269	A	P-OP2	7.65	1.64	1.49
33	N	1257	C	O3'-P	-7.62	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	11	PRO	N-CA	7.46	1.56	1.47
33	N	2588	G	P-OP2	7.46	1.63	1.49
33	N	2543	G	P-OP1	7.46	1.63	1.49
33	N	554	U	O3'-P	-7.45	1.50	1.61
33	N	809	G	O3'-P	-7.44	1.50	1.61
33	N	2550	G	O3'-P	-7.41	1.50	1.61
33	N	2019	A	O3'-P	-7.39	1.50	1.61
33	N	116	C	O3'-P	-7.39	1.50	1.61
33	N	2025	C	O3'-P	-7.38	1.50	1.61
11	W	97	PRO	C-O	7.35	1.33	1.24
33	N	2593	U	O3'-P	-7.35	1.50	1.61
33	N	2576	G	P-OP1	7.35	1.63	1.49
33	N	120	U	P-OP1	7.34	1.63	1.49
17	c	93	ARG	CD-NE	-7.33	1.35	1.46
33	N	2050	C	O3'-P	-7.32	1.50	1.61
33	N	445	C	O3'-P	-7.31	1.50	1.61
30	p	38	GLY	CA-C	-7.30	1.41	1.51
13	Y	19	LEU	C-O	7.26	1.32	1.23
35	0	667	G	O3'-P	-7.26	1.50	1.61
33	N	1664	A	P-OP1	7.25	1.63	1.49
33	N	2714	G	P-OP2	7.23	1.63	1.49
33	N	1152	C	O3'-P	-7.21	1.50	1.61
33	N	2873	A	C6-N1	-7.21	1.21	1.35
33	N	984	A	O3'-P	-7.21	1.50	1.61
35	0	882	C	O3'-P	-7.20	1.50	1.61
33	N	1375	U	O3'-P	-7.19	1.50	1.61
40	5	63	ASN	N-CA	7.18	1.56	1.46
4	P	213	TRP	CZ3-CH2	7.17	1.58	1.40
33	N	2588	G	O3'-P	-7.13	1.50	1.61
16	b	30	ARG	CZ-NH1	7.12	1.42	1.32
33	N	397	U	O3'-P	-7.07	1.50	1.61
33	N	673	C	O3'-P	-7.04	1.50	1.61
33	N	2503	A	P-OP2	7.03	1.63	1.49
15	a	47	VAL	C-O	-7.02	1.15	1.23
12	X	86	LEU	C-O	-7.00	1.15	1.24
33	N	2498	C	P-OP2	6.97	1.62	1.49
6	R	77	ILE	CB-CG1	-6.97	1.39	1.53
33	N	826	U	P-OP1	6.96	1.62	1.49
24	j	14	ARG	C-O	-6.96	1.15	1.23
33	N	1019	U	O3'-P	-6.96	1.50	1.61
33	N	859	G	O3'-P	6.95	1.71	1.61
5	Q	125	TRP	CA-C	-6.94	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	2052	A	O3'-P	-6.93	1.50	1.61
33	N	453	A	P-OP1	6.93	1.62	1.49
28	n	11	SER	N-CA	-6.92	1.38	1.46
33	N	1780	A	P-OP1	6.92	1.62	1.49
33	N	2022	U	P-OP1	6.92	1.62	1.49
11	W	81	ILE	C-O	6.87	1.32	1.24
33	N	1612	C	O3'-P	-6.85	1.50	1.61
4	P	221	ARG	C-O	-6.84	1.15	1.23
33	N	2635	A	O3'-P	-6.84	1.50	1.61
51	G	71	LYS	C-O	-6.83	1.15	1.24
33	N	200	U	O3'-P	-6.82	1.50	1.61
33	N	2698	U	O3'-P	-6.82	1.50	1.61
33	N	1774	C	O3'-P	-6.81	1.50	1.61
46	B	22	PRO	CA-C	6.81	1.62	1.52
15	a	66	ALA	CA-C	-6.79	1.43	1.52
4	P	222	GLY	C-O	-6.78	1.14	1.23
33	N	1658	C	P-OP1	6.76	1.62	1.49
33	N	1994	C	O3'-P	-6.76	1.51	1.61
4	P	86	ASN	C-O	-6.75	1.15	1.24
22	h	68	SER	CB-OG	6.67	1.55	1.42
18	d	49	ASP	CA-C	-6.66	1.43	1.52
33	N	2006	C	P-OP1	6.66	1.62	1.49
33	N	2466	C	O3'-P	-6.66	1.51	1.61
4	P	15	HIS	C-O	-6.66	1.14	1.24
35	0	812	G	O3'-P	6.63	1.71	1.61
35	0	1500	A	O3'-P	-6.62	1.51	1.61
33	N	1782	U	P-OP1	6.62	1.62	1.49
33	N	1751	U	O3'-P	-6.61	1.51	1.61
33	N	1658	C	O3'-P	-6.61	1.51	1.61
33	N	1993	U	O5'-C5'	-6.60	1.32	1.42
33	N	2062	A	P-OP2	6.59	1.62	1.49
33	N	641	U	O3'-P	-6.58	1.51	1.61
33	N	1900	A	O3'-P	6.58	1.71	1.61
15	a	2	ARG	C-N	-6.58	1.24	1.33
33	N	192	C	P-OP1	6.58	1.62	1.49
33	N	1831	G	O3'-P	-6.56	1.51	1.61
28	n	10	ARG	CA-C	6.55	1.61	1.52
18	d	49	ASP	C-O	6.55	1.32	1.24
33	N	1268	A	P-OP1	6.54	1.62	1.49
33	N	2740	A	O3'-P	-6.54	1.51	1.61
33	N	2035	G	O5'-C5'	-6.53	1.33	1.42
33	N	955	U	O3'-P	-6.53	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	1353	A	O3'-P	-6.52	1.51	1.61
33	N	2765	A	C6-N1	-6.49	1.22	1.35
4	P	221	ARG	CB-CG	-6.48	1.33	1.52
33	N	2518	A	P-OP2	6.48	1.61	1.49
12	X	66	LYS	CA-C	-6.47	1.44	1.52
17	c	21	ARG	C-O	-6.46	1.18	1.24
33	N	810	U	P-OP1	6.46	1.61	1.49
14	Z	39	GLY	C-O	-6.46	1.15	1.23
4	P	213	TRP	CB-CG	-6.43	1.30	1.50
15	a	1	MET	C-O	6.41	1.36	1.23
33	N	1254	A	O3'-P	-6.41	1.51	1.61
12	X	7	MET	N-CA	6.40	1.54	1.46
4	P	271	ARG	CZ-NH1	6.39	1.41	1.32
33	N	2489	U	O3'-P	-6.38	1.51	1.61
19	e	79	ARG	C-O	6.37	1.31	1.23
33	N	2605	U	O3'-P	-6.37	1.51	1.61
33	N	1970	A	P-OP2	6.35	1.61	1.49
33	N	1828	G	P-OP1	6.34	1.61	1.49
33	N	2031	A	P-OP1	-6.34	1.36	1.49
33	N	2543	G	O5'-C5'	-6.34	1.32	1.42
4	P	204	VAL	N-CA	-6.33	1.39	1.46
4	P	234	GLY	C-O	-6.33	1.15	1.23
33	N	2437	G	O3'-P	-6.33	1.51	1.61
33	N	2264	C	O3'-P	-6.32	1.51	1.61
13	Y	62	PRO	CA-CB	-6.30	1.45	1.53
33	N	1813	G	O3'-P	-6.29	1.51	1.61
33	N	1678	A	P-OP2	6.29	1.61	1.49
43	8	121	ALA	C-O	-6.29	1.16	1.24
5	Q	126	ASN	CA-C	-6.29	1.45	1.53
33	N	975	A	P-OP2	6.27	1.61	1.49
4	P	220	VAL	CA-CB	-6.25	1.46	1.54
33	N	372	G	O3'-P	6.24	1.70	1.61
33	N	2590	A	O3'-P	-6.24	1.51	1.61
33	N	839	U	O3'-P	-6.23	1.51	1.61
30	p	39	ARG	NE-CZ	6.20	1.39	1.33
17	c	53	ARG	N-CA	-6.20	1.36	1.46
35	0	726	C	O3'-P	-6.20	1.51	1.61
5	Q	163	GLY	N-CA	6.20	1.52	1.45
25	k	22	LEU	C-O	-6.20	1.14	1.23
46	B	114	ARG	C-O	-6.19	1.16	1.24
32	r	37	GLN	CA-C	-6.18	1.44	1.52
13	Y	41	ARG	CA-C	-6.18	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	733	G	O3'-P	-6.18	1.51	1.61
29	o	10	LYS	C-O	-6.17	1.16	1.24
33	N	2265	U	O3'-P	-6.17	1.51	1.61
35	0	24	U	N3-C4	-6.17	1.26	1.38
33	N	1189	A	O3'-P	-6.17	1.51	1.61
33	N	1794	A	O3'-P	-6.15	1.51	1.61
49	E	49	ASP	C-O	6.15	1.31	1.23
33	N	192	C	O3'-P	-6.15	1.51	1.61
15	a	112	TYR	CA-C	-6.14	1.45	1.52
18	d	10	ALA	C-O	6.14	1.31	1.24
33	N	2572	A	O3'-P	-6.14	1.51	1.61
33	N	572	A	P-OP1	6.13	1.61	1.49
33	N	2447	G	O3'-P	-6.12	1.51	1.61
33	N	832	U	O3'-P	-6.12	1.51	1.61
39	4	24	THR	CA-C	-6.12	1.47	1.53
33	N	1778	U	O3'-P	-6.11	1.51	1.61
39	4	24	THR	C-O	-6.09	1.14	1.23
11	W	138	GLN	C-O	-6.08	1.16	1.23
33	N	515	A	O3'-P	-6.08	1.52	1.61
33	N	997	G	O3'-P	-6.08	1.52	1.61
55	K	34	ARG	CZ-NH1	6.07	1.41	1.32
33	N	1790	C	O3'-P	-6.07	1.52	1.61
11	W	84	ILE	CA-C	-6.06	1.46	1.53
33	N	464	U	O3'-P	-6.04	1.52	1.61
11	W	107	GLY	C-O	-6.03	1.17	1.24
33	N	569	U	O3'-P	-6.02	1.52	1.61
4	P	10	SER	CA-CB	6.02	1.62	1.53
11	W	98	GLU	N-CA	-6.02	1.39	1.46
33	N	671	C	P-OP2	6.02	1.60	1.49
13	Y	37	GLY	C-O	-6.01	1.16	1.23
13	Y	51	GLU	N-CA	-6.01	1.39	1.46
33	N	818	G	P-OP2	6.01	1.60	1.49
6	R	75	SER	CA-C	-6.01	1.46	1.53
33	N	1771	C	O3'-P	-6.00	1.52	1.61
33	N	254	G	O3'-P	-6.00	1.52	1.61
33	N	676	A	O3'-P	-6.00	1.52	1.61
4	P	214	ARG	CZ-NH1	6.00	1.41	1.32
33	N	821	A	O3'-P	-5.99	1.52	1.61
55	K	37	PHE	N-CA	5.99	1.53	1.46
33	N	2406	A	P-OP1	5.98	1.60	1.49
33	N	2620	C	O3'-P	-5.98	1.52	1.61
33	N	2822	G	O3'-P	-5.98	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	2081	U	O3'-P	-5.97	1.52	1.61
40	5	51	ILE	C-O	-5.97	1.17	1.24
35	0	1367	C	O3'-P	-5.97	1.52	1.61
33	N	2867	G	O3'-P	5.95	1.70	1.61
13	Y	29	LYS	C-O	5.95	1.31	1.24
33	N	2385	C	P-OP1	5.95	1.60	1.49
4	P	158	ALA	CA-C	-5.95	1.45	1.52
35	0	1393	U	O3'-P	-5.94	1.52	1.61
33	N	2625	G	O3'-P	-5.94	1.52	1.61
33	N	2061	G	C2'-O2'	5.92	1.51	1.42
33	N	2025	C	O5'-C5'	-5.92	1.33	1.42
33	N	2637	U	O3'-P	-5.92	1.52	1.61
44	9	58	ASN	CA-C	-5.92	1.44	1.52
50	F	4	ILE	C-O	-5.91	1.17	1.23
4	P	235	GLY	C-N	-5.91	1.25	1.33
33	N	2072	C	O5'-C5'	-5.91	1.33	1.42
39	4	50	TYR	C-O	5.91	1.31	1.24
37	2	3	GLN	N-CA	-5.91	1.39	1.46
33	N	2499	C	P-OP2	5.90	1.60	1.49
46	B	23	ALA	C-O	-5.88	1.16	1.24
33	N	2072	C	O3'-P	-5.87	1.52	1.61
32	r	36	ARG	CD-NE	-5.87	1.38	1.46
33	N	538	A	O3'-P	-5.86	1.52	1.61
33	N	2232	C	O3'-P	-5.86	1.52	1.61
33	N	2837	A	O3'-P	-5.86	1.52	1.61
29	o	48	ILE	C-O	-5.86	1.17	1.24
33	N	2444	G	O3'-P	-5.85	1.52	1.61
4	P	235	GLY	CA-C	-5.84	1.43	1.51
33	N	566	U	O3'-P	-5.83	1.52	1.61
33	N	730	A	P-OP2	5.83	1.60	1.49
33	N	2359	C	O3'-P	-5.82	1.52	1.61
33	N	2457	U	O3'-P	-5.82	1.52	1.61
4	P	204	VAL	C-N	-5.81	1.25	1.33
33	N	1822	C	O3'-P	-5.81	1.52	1.61
35	0	980	C	P-OP1	5.80	1.60	1.49
4	P	258	ARG	NE-CZ	-5.80	1.26	1.33
33	N	2247	A	O3'-P	-5.79	1.52	1.61
33	N	198	C	O3'-P	-5.79	1.52	1.61
33	N	2062	A	O5'-C5'	-5.78	1.34	1.42
15	a	106	ASP	N-CA	-5.78	1.40	1.46
37	2	2	GLY	N-CA	5.77	1.54	1.45
53	I	6	LYS	N-CA	5.77	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	62	GLN	N-CA	5.76	1.53	1.46
11	W	30	THR	CB-CG2	-5.76	1.33	1.52
35	0	387	U	O3'-P	-5.76	1.52	1.61
33	N	1824	G	P-OP2	5.76	1.60	1.49
49	E	51	HIS	C-O	5.75	1.30	1.24
33	N	2684	U	O3'-P	-5.74	1.52	1.61
35	0	22	G	O3'-P	-5.74	1.52	1.61
33	N	2572	A	P-OP1	-5.74	1.37	1.49
33	N	2598	A	O3'-P	-5.74	1.52	1.61
33	N	2602	A	O3'-P	5.74	1.69	1.61
33	N	1261	C	O3'-P	-5.73	1.52	1.61
33	N	2542	A	O3'-P	-5.72	1.52	1.61
50	F	10	GLY	N-CA	5.72	1.51	1.45
33	N	1298	C	O3'-P	-5.71	1.52	1.61
33	N	2268	A	P-OP1	5.71	1.60	1.49
33	N	966	G	O3'-P	-5.70	1.52	1.61
33	N	1805	A	O3'-P	-5.70	1.52	1.61
14	Z	93	VAL	CA-CB	5.70	1.63	1.54
33	N	2013	A	O3'-P	-5.70	1.52	1.61
24	j	42	GLY	N-CA	5.69	1.55	1.45
33	N	126	A	O3'-P	-5.69	1.52	1.61
33	N	783	A	C4'-O4'	5.69	1.54	1.45
33	N	578	G	P-OP2	5.68	1.60	1.49
12	X	65	THR	C-O	-5.68	1.16	1.23
33	N	940	G	O3'-P	-5.68	1.52	1.61
35	0	814	A	P-OP2	5.68	1.60	1.49
6	R	81	GLY	C-N	-5.68	1.25	1.33
33	N	2499	C	P-OP1	5.67	1.60	1.49
14	Z	11	LYS	C-O	-5.67	1.17	1.24
33	N	1681	G	O3'-P	-5.67	1.52	1.61
4	P	160	THR	C-O	-5.66	1.16	1.24
33	N	29	U	O3'-P	-5.66	1.52	1.61
33	N	1662	U	P-OP2	5.66	1.60	1.49
33	N	571	U	O3'-P	-5.65	1.52	1.61
33	N	2016	U	O3'-P	-5.65	1.52	1.61
30	p	34	ARG	CG-CD	-5.64	1.35	1.52
33	N	25	U	O3'-P	-5.62	1.52	1.61
35	0	505	G	O3'-P	-5.62	1.52	1.61
3	O	83	G	O3'-P	-5.61	1.52	1.61
33	N	1795	C	O3'-P	-5.61	1.52	1.61
12	X	23	LYS	CA-C	-5.61	1.45	1.52
15	a	17	ARG	C-O	5.60	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	205	LEU	N-CA	5.60	1.53	1.46
33	N	773	U	O3'-P	-5.60	1.52	1.61
33	N	796	C	O3'-P	-5.59	1.52	1.61
5	Q	164	GLN	C-O	5.59	1.30	1.24
12	X	41	ILE	C-O	-5.58	1.17	1.23
33	N	1949	G	O3'-P	-5.58	1.52	1.61
33	N	2072	C	P-OP1	5.58	1.60	1.49
33	N	2049	G	O3'-P	-5.57	1.52	1.61
33	N	680	C	O3'-P	-5.57	1.52	1.61
29	o	23	THR	C-O	-5.56	1.20	1.24
33	N	1009	A	P-OP2	5.56	1.60	1.49
33	N	761	A	P-OP1	5.55	1.60	1.49
40	5	99	ALA	CA-C	5.55	1.56	1.52
5	Q	126	ASN	N-CA	5.55	1.54	1.46
46	B	113	ALA	CA-C	-5.54	1.46	1.53
18	d	51	ARG	CA-CB	-5.53	1.44	1.53
33	N	2829	A	O3'-P	-5.51	1.52	1.61
5	Q	162	ALA	C-O	-5.51	1.17	1.23
33	N	1010	A	P-OP2	5.51	1.59	1.49
35	0	764	C	O3'-P	-5.50	1.52	1.61
13	Y	35	HIS	CA-C	-5.50	1.45	1.53
35	0	765	G	O3'-P	-5.49	1.52	1.61
33	N	2051	A	O3'-P	5.49	1.69	1.61
33	N	393	C	P-OP1	5.49	1.59	1.49
33	N	2332	C	O3'-P	-5.49	1.52	1.61
12	X	114	LYS	C-O	-5.48	1.17	1.24
33	N	2436	G	O3'-P	-5.48	1.52	1.61
33	N	2248	C	P-OP2	5.47	1.59	1.49
18	d	32	TYR	C-N	-5.46	1.25	1.33
4	P	198	ALA	C-O	5.46	1.30	1.24
38	3	123	ILE	C-O	-5.46	1.18	1.24
11	W	110	PRO	CA-C	-5.46	1.45	1.52
33	N	1255	U	O5'-C5'	-5.46	1.34	1.42
11	W	80	HIS	CA-C	-5.45	1.45	1.53
19	e	12	HIS	C-O	5.45	1.30	1.23
37	2	166	GLU	C-O	-5.45	1.17	1.24
5	Q	109	VAL	C-O	-5.44	1.18	1.24
33	N	1186	G	P-OP2	5.44	1.59	1.49
33	N	1394	U	O3'-P	-5.43	1.53	1.61
33	N	239	C	O3'-P	-5.43	1.53	1.61
4	P	239	ASN	CA-C	5.43	1.60	1.52
19	e	72	VAL	C-O	-5.42	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	688	U	O3'-P	-5.42	1.53	1.61
55	K	40	LYS	CA-C	5.42	1.59	1.52
33	N	2243	U	P-OP1	5.41	1.59	1.49
33	N	923	G	O3'-P	-5.41	1.53	1.61
40	5	62	MET	C-N	-5.40	1.27	1.33
33	N	784	G	O3'-P	5.39	1.69	1.61
33	N	1671	U	P-OP2	5.38	1.59	1.49
19	e	75	VAL	C-O	-5.37	1.18	1.24
33	N	2048	G	O3'-P	-5.37	1.53	1.61
30	p	34	ARG	C-O	-5.37	1.17	1.24
33	N	503	A	C6-N1	-5.36	1.24	1.35
33	N	2516	A	O3'-P	-5.36	1.53	1.61
33	N	2285	C	O3'-P	-5.36	1.53	1.61
33	N	2554	U	P-OP2	-5.36	1.38	1.49
12	X	35	VAL	C-O	5.36	1.29	1.24
33	N	1782	U	O3'-P	-5.34	1.53	1.61
33	N	1327	A	P-OP2	5.34	1.59	1.49
33	N	419	U	O3'-P	-5.34	1.53	1.61
5	Q	126	ASN	C-O	-5.33	1.16	1.23
24	j	15	ASP	N-CA	-5.33	1.39	1.45
33	N	946	C	P-OP2	5.33	1.59	1.49
4	P	54	ILE	N-CA	5.33	1.52	1.46
4	P	155	ALA	CA-C	-5.33	1.47	1.53
5	Q	170	VAL	CA-C	-5.33	1.46	1.52
33	N	1026	G	P-OP2	-5.32	1.38	1.49
4	P	156	ARG	CD-NE	-5.32	1.38	1.46
33	N	2074	U	O3'-P	-5.31	1.53	1.61
33	N	2045	C	O3'-P	-5.31	1.53	1.61
5	Q	149	ASN	CA-CB	-5.31	1.44	1.53
33	N	1342	A	P-OP2	5.30	1.59	1.49
13	Y	101	ILE	N-CA	-5.30	1.40	1.46
11	W	76	HIS	C-O	-5.29	1.17	1.23
33	N	2260	C	O3'-P	-5.29	1.53	1.61
35	0	1182	G	O3'-P	5.29	1.69	1.61
6	R	45	ALA	N-CA	-5.29	1.40	1.46
35	0	572	A	P-OP1	5.29	1.59	1.49
33	N	2694	G	O3'-P	-5.28	1.53	1.61
33	N	1234	U	O3'-P	-5.28	1.53	1.61
6	R	81	GLY	N-CA	-5.28	1.37	1.45
24	j	72	LYS	C-O	5.28	1.30	1.23
33	N	1649	G	O3'-P	-5.28	1.53	1.61
33	N	1977	A	O3'-P	-5.27	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	1960	A	O3'-P	-5.26	1.53	1.61
33	N	411	G	P-OP1	5.26	1.59	1.49
15	a	8	ARG	NE-CZ	-5.25	1.27	1.33
18	d	49	ASP	CB-CG	5.25	1.65	1.52
33	N	2732	G	C3'-O3'	5.25	1.50	1.42
30	p	42	LEU	N-CA	-5.24	1.41	1.46
33	N	120	U	P-OP2	5.24	1.59	1.49
38	3	39	GLY	N-CA	5.24	1.52	1.45
4	P	195	VAL	CB-CG1	-5.24	1.35	1.52
33	N	698	C	O3'-P	-5.24	1.53	1.61
33	N	2289	G	O3'-P	-5.23	1.53	1.61
5	Q	12	THR	CA-CB	5.23	1.61	1.54
33	N	117	G	O3'-P	-5.23	1.53	1.61
33	N	2682	A	P-OP2	5.23	1.59	1.49
50	F	34	GLU	CA-C	-5.23	1.46	1.52
33	N	193	U	O3'-P	-5.22	1.53	1.61
33	N	2452	C	O3'-P	-5.22	1.53	1.61
4	P	195	VAL	C-O	-5.22	1.17	1.24
33	N	1334	G	O3'-P	-5.22	1.53	1.61
5	Q	150	GLN	N-CA	5.22	1.52	1.46
17	c	92	VAL	CA-C	-5.22	1.46	1.52
18	d	21	ALA	C-O	-5.22	1.16	1.23
20	f	85	ILE	C-O	-5.22	1.18	1.24
55	K	35	ARG	CA-C	-5.21	1.46	1.52
19	e	54	VAL	C-O	5.21	1.29	1.24
29	o	21	TYR	CE2-CZ	-5.21	1.25	1.38
33	N	1432	G	O3'-P	-5.20	1.53	1.61
15	a	10	LEU	CA-C	-5.20	1.45	1.53
33	N	1968	G	P-OP1	5.19	1.59	1.49
4	P	239	ASN	N-CA	-5.19	1.39	1.46
33	N	2028	U	O3'-P	-5.19	1.53	1.61
33	N	2723	C	O3'-P	-5.19	1.53	1.61
33	N	1191	G	O3'-P	-5.18	1.53	1.61
33	N	2727	A	O3'-P	-5.18	1.53	1.61
4	P	175	ARG	CA-C	-5.18	1.46	1.52
20	f	96	ILE	N-CA	-5.18	1.39	1.46
36	1	18	HIS	C-O	-5.18	1.20	1.24
33	N	960	A	O3'-P	-5.18	1.53	1.61
33	N	1153	C	P-OP2	5.17	1.59	1.49
55	K	34	ARG	CA-C	5.16	1.59	1.52
33	N	2426	A	O3'-P	-5.16	1.53	1.61
13	Y	62	PRO	N-CA	-5.16	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Z	73	ILE	C-O	-5.16	1.18	1.24
4	P	213	TRP	CD1-NE1	5.16	1.48	1.37
33	N	1142	A	O3'-P	5.16	1.68	1.61
33	N	2699	C	O3'-P	-5.16	1.53	1.61
33	N	1141	U	N3-C4	-5.16	1.28	1.38
19	e	43	ASN	CA-C	5.15	1.56	1.52
35	0	1110	A	P-OP2	5.15	1.59	1.49
33	N	694	U	O3'-P	-5.15	1.53	1.61
47	C	101	ARG	CZ-NH1	5.14	1.40	1.32
33	N	2262	U	O3'-P	-5.14	1.53	1.61
33	N	1677	A	O3'-P	-5.13	1.53	1.61
35	0	559	A	N1-C2	5.13	1.44	1.34
33	N	1296	G	O3'-P	-5.13	1.53	1.61
33	N	2502	G	O3'-P	-5.12	1.53	1.61
33	N	2503	A	P-OP1	5.11	1.59	1.49
35	0	715	A	O3'-P	-5.11	1.53	1.61
24	j	45	PHE	CA-CB	-5.11	1.45	1.53
33	N	727	A	P-OP1	5.10	1.59	1.49
33	N	1652	A	O3'-P	-5.10	1.53	1.61
33	N	1186	G	O3'-P	-5.10	1.53	1.61
33	N	1680	U	O3'-P	-5.10	1.53	1.61
33	N	963	U	P-OP2	5.10	1.59	1.49
16	b	102	ARG	CZ-NH2	5.09	1.40	1.33
33	N	234	U	N3-C4	-5.09	1.28	1.38
33	N	1648	U	P-OP2	5.09	1.59	1.49
13	Y	63	LYS	N-CA	-5.09	1.39	1.46
33	N	1367	A	O3'-P	-5.08	1.53	1.61
35	0	1062	U	O3'-P	-5.08	1.53	1.61
35	0	368	U	N3-C4	-5.08	1.28	1.38
42	7	106	THR	CA-C	-5.08	1.46	1.53
33	N	745	G	O3'-P	-5.07	1.53	1.61
33	N	632	A	O3'-P	-5.06	1.53	1.61
54	J	10	ARG	CD-NE	-5.06	1.39	1.46
33	N	208	C	O3'-P	-5.05	1.53	1.61
1	s	152	ALA	C-O	5.05	1.30	1.24
33	N	408	G	O3'-P	-5.05	1.53	1.61
9	U	29	PHE	CA-C	-5.05	1.48	1.52
37	2	152	GLU	CA-C	-5.04	1.48	1.53
33	N	1187	G	P-OP2	5.03	1.59	1.49
35	0	37	U	N3-C4	-5.03	1.28	1.38
35	0	19	A	O3'-P	-5.03	1.53	1.61
33	N	247	G	O3'-P	-5.03	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	N	1650	A	O3'-P	-5.03	1.53	1.61
35	O	787	A	O3'-P	-5.03	1.53	1.61
33	N	2000	C	O3'-P	-5.01	1.53	1.61
33	N	1004	U	O3'-P	-5.01	1.53	1.61
6	R	52	VAL	C-O	-5.01	1.18	1.24
39	4	50	TYR	CA-C	-5.00	1.46	1.52

All (365) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	73	C	O3'-P-O5'	18.22	131.32	104.00
5	Q	151	THR	CA-C-N	12.79	134.30	119.47
5	Q	151	THR	C-N-CA	12.79	134.30	119.47
33	N	1936	A	C4'-C3'-O3'	-11.10	96.35	113.00
33	N	2725	A	C3'-C2'-O2'	-10.57	94.84	110.70
33	N	242	G	C4'-C3'-O3'	10.04	124.46	109.40
54	J	10	ARG	CB-CG-CD	-9.41	89.66	111.30
33	N	774	G	C1'-C2'-O2'	-9.39	94.31	108.40
33	N	2251	G	C3'-C2'-O2'	9.33	124.70	110.70
33	N	774	G	C4'-C3'-O3'	-9.29	99.07	113.00
35	O	561	U	C4'-C3'-O3'	-9.15	99.28	113.00
33	N	995	C	C4'-C3'-O3'	-8.84	96.15	109.40
33	N	2776	A	C2'-C3'-O3'	8.73	122.60	109.50
33	N	670	A	C2'-C3'-O3'	8.66	122.50	109.50
4	P	204	VAL	N-CA-C	8.60	120.34	112.43
35	O	1528	U	C1'-C2'-O2'	-8.50	99.05	111.80
33	N	2732	G	C4'-C3'-O3'	-8.47	100.29	113.00
33	N	1937	A	C4'-C3'-O3'	-8.38	100.43	113.00
33	N	2060	A	O3'-P-O5'	8.33	116.49	104.00
33	N	1136	G	P-O5'-C5'	-8.24	108.55	120.90
35	O	1347	G	C4'-C3'-O3'	8.22	121.74	109.40
33	N	784	G	C2'-C3'-O3'	8.22	126.03	113.70
35	O	717	U	C4'-C3'-O3'	-8.07	100.89	113.00
33	N	1236	G	C4'-C3'-O3'	-8.06	100.92	113.00
33	N	2324	U	C4'-C3'-O3'	-8.03	100.96	113.00
35	O	1345	U	C4'-C3'-O3'	7.99	121.39	109.40
4	P	221	ARG	CG-CD-NE	-7.95	94.50	112.00
33	N	746	U	C4'-C3'-O3'	-7.91	101.13	113.00
4	P	232	HIS	O-C-N	-7.86	113.84	123.04
33	N	1141	U	C2'-C3'-O3'	7.78	121.18	109.50
12	X	94	PRO	N-CA-C	7.72	122.82	110.40
33	N	2266	A	C4'-C3'-O3'	-7.65	97.93	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	5	90	MET	CA-C-N	7.60	136.06	121.54
40	5	90	MET	C-N-CA	7.60	136.06	121.54
3	O	44	G	C4'-C3'-O3'	-7.52	101.72	113.00
33	N	2406	A	C2'-C3'-O3'	-7.50	102.44	113.70
35	0	115	G	C2'-C3'-O3'	7.44	120.66	109.50
12	X	35	VAL	O-C-N	7.42	129.88	121.94
35	0	518	C	C4'-C3'-O3'	7.41	120.51	109.40
6	R	81	GLY	O-C-N	-7.40	113.08	122.70
31	q	8	ARG	CD-NE-CZ	-7.39	114.06	124.40
33	N	1142	A	C2'-C3'-O3'	7.36	120.53	109.50
16	b	101	GLY	O-C-N	7.33	125.95	121.85
35	0	1278	G	C4'-C3'-O3'	-7.25	102.12	113.00
53	I	5	LEU	CB-CG-CD2	7.25	132.44	110.70
33	N	2543	G	P-O5'-C5'	-7.25	110.03	120.90
33	N	2497	A	C5'-C4'-C3'	-7.22	104.37	115.20
6	R	81	GLY	CA-C-N	-7.17	107.36	121.41
6	R	81	GLY	C-N-CA	-7.17	107.36	121.41
35	0	752	G	C4'-C3'-O3'	-7.14	102.30	113.00
33	N	33	C	C4'-C3'-O3'	-7.09	102.37	113.00
4	P	239	ASN	N-CA-C	7.07	125.87	110.80
33	N	2225	A	C2'-C3'-O3'	7.06	120.09	109.50
45	A	126	LYS	N-CA-C	7.02	120.74	109.79
33	N	227	A	C4'-C3'-O3'	-7.02	102.47	113.00
6	R	65	THR	O-C-N	-7.01	114.59	122.86
35	0	1362	A	C4'-C3'-O3'	-7.01	102.49	113.00
35	0	878	A	C3'-C2'-O2'	7.00	121.19	110.70
30	p	39	ARG	NE-CZ-NH2	-6.98	112.91	119.20
33	N	1648	U	P-O5'-C5'	-6.98	110.43	120.90
39	4	111	MET	CG-SD-CE	-6.97	85.56	100.90
33	N	2732	G	C1'-C2'-O2'	-6.97	97.95	108.40
24	j	14	ARG	CG-CD-NE	-6.93	96.75	112.00
4	P	157	SER	N-CA-C	-6.88	100.62	110.59
33	N	1865	U	C4'-C3'-O3'	-6.87	102.69	113.00
33	N	1993	U	C3'-C2'-O2'	-6.86	100.41	110.70
18	d	22	LYS	N-CA-C	-6.85	100.34	110.48
30	p	39	ARG	NE-CZ-NH1	6.85	128.35	121.50
33	N	1666	G	C3'-C2'-O2'	6.85	120.97	110.70
35	0	1279	G	N9-C1'-C2'	6.85	122.27	112.00
5	Q	13	ARG	NE-CZ-NH2	6.84	125.36	119.20
2	M	73	C	OP1-P-O3'	-6.83	87.52	108.00
18	d	6	ARG	NE-CZ-NH2	6.80	125.33	119.20
33	N	989	G	C4'-C3'-O3'	-6.77	102.85	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	241	GLY	N-CA-C	6.74	124.66	114.61
33	N	995	C	C2'-C3'-O3'	6.74	119.61	109.50
41	6	109	ARG	CG-CD-NE	-6.73	97.20	112.00
33	N	2061	G	C4'-C3'-O3'	-6.71	102.93	113.00
33	N	1313	U	N1-C1'-C2'	6.70	122.05	112.00
35	0	1190	G	C1'-C2'-O2'	-6.70	101.75	111.80
33	N	2832	U	C4'-C3'-O3'	-6.69	102.96	113.00
33	N	974	G	N9-C1'-C2'	6.68	124.01	114.00
33	N	2238	G	C2'-C3'-O3'	6.67	119.50	109.50
17	c	93	ARG	CG-CD-NE	-6.61	97.45	112.00
3	O	108	A	C2'-C3'-O3'	-6.61	103.79	113.70
33	N	421	C	C2'-C3'-O3'	6.59	119.38	109.50
35	0	1190	G	C4'-C3'-O3'	-6.59	99.52	109.40
30	p	34	ARG	NE-CZ-NH1	-6.56	114.94	121.50
33	N	1666	G	O4'-C4'-C3'	-6.55	97.45	104.00
43	8	18	ARG	CB-CG-CD	-6.54	96.25	111.30
35	0	388	G	C2'-C3'-O3'	6.54	119.30	109.50
33	N	2509	G	C3'-C2'-O2'	6.53	120.50	110.70
33	N	2071	A	C3'-C2'-O2'	6.52	120.48	110.70
16	b	102	ARG	NE-CZ-NH2	6.51	125.06	119.20
34	L	54	GLY	N-CA-C	6.50	120.97	112.25
35	0	665	A	C2'-C3'-O3'	-6.50	103.95	113.70
13	Y	68	SER	N-CA-C	6.49	118.43	111.36
35	0	1145	A	C4'-C3'-O3'	-6.47	103.30	113.00
35	0	1301	U	N1-C1'-C2'	6.46	121.69	112.00
35	0	1151	A	C4'-C3'-O3'	-6.45	103.32	113.00
13	Y	30	THR	N-CA-CB	6.45	121.38	110.49
54	J	69	LYS	N-CA-C	6.45	124.53	110.80
33	N	1452	G	C4'-C3'-O3'	-6.42	103.36	113.00
35	0	818	G	C4'-C3'-O3'	-6.39	103.42	113.00
17	c	73	VAL	N-CA-CB	6.38	117.67	110.72
13	Y	47	ARG	NE-CZ-NH2	6.36	124.92	119.20
33	N	1212	G	C4'-C3'-O3'	-6.35	103.48	113.00
25	k	57	ARG	NE-CZ-NH2	6.34	124.91	119.20
28	n	25	VAL	CA-C-N	6.32	133.08	121.70
28	n	25	VAL	C-N-CA	6.32	133.08	121.70
50	F	43	ALA	CA-C-N	6.31	133.60	121.54
50	F	43	ALA	C-N-CA	6.31	133.60	121.54
33	N	404	A	C4'-C3'-O3'	6.30	118.86	109.40
52	H	57	ARG	CA-CB-CG	6.30	126.70	114.10
39	4	127	ALA	N-CA-C	6.29	119.48	110.24
24	j	41	ARG	CD-NE-CZ	6.28	133.19	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	2443	C	O4'-C4'-C3'	-6.28	97.72	104.00
35	0	1213	A	C4'-C3'-O3'	-6.27	103.59	113.00
4	P	11	PRO	CB-CA-C	-6.26	103.37	111.39
3	O	44	G	N9-C1'-C2'	6.25	121.38	112.00
33	N	2364	C	O4'-C4'-C3'	-6.24	97.76	104.00
37	2	167	TRP	N-CA-C	6.21	119.68	110.48
33	N	859	G	C1'-C2'-O2'	-6.20	102.49	111.80
33	N	446	G	C2'-C3'-O3'	6.19	118.78	109.50
33	N	2728	U	C2'-C3'-O3'	-6.19	104.42	113.70
33	N	2501	C	C4'-C3'-O3'	-6.18	103.73	113.00
46	B	22	PRO	O-C-N	-6.13	114.36	122.64
35	0	1201	A	C2'-C3'-O3'	6.12	118.69	109.50
24	j	41	ARG	CB-CG-CD	6.11	125.35	111.30
35	0	818	G	N9-C1'-C2'	6.10	121.16	112.00
33	N	2728	U	C4'-C3'-O3'	-6.09	103.86	113.00
9	U	27	ARG	NE-CZ-NH1	-6.07	115.43	121.50
30	p	12	ARG	CA-CB-CG	6.07	126.24	114.10
45	A	124	PRO	CA-C-N	6.07	129.02	120.28
45	A	124	PRO	C-N-CA	6.07	129.02	120.28
13	Y	78	ARG	NE-CZ-NH2	6.05	124.65	119.20
39	4	138	ARG	N-CA-CB	6.05	120.72	110.49
33	N	2725	A	C1'-C2'-O2'	-6.04	99.33	108.40
46	B	44	LYS	N-CA-C	6.04	120.44	112.35
33	N	1352	U	O4'-C1'-C2'	-6.02	101.58	107.60
33	N	2034	U	C4'-C3'-O3'	-6.02	103.97	113.00
4	P	221	ARG	N-CA-CB	6.01	120.08	110.46
15	a	69	ARG	NE-CZ-NH2	6.01	124.61	119.20
33	N	2319	G	C4'-C3'-O3'	-5.99	104.01	113.00
15	a	70	THR	N-CA-C	5.99	123.55	110.80
50	F	44	SER	N-CA-C	-5.98	98.06	110.80
33	N	827	U	C2'-C3'-O3'	-5.97	104.74	113.70
33	N	2518	A	C1'-C2'-O2'	-5.94	102.89	111.80
33	N	2246	G	O4'-C4'-C3'	-5.93	98.07	104.00
27	m	32	ILE	N-CA-CB	5.93	116.99	110.53
33	N	782	A	C4'-C3'-O3'	-5.92	100.53	109.40
33	N	1567	G	C1'-C2'-O2'	-5.92	102.93	111.80
33	N	2468	A	C4'-C3'-O3'	-5.91	104.13	113.00
35	0	64	G	C2'-C3'-O3'	-5.91	104.83	113.70
33	N	2543	G	C5'-C4'-C3'	-5.90	107.15	116.00
33	N	974	G	C4'-C3'-O3'	-5.90	100.56	109.40
24	j	19	LYS	N-CA-C	5.89	120.47	113.16
33	N	871	U	P-O5'-C5'	-5.88	112.07	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	1626	A	C2'-C3'-O3'	-5.87	104.89	113.70
33	N	1254	A	C4'-C3'-O3'	-5.87	104.19	113.00
24	j	41	ARG	N-CA-C	5.86	120.72	112.93
35	0	330	C	P-O5'-C5'	-5.84	112.14	120.90
32	r	36	ARG	NE-CZ-NH1	-5.84	115.66	121.50
33	N	820	A	O4'-C4'-C3'	-5.84	98.16	104.00
33	N	2035	G	C4'-C3'-O3'	-5.84	100.65	109.40
4	P	31	ALA	CA-C-N	-5.83	114.89	120.83
4	P	31	ALA	C-N-CA	-5.83	114.89	120.83
4	P	258	ARG	NE-CZ-NH1	-5.81	115.69	121.50
33	N	301	G	C4'-C3'-O3'	-5.81	104.29	113.00
33	N	2873	A	P-O5'-C5'	-5.80	112.19	120.90
5	Q	113	SER	N-CA-C	5.80	117.54	110.41
33	N	974	G	C2'-C3'-O3'	5.80	118.19	109.50
5	Q	151	THR	O-C-N	-5.79	114.95	121.43
28	n	25	VAL	N-CA-C	5.79	116.43	110.82
33	N	1970	A	C2'-C3'-O3'	5.79	118.18	109.50
39	4	38	VAL	CG1-CB-CG2	-5.75	98.14	110.80
4	P	238	ARG	N-CA-C	5.75	123.04	110.80
19	e	79	ARG	CD-NE-CZ	-5.73	116.38	124.40
33	N	782	A	C2'-C3'-O3'	5.73	118.09	109.50
33	N	2267	A	N9-C1'-C2'	5.73	120.59	112.00
4	P	177	ARG	CG-CD-NE	-5.72	99.41	112.00
18	d	33	ARG	CB-CG-CD	-5.72	98.15	111.30
33	N	512	G	P-O3'-C3'	5.71	128.77	120.20
33	N	2447	G	P-O3'-C3'	5.71	128.77	120.20
33	N	140	C	N1-C1'-C2'	5.71	120.56	112.00
39	4	24	THR	N-CA-C	5.69	117.57	110.91
35	0	971	G	C2'-C3'-O3'	-5.69	105.17	113.70
28	n	7	LYS	CD-CE-NZ	5.69	130.10	111.90
33	N	2035	G	C1'-C2'-O2'	-5.68	103.28	111.80
4	P	156	ARG	CB-CG-CD	-5.68	98.24	111.30
33	N	2049	G	C3'-C2'-O2'	5.68	119.22	110.70
35	0	96	U	C2'-C3'-O3'	5.67	122.21	113.70
33	N	2543	G	O5'-C5'-C4'	5.67	120.00	111.50
33	N	1261	C	O4'-C4'-C3'	-5.66	98.34	104.00
35	0	1280	A	C4'-C3'-O3'	-5.66	104.50	113.00
3	O	88	C	C4'-C3'-O3'	-5.65	104.53	113.00
37	2	6	HIS	N-CA-C	-5.64	102.55	109.65
18	d	13	ARG	NE-CZ-NH2	5.63	124.27	119.20
33	N	555	G	C4'-C3'-O3'	-5.63	104.55	113.00
37	2	3	GLN	N-CA-C	5.63	122.08	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	1900	A	P-O3'-C3'	5.63	128.64	120.20
33	N	2776	A	C4'-N9-C1'	5.63	143.18	126.30
33	N	2776	A	C8-N9-C1'	-5.62	110.83	127.70
33	N	301	G	N9-C1'-C2'	5.61	120.42	112.00
16	b	100	HIS	CA-C-N	-5.61	115.54	123.95
16	b	100	HIS	C-N-CA	-5.61	115.54	123.95
17	c	53	ARG	CB-CG-CD	-5.61	98.41	111.30
3	O	24	G	C2'-C3'-O3'	-5.60	105.30	113.70
35	0	1432	G	C4'-C3'-O3'	-5.60	104.60	113.00
15	a	69	ARG	CG-CD-NE	5.59	124.31	112.00
33	N	1661	G	C3'-C2'-O2'	5.59	119.09	110.70
33	N	2034	U	O3'-P-O5'	-5.59	95.62	104.00
33	N	1565	C	C2'-C3'-O3'	5.59	117.88	109.50
35	0	1196	A	C4'-C3'-O3'	-5.58	104.63	113.00
33	N	752	A	N9-C1'-C2'	5.58	122.36	114.00
16	b	102	ARG	NE-CZ-NH1	-5.57	115.93	121.50
33	N	2019	A	C3'-C2'-O2'	5.57	119.05	110.70
31	q	8	ARG	CG-CD-NE	5.56	124.22	112.00
33	N	2517	C	O3'-P-O5'	-5.55	95.67	104.00
28	n	55	ILE	N-CA-C	5.54	120.86	109.34
33	N	1205	A	C4'-C3'-O3'	5.54	117.71	109.40
43	8	126	GLN	CA-C-O	-5.53	114.96	121.16
35	0	665	A	C3'-C2'-O2'	5.53	119.00	110.70
33	N	1565	C	C5'-C4'-C3'	-5.53	106.91	115.20
33	N	784	G	P-O3'-C3'	5.52	128.48	120.20
40	5	63	ASN	N-CA-C	5.52	117.37	110.91
35	0	686	U	C4'-C3'-O3'	-5.51	104.73	113.00
33	N	727	A	N9-C1'-C2'	5.50	120.25	112.00
33	N	2751	G	C2'-C3'-O3'	-5.50	105.45	113.70
33	N	2645	G	C5'-C4'-C3'	-5.50	106.95	115.20
33	N	2645	G	P-O5'-C5'	-5.48	112.67	120.90
36	1	17	GLY	CA-C-O	-5.48	117.85	122.29
33	N	1428	C	C2'-C3'-O3'	-5.48	105.49	113.70
33	N	372	G	C1'-C2'-O2'	-5.47	103.59	111.80
33	N	645	C	N1-C1'-C2'	5.47	120.21	112.00
5	Q	160	LYS	CG-CD-CE	5.46	123.86	111.30
33	N	947	A	C3'-C2'-O2'	-5.46	102.52	110.70
33	N	2724	U	C2'-C3'-O3'	-5.45	105.53	113.70
35	0	1125	U	N1-C1'-C2'	5.44	120.16	112.00
33	N	923	G	C3'-C2'-O2'	5.44	118.86	110.70
33	N	962	G	C3'-C2'-O2'	5.44	118.86	110.70
35	0	1491	G	C4'-C3'-O3'	5.44	121.16	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	157	ARG	NE-CZ-NH1	-5.43	116.07	121.50
33	N	1012	U	C2'-C3'-O3'	-5.42	105.56	113.70
51	G	71	LYS	N-CA-C	5.42	122.35	110.80
33	N	2038	G	C3'-C2'-O2'	5.42	118.82	110.70
35	0	1211	U	C2'-C3'-O3'	-5.40	105.59	113.70
17	c	21	ARG	NE-CZ-NH1	-5.40	116.10	121.50
33	N	2820	A	C4'-C3'-O3'	-5.40	104.90	113.00
28	n	7	LYS	CG-CD-CE	-5.39	98.89	111.30
35	0	813	U	C4'-C3'-O3'	-5.39	104.92	113.00
33	N	1819	A	C1'-C2'-O2'	-5.39	103.72	111.80
32	r	1	MET	CB-CG-SD	-5.38	96.57	112.70
35	0	563	A	N9-C1'-C2'	5.37	120.06	112.00
33	N	51	G	C4'-C3'-O3'	-5.37	104.95	113.00
33	N	983	A	C5'-C4'-O4'	-5.37	101.75	109.80
33	N	2645	G	C2'-C3'-O3'	5.37	117.55	109.50
33	N	2497	A	C2'-C3'-O3'	5.35	117.53	109.50
33	N	783	A	O4'-C1'-C2'	-5.35	102.25	107.60
33	N	1937	A	N9-C1'-C2'	5.35	120.02	112.00
35	0	5	U	C2'-C3'-O3'	-5.34	105.69	113.70
33	N	310	A	C1'-C2'-O2'	-5.33	100.40	108.40
44	9	42	LEU	CA-C-N	5.33	126.50	119.84
44	9	42	LEU	C-N-CA	5.33	126.50	119.84
33	N	1770	G	C3'-C2'-O2'	5.32	118.68	110.70
33	N	2394	C	O4'-C4'-C3'	-5.32	98.68	104.00
30	p	12	ARG	CB-CG-CD	-5.31	99.08	111.30
24	j	41	ARG	NH1-CZ-NH2	-5.31	112.39	119.30
33	N	2430	A	C3'-C2'-O2'	5.31	118.67	110.70
33	N	2552	U	C3'-C2'-O2'	5.31	118.67	110.70
13	Y	29	LYS	CD-CE-NZ	-5.31	94.92	111.90
33	N	1236	G	P-O3'-C3'	5.30	128.16	120.20
33	N	2354	C	C5'-C4'-C3'	-5.29	108.06	116.00
33	N	1620	G	C3'-C2'-O2'	5.28	118.62	110.70
35	0	388	G	O3'-P-O5'	-5.27	96.09	104.00
33	N	2092	U	P-O5'-C5'	-5.27	113.00	120.90
14	Z	118	LYS	CB-CG-CD	-5.26	99.19	111.30
33	N	1977	A	C2'-C3'-O3'	-5.26	105.81	113.70
33	N	669	G	N9-C1'-C2'	5.26	119.89	112.00
35	0	1094	G	C4'-C3'-O3'	-5.26	105.11	113.00
33	N	1650	A	C3'-C2'-O2'	5.26	118.58	110.70
4	P	226	ASN	CA-C-N	-5.25	114.25	119.56
4	P	226	ASN	C-N-CA	-5.25	114.25	119.56
33	N	2498	C	C3'-C2'-O2'	5.25	118.58	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	114	LYS	CA-CB-CG	5.25	124.60	114.10
33	N	2497	A	C4'-C3'-O3'	-5.25	101.53	109.40
25	k	28	ARG	NE-CZ-NH2	-5.24	114.48	119.20
35	0	652	U	C2'-C3'-O3'	-5.24	105.85	113.70
33	N	2502	G	C3'-C2'-O2'	-5.23	102.85	110.70
49	E	64	ARG	CG-CD-NE	-5.23	100.49	112.00
13	Y	18	ARG	NE-CZ-NH2	-5.22	114.50	119.20
33	N	785	G	P-O5'-C5'	-5.21	113.09	120.90
33	N	1343	G	N9-C1'-C2'	5.21	119.81	112.00
4	P	156	ARG	CG-CD-NE	5.20	123.45	112.00
12	X	29	HIS	CB-CA-C	-5.20	103.49	111.66
5	Q	12	THR	N-CA-C	-5.20	101.48	108.19
33	N	372	G	C2'-C3'-O3'	5.20	117.29	109.50
33	N	2849	U	P-O5'-C5'	5.20	128.69	120.90
33	N	2474	U	N1-C1'-C2'	5.19	119.79	112.00
46	B	12	ARG	NE-CZ-NH1	-5.19	116.31	121.50
20	f	11	ARG	N-CA-CB	5.19	118.05	110.58
33	N	421	C	C4'-C3'-O3'	5.19	117.18	109.40
33	N	2596	U	C2'-C3'-O3'	-5.19	105.92	113.70
3	O	41	G	C4'-C3'-O3'	-5.18	105.22	113.00
38	3	5	LEU	CB-CA-C	-5.18	104.55	112.11
15	a	69	ARG	N-CA-C	-5.18	103.20	110.50
35	0	812	G	C1'-C2'-O2'	-5.17	100.64	108.40
35	0	1530	G	C4'-C3'-O3'	-5.17	105.24	113.00
33	N	27	G	C5'-C4'-O4'	-5.17	102.04	109.80
33	N	1180	U	N1-C1'-C2'	5.17	119.76	112.00
33	N	2638	G	C4'-C3'-O3'	-5.17	105.25	113.00
33	N	2311	A	P-O3'-C3'	5.16	127.94	120.20
13	Y	41	ARG	CA-CB-CG	-5.16	103.78	114.10
12	X	35	VAL	CA-C-O	-5.16	115.20	121.18
33	N	278	A	N9-C1'-C2'	5.16	119.73	112.00
35	0	1303	C	N1-C1'-C2'	5.16	119.73	112.00
33	N	2867	G	C4'-C3'-O3'	5.15	117.12	109.40
33	N	2035	G	C2'-C3'-O3'	5.14	117.22	109.50
33	N	2062	A	O4'-C4'-C3'	-5.14	100.96	106.10
33	N	2621	G	C3'-C2'-O2'	5.14	118.41	110.70
33	N	2580	U	N1-C1'-C2'	5.14	119.71	112.00
33	N	1676	A	C3'-C2'-O2'	5.13	118.40	110.70
55	K	33	ARG	CA-CB-CG	5.13	124.37	114.10
18	d	3	ARG	NE-CZ-NH1	-5.13	116.37	121.50
26	l	52	ARG	NE-CZ-NH1	-5.13	116.37	121.50
6	R	49	ARG	NE-CZ-NH1	-5.12	116.38	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	100	G	C3'-C2'-O2'	5.12	118.38	110.70
5	Q	128	ARG	CA-C-N	5.12	127.98	120.71
5	Q	128	ARG	C-N-CA	5.12	127.98	120.71
33	N	481	G	C2'-C3'-O3'	-5.12	106.02	113.70
33	N	1998	A	O4'-C4'-C3'	-5.12	98.88	104.00
33	N	2019	A	C2'-C3'-O3'	-5.12	106.03	113.70
33	N	566	U	C2'-C3'-O3'	-5.11	106.03	113.70
33	N	2049	G	O4'-C4'-C3'	-5.11	98.89	104.00
18	d	32	TYR	CA-C-O	5.10	125.86	120.10
33	N	123	G	C3'-C2'-O2'	5.09	118.34	110.70
32	r	36	ARG	CG-CD-NE	-5.09	100.80	112.00
33	N	1997	C	O4'-C4'-C3'	-5.09	98.91	104.00
33	N	2732	G	C3'-C2'-O2'	-5.09	103.07	110.70
50	F	42	ILE	CA-C-N	5.08	131.24	121.54
50	F	42	ILE	C-N-CA	5.08	131.24	121.54
35	0	971	G	P-O5'-C5'	-5.08	113.28	120.90
35	0	595	A	C4'-C3'-O3'	5.07	117.01	109.40
35	0	812	G	P-O3'-C3'	5.07	127.81	120.20
38	3	23	SER	O-C-N	5.07	127.99	122.11
33	N	1253	A	C2'-C3'-O3'	5.07	117.10	109.50
33	N	2238	G	C4'-C3'-O3'	-5.07	101.80	109.40
33	N	1131	G	O3'-P-O5'	-5.05	96.42	104.00
33	N	2502	G	P-O5'-C5'	5.05	128.47	120.90
35	0	801	U	C2'-C3'-O3'	-5.05	106.12	113.70
2	M	9	C	C2'-C3'-O3'	-5.05	106.13	113.70
33	N	683	U	N1-C1'-C2'	5.05	119.57	112.00
18	d	53	ARG	NE-CZ-NH1	5.03	126.53	121.50
33	N	1928	A	C3'-C2'-O2'	5.03	118.25	110.70
33	N	995	C	C1'-C2'-O2'	-5.03	104.25	111.80
36	1	103	ASN	N-CA-CB	5.03	119.91	110.56
33	N	2049	G	C2'-C3'-O3'	-5.02	106.17	113.70
33	N	60	G	C1'-C2'-O2'	-5.02	104.27	111.80
14	Z	8	LYS	CB-CG-CD	-5.02	99.76	111.30
15	a	1	MET	CB-CG-SD	-5.02	97.65	112.70
18	d	9	ILE	N-CA-C	5.02	117.36	111.09
33	N	1968	G	O4'-C4'-C3'	-5.02	98.98	104.00
18	d	32	TYR	N-CA-C	5.01	117.47	111.71
39	4	30	ILE	CB-CA-C	5.01	117.65	110.33
33	N	820	A	O4'-C1'-C2'	-5.01	102.59	107.60

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	0	24	U	Sidechain
35	0	368	U	Sidechain
35	0	559	A	Sidechain
35	0	571	U	Sidechain
35	0	864	A	Sidechain
36	1	10	LEU	Peptide
36	1	102	THR	Peptide
36	1	14	VAL	Peptide
37	2	79	LYS	Peptide
37	2	80	LYS	Peptide
39	4	102	GLY	Peptide
39	4	136	VAL	Peptide
39	4	137	VAL	Peptide
39	4	142	ASP	Peptide
39	4	89	HIS	Peptide
40	5	52	ASN	Peptide
40	5	93	LYS	Peptide
43	8	128	SER	Peptide
43	8	53	GLU	Peptide
43	8	54	LEU	Peptide
43	8	55	VAL	Peptide
45	A	125	LYS	Peptide
46	B	22	PRO	Peptide
46	B	77	HIS	Peptide
51	G	17	MET	Peptide
51	G	69	LYS	Peptide
53	I	37	ARG	Peptide
54	J	3	ASN	Peptide
55	K	34	ARG	Peptide
33	N	1802	A	Sidechain
33	N	2105	U	Sidechain
33	N	2522	U	Sidechain
33	N	2765	A	Sidechain
33	N	586	A	Sidechain
33	N	850	U	Sidechain
33	N	927	A	Sidechain
4	P	195	VAL	Peptide
4	P	234	GLY	Peptide
4	P	238	ARG	Peptide
5	Q	151	THR	Peptide
7	S	174	ASP	Peptide
7	S	175	PHE	Peptide
9	U	34	GLY	Peptide

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Mol	Chain	Res	Type	Group
10	V	11	LEU	Peptide
13	Y	114	GLY	Peptide
13	Y	82	LEU	Peptide
14	Z	57	VAL	Peptide,Mainchain
22	h	52	LEU	Peptide
31	q	31	HIS	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	s	316	0	283	8	0
2	M	1594	0	809	17	0
3	O	2529	0	1281	15	0
4	P	2082	0	2154	38	0
5	Q	1564	0	1616	25	0
6	R	1552	0	1619	20	0
7	S	1410	0	1444	23	0
8	T	1322	0	1371	13	0
9	U	359	0	381	6	0
10	V	1031	0	1085	19	0
11	W	1128	0	1162	15	0
12	X	938	0	1012	15	0
13	Y	1044	0	1117	18	0
14	Z	1073	0	1157	16	0
15	a	960	0	1000	15	0
16	b	891	0	923	9	0
17	c	915	0	958	15	0
18	d	946	0	1019	21	0
19	e	815	0	839	18	0
20	f	857	0	922	11	0
21	g	738	0	807	5	0
22	h	779	0	831	10	0
23	i	752	0	780	9	0
24	j	568	0	581	10	0
25	k	624	0	652	13	0
26	l	508	0	543	8	0
27	m	448	0	488	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	n	443	0	458	12	0
29	o	409	0	440	5	0
30	p	376	0	418	17	0
31	q	503	0	572	11	0
32	r	301	0	341	8	0
33	N	62215	0	31280	338	0
34	L	522	0	524	12	0
35	0	33015	0	16607	168	0
36	1	1704	0	1732	29	0
37	2	1624	0	1696	20	0
38	3	1642	0	1707	22	0
39	4	1105	0	1148	22	0
40	5	817	0	808	15	0
41	6	1181	0	1238	19	0
42	7	978	0	1031	6	0
43	8	1021	0	1070	22	0
44	9	786	0	828	21	0
45	A	876	0	887	22	0
46	B	954	0	1016	17	0
47	C	883	0	941	18	0
48	D	773	0	824	12	0
49	E	709	0	728	5	0
50	F	648	0	666	10	0
51	G	648	0	691	6	0
52	H	455	0	478	12	0
53	I	637	0	665	11	0
54	J	664	0	714	17	0
55	K	425	0	449	13	0
56	t	85	0	44	0	0
All	All	144142	0	96835	1014	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 4.

All (1014) 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)
33:N:306:U:H3	33:N:310:A:N6	1.15	1.39
35:0:1238:A:N6	35:0:1301:U:H3	1.22	1.31
33:N:499:U:H3	33:N:503:A:N6	1.39	1.19
2:M:75:A:N1	33:N:2450:A:O2'	1.74	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:306:U:N3	33:N:310:A:N6	1.86	1.01
2:M:15:G:H5''	2:M:15:G:H8	1.31	0.95
2:M:15:G:H5''	2:M:15:G:C8	2.02	0.93
35:0:1060:U:C5	37:2:2:GLY:HA3	2.07	0.90
4:P:35:GLU:OE2	33:N:1816:C:N4	2.10	0.85
33:N:2304:G:H22	33:N:2312:U:H3	1.23	0.83
44:9:83:THR:O	44:9:87:LEU:HB2	1.79	0.83
33:N:499:U:N3	33:N:503:A:N6	2.11	0.81
45:A:109:ASN:OD1	55:K:7:ARG:HG2	1.80	0.81
2:M:15:G:H5'	2:M:16:C:OP2	1.81	0.80
33:N:284:U:H3	33:N:356:G:H1	1.30	0.79
35:0:1238:A:N7	35:0:1301:U:O4	2.18	0.77
15:a:53:THR:HG21	33:N:2840:C:H5''	1.66	0.77
47:C:101:ARG:NH1	47:C:104:THR:OG1	2.16	0.77
35:0:1279:G:OP1	44:9:9:ARG:NH2	2.18	0.76
2:M:16:C:H3'	2:M:17:G:H5'	1.68	0.76
9:U:11:ASN:HD22	33:N:2095:A:H5''	1.50	0.76
39:4:101:GLU:OE2	39:4:103:THR:OG1	2.05	0.75
32:r:3:VAL:HG21	33:N:2539:C:H5'	1.66	0.75
33:N:306:U:C2	33:N:310:A:N6	2.54	0.75
4:P:221:ARG:NH1	33:N:1789:A:OP2	2.20	0.74
47:C:87:ARG:O	47:C:91:HIS:HB2	1.87	0.74
35:0:673:A:O3'	40:5:86:ARG:NH2	2.20	0.73
53:I:30:PRO:HA	53:I:48:THR:O	1.88	0.73
35:0:1527:U:OP2	55:K:39:GLU:OE1	2.07	0.73
44:9:65:TYR:HB3	48:D:96:LEU:HD11	1.69	0.73
5:Q:14:ILE:HA	17:c:12:GLN:HE22	1.52	0.73
53:I:6:LYS:HG3	53:I:7:LYS:HG2	1.70	0.73
33:N:1093:G:N2	33:N:1098:A:H62	1.85	0.73
35:0:1147:C:O2	43:8:18:ARG:NH2	2.22	0.73
33:N:1093:G:H21	33:N:1098:A:N6	1.87	0.72
2:M:16:C:C3'	2:M:17:G:H5'	2.20	0.71
35:0:1081:A:OP2	39:4:52:LYS:NZ	2.23	0.71
15:a:77:ALA:O	15:a:81:ASN:HB2	1.90	0.71
39:4:81:LEU:HD13	39:4:123:VAL:HG11	1.72	0.71
48:D:47:LYS:HB3	53:I:13:LEU:HD12	1.72	0.71
35:0:404:G:O2'	35:0:498:A:N1	2.23	0.70
20:f:15:GLN:HE22	33:N:1266:G:H5''	1.56	0.70
31:q:8:ARG:NH2	33:N:243:U:OP1	2.24	0.70
35:0:664:G:H22	35:0:741:G:H1	1.37	0.70
33:N:2637:U:N3	33:N:2776:A:N6	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:O:1309:G:OP2	47:C:98:ARG:NH1	2.25	0.70
7:S:37:ASN:ND2	33:N:2312:U:O2	2.24	0.70
6:R:163:ASN:ND2	33:N:323:C:H2'	2.07	0.69
4:P:258:ARG:NH1	4:P:264:ASP:OD1	2.23	0.69
35:O:501:C:OP1	46:B:114:ARG:NH2	2.26	0.69
4:P:87:ARG:NH2	33:N:1817:G:OP1	2.26	0.68
3:O:48:U:OP1	16:b:30:ARG:NH2	2.26	0.68
43:8:84:THR:HG21	43:8:103:PHE:HB3	1.75	0.68
21:g:46:ALA:O	21:g:50:LEU:HB2	1.94	0.68
33:N:613:A:N7	33:N:616:A:N1	2.41	0.68
11:W:113:PRO:HD2	33:N:558:U:OP1	1.94	0.67
5:Q:45:TYR:HH	33:N:2636:C:HO2'	1.41	0.67
47:C:29:ARG:HH21	47:C:63:PHE:HB2	1.59	0.67
33:N:499:U:C2	33:N:503:A:N6	2.63	0.67
35:O:1064:G:N2	35:O:1190:G:O2'	2.28	0.67
36:1:209:ALA:O	36:1:213:TYR:HB2	1.94	0.67
48:D:26:GLU:HG2	48:D:30:ILE:HD12	1.77	0.66
8:T:67:THR:HG21	33:N:2757:A:N1	2.10	0.66
33:N:962:G:H21	33:N:2250:G:H1	1.41	0.66
35:O:427:U:OP1	38:3:13:ARG:NH2	2.28	0.66
4:P:29:PRO:HG2	4:P:34:LEU:HD11	1.78	0.66
2:M:74:C:H2'	2:M:75:A:H1'	1.78	0.65
35:O:554:A:H5'	46:B:26:ALA:HB1	1.78	0.65
33:N:140:C:OP1	33:N:141:G:N2	2.30	0.65
33:N:1019:U:H3	33:N:1142:A:N6	1.95	0.65
42:7:75:ILE:HD13	42:7:129:VAL:HG22	1.79	0.65
31:q:8:ARG:NH2	33:N:243:U:P	2.70	0.65
33:N:1311:G:H21	33:N:1603:A:H62	1.45	0.65
30:p:37:LYS:HE2	33:N:469:G:O6	1.97	0.64
35:O:458:U:H3	35:O:474:G:H1	1.44	0.64
35:O:974:A:OP1	48:D:69:ARG:NH2	2.30	0.64
42:7:15:ARG:NH1	42:7:75:ILE:O	2.30	0.64
7:S:88:LYS:HD3	33:N:2313:C:H5''	1.80	0.64
35:O:1060:U:OP1	48:D:85:ARG:NH2	2.30	0.64
43:8:123:ARG:NH1	43:8:124:ARG:O	2.31	0.64
45:A:24:HIS:HB3	45:A:31:ILE:HG23	1.78	0.64
33:N:2405:G:O2'	33:N:2411:A:N6	2.30	0.64
33:N:2637:U:H3	33:N:2776:A:N6	1.96	0.64
35:O:437:U:OP1	38:3:152:GLN:NE2	2.30	0.64
43:8:46:MET:HE2	43:8:50:GLN:HE21	1.63	0.64
33:N:1315:C:O2'	33:N:1392:A:N3	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:2:ILE:HB	12:X:33:ALA:HB3	1.80	0.63
18:d:6:ARG:NH1	33:N:585:G:N7	2.47	0.63
51:G:9:GLN:HG2	51:G:60:GLU:HG2	1.81	0.63
53:I:11:ILE:HG22	53:I:38:SER:HB3	1.81	0.63
35:0:972:C:OP2	44:9:59:LYS:HD3	1.98	0.63
3:O:31:C:H4'	7:S:26:MET:HE1	1.79	0.63
41:6:147:ALA:O	45:A:56:ARG:NH2	2.32	0.63
12:X:92:GLU:O	12:X:93:GLN:HB2	1.99	0.63
14:Z:55:ARG:NH2	33:N:2469:A:O2'	2.32	0.63
30:p:44:VAL:HG13	30:p:44:VAL:O	1.98	0.63
43:8:25:ASN:HA	43:8:59:GLU:HG3	1.81	0.63
35:0:1086:U:H3	35:0:1099:G:H22	1.46	0.63
33:N:1105:U:H2'	33:N:1106:G:H8	1.64	0.62
35:0:1527:U:OP2	55:K:39:GLU:CD	2.42	0.62
1:s:132:TYR:OH	6:R:67:ARG:NH1	2.32	0.62
5:Q:49:GLN:HE21	5:Q:79:LEU:HB3	1.64	0.62
8:T:86:LYS:HG3	8:T:132:VAL:HG22	1.81	0.62
5:Q:38:LYS:O	5:Q:46:ARG:HA	1.97	0.62
33:N:2849:U:O2'	33:N:2866:U:O2	2.15	0.62
14:Z:20:LEU:HD13	23:i:81:PRO:HG2	1.82	0.62
33:N:1066:U:O2'	33:N:1074:G:N2	2.32	0.62
31:q:12:LYS:NZ	33:N:249:C:O2	2.33	0.62
25:k:16:ASN:HA	25:k:25:THR:O	2.01	0.61
21:g:28:ASN:OD1	21:g:91:GLN:NE2	2.31	0.61
23:i:51:GLN:HE22	23:i:86:LEU:HD21	1.65	0.61
43:8:52:LEU:HB3	43:8:57:MET:HB3	1.81	0.61
25:k:12:PRO:HB3	25:k:30:LEU:HD23	1.82	0.61
16:b:16:ARG:NH2	16:b:19:GLN:OE1	2.33	0.61
20:f:15:GLN:NE2	33:N:1266:G:H5''	2.16	0.61
34:L:20:ASN:ND2	34:L:37:CYS:SG	2.73	0.61
55:K:4:ILE:O	55:K:20:LYS:NZ	2.33	0.61
2:M:75:A:C2	33:N:2450:A:O2'	2.40	0.60
3:O:24:G:O2'	3:O:27:C:N4	2.34	0.60
10:V:135:SER:OG	33:N:1062:G:N3	2.34	0.60
33:N:2506[A]:U:OP2	33:N:2576:G:N1	2.33	0.60
44:9:19:ASP:HA	44:9:22:THR:HG22	1.83	0.60
9:U:5:LEU:HD13	9:U:13:GLY:HA2	1.82	0.60
33:N:613:A:H62	33:N:616:A:H61	1.50	0.60
35:0:1055:A:H1'	37:2:156:ARG:HH21	1.66	0.60
30:p:9:VAL:HG23	33:N:1309:G:OP1	2.01	0.60
33:N:475:C:O2	33:N:479:A:N6	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:1019:U:N3	33:N:1142:A:N6	2.50	0.60
33:N:1068:G:N1	33:N:1073:A:N6	2.50	0.60
35:0:933:G:N7	41:6:3:ARG:NH1	2.49	0.60
5:Q:156:PHE:CE1	11:W:81:ILE:HD12	2.37	0.60
33:N:1779:U:H5	33:N:1784:A:N7	1.99	0.60
35:0:769:G:H4'	35:0:1513:A:H4'	1.84	0.59
35:0:1238:A:N6	35:0:1301:U:N3	2.01	0.59
35:0:1238:A:N6	35:0:1301:U:C2	2.68	0.59
53:I:31:LEU:HB2	53:I:49:ILE:HG22	1.84	0.59
4:P:236:GLU:HG2	33:N:2600:A:N7	2.18	0.59
24:j:18:ALA:O	24:j:20:ARG:NH1	2.35	0.59
31:q:16:LYS:HE2	31:q:20:GLY:HA2	1.84	0.59
35:0:1526:G:H3'	55:K:39:GLU:OE1	2.03	0.59
1:s:124:TRP:HB2	20:f:85:ILE:HD11	1.84	0.59
46:B:50:ARG:NH1	46:B:89:ASP:OD2	2.35	0.59
33:N:1726:C:N4	33:N:1735:A:N6	2.51	0.59
35:0:675:A:H1'	45:A:118:HIS:CD2	2.38	0.59
5:Q:46:ARG:NH2	5:Q:88:GLU:O	2.36	0.59
33:N:1019:U:C4	33:N:1142:A:N6	2.71	0.58
33:N:2134:A:H1'	33:N:2159:G:H1'	1.84	0.58
18:d:92:ARG:HG2	33:N:997:G:OP1	2.03	0.58
24:j:15:ASP:OD1	33:N:2263:C:N4	2.35	0.58
35:0:946:A:H2'	35:0:947:G:C8	2.38	0.58
38:3:60:LYS:HE3	38:3:195:ILE:HG22	1.84	0.58
11:W:32:LEU:HD22	11:W:54:ILE:HG21	1.85	0.58
35:0:693:G:OP1	45:A:127:ARG:NH2	2.36	0.58
52:H:26:ILE:O	52:H:30:LYS:HB2	2.02	0.58
35:0:579:A:O2'	49:E:54:ARG:NH1	2.36	0.58
36:1:81:LYS:O	36:1:85:LEU:HB2	2.04	0.58
45:A:93:ARG:HH12	55:K:25:LYS:HD3	1.68	0.58
35:0:1224:U:O2'	35:0:1322:C:OP1	2.21	0.58
35:0:1302:C:C5	47:C:17:ILE:HD13	2.38	0.58
37:2:40:ARG:NH1	37:2:55:ILE:O	2.36	0.58
46:B:68:GLY:O	46:B:99:ARG:NH1	2.36	0.58
14:Z:45:GLN:NE2	33:N:2485:G:OP1	2.34	0.58
49:E:46:HIS:O	49:E:48:LYS:N	2.36	0.58
31:q:5:LYS:HE2	33:N:254:G:N7	2.19	0.58
33:N:1093:G:N2	33:N:1098:A:N6	2.48	0.58
35:0:246:A:N1	35:0:278:G:O2'	2.35	0.58
35:0:812:G:OP1	35:0:902:G:N2	2.34	0.58
18:d:88:VAL:HA	19:e:49:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:693:A:O2'	33:N:1353:A:N3	2.33	0.58
33:N:1212:G:O2'	33:N:1237:A:N6	2.36	0.58
35:0:890:G:O2'	35:0:906:A:N6	2.36	0.58
35:0:1316:G:H22	35:0:1319:A:H5''	1.69	0.58
45:A:112:ASP:HB3	55:K:20:LYS:HE2	1.84	0.58
3:O:43:C:O2	7:S:92:ARG:NH2	2.36	0.57
12:X:70:ARG:NH1	33:N:2684:U:O4'	2.37	0.57
33:N:481:G:O2'	33:N:506:G:N2	2.37	0.57
33:N:2106:U:H2'	33:N:2107:G:H8	1.68	0.57
35:0:927:G:O2'	35:0:1503:A:N7	2.35	0.57
35:0:1368:A:OP2	43:8:114:LYS:HD3	2.05	0.57
36:1:141:LEU:O	36:1:145:GLU:HB2	2.03	0.57
38:3:91:LEU:HD13	38:3:191:LEU:HD11	1.86	0.57
4:P:144:VAL:HB	4:P:154:LEU:HB2	1.86	0.57
23:i:62:THR:HG22	23:i:71:LYS:HG2	1.86	0.57
30:p:34:ARG:HD3	33:N:467:G:OP2	2.05	0.57
33:N:370:G:O2'	33:N:424:G:OP1	2.22	0.57
35:0:1261:A:N6	35:0:1274:A:O2'	2.35	0.57
47:C:83:LEU:HD21	53:I:65:GLU:HG2	1.85	0.57
44:9:27:GLU:O	44:9:31:ARG:HB2	2.04	0.57
11:W:135:GLN:NE2	33:N:6:A:N3	2.53	0.57
24:j:23:VAL:HG22	24:j:38:VAL:HG22	1.87	0.57
40:5:38:ARG:HG2	40:5:63:ASN:HB2	1.85	0.57
10:V:34:ASN:H	10:V:67:PHE:HE1	1.52	0.57
25:k:10:LYS:NZ	33:N:396:G:OP2	2.37	0.57
6:R:69:ARG:HG3	33:N:674:G:O2'	2.05	0.57
8:T:24:ILE:HD11	8:T:43:VAL:HG11	1.87	0.57
33:N:805:G:N2	33:N:829:A:OP1	2.38	0.57
37:2:156:ARG:HD3	37:2:193:TYR:HB3	1.86	0.57
33:N:2848:G:O2'	33:N:2867:G:N2	2.36	0.56
33:N:1726:C:H42	33:N:1735:A:N6	2.04	0.56
14:Z:50:ARG:HD3	14:Z:65:ILE:HD11	1.87	0.56
14:Z:66:ARG:NH1	14:Z:104:GLU:OE2	2.36	0.56
33:N:987:C:O2'	33:N:1000:A:N3	2.36	0.56
43:8:36:GLU:HA	43:8:40:GLY:HA3	1.88	0.56
25:k:6:GLN:O	25:k:74:ARG:NH1	2.37	0.56
3:O:42:C:C5	7:S:66:LEU:HD22	2.40	0.56
35:0:451:A:H61	35:0:481:G:H5'	1.70	0.56
33:N:1070:A:N7	33:N:1096:A:O2'	2.36	0.56
37:2:36:ASP:OD1	37:2:59:ARG:NH2	2.34	0.56
45:A:93:ARG:NH2	45:A:112:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:235:GLY:O	4:P:239:ASN:ND2	2.39	0.56
10:V:31:GLN:NE2	33:N:1097:U:O4	2.34	0.56
15:a:53:THR:HA	15:a:56:LYS:HD3	1.88	0.56
28:n:43:ILE:HG22	28:n:49:TYR:HB2	1.88	0.56
33:N:1332:G:N7	33:N:1609:A:O2'	2.38	0.56
13:Y:111:ILE:HD12	13:Y:111:ILE:H	1.70	0.55
35:0:796:C:O3'	45:A:127:ARG:NH1	2.38	0.55
33:N:413:C:HO2'	33:N:1880:U:HO2'	1.54	0.55
35:0:409:U:OP1	38:3:24:GLY:HA3	2.06	0.55
11:W:56:VAL:HB	11:W:124:VAL:HG12	1.88	0.55
35:0:673:A:H2'	35:0:674:G:C8	2.42	0.55
45:A:30:THR:HG21	45:A:92:GLY:HA3	1.89	0.55
33:N:1980:G:O2'	33:N:1982:U:OP2	2.22	0.55
41:6:40:GLU:OE2	43:8:43:THR:HG23	2.06	0.55
7:S:140:GLU:OE2	34:L:27:THR:HG23	2.07	0.55
10:V:97:LYS:HD2	10:V:139:VAL:HG21	1.87	0.55
39:4:13:GLU:OE1	39:4:68:ARG:NH2	2.39	0.55
44:9:10:LEU:HG	44:9:98:VAL:HG12	1.88	0.55
1:s:150:TYR:O	1:s:154:ASN:ND2	2.35	0.55
19:e:49:ILE:HB	19:e:52:PRO:HA	1.89	0.55
25:k:37:ARG:NH2	33:N:2200:C:OP2	2.39	0.55
33:N:1724:G:O6	33:N:1737:G:C2	2.59	0.55
35:0:401:C:O2'	35:0:621:A:N3	2.39	0.55
35:0:1166:G:N1	35:0:1169:A:OP2	2.40	0.55
33:N:837:C:N3	33:N:941:A:N6	2.54	0.55
35:0:993:G:O2'	35:0:994:A:N7	2.40	0.55
47:C:77:ILE:HG22	47:C:81:MET:HE2	1.89	0.55
6:R:149:ILE:HD12	6:R:175:ILE:HG21	1.88	0.54
28:n:53:LYS:HE2	28:n:56:ALA:HB2	1.89	0.54
33:N:2850:A:N7	33:N:2868:A:O2'	2.35	0.54
3:O:72:G:H21	3:O:104:A:H62	1.55	0.54
39:4:99:ALA:O	39:4:102:GLY:N	2.39	0.54
4:P:2:ALA:N	4:P:199:GLU:OE1	2.39	0.54
8:T:33:LEU:HD22	8:T:75:MET:HG2	1.89	0.54
12:X:43:ILE:HD12	12:X:56:ASP:HB2	1.89	0.54
30:p:31:LEU:HD22	30:p:42:LEU:HD23	1.88	0.54
33:N:306:U:O4	33:N:310:A:N7	2.41	0.54
33:N:1417:C:HO2'	33:N:1587:G:HO2'	1.55	0.54
36:1:117:LEU:HB3	36:1:141:LEU:HD11	1.89	0.54
35:0:1522:U:OP1	45:A:128:ARG:NH1	2.40	0.54
48:D:41:ARG:NH1	48:D:42:TRP:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:204:VAL:O	4:P:206:GLY:N	2.40	0.54
32:r:3:VAL:HG12	32:r:36:ARG:HE	1.73	0.54
33:N:1297:C:O2'	33:N:1302:A:N1	2.39	0.54
33:N:2107:G:O6	33:N:2182:U:O2	2.26	0.54
5:Q:13:ARG:NH1	33:N:2683:C:H4'	2.22	0.54
18:d:37:GLN:HE21	33:N:1252:G:H1	1.55	0.54
25:k:45:ARG:HH21	25:k:47:VAL:HG22	1.71	0.54
32:r:36:ARG:HD2	32:r:37:GLN:HB2	1.88	0.54
33:N:1450:G:N2	33:N:1452:G:O6	2.41	0.54
13:Y:76:GLU:OE2	33:N:627:A:O2'	2.23	0.54
20:f:73:LYS:HB2	20:f:106:VAL:HB	1.90	0.54
2:M:16:C:O2	2:M:16:C:H5''	2.07	0.53
10:V:100:LYS:HA	10:V:139:VAL:O	2.08	0.53
14:Z:74:THR:HA	14:Z:88:ASN:O	2.07	0.53
33:N:1936:A:H2	33:N:1943:U:H3	1.56	0.53
12:X:77:ILE:HG12	17:c:72:ARG:HD2	1.90	0.53
15:a:22:ARG:HG3	15:a:70:THR:HA	1.91	0.53
33:N:28:A:N6	33:N:512:G:H1'	2.23	0.53
35:0:768:A:N3	35:0:1512:U:O2'	2.40	0.53
6:R:178:VAL:O	6:R:182:ALA:HB2	2.08	0.53
33:N:1536:C:O2	33:N:1537:G:N2	2.41	0.53
35:0:979:C:O2	48:D:59:ARG:NH1	2.36	0.53
35:0:1006:G:O6	35:0:1023:U:O2	2.27	0.53
40:5:41:ASP:OD1	40:5:58:HIS:NE2	2.41	0.53
53:I:36:ARG:NH2	53:I:75:ALA:O	2.42	0.53
15:a:114:GLU:OE1	15:a:118:ARG:NH2	2.42	0.53
19:e:1:MET:HA	19:e:42:ALA:O	2.07	0.53
35:0:676:A:H5''	45:A:115:PRO:HB3	1.90	0.53
40:5:11:HIS:HD2	40:5:12:PRO:HD2	1.72	0.53
2:M:74:C:H2'	2:M:75:A:C1'	2.38	0.53
3:O:89:U:H6	33:N:958:U:H2'	1.74	0.53
33:N:1939:U:OP1	33:N:2604:U:O2'	2.27	0.53
7:S:116:GLY:HA3	7:S:178:ARG:HB3	1.91	0.53
31:q:32:ILE:O	31:q:36:LYS:NZ	2.35	0.53
49:E:46:HIS:C	49:E:48:LYS:H	2.17	0.53
28:n:17:ARG:NE	33:N:1266:G:OP2	2.40	0.53
35:0:1003:G:H21	35:0:1005:A:H5'	1.73	0.53
44:9:8:ILE:HA	44:9:99:GLN:O	2.08	0.53
47:C:39:ILE:HD12	47:C:52:GLN:HE21	1.73	0.53
25:k:72:ARG:NH2	25:k:78:TYR:OH	2.33	0.53
33:N:1070:A:H2'	33:N:1097:U:H4'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:0:502:A:OP1	46:B:115:SER:HB3	2.09	0.53
54:J:59:ASP:OD1	54:J:76:LYS:NZ	2.33	0.53
13:Y:21:ARG:HA	33:N:811:U:H2'	1.90	0.52
18:d:88:VAL:HG22	19:e:49:ILE:O	2.09	0.52
13:Y:76:GLU:HG3	13:Y:111:ILE:HD13	1.91	0.52
19:e:74:ILE:HD13	33:N:992:C:H4'	1.90	0.52
22:h:86:ARG:NH1	22:h:100:SER:OG	2.42	0.52
30:p:29:GLN:NE2	33:N:210:C:OP1	2.40	0.52
30:p:12:ARG:NH1	33:N:465:G:OP1	2.42	0.52
33:N:1726:C:N4	33:N:1735:A:H61	2.06	0.52
36:1:80:VAL:HG12	36:1:214:LEU:HD21	1.91	0.52
46:B:34:CYS:SG	46:B:78:SER:OG	2.67	0.52
54:J:28:MET:HE1	54:J:67:ILE:HG12	1.91	0.52
4:P:48:ARG:HD3	33:N:773:U:O2'	2.09	0.52
43:8:19:VAL:HA	43:8:65:ILE:HG22	1.92	0.52
44:9:80:THR:HG22	44:9:82:LYS:H	1.74	0.52
6:R:144:GLU:HG2	6:R:166:LYS:HD2	1.92	0.52
10:V:12:GLN:HE21	10:V:55:ILE:H	1.57	0.52
33:N:51:G:O2'	33:N:118:A:N6	2.42	0.52
36:1:67:ILE:HD12	36:1:160:ALA:HB3	1.91	0.52
6:R:163:ASN:HD21	33:N:323:C:H2'	1.74	0.52
22:h:86:ARG:NH2	22:h:102:THR:OG1	2.43	0.52
10:V:76:ALA:HA	10:V:79:LEU:HB3	1.91	0.52
4:P:160:THR:HG23	4:P:177:ARG:HG2	1.91	0.52
21:g:8:LEU:HD23	21:g:50:LEU:HD21	1.91	0.52
33:N:877:A:O2'	33:N:900:A:N6	2.43	0.52
37:2:55:ILE:HG22	37:2:68:ILE:HG12	1.92	0.52
21:g:18:GLU:OE2	33:N:1392:A:N6	2.43	0.52
35:0:76:G:H1	35:0:93:U:H3	1.56	0.52
24:j:41:ARG:HH11	33:N:2387:U:H1'	1.74	0.52
31:q:8:ARG:HH21	33:N:243:U:P	2.33	0.52
35:0:835:U:OP1	52:H:53:ARG:NH2	2.32	0.52
2:M:15:G:C8	2:M:15:G:C5'	2.86	0.51
6:R:2:GLU:HB3	6:R:11:ALA:HB1	1.92	0.51
11:W:13:ARG:NH1	11:W:49:ASP:O	2.39	0.51
35:0:1076:U:OP1	36:1:174:LYS:NZ	2.43	0.51
51:G:17:MET:HG3	51:G:20:SER:HB3	1.92	0.51
4:P:220:VAL:HG21	33:N:782:A:N7	2.26	0.51
33:N:503:A:O2'	33:N:506:G:OP2	2.28	0.51
33:N:639:U:H2'	33:N:640:C:C6	2.45	0.51
37:2:156:ARG:NH1	37:2:160:ALA:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:16:C:H4'	2:M:17:G:OP2	2.10	0.51
6:R:176:ASP:OD1	6:R:176:ASP:N	2.40	0.51
8:T:24:ILE:HG21	8:T:72:LEU:HD21	1.91	0.51
35:0:263:A:OP2	54:J:74:ARG:NH1	2.42	0.51
44:9:15:HIS:HA	44:9:18:ILE:HG22	1.93	0.51
12:X:77:ILE:HG12	17:c:72:ARG:CD	2.41	0.51
19:e:57:GLY:HA2	19:e:102:SER:O	2.10	0.51
33:N:81:G:HO2'	33:N:295:G:HO2'	1.58	0.51
33:N:270:A:N1	33:N:369:U:O2'	2.39	0.51
6:R:19:PHE:HE1	6:R:109:LEU:HD13	1.75	0.51
26:l:54:LYS:HE3	33:N:72:U:OP2	2.11	0.51
35:0:1527:U:OP2	55:K:39:GLU:OE2	2.28	0.51
40:5:90:MET:SD	52:H:61:ARG:NH1	2.83	0.51
28:n:4:GLN:HA	33:N:2615:U:C2	2.45	0.51
52:H:42:SER:HB3	52:H:52:GLN:HE21	1.75	0.51
33:N:612:G:N2	33:N:614:A:O2'	2.44	0.51
45:A:35:THR:OG1	45:A:36:ASP:N	2.44	0.51
12:X:76:VAL:HG12	17:c:73:VAL:HG22	1.93	0.51
17:c:37:LYS:HD2	17:c:39:ARG:HH11	1.75	0.51
33:N:698:C:O2'	33:N:734:A:N6	2.44	0.51
35:0:976:G:OP2	35:0:1358:U:O2'	2.29	0.51
36:1:54:LEU:HG	36:1:220:THR:HG21	1.92	0.51
2:M:16:C:H3'	2:M:17:G:C5'	2.40	0.51
9:U:38:PRO:O	9:U:43:ASN:ND2	2.41	0.51
10:V:124:ALA:HB1	33:N:1081:U:H4'	1.93	0.51
15:a:41:ALA:HB1	15:a:97:ILE:HD12	1.92	0.51
24:j:19:LYS:NZ	33:N:2261:C:OP1	2.33	0.51
33:N:948:C:O2	33:N:984:A:O2'	2.28	0.51
36:1:68:LEU:HD12	36:1:154:MET:HE1	1.92	0.51
37:2:77:ILE:HA	37:2:84:VAL:HG23	1.92	0.51
41:6:109:ARG:O	41:6:119:ARG:NH2	2.44	0.51
4:P:3:VAL:HG12	4:P:19:VAL:HG22	1.92	0.50
22:h:34:VAL:HG13	22:h:67:VAL:HG22	1.93	0.50
50:F:6:LEU:HG	50:F:17:TYR:HB3	1.93	0.50
6:R:21:ARG:HD3	6:R:106:LYS:HB3	1.93	0.50
33:N:527:C:N4	33:N:2779:U:OP2	2.44	0.50
3:O:44:G:OP2	34:L:1:MET:N	2.40	0.50
4:P:165:VAL:HG21	4:P:181:MET:HE1	1.93	0.50
22:h:51:ALA:O	22:h:54:GLN:NE2	2.44	0.50
35:0:552:U:H5'	46:B:83:ARG:HH11	1.76	0.50
45:A:72:ASP:O	45:A:73:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:16:C:O2	2:M:16:C:H2'	2.11	0.50
38:3:58:LYS:NZ	38:3:69:GLU:OE1	2.44	0.50
10:V:117:MET:HA	33:N:1058:U:O2'	2.11	0.50
39:4:99:ALA:HB2	39:4:124:LEU:HG	1.93	0.50
43:8:55:VAL:O	43:8:60:LYS:NZ	2.43	0.50
12:X:99:ILE:HD12	12:X:118:LEU:HB2	1.93	0.50
19:e:76:LYS:O	19:e:84:ARG:HA	2.11	0.50
22:h:7:ARG:NH2	22:h:26:LYS:O	2.45	0.50
33:N:2140:G:O6	33:N:2151:U:O2	2.29	0.50
37:2:172:ARG:NH2	37:2:206:GLU:OE2	2.44	0.50
47:C:10:PRO:HB2	47:C:18:ALA:HB1	1.94	0.50
10:V:55:ILE:HG22	10:V:57:VAL:HB	1.94	0.50
22:h:11:VAL:HG12	22:h:72:ILE:HG22	1.94	0.50
35:0:843:U:OP1	35:0:844:G:N2	2.43	0.50
15:a:32:GLU:HG2	15:a:115:LEU:HD12	1.93	0.50
33:N:2638:G:O2'	33:N:2778:A:N6	2.44	0.50
19:e:7:SER:OG	19:e:8:GLY:N	2.45	0.50
26:l:6:LEU:HD13	26:l:56:LEU:HD22	1.93	0.50
34:L:37:CYS:SG	34:L:38:SER:N	2.85	0.50
43:8:120:LYS:HG2	43:8:123:ARG:HB3	1.94	0.50
44:9:11:LYS:HA	44:9:70:HIS:O	2.12	0.50
51:G:59:VAL:HG21	51:G:75:LEU:HD22	1.92	0.50
35:0:542:G:H5'	38:3:39:GLY:HA3	1.94	0.49
45:A:110:ILE:HG22	55:K:17:ARG:NH1	2.27	0.49
52:H:32:TYR:HB3	52:H:55:LEU:HD21	1.93	0.49
9:U:7:ASP:HB3	9:U:9:VAL:HG23	1.94	0.49
16:b:31:THR:O	16:b:102:ARG:NH1	2.41	0.49
31:q:8:ARG:NH2	33:N:243:U:OP2	2.44	0.49
33:N:1534:U:O2'	33:N:1537:G:O6	2.29	0.49
41:6:57:SER:HB3	41:6:60:GLU:HG2	1.93	0.49
4:P:207:LYS:HB2	33:N:729:G:C6	2.48	0.49
6:R:58:LYS:HG3	6:R:71:GLY:HA2	1.95	0.49
27:m:3:LYS:HE2	27:m:40:ASP:HB3	1.94	0.49
33:N:372:G:HO2'	33:N:400:G:H1	1.60	0.49
39:4:153:VAL:HG12	39:4:156:LYS:HZ1	1.76	0.49
26:l:2:LYS:HD3	33:N:77:G:OP1	2.13	0.49
33:N:160:A:N3	33:N:2208:C:O2'	2.44	0.49
36:1:141:LEU:O	36:1:145:GLU:CB	2.61	0.49
10:V:127:ARG:HA	10:V:130:GLU:HB2	1.94	0.49
30:p:1:MET:SD	33:N:752:A:H3'	2.53	0.49
33:N:1047:G:O2'	33:N:1111:A:N6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:2125:G:N1	33:N:2171:A:OP2	2.41	0.49
15:a:61:ALA:O	15:a:65:LEU:HB2	2.13	0.49
16:b:40:ILE:HG12	16:b:47:VAL:HG12	1.94	0.49
35:0:972:C:P	44:9:59:LYS:HD3	2.53	0.49
6:R:83:VAL:HB	6:R:86:ALA:HB2	1.95	0.49
19:e:71:LYS:NZ	33:N:1223:G:N7	2.61	0.49
35:0:812:G:HO2'	35:0:813:U:H6	1.60	0.49
44:9:27:GLU:O	44:9:31:ARG:CB	2.60	0.49
3:O:74:U:O2	23:i:29:ILE:HD13	2.13	0.49
23:i:6:ALA:HB1	23:i:40:ILE:HG23	1.95	0.49
33:N:1783:A:H5'	33:N:2608:G:H4'	1.95	0.49
44:9:83:THR:O	44:9:87:LEU:CB	2.58	0.49
54:J:69:LYS:O	54:J:72:ALA:HB3	2.12	0.49
28:n:3:VAL:HG23	33:N:2015:A:C6	2.47	0.49
33:N:306:U:H3	33:N:310:A:H62	0.61	0.49
36:1:176:ALA:HB1	36:1:181:ILE:HB	1.94	0.49
22:h:45:HIS:HB3	22:h:58:ILE:HG12	1.95	0.48
33:N:299:A:N3	33:N:319:G:O2'	2.37	0.48
35:0:705:G:H21	45:A:31:ILE:HD11	1.78	0.48
35:0:1074:G:O2'	35:0:1101:A:N1	2.44	0.48
38:3:141:ASP:O	38:3:181:THR:HA	2.12	0.48
51:G:31:HIS:HD2	51:G:34:TYR:H	1.60	0.48
2:M:37:U:O2'	35:0:790:A:OP1	2.27	0.48
33:N:355:U:H2'	33:N:356:G:H8	1.78	0.48
33:N:1363:C:O2'	33:N:1809:A:N3	2.41	0.48
2:M:1:U:H2'	2:M:2:G:H8	1.78	0.48
30:p:18:PHE:HA	30:p:43:THR:HG21	1.95	0.48
11:W:108:MET:HE2	33:N:1138:G:N3	2.27	0.48
13:Y:51:GLU:OE1	13:Y:60:ARG:NH1	2.46	0.48
35:0:197:A:N1	35:0:220:G:O2'	2.45	0.48
39:4:122:ASN:N	39:4:122:ASN:OD1	2.42	0.48
41:6:142:HIS:O	41:6:146:GLU:HB2	2.13	0.48
46:B:64:THR:HG23	46:B:93:VAL:HG12	1.95	0.48
9:U:27:ARG:NH2	25:k:56:MET:HE2	2.29	0.48
29:o:35:GLU:HA	29:o:49:TYR:O	2.13	0.48
33:N:2127:G:H21	33:N:2173:A:H1'	1.78	0.48
36:1:81:LYS:O	36:1:85:LEU:CB	2.62	0.48
33:N:1724:G:C6	33:N:1737:G:N2	2.81	0.48
35:0:757:U:O2'	35:0:879:C:O2	2.31	0.48
54:J:54:MET:HE3	54:J:58:VAL:HG21	1.94	0.48
4:P:235:GLY:O	33:N:2599:G:N7	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:33:LEU:HD13	14:Z:117:PHE:HB3	1.95	0.48
33:N:2540:C:O2'	33:N:2740:A:N3	2.42	0.48
35:0:642:A:C5	42:7:107:SER:HA	2.49	0.48
13:Y:57:LEU:HD22	31:q:54:ASP:HB3	1.96	0.48
13:Y:67:THR:HG21	33:N:244:A:H5''	1.95	0.48
18:d:4:VAL:HG22	33:N:1199:U:H1'	1.95	0.48
33:N:1868:C:N4	33:N:1869:G:O6	2.46	0.48
43:8:28:ILE:HD11	43:8:57:MET:HE1	1.96	0.48
15:a:82:GLU:OE2	15:a:86:ARG:NH2	2.47	0.48
33:N:2167:U:O2'	33:N:2169:A:N7	2.46	0.48
35:0:261:U:OP2	54:J:74:ARG:NH2	2.47	0.48
37:2:108:LYS:HD3	37:2:111:LEU:HD12	1.96	0.48
47:C:8:ASN:HD22	47:C:22:ILE:HG13	1.78	0.48
4:P:66:ASP:OD2	4:P:102:ARG:NH1	2.46	0.48
33:N:33:C:O2	33:N:447:A:N6	2.47	0.48
35:0:677:U:H3	35:0:713:G:H22	1.62	0.48
35:0:812:G:O2'	35:0:813:U:H6	1.96	0.48
40:5:88:MET:HE3	52:H:64:TYR:CD2	2.49	0.48
13:Y:111:ILE:HD11	33:N:636:G:C6	2.49	0.47
24:j:65:GLY:HA3	24:j:83:GLU:O	2.14	0.47
33:N:749:A:N1	33:N:753:A:O2'	2.43	0.47
40:5:51:ILE:HD13	40:5:51:ILE:HG21	1.64	0.47
8:T:67:THR:HG22	33:N:2748:A:H1'	1.95	0.47
18:d:51:ARG:HG2	33:N:1156:A:C8	2.48	0.47
24:j:41:ARG:NH1	33:N:2262:U:OP1	2.47	0.47
45:A:16:VAL:HG12	45:A:77:TYR:HB3	1.96	0.47
45:A:23:ILE:HG22	45:A:32:VAL:HG13	1.96	0.47
47:C:3:ARG:O	47:C:57:ARG:NH1	2.38	0.47
11:W:114:LEU:HG	11:W:118:MET:HE3	1.97	0.47
17:c:26:VAL:O	17:c:44:GLU:HA	2.14	0.47
33:N:1187:G:N2	33:N:1188:U:O4	2.47	0.47
33:N:2092:U:N3	33:N:2226:C:OP2	2.44	0.47
35:0:618:C:O2'	50:F:14:ARG:NH2	2.47	0.47
35:0:1130:A:H61	35:0:1144:G:H1'	1.79	0.47
38:3:95:GLU:HA	38:3:100:ASN:ND2	2.29	0.47
39:4:105:ILE:HD11	39:4:115:LEU:HD23	1.96	0.47
14:Z:42:THR:HG22	14:Z:93:VAL:HG12	1.97	0.47
14:Z:57:VAL:HG13	14:Z:116:ALA:HB2	1.96	0.47
18:d:37:GLN:HE21	33:N:1252:G:H22	1.62	0.47
35:0:1006:G:O6	35:0:1023:U:C2	2.67	0.47
10:V:30:GLN:OE1	33:N:1095:A:N6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:81:ASP:HB2	13:Y:100:ILE:HD11	1.96	0.47
30:p:19:ARG:HG2	33:N:126:A:O5'	2.14	0.47
35:0:35:G:O2'	46:B:115:SER:O	2.31	0.47
52:H:34:THR:HG23	52:H:36:SER:H	1.79	0.47
4:P:132:MET:HG2	4:P:135:ILE:HD12	1.96	0.47
10:V:33:VAL:HG13	10:V:59:ILE:HG21	1.97	0.47
33:N:476:G:N1	33:N:479:A:OP2	2.46	0.47
33:N:1724:G:O6	33:N:1737:G:N2	2.47	0.47
43:8:38:TYR:HD2	43:8:39:PHE:HD1	1.61	0.47
48:D:89:MET:HE1	48:D:98:LYS:HD3	1.96	0.47
55:K:37:PHE:HB3	55:K:39:GLU:H	1.79	0.47
13:Y:41:ARG:NH1	33:N:807:U:OP2	2.48	0.47
20:f:90:LYS:NZ	33:N:746:U:O2'	2.47	0.47
22:h:41:LEU:HA	22:h:61:LYS:O	2.15	0.47
33:N:299:A:N1	33:N:322:A:O2'	2.46	0.47
33:N:503:A:H4'	33:N:504:A:H5'	1.97	0.47
35:0:254:G:O3'	51:G:71:LYS:NZ	2.47	0.47
35:0:999:C:N3	35:0:1042:A:N6	2.63	0.47
35:0:1227:A:OP2	47:C:95:LEU:HD21	2.15	0.47
28:n:6:ASN:ND2	33:N:2020:A:H62	2.12	0.47
33:N:84:A:N1	33:N:98:G:O2'	2.46	0.47
33:N:910:A:H2'	33:N:911:A:C8	2.50	0.47
33:N:2243:U:H2'	33:N:2244:U:C6	2.50	0.47
35:0:674:G:P	40:5:86:ARG:HH22	2.38	0.47
35:0:1302:C:C6	47:C:17:ILE:HD13	2.50	0.47
36:1:136:MET:SD	36:1:139:ARG:NH2	2.87	0.47
4:P:155:ALA:HB2	4:P:162:VAL:HG23	1.97	0.47
7:S:42:GLU:OE1	7:S:148:ARG:NH1	2.48	0.47
7:S:112:ARG:HB2	47:C:7:ILE:HG12	1.95	0.47
33:N:2776:A:O5'	33:N:2776:A:H8	1.97	0.47
35:0:1363:A:O2'	35:0:1365:G:N7	2.42	0.47
36:1:207:ILE:HA	36:1:210:VAL:HG22	1.96	0.47
4:P:260:ASN:ND2	4:P:263:THR:OG1	2.48	0.47
14:Z:136:MET:HE3	23:i:57:TYR:HB3	1.96	0.47
17:c:29:LYS:HD3	17:c:40:LEU:HD21	1.97	0.47
21:g:22:THR:O	21:g:26:LYS:HB3	2.15	0.47
30:p:12:ARG:CZ	30:p:44:VAL:HG21	2.45	0.47
30:p:33:ARG:NH2	33:N:467:G:OP1	2.46	0.47
32:r:36:ARG:HH11	32:r:36:ARG:HD3	1.53	0.47
33:N:528:A:C2	33:N:2042:A:H2'	2.50	0.47
50:F:46:LYS:HG3	50:F:47:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:H:51:TYR:O	52:H:55:LEU:HB2	2.15	0.47
7:S:24:SER:HB3	7:S:27:GLN:HB2	1.97	0.46
33:N:45:G:H5''	33:N:46:G:H5'	1.98	0.46
11:W:31:GLU:HG2	11:W:142:ILE:HG12	1.97	0.46
11:W:81:ILE:O	33:N:1131:G:OP1	2.32	0.46
31:q:5:LYS:CE	33:N:254:G:N7	2.79	0.46
33:N:548:G:H5''	33:N:549:G:H5'	1.97	0.46
33:N:1853:A:N3	33:N:2233:U:O2'	2.43	0.46
33:N:2006:C:O2'	33:N:2823:A:N3	2.48	0.46
35:0:1073:U:O2	36:1:103:ASN:ND2	2.48	0.46
36:1:104:TRP:O	36:1:108:ARG:N	2.47	0.46
5:Q:35:THR:HG22	5:Q:73:VAL:HG11	1.96	0.46
10:V:107:GLN:O	10:V:111:GLN:HB2	2.15	0.46
32:r:11:CYS:SG	32:r:14:CYS:N	2.88	0.46
33:N:1509:A:H2'	33:N:1510:G:C8	2.50	0.46
33:N:2126:A:N3	33:N:2173:A:N6	2.64	0.46
33:N:284:U:O4	33:N:356:G:O6	2.33	0.46
33:N:1733:G:H2'	33:N:1734:G:C8	2.51	0.46
33:N:1999:C:O3'	33:N:2722:G:N2	2.48	0.46
35:0:1270:G:O2'	35:0:1313:U:O2'	2.31	0.46
38:3:58:LYS:HD3	38:3:203:LEU:HD23	1.98	0.46
9:U:24:GLY:O	9:U:28:ASN:HB2	2.15	0.46
28:n:25:VAL:HG21	28:n:28:LEU:HD23	1.97	0.46
33:N:1475:G:H1'	33:N:1732:C:H41	1.79	0.46
35:0:1096:C:O2	35:0:1170:A:O2'	2.34	0.46
20:f:38:TYR:CD2	28:n:28:LEU:HD22	2.51	0.46
33:N:1176:U:H2'	33:N:1177:G:C8	2.51	0.46
35:0:1006:G:C6	35:0:1023:U:O2	2.68	0.46
39:4:18:VAL:HA	39:4:34:THR:O	2.16	0.46
13:Y:54:GLN:HE21	33:N:2428:G:N2	2.14	0.46
14:Z:9:PHE:HZ	33:N:911:A:H2'	1.80	0.46
33:N:881:G:N2	33:N:895:U:O2	2.49	0.46
33:N:2533:U:OP1	33:N:2665:A:O2'	2.29	0.46
35:0:1356:G:H2'	35:0:1357:A:C8	2.51	0.46
39:4:89:HIS:CD2	39:4:90:THR:H	2.33	0.46
7:S:74:VAL:HG22	7:S:79:ILE:HD11	1.97	0.46
14:Z:55:ARG:NH2	33:N:2469:A:O3'	2.49	0.46
35:0:523:A:N1	46:B:89:ASP:HB2	2.31	0.46
4:P:167:ARG:HG2	4:P:172:VAL:HG12	1.96	0.46
33:N:2273:A:H2'	33:N:2274:A:C8	2.50	0.46
7:S:131:GLY:HA3	33:N:2305:U:H5''	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:35:ARG:HG3	30:p:42:LEU:HD21	1.98	0.46
33:N:1847:A:O2'	33:N:1848:A:H8	1.98	0.46
35:0:1315:U:O2'	35:0:1360:A:N3	2.47	0.46
10:V:11:LEU:HD23	33:N:1097:U:O2	2.16	0.45
19:e:34:GLU:HG2	19:e:60:LYS:HG2	1.98	0.45
33:N:499:U:O4	33:N:503:A:N7	2.49	0.45
33:N:1900:A:H1'	33:N:1970:A:H2'	1.97	0.45
1:s:155:SER:HB3	33:N:2061:G:H22	1.81	0.45
18:d:16:LYS:NZ	33:N:1227:G:OP2	2.48	0.45
25:k:37:ARG:HG2	25:k:46:PHE:HB3	1.98	0.45
33:N:1064:C:N4	33:N:1070:A:OP2	2.49	0.45
33:N:1077:A:N6	33:N:1089:A:OP1	2.46	0.45
33:N:1078:U:O2'	33:N:1088:A:OP1	2.34	0.45
33:N:2514:U:H2'	33:N:2515:C:C6	2.51	0.45
34:L:13:THR:HA	34:L:23:LYS:HA	1.97	0.45
38:3:140:ASN:N	38:3:182:PHE:O	2.49	0.45
53:I:50:ALA:HB1	53:I:57:HIS:HB3	1.97	0.45
10:V:11:LEU:HD11	10:V:28:LEU:HB3	1.99	0.45
13:Y:33:ARG:NH1	33:N:587:C:O2	2.46	0.45
23:i:48:MET:SD	23:i:51:GLN:NE2	2.89	0.45
32:r:1:MET:HE2	32:r:34:LYS:HD3	1.98	0.45
33:N:2139:U:O2	33:N:2152:G:O6	2.34	0.45
35:0:1126:U:OP1	44:9:7:ARG:NH2	2.49	0.45
36:1:53:ALA:O	36:1:57:LEU:HB2	2.16	0.45
6:R:148:ILE:HB	6:R:169:VAL:HG22	1.98	0.45
19:e:27:ILE:O	19:e:66:HIS:NE2	2.42	0.45
35:0:1101:A:H61	36:1:102:THR:HG21	1.81	0.45
36:1:100:MET:HA	36:1:107:VAL:HG21	1.99	0.45
40:5:62:MET:HG2	40:5:64:VAL:HG23	1.97	0.45
4:P:251:GLN:NE2	4:P:252:THR:O	2.48	0.45
11:W:82:GLY:HA2	33:N:1131:G:OP1	2.17	0.45
14:Z:123:LYS:HE3	33:N:2483:C:N3	2.32	0.45
18:d:37:GLN:NE2	33:N:1252:G:H22	2.14	0.45
39:4:133:PRO:HA	39:4:136:VAL:HG12	1.98	0.45
41:6:56:LYS:HE3	41:6:60:GLU:HG3	1.99	0.45
4:P:182:ARG:NH1	33:N:1800:C:OP2	2.49	0.45
17:c:92:VAL:HG21	17:c:97:LEU:HD21	1.98	0.45
13:Y:82:LEU:HA	13:Y:85:VAL:HG13	1.99	0.45
33:N:499:U:H3	33:N:503:A:H62	0.54	0.45
33:N:1311:G:N2	33:N:1603:A:H62	2.14	0.45
33:N:2134:A:N6	33:N:2157:G:O2'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:0:309:A:H2'	35:0:310:G:H8	1.81	0.45
37:2:65:ARG:O	37:2:65:ARG:HG3	2.16	0.45
40:5:70:VAL:HA	40:5:73:GLU:HG2	1.99	0.45
44:9:10:LEU:O	44:9:71:LEU:HA	2.15	0.45
45:A:49:GLY:O	45:A:69:ARG:NH1	2.50	0.45
5:Q:149:ASN:HD22	33:N:2572:A:H2'	1.82	0.45
35:0:1379:G:O6	41:6:2:PRO:HB2	2.17	0.45
36:1:163:VAL:HG21	36:1:173:ILE:HD11	1.98	0.45
37:2:155:GLY:HA2	37:2:163:ALA:HB1	1.98	0.45
46:B:38:TYR:HB2	46:B:52:VAL:O	2.15	0.45
1:s:153:LEU:HD21	33:N:2585:U:O2'	2.17	0.45
18:d:31:VAL:HG13	33:N:580:U:O3'	2.17	0.45
33:N:613:A:N7	33:N:616:A:C6	2.85	0.45
33:N:2153:C:H2'	33:N:2154:A:H8	1.82	0.45
39:4:107:ALA:HA	39:4:125:ALA:HB3	1.99	0.45
43:8:106:ARG:NH1	43:8:107:ASP:O	2.50	0.45
5:Q:43:ASP:OD1	33:N:2784:U:H4'	2.17	0.45
5:Q:45:TYR:OH	33:N:2636:C:O2'	2.07	0.45
15:a:44:LEU:HD23	15:a:113:ILE:HD13	1.97	0.45
33:N:1794:A:H2'	33:N:1795:C:C6	2.52	0.45
35:0:1106:G:O2'	37:2:169:ARG:NH1	2.50	0.45
50:F:38:PHE:CE1	50:F:51:ARG:HG2	2.52	0.45
3:O:7:G:H5'	16:b:29:HIS:CE1	2.52	0.44
4:P:141:VAL:HG13	4:P:190:ALA:HB1	1.99	0.44
7:S:140:GLU:CD	34:L:27:THR:HG23	2.41	0.44
26:l:13:GLU:HA	26:l:16:THR:HG22	1.99	0.44
28:n:4:GLN:NE2	33:N:2016:U:O2	2.49	0.44
33:N:1072:C:H42	33:N:1098:A:N6	2.15	0.44
35:0:928:G:O2'	35:0:1533:C:OP1	2.34	0.44
35:0:1218:C:H2'	35:0:1219:A:C8	2.51	0.44
4:P:145:GLU:HB2	4:P:188:CYS:HB3	1.98	0.44
5:Q:146:ILE:HG21	5:Q:146:ILE:HD13	1.62	0.44
30:p:16:HIS:ND1	33:N:684:G:OP1	2.48	0.44
33:N:857:G:N2	33:N:2269:G:O4'	2.49	0.44
35:0:362:G:N1	35:0:365:U:OP2	2.43	0.44
35:0:1113:C:H4'	37:2:14:ILE:HD12	1.97	0.44
50:F:6:LEU:HD12	50:F:19:VAL:HB	1.99	0.44
10:V:79:LEU:HD21	10:V:109:ILE:HG21	1.99	0.44
18:d:113:ALA:O	18:d:117:LEU:HB2	2.18	0.44
33:N:700:G:O2'	33:N:1632:A:N3	2.48	0.44
33:N:2506[A]:U:OP2	33:N:2576:G:N2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:0:71:A:H61	35:0:99:C:H1'	1.83	0.44
52:H:71:THR:HG23	52:H:73:ARG:H	1.82	0.44
1:s:153:LEU:C	1:s:153:LEU:HD23	2.43	0.44
35:0:723:U:C5'	55:K:49:LYS:HE2	2.48	0.44
35:0:825:A:H4'	42:7:3:MET:HE2	1.99	0.44
54:J:12:ILE:HG21	54:J:12:ILE:HD13	1.72	0.44
8:T:66:GLY:O	8:T:69:ARG:HB3	2.17	0.44
10:V:133:ALA:O	10:V:138:LEU:N	2.51	0.44
17:c:29:LYS:HB2	17:c:83:SER:HB2	1.98	0.44
26:l:56:LEU:HD23	26:l:56:LEU:HA	1.86	0.44
32:r:7:VAL:HG22	32:r:38:GLY:HA3	1.99	0.44
33:N:1826:G:O2'	33:N:1971:U:OP2	2.34	0.44
35:0:296:U:O2'	35:0:556:C:O2	2.33	0.44
35:0:1317:C:H4'	48:D:49:GLN:HE21	1.83	0.44
39:4:80:THR:OG1	39:4:81:LEU:N	2.50	0.44
39:4:114:VAL:O	39:4:118:ALA:HB2	2.18	0.44
46:B:114:ARG:HG2	46:B:119:VAL:HB	1.99	0.44
5:Q:4:LEU:HD21	5:Q:96:ILE:HG22	1.99	0.44
5:Q:13:ARG:HD2	5:Q:15:PHE:CZ	2.53	0.44
6:R:165:HIS:CD2	33:N:1205:A:C6	3.05	0.44
14:Z:9:PHE:CZ	33:N:911:A:H2'	2.52	0.44
35:0:1062:U:H2'	35:0:1063:C:C6	2.52	0.44
35:0:1321:U:O2'	53:I:78:ARG:NH1	2.51	0.44
38:3:100:ASN:OD1	38:3:111:ARG:NH1	2.51	0.44
47:C:16:VAL:HG23	47:C:17:ILE:HG13	2.00	0.44
4:P:19:VAL:HG23	4:P:203:ARG:HB3	1.99	0.44
10:V:24:VAL:HG12	33:N:1070:A:H61	1.83	0.44
12:X:63:VAL:HG12	12:X:107:LEU:HD21	2.00	0.44
19:e:3:ALA:HA	19:e:40:MET:O	2.17	0.44
33:N:2777:G:OP2	33:N:2781:A:O2'	2.26	0.44
35:0:71:A:N1	35:0:99:C:O2'	2.47	0.44
35:0:1178:G:C5	43:8:99:ARG:NH2	2.86	0.44
41:6:144:MET:HE3	41:6:144:MET:HB3	1.91	0.44
44:9:12:ALA:HB3	44:9:18:ILE:HB	1.98	0.44
53:I:4:SER:HB3	53:I:5:LEU:HD12	2.00	0.44
8:T:9:VAL:HB	8:T:50:LEU:HB2	2.00	0.44
12:X:99:ILE:HD13	12:X:115:ILE:HG23	1.99	0.44
14:Z:40:ARG:HD3	14:Z:93:VAL:HG21	2.00	0.44
17:c:63:LYS:HE3	17:c:65:SER:HB2	2.00	0.44
22:h:10:GLU:OE2	22:h:22:ARG:NH2	2.48	0.44
30:p:34:ARG:HD3	30:p:34:ARG:HH11	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:0:971:G:O6	35:0:1364:U:O2'	2.35	0.44
35:0:1380:U:O2	35:0:1382:C:N4	2.49	0.44
36:1:53:ALA:O	36:1:57:LEU:CB	2.65	0.44
50:F:70:ARG:HD2	50:F:70:ARG:HA	1.62	0.44
29:o:9:ILE:HG22	29:o:53:LYS:HB2	2.00	0.44
33:N:2107:G:C6	33:N:2182:U:O2	2.71	0.44
35:0:9:G:OP2	39:4:126:LYS:HD2	2.18	0.44
38:3:95:GLU:HG3	38:3:191:LEU:HD22	2.00	0.44
5:Q:59:ARG:NH1	33:N:2831:G:OP2	2.42	0.43
19:e:80:ARG:NH2	33:N:572:A:OP2	2.47	0.43
33:N:569:U:H5''	33:N:821:A:C2	2.52	0.43
35:0:1080:A:OP1	39:4:52:LYS:HD2	2.18	0.43
41:6:71:PRO:O	41:6:96:ARG:NH1	2.51	0.43
43:8:16:ALA:O	43:8:67:VAL:HA	2.17	0.43
17:c:53:ARG:NH2	33:N:2720:U:OP1	2.51	0.43
29:o:40:ASP:O	29:o:44:ARG:N	2.50	0.43
38:3:109:ALA:HA	38:3:161:LEU:HD11	2.00	0.43
41:6:59:LEU:O	41:6:63:GLU:HB2	2.18	0.43
6:R:77:ILE:HG21	6:R:77:ILE:HD13	1.24	0.43
6:R:108:ILE:HD13	6:R:108:ILE:HG21	1.72	0.43
33:N:285:G:O6	33:N:355:U:O2	2.36	0.43
33:N:828:U:H2'	33:N:829:A:C8	2.53	0.43
37:2:55:ILE:HD13	37:2:55:ILE:HG21	1.65	0.43
39:4:106:ILE:HG21	39:4:106:ILE:HD13	1.75	0.43
6:R:165:HIS:CD2	33:N:1205:A:C5	3.06	0.43
12:X:70:ARG:NH2	33:N:2683:C:O2	2.52	0.43
15:a:3:HIS:O	15:a:4:ARG:HB2	2.17	0.43
18:d:49:ASP:OD2	33:N:534:U:O2'	2.20	0.43
29:o:21:TYR:HE2	29:o:38:LYS:HB3	1.83	0.43
33:N:514:A:N3	33:N:581:C:O2'	2.44	0.43
34:L:11:GLU:HA	34:L:25:ARG:HA	2.01	0.43
35:0:946:A:O2'	35:0:1333:A:N3	2.45	0.43
35:0:1026:G:C6	35:0:1035:A:C6	3.06	0.43
35:0:1507:A:H2'	35:0:1508:A:C8	2.53	0.43
38:3:159:LEU:HD13	38:3:175:ALA:HB1	2.01	0.43
4:P:85:PRO:HG3	33:N:1567:G:H2'	2.00	0.43
5:Q:25:THR:HG21	5:Q:193:VAL:HG22	2.00	0.43
6:R:69:ARG:NH2	33:N:2445:G:OP1	2.47	0.43
13:Y:100:ILE:HG21	13:Y:100:ILE:HD13	1.75	0.43
18:d:48:ARG:NE	18:d:49:ASP:OD1	2.49	0.43
28:n:16:ARG:HA	33:N:2046:G:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:q:33:LEU:HB2	33:N:2420:C:OP2	2.19	0.43
35:0:714:G:H2'	35:0:715:A:C8	2.53	0.43
54:J:67:ILE:HG13	54:J:71:LYS:HD3	2.00	0.43
4:P:61:ALA:O	4:P:63:ARG:NH2	2.52	0.43
5:Q:1:MET:HG2	5:Q:205:PRO:HG2	2.00	0.43
5:Q:37:VAL:HG22	5:Q:48:ILE:HG22	2.00	0.43
13:Y:77:ILE:CD1	13:Y:108:ALA:HB1	2.48	0.43
15:a:37:THR:HG22	15:a:110:MET:HE1	2.00	0.43
15:a:90:ARG:HD2	33:N:2880:C:O2'	2.18	0.43
33:N:964:C:O2'	33:N:2273:A:N3	2.49	0.43
35:0:228:A:H5'	50:F:63:GLN:NE2	2.34	0.43
35:0:552:U:H5'	46:B:83:ARG:NH1	2.32	0.43
35:0:620:C:C2	38:3:132:ILE:HD13	2.53	0.43
7:S:105:THR:HG21	34:L:22:MET:SD	2.59	0.43
18:d:88:VAL:HA	19:e:49:ILE:CD1	2.47	0.43
33:N:219:A:N3	33:N:234:U:O2'	2.40	0.43
33:N:221:A:N1	33:N:265:A:O2'	2.51	0.43
33:N:2602:A:H4'	33:N:2603:G:H5'	2.01	0.43
33:N:2726:A:O2'	33:N:2727:A:O5'	2.34	0.43
35:0:1143:G:H2'	35:0:1144:G:H8	1.83	0.43
52:H:26:ILE:HG21	52:H:67:LEU:HB3	2.01	0.43
4:P:201:MET:HG3	4:P:202:LEU:HD12	2.01	0.43
7:S:37:ASN:ND2	33:N:2313:C:O4'	2.52	0.43
11:W:113:PRO:HD2	33:N:558:U:P	2.58	0.43
15:a:28:LEU:HD23	15:a:48:VAL:HG21	2.01	0.43
24:j:33:ALA:N	24:j:64:ASP:OD1	2.51	0.43
26:l:1:MET:HG2	26:l:4:LYS:HD3	2.00	0.43
35:0:537:G:H5''	46:B:110:ARG:HH12	1.84	0.43
36:1:74:ARG:HA	36:1:75:ALA:HA	1.80	0.43
38:3:157:ALA:O	38:3:160:GLU:HB3	2.19	0.43
40:5:51:ILE:N	40:5:53:LYS:O	2.52	0.43
54:J:51:PHE:HA	54:J:54:MET:HG2	2.01	0.43
4:P:153:GLN:O	33:N:1818:U:O2'	2.30	0.43
33:N:373:U:H2'	33:N:374:A:H8	1.84	0.43
33:N:1447:C:O2'	33:N:1544:A:N3	2.39	0.43
35:0:269:C:H2'	35:0:270:A:C8	2.54	0.43
35:0:1064:G:O2'	35:0:1190:G:N2	2.51	0.43
42:7:49:PHE:HA	42:7:60:GLU:O	2.19	0.43
7:S:140:GLU:HA	34:L:28:VAL:HG22	2.01	0.43
18:d:112:LYS:HG3	19:e:48:LYS:HE2	2.01	0.43
26:l:20:ASN:HB3	26:l:50:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:0:723:U:H5''	55:K:49:LYS:HE2	2.01	0.43
35:0:746:A:H2'	35:0:747:A:C8	2.54	0.43
35:0:766:A:OP2	35:0:812:G:N2	2.50	0.43
36:1:15:HIS:HB2	36:1:203:ASN:HD22	1.84	0.43
36:1:166:ALA:HB3	36:1:191:SER:HB3	2.00	0.43
38:3:62:ARG:HH21	38:3:68:LEU:HA	1.82	0.43
41:6:73:VAL:HG12	41:6:90:GLU:HA	2.00	0.43
41:6:105:VAL:O	41:6:109:ARG:HG2	2.19	0.43
50:F:76:LYS:HE3	50:F:76:LYS:HB3	1.87	0.43
1:s:153:LEU:O	33:N:2585:U:O2	2.37	0.42
5:Q:109:VAL:HG22	5:Q:203:VAL:HG22	2.00	0.42
8:T:22:GLN:HE22	8:T:55:ARG:HH21	1.66	0.42
8:T:85:LYS:HG2	8:T:141:ILE:HD12	1.99	0.42
11:W:96:ARG:HH21	11:W:99:ARG:HG2	1.84	0.42
12:X:38:ILE:HD11	12:X:112:PHE:HZ	1.84	0.42
16:b:29:HIS:HB3	16:b:36:TYR:HB2	2.00	0.42
17:c:114:LEU:HD21	35:0:1441:A:C2	2.54	0.42
33:N:1509:A:H2'	33:N:1510:G:H8	1.84	0.42
34:L:30:HIS:ND1	34:L:31:ASP:O	2.52	0.42
35:0:481:G:O2'	35:0:483:C:N4	2.50	0.42
35:0:713:G:H2'	35:0:714:G:C8	2.54	0.42
43:8:129:LYS:HB2	43:8:129:LYS:HE3	1.71	0.42
47:C:96:PRO:HA	47:C:109:ARG:HG2	2.01	0.42
4:P:247:PRO:HD3	33:N:1824:G:O3'	2.19	0.42
13:Y:30:THR:O	13:Y:32:GLY:N	2.52	0.42
25:k:17:ASN:HB2	25:k:25:THR:HB	1.99	0.42
33:N:320:A:H4'	33:N:322:A:C8	2.54	0.42
33:N:1067:A:OP1	33:N:1068:G:N2	2.49	0.42
35:0:228:A:C4'	50:F:63:GLN:HE21	2.32	0.42
35:0:1118:U:H2'	35:0:1119:C:C6	2.54	0.42
54:J:79:LEU:HD23	54:J:79:LEU:HA	1.83	0.42
8:T:94:TYR:HA	8:T:106:SER:O	2.19	0.42
15:a:3:HIS:CD2	33:N:2820:A:H4'	2.54	0.42
35:0:1060:U:P	48:D:85:ARG:HH22	2.41	0.42
35:0:1118:U:H2'	35:0:1119:C:H6	1.85	0.42
36:1:186:ILE:HB	36:1:213:TYR:CZ	2.54	0.42
49:E:35:GLN:HE21	49:E:39:LEU:HD13	1.84	0.42
5:Q:154:LYS:HE2	33:N:2024:G:O3'	2.20	0.42
20:f:77:ASP:HB2	20:f:102:HIS:HB2	2.00	0.42
24:j:41:ARG:HH12	33:N:2262:U:H5''	1.84	0.42
33:N:247:G:OP2	33:N:249:C:N4	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:2291:U:H2'	33:N:2292:U:C6	2.54	0.42
36:1:21:ARG:HG3	36:1:22:TYR:CD2	2.55	0.42
38:3:72:PHE:HE1	38:3:94:LEU:HD11	1.85	0.42
41:6:78:ARG:HB3	41:6:80:VAL:HG23	2.01	0.42
54:J:33:LYS:O	54:J:37:ALA:HB3	2.19	0.42
2:M:1:U:H2'	2:M:2:G:C8	2.54	0.42
7:S:112:ARG:NH2	7:S:113:ASP:OD2	2.53	0.42
18:d:97:ASP:OD2	19:e:13:ARG:NE	2.47	0.42
20:f:85:ILE:HA	20:f:94:ASP:O	2.19	0.42
23:i:75:GLN:HB2	23:i:92:VAL:HG23	2.01	0.42
33:N:1779:U:OP2	33:N:1784:A:N6	2.50	0.42
33:N:2866:U:H4'	33:N:2867:G:H5'	2.02	0.42
35:0:555:U:H2'	35:0:556:C:C6	2.55	0.42
35:0:1516:G:N2	35:0:1519:A:OP2	2.48	0.42
5:Q:19:GLY:HA3	17:c:80:VAL:HG23	2.01	0.42
28:n:8:PRO:HD2	33:N:1263:U:O2'	2.19	0.42
33:N:1769:U:O2'	33:N:1958:C:OP1	2.36	0.42
35:0:1101:A:H61	36:1:102:THR:CG2	2.32	0.42
41:6:107:ALA:HB1	41:6:133:THR:HB	2.00	0.42
54:J:56:PRO:O	54:J:60:ARG:HB2	2.20	0.42
3:O:89:U:H1'	33:N:958:U:H2'	2.02	0.42
32:r:3:VAL:HG12	32:r:36:ARG:HB3	2.02	0.42
37:2:153:VAL:HG12	37:2:198:VAL:HG22	2.01	0.42
4:P:146:MET:HE1	33:N:1800:C:H5'	2.02	0.42
20:f:24:ILE:HD13	20:f:36:LEU:HD11	2.02	0.42
22:h:16:GLY:C	22:h:18:ASP:H	2.28	0.42
33:N:1075:C:H2'	33:N:1076:C:C6	2.54	0.42
33:N:2127:G:H2'	33:N:2128:G:C8	2.55	0.42
36:1:164:ILE:HD11	36:1:210:VAL:HB	2.02	0.42
40:5:42:TRP:HB2	40:5:59:TYR:HB2	2.01	0.42
46:B:34:CYS:HA	46:B:55:VAL:HA	2.01	0.42
49:E:26:GLU:OE2	49:E:77:ARG:NE	2.53	0.42
7:S:33:LYS:HD3	7:S:92:ARG:NH1	2.35	0.42
13:Y:109:LYS:HE2	13:Y:128:THR:HG22	2.02	0.42
30:p:19:ARG:NH2	33:N:125:A:OP2	2.53	0.42
33:N:500:G:N1	33:N:503:A:OP2	2.42	0.42
39:4:72:ILE:HG21	39:4:72:ILE:HD13	1.83	0.42
52:H:21:ILE:HD12	52:H:22:ASP:HB2	2.01	0.42
35:0:96:U:H2'	35:0:97:G:C8	2.54	0.42
35:0:677:U:O2	35:0:777:A:O2'	2.38	0.42
35:0:1041:G:H2'	35:0:1042:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3:95:GLU:HA	38:3:100:ASN:HD22	1.84	0.42
39:4:112:ARG:O	39:4:116:GLU:HB2	2.20	0.42
44:9:22:THR:HA	44:9:25:ILE:HG22	2.02	0.42
5:Q:152:PRO:HG2	5:Q:156:PHE:CZ	2.55	0.41
7:S:153:ASP:N	7:S:153:ASP:OD1	2.53	0.41
12:X:7:MET:HB3	12:X:18:ARG:HD2	2.02	0.41
18:d:33:ARG:HG2	33:N:1252:G:N3	2.35	0.41
33:N:372:G:H1'	33:N:373:U:H5	1.85	0.41
33:N:526:A:O2'	33:N:2043:C:O2	2.34	0.41
33:N:2163:A:OP1	33:N:2171:A:N6	2.53	0.41
35:0:1119:C:H2'	35:0:1120:C:H6	1.84	0.41
35:0:1380:U:C5	41:6:3:ARG:HA	2.54	0.41
42:7:18:GLN:NE2	42:7:70:ALA:HB1	2.35	0.41
8:T:16:ASP:O	8:T:26:ILE:HA	2.19	0.41
14:Z:136:MET:SD	23:i:75:GLN:O	2.78	0.41
29:o:5:ILE:HG21	29:o:28:ARG:HH12	1.86	0.41
33:N:1044:C:O2'	33:N:1111:A:N1	2.48	0.41
33:N:2458:G:O2'	33:N:2460:U:O4	2.34	0.41
35:0:1306:A:N6	35:0:1331:G:H1'	2.35	0.41
37:2:134:MET:HE2	37:2:134:MET:HB3	1.91	0.41
4:P:161:TYR:HB3	4:P:194:GLU:HB3	2.01	0.41
20:f:93:ALA:HB2	33:N:1614:A:C2	2.55	0.41
28:n:16:ARG:NE	33:N:1266:G:OP1	2.37	0.41
33:N:307:G:N1	33:N:310:A:OP2	2.50	0.41
33:N:493:G:H2'	33:N:494:G:O4'	2.21	0.41
33:N:2328:A:H2'	33:N:2329:U:C6	2.55	0.41
33:N:2554:U:H2'	33:N:2555:U:C6	2.56	0.41
35:0:135:C:O2	50:F:1:MET:HB2	2.20	0.41
43:8:40:GLY:O	43:8:45:ARG:NH2	2.36	0.41
45:A:31:ILE:HG21	45:A:31:ILE:HD13	1.70	0.41
4:P:146:MET:HE1	33:N:1800:C:C5'	2.50	0.41
5:Q:156:PHE:CD1	11:W:81:ILE:HD12	2.55	0.41
12:X:116:ILE:HD13	12:X:116:ILE:HG21	1.86	0.41
25:k:31:PRO:HG2	25:k:33:LEU:HD13	2.01	0.41
33:N:1437:C:O2'	33:N:1516:G:O2'	2.35	0.41
35:0:254:G:H5''	51:G:71:LYS:HE3	2.02	0.41
35:0:352:C:O2'	35:0:354:G:OP1	2.32	0.41
35:0:1255:G:O2'	35:0:1258:G:N3	2.46	0.41
40:5:6:ILE:HB	40:5:62:MET:HB3	2.03	0.41
4:P:236:GLU:HB3	33:N:2599:G:N7	2.35	0.41
33:N:537:G:O2'	33:N:556:A:N6	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:0:1371:G:O3'	43:8:71:GLY:HA3	2.20	0.41
35:0:1530:G:H2'	35:0:1531:A:C8	2.54	0.41
36:1:128:LYS:HG3	36:1:129:LEU:HG	2.01	0.41
7:S:140:GLU:OE1	34:L:27:THR:HG23	2.21	0.41
17:c:58:ALA:HA	17:c:74:PHE:O	2.20	0.41
24:j:37:ILE:HG22	24:j:38:VAL:HG23	2.01	0.41
33:N:214:G:N2	33:N:216:A:N3	2.68	0.41
33:N:1919:A:N1	35:0:1495:U:O2'	2.47	0.41
33:N:2087:G:H2'	33:N:2088:A:H8	1.86	0.41
33:N:2469:A:N6	33:N:2481:G:O2'	2.50	0.41
33:N:2541:A:HO2'	33:N:2765:A:H2	1.68	0.41
35:0:331:G:H2'	54:J:5:LYS:NZ	2.35	0.41
35:0:1071:C:H2'	35:0:1072:G:H8	1.86	0.41
54:J:33:LYS:O	54:J:37:ALA:CB	2.68	0.41
4:P:107:PRO:HA	4:P:195:VAL:HA	2.03	0.41
5:Q:149:ASN:ND2	33:N:2572:A:H2'	2.35	0.41
12:X:121:GLU:HG3	17:c:66:ASN:HD21	1.85	0.41
18:d:24:TYR:CD1	33:N:533:G:H5'	2.55	0.41
26:l:14:LEU:HD23	26:l:14:LEU:HA	1.94	0.41
33:N:33:C:N4	33:N:446:G:O2'	2.46	0.41
33:N:2532:G:O2'	33:N:2657:A:N1	2.52	0.41
37:2:24:ALA:HB1	37:2:28:GLU:HG2	2.02	0.41
43:8:96:SER:O	43:8:99:ARG:HB3	2.21	0.41
48:D:25:ALA:O	48:D:28:LYS:HG2	2.21	0.41
54:J:57:ILE:HD12	54:J:57:ILE:HA	1.95	0.41
8:T:90:VAL:O	8:T:160:LYS:HA	2.21	0.41
33:N:1058:U:H2'	33:N:1059:G:C8	2.55	0.41
33:N:1173:U:H3'	33:N:1174:U:H4'	2.02	0.41
35:0:1081:A:H5'	39:4:23:LYS:HG3	2.01	0.41
53:I:58:VAL:HA	53:I:59:PRO:HD3	1.94	0.41
5:Q:81:GLU:OE1	33:N:2635:A:O2'	2.30	0.41
6:R:125:SER:O	6:R:137:LYS:NZ	2.54	0.41
18:d:15:LYS:HB2	18:d:15:LYS:HE2	1.80	0.41
19:e:81:LYS:HD2	33:N:973:A:OP2	2.20	0.41
30:p:24:THR:HG23	30:p:27:GLY:H	1.86	0.41
33:N:355:U:H2'	33:N:356:G:C8	2.56	0.41
33:N:568:U:O5'	33:N:945:A:N6	2.54	0.41
33:N:629:G:N3	33:N:639:U:O2'	2.52	0.41
33:N:632:A:H2'	33:N:633:A:C8	2.56	0.41
33:N:927:A:H2'	33:N:928:A:C8	2.56	0.41
33:N:2627:G:O2'	33:N:2781:A:N1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:2788:C:H2'	33:N:2789:C:C6	2.56	0.41
35:0:384:G:H2'	35:0:385:C:C6	2.56	0.41
35:0:501:C:H2'	35:0:502:A:C8	2.56	0.41
35:0:1300:G:O2'	35:0:1301:U:O5'	2.38	0.41
35:0:1328:C:H5''	47:C:28:THR:HG21	2.03	0.41
37:2:80:LYS:O	37:2:82:GLU:N	2.54	0.41
41:6:27:VAL:HG12	41:6:43:VAL:HG21	2.02	0.41
43:8:20:PHE:HB2	43:8:64:TYR:O	2.21	0.41
44:9:37:ARG:HA	44:9:37:ARG:HD3	1.89	0.41
44:9:71:LEU:O	44:9:72:ARG:NH1	2.46	0.41
46:B:50:ARG:HG3	46:B:90:LEU:HD11	2.01	0.41
54:J:28:MET:HE3	54:J:58:VAL:HG22	2.02	0.41
54:J:62:ALA:HA	54:J:67:ILE:HG22	2.02	0.41
1:s:150:TYR:OH	33:N:2609:U:H5'	2.21	0.41
7:S:112:ARG:HD3	47:C:7:ILE:CG1	2.51	0.41
11:W:110:PRO:O	11:W:115:GLY:HA3	2.20	0.41
16:b:24:THR:HG22	16:b:42:PRO:HD3	2.03	0.41
16:b:94:ARG:HH12	33:N:2294:G:P	2.43	0.41
20:f:85:ILE:HG23	20:f:93:ALA:HB1	2.03	0.41
33:N:675:A:N3	33:N:2443:C:O2'	2.47	0.41
33:N:1212:G:H2'	33:N:1236:G:H22	1.85	0.41
33:N:1236:G:O2'	33:N:1237:A:O5'	2.37	0.41
33:N:2572:A:OP1	33:N:2574:G:H4'	2.20	0.41
35:0:109:A:H5'	35:0:110:C:C5	2.56	0.41
35:0:1524:C:H2'	35:0:1525:G:C8	2.56	0.41
40:5:3:HIS:CE1	40:5:95:ALA:HB2	2.55	0.41
40:5:90:MET:HE1	52:H:23:TYR:CE1	2.56	0.41
3:O:72:G:N2	3:O:104:A:H62	2.18	0.40
3:O:89:U:O2'	33:N:958:U:O2	2.38	0.40
13:Y:35:HIS:O	13:Y:36:LYS:O	2.39	0.40
25:k:3:ARG:HD3	33:N:1365:A:OP1	2.21	0.40
34:L:8:LYS:HA	34:L:8:LYS:HD3	1.82	0.40
38:3:200:ILE:HG21	38:3:200:ILE:HD13	1.76	0.40
3:O:42:C:C6	7:S:66:LEU:HB2	2.56	0.40
4:P:178:SER:HB2	33:N:1799:G:N7	2.36	0.40
19:e:10:LYS:HE3	19:e:10:LYS:HB3	1.92	0.40
33:N:1105:U:H2'	33:N:1106:G:C8	2.51	0.40
33:N:1746:A:H2'	33:N:1747:U:C6	2.56	0.40
33:N:2500:U:O2'	33:N:2504:U:OP1	2.39	0.40
35:0:552:U:O2'	46:B:83:ARG:O	2.40	0.40
35:0:1095:U:P	35:0:1108:G:H1	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:0:1251:A:N3	35:0:1369:C:O2'	2.51	0.40
7:S:10:ASP:OD1	7:S:11:GLU:N	2.54	0.40
18:d:24:TYR:CE1	33:N:533:G:H5'	2.56	0.40
25:k:37:ARG:HG3	25:k:48:THR:HB	2.02	0.40
33:N:704:G:H1'	33:N:727:A:N6	2.36	0.40
33:N:1009:A:N3	33:N:1153:C:O2'	2.53	0.40
33:N:2114:A:N1	33:N:2119:A:N6	2.69	0.40
35:0:321:A:N7	35:0:328:C:O2'	2.52	0.40
35:0:752:G:H1'	35:0:754:C:H41	1.86	0.40
39:4:150:PRO:HA	39:4:153:VAL:HG22	2.03	0.40
41:6:75:VAL:HA	41:6:87:VAL:O	2.21	0.40
45:A:110:ILE:HG22	55:K:17:ARG:CZ	2.51	0.40
33:N:1394:U:H4'	33:N:1603:A:H4'	2.02	0.40
33:N:2724:U:H2'	33:N:2725:A:C8	2.56	0.40
35:0:1523:G:OP1	45:A:125:LYS:CE	2.70	0.40
37:2:22:TRP:NE1	37:2:36:ASP:OD2	2.50	0.40
41:6:44:TYR:O	41:6:48:GLU:HB2	2.21	0.40
3:O:8:C:O3'	16:b:25:ARG:NH1	2.54	0.40
33:N:141:G:H5'	33:N:142:A:C8	2.57	0.40
33:N:624:C:O2'	33:N:657:U:OP1	2.33	0.40
33:N:1047:G:H5'	33:N:1048:A:H5'	2.04	0.40
33:N:1858:A:H61	33:N:1884:G:H1'	1.86	0.40
35:0:1021:A:H2'	35:0:1022:A:C8	2.57	0.40
35:0:1216:A:H5''	48:D:5:SER:HB2	2.02	0.40
38:3:124:MET:HE3	38:3:146:ARG:HG2	2.03	0.40
44:9:36:VAL:HG22	44:9:76:ILE:HG12	2.03	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	
1	s	35/179 (20%)	32 (91%)	3 (9%)	0	100	100
4	P	269/273 (98%)	247 (92%)	18 (7%)	4 (2%)	8	28
5	Q	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	24	54
6	R	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
7	S	175/179 (98%)	163 (93%)	11 (6%)	1 (1%)	21	51
8	T	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
9	U	45/149 (30%)	35 (78%)	9 (20%)	1 (2%)	5	20
10	V	139/142 (98%)	112 (81%)	27 (19%)	0	100	100
11	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
12	X	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	7	26
13	Y	141/144 (98%)	121 (86%)	16 (11%)	4 (3%)	4	15
14	Z	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	2	11
15	a	118/127 (93%)	102 (86%)	14 (12%)	2 (2%)	7	26
16	b	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
17	c	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
18	d	115/118 (98%)	115 (100%)	0	0	100	100
19	e	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	12	39
20	f	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	41
21	g	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	20
22	h	100/104 (96%)	84 (84%)	14 (14%)	2 (2%)	6	22
23	i	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
24	j	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
25	k	75/78 (96%)	71 (95%)	3 (4%)	1 (1%)	9	32
26	l	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
27	m	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
28	n	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	23
29	o	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
30	p	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
31	q	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	7	27
32	r	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	L	64/70 (91%)	56 (88%)	7 (11%)	1 (2%)	7	27
36	1	216/233 (93%)	187 (87%)	28 (13%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2	204/233 (88%)	186 (91%)	16 (8%)	2 (1%)	12	39
38	3	203/206 (98%)	182 (90%)	21 (10%)	0	100	100
39	4	148/166 (89%)	116 (78%)	30 (20%)	2 (1%)	9	30
40	5	98/131 (75%)	81 (83%)	11 (11%)	6 (6%)	1	4
41	6	149/156 (96%)	139 (93%)	10 (7%)	0	100	100
42	7	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
43	8	125/130 (96%)	103 (82%)	20 (16%)	2 (2%)	7	27
44	9	96/103 (93%)	84 (88%)	9 (9%)	3 (3%)	3	14
45	A	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
46	B	121/124 (98%)	104 (86%)	15 (12%)	2 (2%)	7	26
47	C	112/118 (95%)	103 (92%)	8 (7%)	1 (1%)	14	41
48	D	92/101 (91%)	77 (84%)	14 (15%)	1 (1%)	11	36
49	E	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
50	F	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	9	32
51	G	78/84 (93%)	66 (85%)	9 (12%)	3 (4%)	2	10
52	H	53/75 (71%)	49 (92%)	3 (6%)	1 (2%)	6	23
53	I	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
54	J	83/87 (95%)	78 (94%)	4 (5%)	1 (1%)	10	34
55	K	49/71 (69%)	40 (82%)	9 (18%)	0	100	100
All	All	5614/6198 (91%)	5069 (90%)	489 (9%)	56 (1%)	15	39

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	239	ASN
13	Y	36	LYS
14	Z	58	LYS
19	e	53	PHE
28	n	55	ILE
31	q	32	ILE
40	5	53	LYS
44	9	58	ASN
50	F	44	SER
51	G	70	THR
14	Z	59	ARG

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Mol	Chain	Res	Type
15	a	3	HIS
37	2	81	GLY
40	5	56	LYS
40	5	91	ARG
43	8	55	VAL
46	B	23	ALA
51	G	18	GLU
54	J	69	LYS
4	P	235	GLY
14	Z	39	GLY
21	g	77	ARG
21	g	78	SER
22	h	99	ASN
25	k	3	ARG
37	2	80	LYS
40	5	54	LEU
40	5	94	HIS
44	9	43	PRO
46	B	78	SER
51	G	71	LYS
52	H	48	ARG
4	P	10	SER
4	P	238	ARG
5	Q	149	ASN
7	S	175	PHE
9	U	35	LYS
12	X	93	GLN
13	Y	29	LYS
13	Y	30	THR
13	Y	31	GLY
14	Z	69	PRO
34	L	3	LYS
39	4	51	GLY
40	5	86	ARG
47	C	66	GLU
15	a	88	ALA
20	f	64	ALA
22	h	53	ASN
36	1	194	ASP
39	4	90	THR
48	D	4	GLN
44	9	42	LEU

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Mol	Chain	Res	Type
14	Z	87	GLY
43	8	10	GLY
12	X	119	ALA

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 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	
1	s	34/158 (22%)	34 (100%)	0	100	100
4	P	216/218 (99%)	213 (99%)	3 (1%)	59	85
5	Q	164/164 (100%)	159 (97%)	5 (3%)	36	70
6	R	165/165 (100%)	162 (98%)	3 (2%)	51	80
7	S	148/150 (99%)	147 (99%)	1 (1%)	76	92
8	T	137/138 (99%)	137 (100%)	0	100	100
9	U	38/114 (33%)	37 (97%)	1 (3%)	40	73
10	V	109/110 (99%)	109 (100%)	0	100	100
11	W	116/116 (100%)	115 (99%)	1 (1%)	70	90
12	X	103/104 (99%)	101 (98%)	2 (2%)	50	79
13	Y	102/103 (99%)	100 (98%)	2 (2%)	48	78
14	Z	109/109 (100%)	108 (99%)	1 (1%)	70	90
15	a	100/103 (97%)	98 (98%)	2 (2%)	48	78
16	b	86/87 (99%)	85 (99%)	1 (1%)	63	86
17	c	98/100 (98%)	94 (96%)	4 (4%)	27	61
18	d	89/90 (99%)	87 (98%)	2 (2%)	45	77
19	e	84/84 (100%)	83 (99%)	1 (1%)	63	86
20	f	93/93 (100%)	93 (100%)	0	100	100
21	g	80/84 (95%)	79 (99%)	1 (1%)	61	86
22	h	83/85 (98%)	81 (98%)	2 (2%)	43	75
23	i	78/78 (100%)	77 (99%)	1 (1%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	j	56/63 (89%)	55 (98%)	1 (2%)	51	80
25	k	67/68 (98%)	67 (100%)	0	100	100
26	l	55/55 (100%)	54 (98%)	1 (2%)	51	80
27	m	48/49 (98%)	48 (100%)	0	100	100
28	n	47/48 (98%)	46 (98%)	1 (2%)	47	77
29	o	45/49 (92%)	45 (100%)	0	100	100
30	p	38/38 (100%)	38 (100%)	0	100	100
31	q	51/52 (98%)	49 (96%)	2 (4%)	28	63
32	r	34/34 (100%)	33 (97%)	1 (3%)	37	71
34	L	59/62 (95%)	59 (100%)	0	100	100
36	1	180/192 (94%)	179 (99%)	1 (1%)	78	93
37	2	170/190 (90%)	167 (98%)	3 (2%)	51	80
38	3	172/173 (99%)	170 (99%)	2 (1%)	63	86
39	4	113/125 (90%)	107 (95%)	6 (5%)	20	52
40	5	87/112 (78%)	87 (100%)	0	100	100
41	6	124/129 (96%)	123 (99%)	1 (1%)	73	90
42	7	104/105 (99%)	101 (97%)	3 (3%)	37	71
43	8	105/107 (98%)	104 (99%)	1 (1%)	68	89
44	9	86/90 (96%)	85 (99%)	1 (1%)	63	86
45	A	90/99 (91%)	89 (99%)	1 (1%)	65	88
46	B	103/104 (99%)	103 (100%)	0	100	100
47	C	92/96 (96%)	90 (98%)	2 (2%)	45	77
48	D	79/84 (94%)	79 (100%)	0	100	100
49	E	75/77 (97%)	75 (100%)	0	100	100
50	F	65/65 (100%)	64 (98%)	1 (2%)	57	84
51	G	74/78 (95%)	73 (99%)	1 (1%)	59	85
52	H	48/65 (74%)	47 (98%)	1 (2%)	47	77
53	I	70/79 (89%)	66 (94%)	4 (6%)	18	49
54	J	65/66 (98%)	65 (100%)	0	100	100
55	K	44/61 (72%)	43 (98%)	1 (2%)	44	76
All	All	4678/5068 (92%)	4610 (98%)	68 (2%)	55	84

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P	141	VAL
4	P	165	VAL
4	P	218	PRO
5	Q	48	ILE
5	Q	73	VAL
5	Q	177	VAL
5	Q	202	ILE
5	Q	205	PRO
6	R	69	ARG
6	R	149	ILE
6	R	163	ASN
7	S	31	VAL
9	U	27	ARG
11	W	57	LEU
12	X	58	LEU
12	X	86	LEU
13	Y	77	ILE
13	Y	94	THR
14	Z	128	THR
15	a	50	PRO
15	a	70	THR
16	b	3	LYS
17	c	32	VAL
17	c	53	ARG
17	c	73	VAL
17	c	93	ARG
18	d	16	LYS
18	d	33	ARG
19	e	49	ILE
21	g	32	LEU
22	h	28	VAL
22	h	68	SER
23	i	65	VAL
24	j	41	ARG
26	l	6	LEU
28	n	28	LEU
31	q	2	PRO
31	q	32	ILE
32	r	26	ILE
36	1	207	ILE
37	2	55	ILE
37	2	75	ILE

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Mol	Chain	Res	Type
37	2	200	VAL
38	3	5	LEU
38	3	143	VAL
39	4	15	LEU
39	4	115	LEU
39	4	120	VAL
39	4	123	VAL
39	4	141	ILE
39	4	157	ARG
41	6	25	LYS
42	7	51	VAL
42	7	121	LEU
42	7	125	ILE
43	8	120	LYS
44	9	17	LEU
45	A	31	ILE
47	C	25	VAL
47	C	98	ARG
50	F	19	VAL
51	G	61	ILE
52	H	21	ILE
53	I	5	LEU
53	I	11	ILE
53	I	49	ILE
53	I	58	VAL
55	K	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	s	126	HIS
4	P	53	HIS
4	P	86	ASN
4	P	239	ASN
4	P	260	ASN
5	Q	32	ASN
5	Q	49	GLN
5	Q	149	ASN
5	Q	150	GLN
6	R	136	GLN
6	R	163	ASN
6	R	165	HIS

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Mol	Chain	Res	Type
8	T	22	GLN
8	T	73	ASN
8	T	143	GLN
9	U	2	GLN
9	U	11	ASN
10	V	12	GLN
11	W	40	HIS
11	W	86	GLN
15	a	3	HIS
15	a	73	ASN
17	c	12	GLN
17	c	15	GLN
17	c	52	ASN
18	d	37	GLN
20	f	15	GLN
23	i	51	GLN
24	j	57	HIS
25	k	36	HIS
28	n	6	ASN
28	n	19	HIS
28	n	38	HIS
28	n	42	HIS
29	o	19	HIS
34	L	20	ASN
34	L	61	ASN
36	1	15	HIS
36	1	177	ASN
36	1	203	ASN
37	2	8	ASN
37	2	123	GLN
37	2	190	HIS
39	4	73	ASN
39	4	89	HIS
39	4	121	HIS
40	5	11	HIS
40	5	55	HIS
41	6	28	ASN
41	6	148	ASN
43	8	25	ASN
43	8	50	GLN
43	8	81	HIS
44	9	56	HIS

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Mol	Chain	Res	Type
44	9	58	ASN
45	A	118	HIS
47	C	8	ASN
48	D	49	GLN
48	D	66	GLN
48	D	71	HIS
49	E	35	GLN
49	E	37	ASN
50	F	63	GLN
51	G	31	HIS
52	H	52	GLN
52	H	54	GLN
53	I	56	GLN
54	J	20	HIS
54	J	48	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	M	74/75 (98%)	11 (14%)	0
3	O	117/120 (97%)	21 (17%)	1 (0%)
33	N	2894/2903 (99%)	537 (18%)	34 (1%)
35	0	1538/1539 (99%)	281 (18%)	22 (1%)
56	t	3/4 (75%)	1 (33%)	0
All	All	4626/4641 (99%)	851 (18%)	57 (1%)

All (851) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	M	9	C
2	M	10	G
2	M	15	G
2	M	16	C
2	M	17	G
2	M	19	U
2	M	20	A
2	M	42	G
2	M	47	C
2	M	74	C
2	M	75	A
3	O	13	G

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Mol	Chain	Res	Type
3	O	25	U
3	O	31	C
3	O	35	C
3	O	41	G
3	O	44	G
3	O	45	A
3	O	51	G
3	O	53	A
3	O	56	G
3	O	57	A
3	O	64	G
3	O	66	A
3	O	67	G
3	O	88	C
3	O	89	U
3	O	90	C
3	O	91	C
3	O	99	A
3	O	108	A
3	O	109	A
33	N	10	A
33	N	23	G
33	N	28	A
33	N	35	G
33	N	36	G
33	N	42	A
33	N	46	G
33	N	51	G
33	N	55	G
33	N	60	G
33	N	61	C
33	N	63	A
33	N	71	A
33	N	74	A
33	N	75	G
33	N	84	A
33	N	96	C
33	N	101	A
33	N	102	U
33	N	103	A
33	N	118	A
33	N	119	A

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Mol	Chain	Res	Type
33	N	120	U
33	N	125	A
33	N	138	U
33	N	139	U
33	N	140	C
33	N	141	G
33	N	142	A
33	N	162	U
33	N	163	C
33	N	165	A
33	N	166	U
33	N	188	G
33	N	196	A
33	N	199	A
33	N	201	C
33	N	215	G
33	N	216	A
33	N	221	A
33	N	222	A
33	N	223	A
33	N	224	U
33	N	228	C
33	N	241	A
33	N	242	G
33	N	243	U
33	N	248	G
33	N	255	A
33	N	265	A
33	N	266	G
33	N	267	C
33	N	271	G
33	N	272	A
33	N	276	U
33	N	278	A
33	N	281	C
33	N	284	U
33	N	294	A
33	N	301	G
33	N	311	A
33	N	323	C
33	N	329	G
33	N	330	A

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Mol	Chain	Res	Type
33	N	332	A
33	N	346	A
33	N	361	G
33	N	362	A
33	N	371	A
33	N	372	G
33	N	373	U
33	N	386	G
33	N	396	G
33	N	399	U
33	N	403	U
33	N	404	A
33	N	405	U
33	N	406	G
33	N	411	G
33	N	412	A
33	N	421	C
33	N	422	A
33	N	424	G
33	N	435	C
33	N	447	A
33	N	455	C
33	N	456	C
33	N	457	A
33	N	467	G
33	N	471	A
33	N	473	G
33	N	481	G
33	N	491	G
33	N	501	A
33	N	504	A
33	N	505	A
33	N	509	C
33	N	513	A
33	N	529	A
33	N	531	C
33	N	532	A
33	N	543	G
33	N	544	C
33	N	546	U
33	N	548	G
33	N	549	G

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Mol	Chain	Res	Type
33	N	550	C
33	N	556	A
33	N	563	A
33	N	573	U
33	N	575	A
33	N	578	G
33	N	586	A
33	N	603	A
33	N	613	A
33	N	614	A
33	N	616	A
33	N	622	G
33	N	627	A
33	N	637	A
33	N	645	C
33	N	646	U
33	N	647	G
33	N	648	G
33	N	654	A
33	N	655	A
33	N	669	G
33	N	670	A
33	N	671	C
33	N	677	A
33	N	686	U
33	N	695	G
33	N	696	G
33	N	717	C
33	N	729	G
33	N	730	A
33	N	738	G
33	N	747	U
33	N	764	A
33	N	765	C
33	N	775	G
33	N	776	G
33	N	782	A
33	N	783	A
33	N	784	G
33	N	785	G
33	N	792	A
33	N	800	A

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Mol	Chain	Res	Type
33	N	805	G
33	N	806	C
33	N	812	C
33	N	819	A
33	N	827	U
33	N	828	U
33	N	829	A
33	N	845	A
33	N	846	U
33	N	858	G
33	N	860	U
33	N	866	A
33	N	869	G
33	N	878	A
33	N	885	C
33	N	896	A
33	N	897	C
33	N	907	G
33	N	910	A
33	N	914	G
33	N	919	U
33	N	932	U
33	N	941	A
33	N	945	A
33	N	946	C
33	N	953	G
33	N	961	C
33	N	973	A
33	N	974	G
33	N	983	A
33	N	985	C
33	N	989	G
33	N	995	C
33	N	996	A
33	N	997	G
33	N	1004	U
33	N	1012	U
33	N	1013	C
33	N	1020	A
33	N	1021	A
33	N	1022	G
33	N	1023	U

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Mol	Chain	Res	Type
33	N	1025	G
33	N	1026	G
33	N	1033	U
33	N	1046	A
33	N	1047	G
33	N	1057	A
33	N	1060	U
33	N	1062	G
33	N	1064	C
33	N	1066	U
33	N	1067	A
33	N	1068	G
33	N	1070	A
33	N	1077	A
33	N	1082	U
33	N	1083	U
33	N	1088	A
33	N	1089	A
33	N	1090	A
33	N	1094	U
33	N	1096	A
33	N	1097	U
33	N	1100	C
33	N	1104	C
33	N	1110	G
33	N	1111	A
33	N	1112	G
33	N	1119	U
33	N	1122	G
33	N	1130	U
33	N	1132	U
33	N	1133	A
33	N	1135	C
33	N	1136	G
33	N	1141	U
33	N	1142	A
33	N	1143	A
33	N	1155	A
33	N	1168	G
33	N	1171	G
33	N	1173	U
33	N	1174	U

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Mol	Chain	Res	Type
33	N	1175	A
33	N	1180	U
33	N	1186	G
33	N	1195	G
33	N	1204	A
33	N	1205	A
33	N	1206	G
33	N	1210	G
33	N	1212	G
33	N	1237	A
33	N	1238	G
33	N	1250	G
33	N	1251	C
33	N	1253	A
33	N	1256	G
33	N	1257	C
33	N	1265	A
33	N	1266	G
33	N	1268	A
33	N	1271	G
33	N	1272	A
33	N	1275	A
33	N	1300	G
33	N	1301	A
33	N	1321	A
33	N	1329	U
33	N	1332	G
33	N	1345	C
33	N	1352	U
33	N	1365	A
33	N	1368	G
33	N	1376	C
33	N	1379	U
33	N	1383	A
33	N	1386	C
33	N	1395	A
33	N	1403	A
33	N	1416	G
33	N	1419	A
33	N	1420	A
33	N	1421	G
33	N	1427	A

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Mol	Chain	Res	Type
33	N	1428	C
33	N	1434	A
33	N	1437	C
33	N	1453	A
33	N	1458	U
33	N	1461	C
33	N	1478	G
33	N	1482	G
33	N	1504	A
33	N	1508	A
33	N	1509	A
33	N	1515	A
33	N	1524	G
33	N	1529	G
33	N	1535	A
33	N	1536	C
33	N	1537	G
33	N	1538	G
33	N	1554	U
33	N	1565	C
33	N	1566	A
33	N	1569	A
33	N	1578	U
33	N	1583	A
33	N	1584	U
33	N	1585	C
33	N	1587	G
33	N	1607	C
33	N	1608	A
33	N	1610	A
33	N	1613	G
33	N	1622	G
33	N	1647	U
33	N	1648	U
33	N	1651	G
33	N	1674	G
33	N	1675	C
33	N	1676	A
33	N	1698	A
33	N	1699	G
33	N	1713	A
33	N	1715	G

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Mol	Chain	Res	Type
33	N	1728	C
33	N	1729	U
33	N	1730	C
33	N	1733	G
33	N	1738	G
33	N	1757	A
33	N	1758	U
33	N	1760	C
33	N	1764	C
33	N	1773	A
33	N	1784	A
33	N	1787	A
33	N	1800	C
33	N	1801	A
33	N	1802	A
33	N	1808	A
33	N	1811	G
33	N	1816	C
33	N	1829	A
33	N	1833	C
33	N	1835	G
33	N	1857	G
33	N	1869	G
33	N	1870	C
33	N	1900	A
33	N	1901	A
33	N	1905	C
33	N	1906	G
33	N	1913	A
33	N	1919	A
33	N	1927	A
33	N	1929	G
33	N	1930	G
33	N	1931	U
33	N	1938	A
33	N	1955	U
33	N	1964	G
33	N	1967	C
33	N	1970	A
33	N	1971	U
33	N	1972	G
33	N	1991	U

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Mol	Chain	Res	Type
33	N	1993	U
33	N	1997	C
33	N	2004	G
33	N	2006	C
33	N	2020	A
33	N	2022	U
33	N	2023	C
33	N	2031	A
33	N	2033	A
33	N	2043	C
33	N	2046	G
33	N	2055	C
33	N	2056	G
33	N	2060	A
33	N	2061	G
33	N	2062	A
33	N	2063	C
33	N	2069	G
33	N	2072	C
33	N	2077	A
33	N	2092	U
33	N	2093	G
33	N	2097	A
33	N	2098	U
33	N	2102	G
33	N	2106	U
33	N	2110	G
33	N	2111	U
33	N	2112	G
33	N	2113	U
33	N	2118	U
33	N	2119	A
33	N	2121	G
33	N	2123	G
33	N	2125	G
33	N	2128	G
33	N	2131	U
33	N	2132	U
33	N	2133	G
33	N	2137	U
33	N	2139	U
33	N	2146	C

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Mol	Chain	Res	Type
33	N	2149	U
33	N	2158	A
33	N	2159	G
33	N	2161	C
33	N	2162	G
33	N	2163	A
33	N	2164	C
33	N	2165	C
33	N	2170	A
33	N	2172	U
33	N	2173	A
33	N	2174	C
33	N	2178	C
33	N	2186	G
33	N	2189	U
33	N	2198	A
33	N	2203	U
33	N	2204	G
33	N	2211	A
33	N	2212	A
33	N	2214	C
33	N	2225	A
33	N	2226	C
33	N	2238	G
33	N	2239	G
33	N	2266	A
33	N	2278	A
33	N	2279	G
33	N	2283	C
33	N	2286	G
33	N	2287	A
33	N	2288	A
33	N	2297	A
33	N	2305	U
33	N	2307	G
33	N	2309	A
33	N	2312	U
33	N	2325	G
33	N	2333	A
33	N	2334	U
33	N	2345	G
33	N	2347	C

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Mol	Chain	Res	Type
33	N	2350	C
33	N	2354	C
33	N	2357	G
33	N	2361	G
33	N	2383	G
33	N	2385	C
33	N	2391	G
33	N	2402	U
33	N	2403	C
33	N	2406	A
33	N	2407	A
33	N	2422	C
33	N	2423	U
33	N	2425	A
33	N	2426	A
33	N	2427	C
33	N	2429	G
33	N	2430	A
33	N	2431	U
33	N	2435	A
33	N	2441	U
33	N	2448	A
33	N	2470	G
33	N	2476	A
33	N	2498	C
33	N	2502	G
33	N	2503	A
33	N	2504	U
33	N	2505	G
33	N	2518	A
33	N	2520	C
33	N	2529	G
33	N	2535	G
33	N	2547	A
33	N	2554	U
33	N	2566	A
33	N	2567	G
33	N	2572	A
33	N	2573	C
33	N	2574	G
33	N	2578	G
33	N	2585	U

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Mol	Chain	Res	Type
33	N	2602	A
33	N	2603	G
33	N	2609	U
33	N	2613	U
33	N	2615	U
33	N	2629	U
33	N	2630	G
33	N	2636	C
33	N	2645	G
33	N	2646	C
33	N	2655	G
33	N	2656	U
33	N	2661	G
33	N	2663	G
33	N	2682	A
33	N	2689	U
33	N	2690	U
33	N	2714	G
33	N	2716	C
33	N	2718	G
33	N	2724	U
33	N	2727	A
33	N	2733	A
33	N	2748	A
33	N	2751	G
33	N	2752	C
33	N	2765	A
33	N	2776	A
33	N	2777	G
33	N	2778	A
33	N	2779	U
33	N	2791	G
33	N	2792	A
33	N	2798	U
33	N	2801	G
33	N	2818	U
33	N	2820	A
33	N	2833	U
33	N	2834	G
33	N	2836	U
33	N	2849	U
33	N	2850	A

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Mol	Chain	Res	Type
33	N	2859	G
33	N	2867	G
33	N	2868	A
33	N	2872	A
33	N	2873	A
33	N	2874	C
33	N	2880	C
33	N	2884	U
33	N	2887	A
33	N	2891	U
33	N	2903	U
35	0	4	U
35	0	6	G
35	0	9	G
35	0	32	A
35	0	39	G
35	0	44	A
35	0	47	C
35	0	48	C
35	0	50	A
35	0	51	A
35	0	52	C
35	0	58	C
35	0	65	A
35	0	69	G
35	0	71	A
35	0	72	A
35	0	83	C
35	0	84	U
35	0	85	U
35	0	86	G
35	0	87	C
35	0	92	U
35	0	97	G
35	0	108	G
35	0	115	G
35	0	116	A
35	0	122	G
35	0	130	A
35	0	141	G
35	0	143	A
35	0	144	G

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Mol	Chain	Res	Type
35	0	149	A
35	0	156	C
35	0	163	C
35	0	174	A
35	0	177	G
35	0	182	A
35	0	183	C
35	0	184	G
35	0	197	A
35	0	209	U
35	0	210	C
35	0	211	G
35	0	226	G
35	0	245	U
35	0	247	G
35	0	251	G
35	0	266	G
35	0	267	C
35	0	280	C
35	0	281	G
35	0	289	G
35	0	298	A
35	0	306	A
35	0	321	A
35	0	328	C
35	0	332	G
35	0	347	G
35	0	351	G
35	0	352	C
35	0	354	G
35	0	358	U
35	0	367	U
35	0	372	C
35	0	375	U
35	0	384	G
35	0	388	G
35	0	389	A
35	0	397	A
35	0	398	U
35	0	406	G
35	0	412	A
35	0	413	G

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Mol	Chain	Res	Type
35	0	421	U
35	0	422	C
35	0	423	G
35	0	424	G
35	0	429	U
35	0	430	A
35	0	439	U
35	0	451	A
35	0	458	U
35	0	459	A
35	0	467	U
35	0	468	A
35	0	474	G
35	0	478	A
35	0	479	U
35	0	481	G
35	0	484	G
35	0	485	U
35	0	486	U
35	0	495	A
35	0	497	G
35	0	511	C
35	0	518	C
35	0	519	C
35	0	521	G
35	0	527	G
35	0	531	U
35	0	532	A
35	0	533	A
35	0	547	A
35	0	559	A
35	0	562	U
35	0	572	A
35	0	573	A
35	0	576	C
35	0	595	A
35	0	596	A
35	0	607	A
35	0	633	G
35	0	639	G
35	0	650	G
35	0	652	U

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Mol	Chain	Res	Type
35	0	665	A
35	0	675	A
35	0	688	G
35	0	695	A
35	0	701	U
35	0	702	A
35	0	703	G
35	0	718	A
35	0	721	G
35	0	723	U
35	0	724	G
35	0	731	G
35	0	734	G
35	0	747	A
35	0	755	G
35	0	777	A
35	0	793	U
35	0	794	A
35	0	813	U
35	0	815	A
35	0	817	C
35	0	818	G
35	0	819	A
35	0	821	G
35	0	828	U
35	0	832	G
35	0	836	G
35	0	841	C
35	0	843	U
35	0	844	G
35	0	846	G
35	0	849	G
35	0	859	G
35	0	864	A
35	0	885	G
35	0	889	A
35	0	890	G
35	0	891	U
35	0	902	G
35	0	914	A
35	0	922	G
35	0	926	G

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Mol	Chain	Res	Type
35	0	934	C
35	0	935	A
35	0	960	U
35	0	965	U
35	0	966	G
35	0	969	A
35	0	971	G
35	0	972	C
35	0	975	A
35	0	976	G
35	0	977	A
35	0	989	U
35	0	993	G
35	0	996	A
35	0	999	C
35	0	1000	A
35	0	1004	A
35	0	1008	U
35	0	1009	U
35	0	1017	U
35	0	1018	G
35	0	1020	G
35	0	1022	A
35	0	1024	G
35	0	1025	U
35	0	1026	G
35	0	1027	C
35	0	1030	U
35	0	1031	C
35	0	1032	G
35	0	1043	G
35	0	1044	A
35	0	1053	G
35	0	1056	U
35	0	1065	U
35	0	1085	U
35	0	1092	A
35	0	1094	G
35	0	1095	U
35	0	1101	A
35	0	1125	U
35	0	1130	A

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Mol	Chain	Res	Type
35	0	1132	C
35	0	1136	C
35	0	1137	C
35	0	1138	G
35	0	1139	G
35	0	1140	C
35	0	1146	A
35	0	1158	C
35	0	1159	U
35	0	1168	U
35	0	1171	A
35	0	1182	G
35	0	1183	U
35	0	1184	G
35	0	1190	G
35	0	1196	A
35	0	1200	C
35	0	1201	A
35	0	1202	U
35	0	1212	U
35	0	1213	A
35	0	1227	A
35	0	1238	A
35	0	1253	G
35	0	1256	A
35	0	1257	A
35	0	1258	G
35	0	1260	G
35	0	1261	A
35	0	1274	A
35	0	1275	A
35	0	1278	G
35	0	1280	A
35	0	1281	C
35	0	1287	A
35	0	1297	G
35	0	1298	U
35	0	1300	G
35	0	1301	U
35	0	1302	C
35	0	1305	G
35	0	1317	C

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Mol	Chain	Res	Type
35	0	1318	A
35	0	1319	A
35	0	1320	C
35	0	1322	C
35	0	1323	G
35	0	1331	G
35	0	1332	A
35	0	1340	A
35	0	1346	A
35	0	1347	G
35	0	1348	U
35	0	1353	G
35	0	1363	A
35	0	1364	U
35	0	1370	G
35	0	1379	G
35	0	1383	C
35	0	1394	A
35	0	1400	C
35	0	1419	G
35	0	1422	G
35	0	1433	A
35	0	1441	A
35	0	1446	A
35	0	1451	U
35	0	1452	C
35	0	1487	G
35	0	1492	A
35	0	1494	G
35	0	1497	G
35	0	1503	A
35	0	1506	U
35	0	1517	G
35	0	1519	A
35	0	1529	G
35	0	1530	G
35	0	1531	A
35	0	1534	A
35	0	1535	C
35	0	1537	U
56	t	466	C

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	O	52	A
33	N	60	G
33	N	227	A
33	N	242	G
33	N	249	C
33	N	372	G
33	N	404	A
33	N	421	C
33	N	446	G
33	N	456	C
33	N	474	G
33	N	503	A
33	N	512	G
33	N	555	G
33	N	670	A
33	N	774	G
33	N	784	G
33	N	859	G
33	N	995	C
33	N	1020	A
33	N	1134	A
33	N	1141	U
33	N	1142	A
33	N	1236	G
33	N	1900	A
33	N	2062	A
33	N	2225	A
33	N	2282	G
33	N	2286	G
33	N	2311	A
33	N	2405	G
33	N	2655	G
33	N	2776	A
33	N	2867	G
33	N	2873	A
35	0	64	G
35	0	85	U
35	0	96	U
35	0	115	G
35	0	388	G
35	0	429	U
35	0	518	C
35	0	595	A

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Mol	Chain	Res	Type
35	0	812	G
35	0	890	G
35	0	965	U
35	0	1124	G
35	0	1145	A
35	0	1182	G
35	0	1190	G
35	0	1201	A
35	0	1300	G
35	0	1345	U
35	0	1347	G
35	0	1491	G
35	0	1493	A
35	0	1528	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

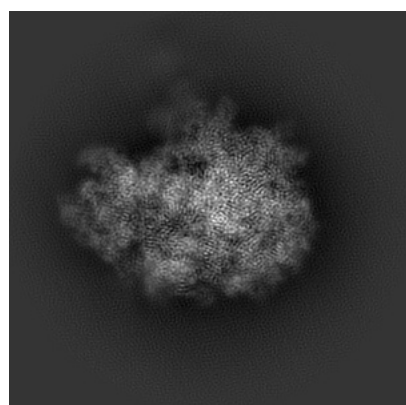
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3713. These allow visual inspection of the internal detail of the map and identification of artifacts.

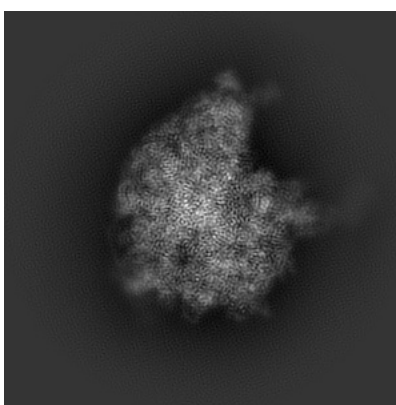
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

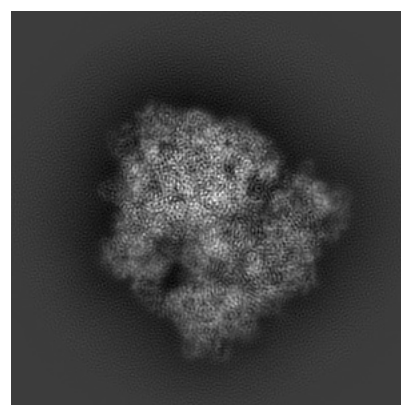
6.1.1 Primary map



X



Y

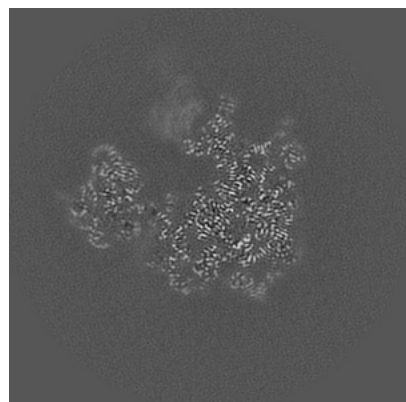


Z

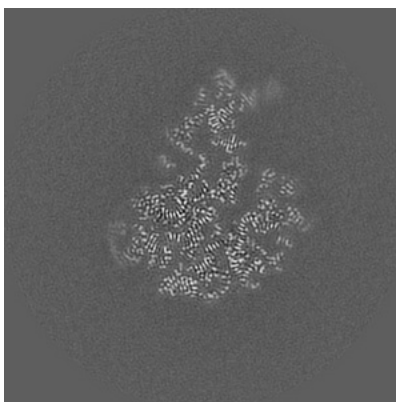
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

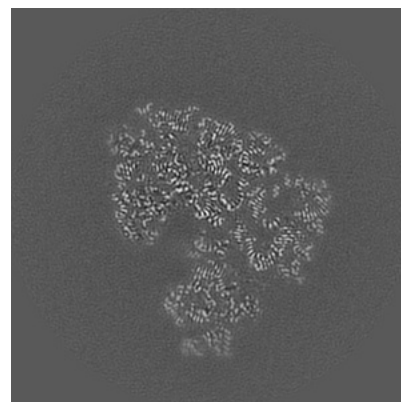
6.2.1 Primary map



X Index: 184



Y Index: 184

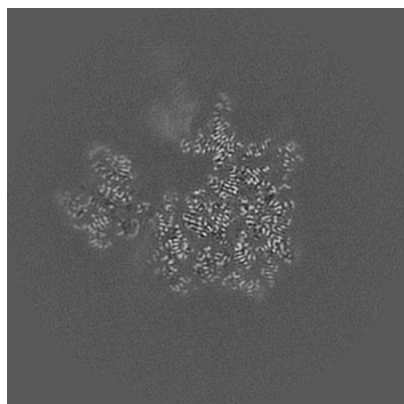


Z Index: 184

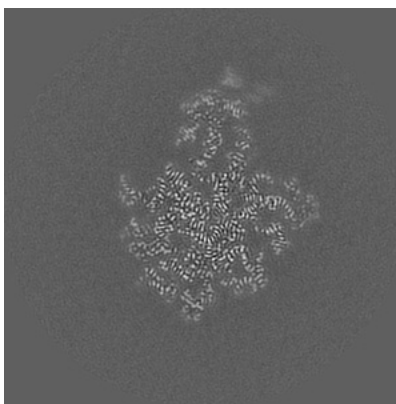
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

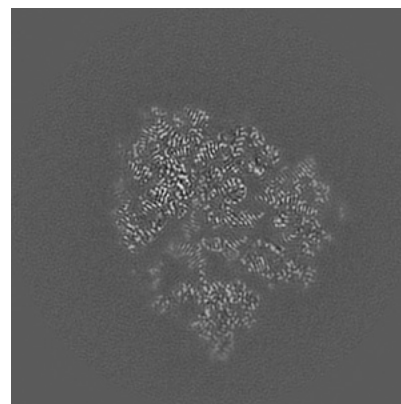
6.3.1 Primary map



X Index: 187



Y Index: 199

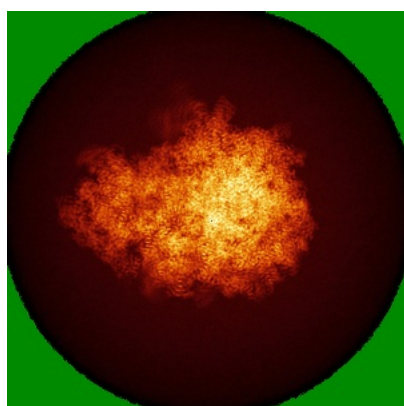


Z Index: 193

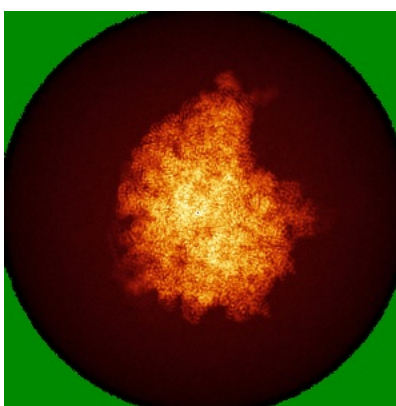
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

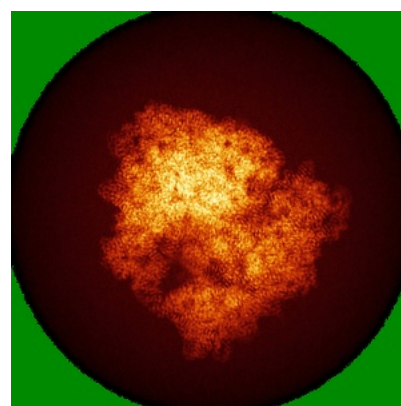
6.4.1 Primary map



X



Y



Z

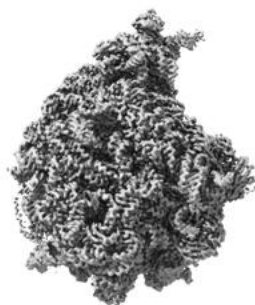
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

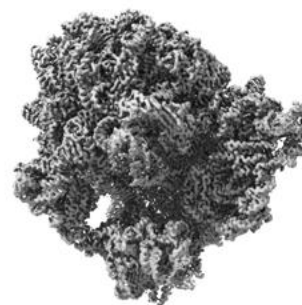
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

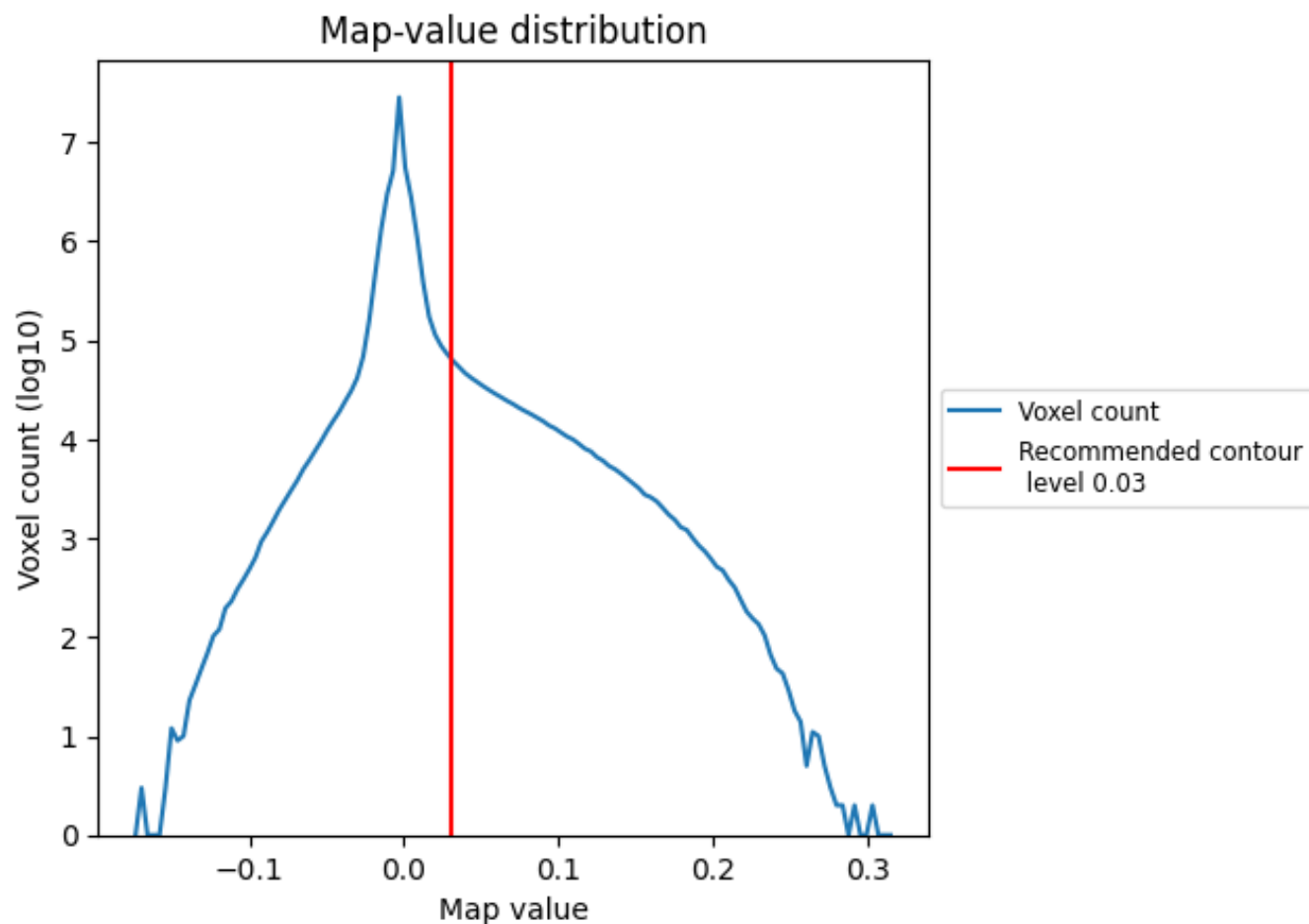
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

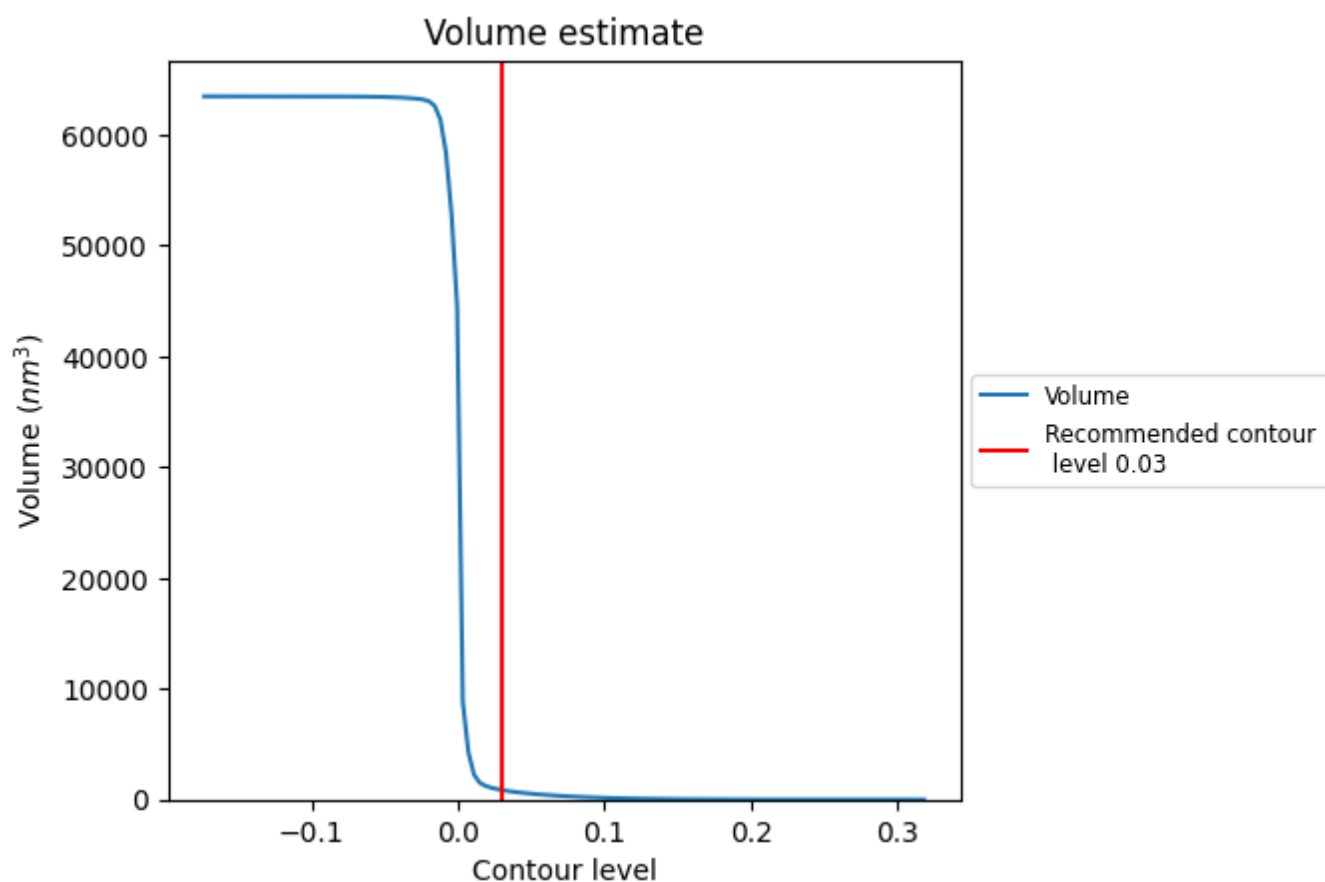
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

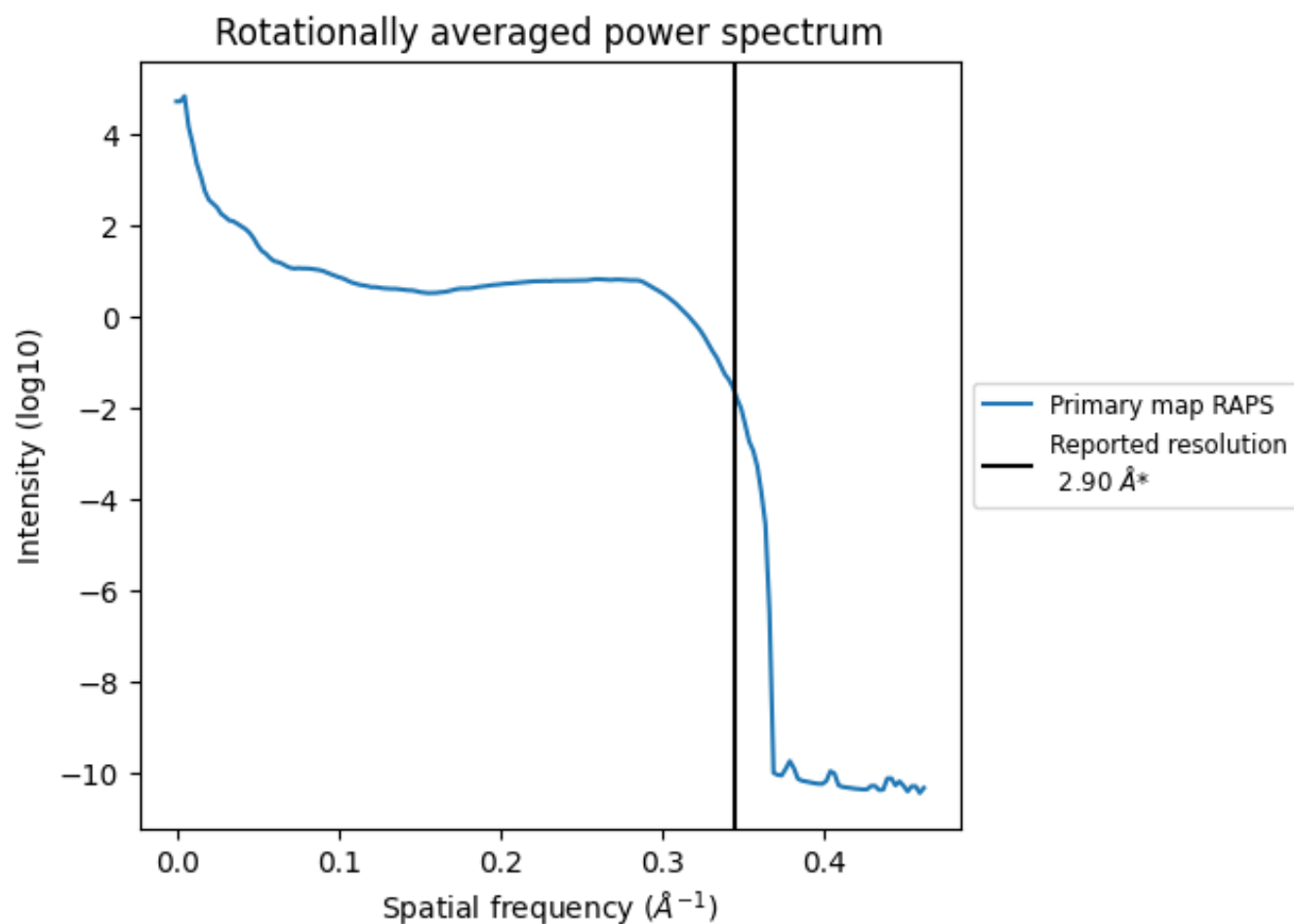
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 859 nm³; this corresponds to an approximate mass of 776 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

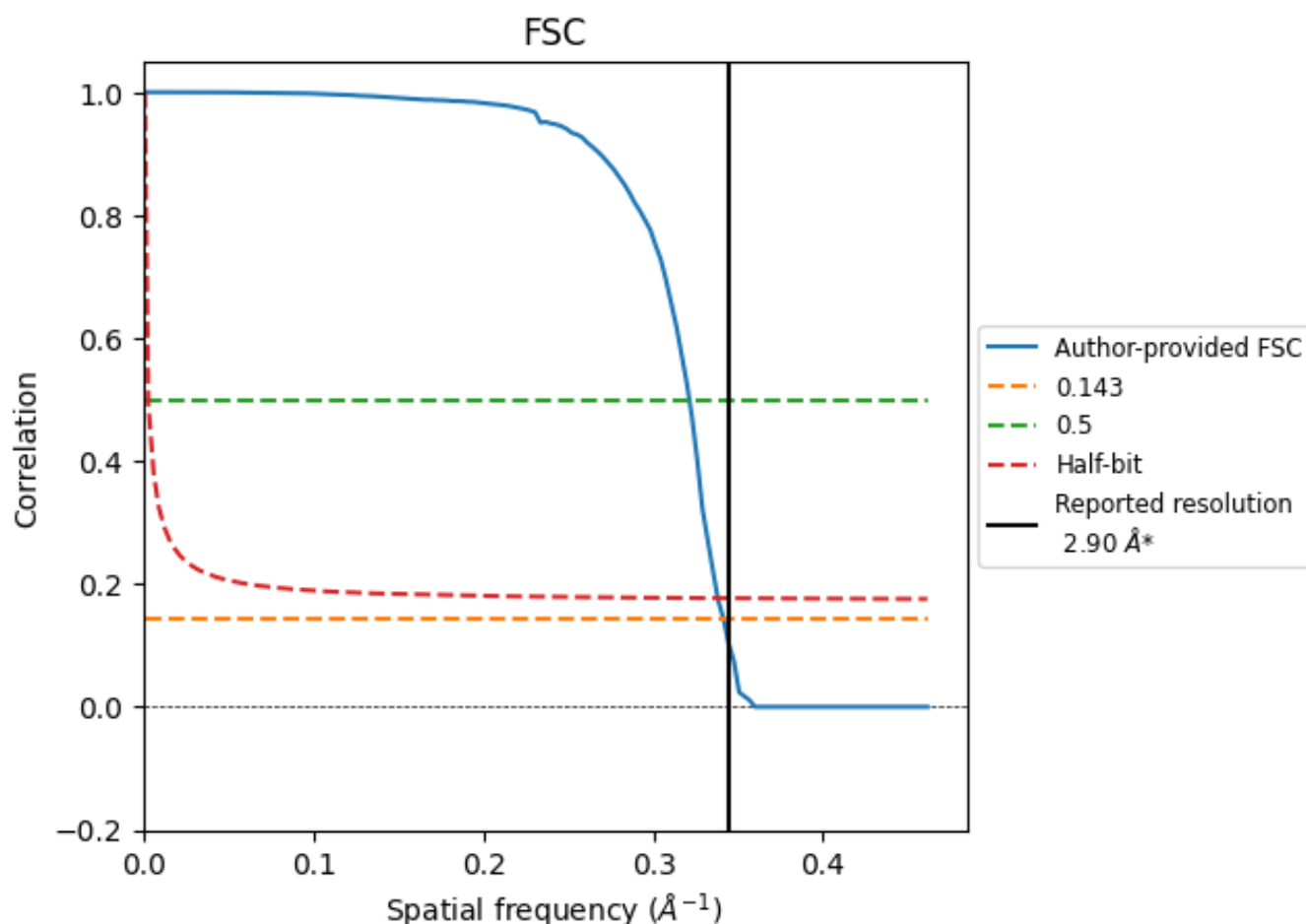


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

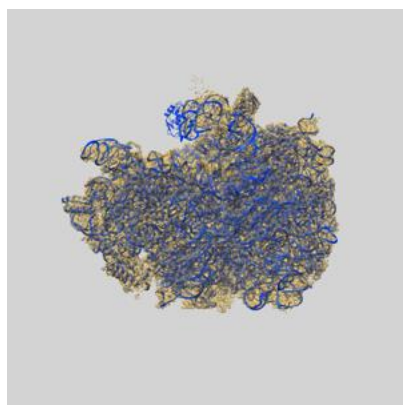
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.11	2.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

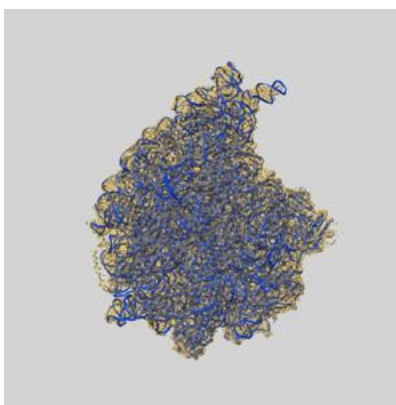
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3713 and PDB model 5NWY. Per-residue inclusion information can be found in section [3](#) on page [16](#).

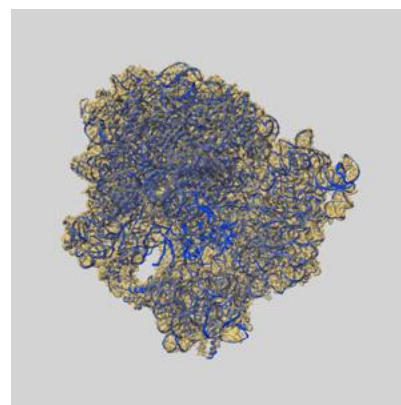
9.1 Map-model overlay [i](#)



X



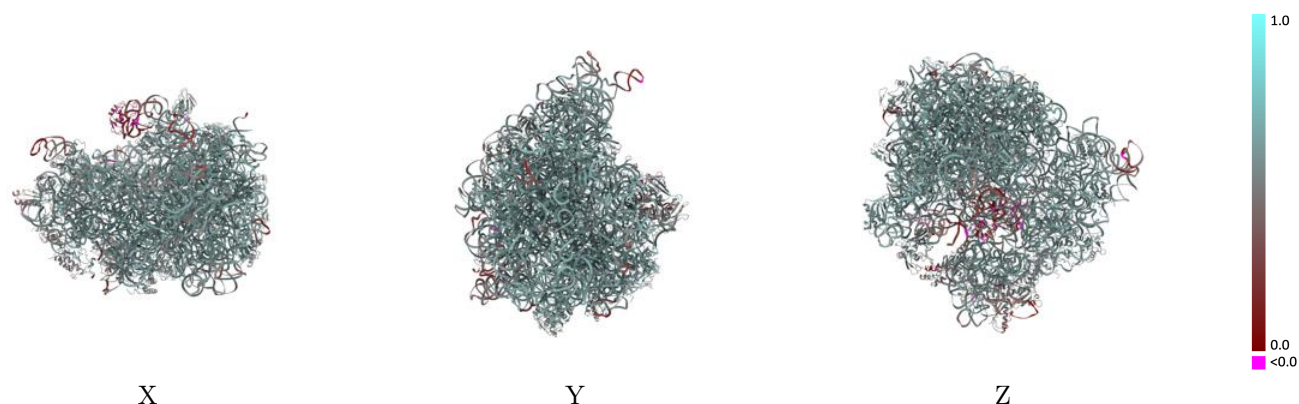
Y



Z

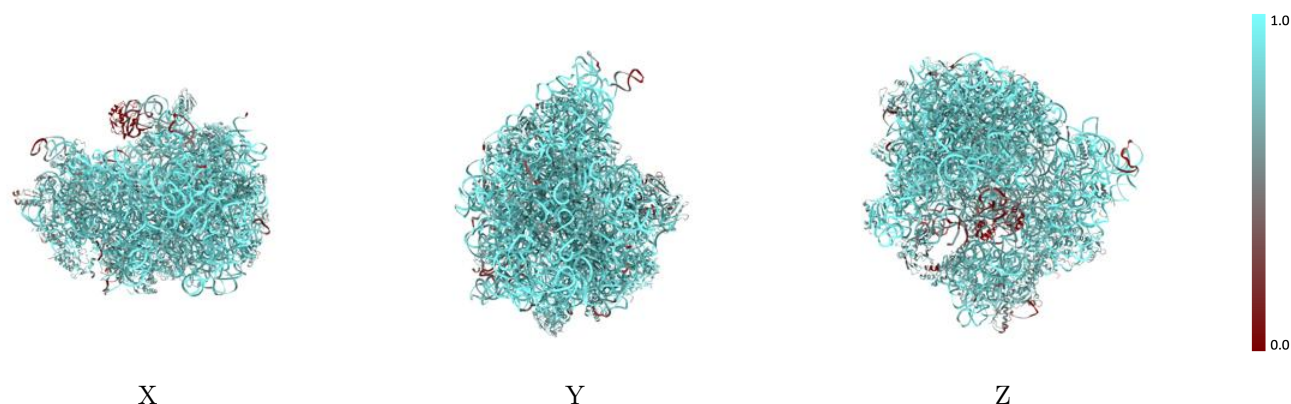
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



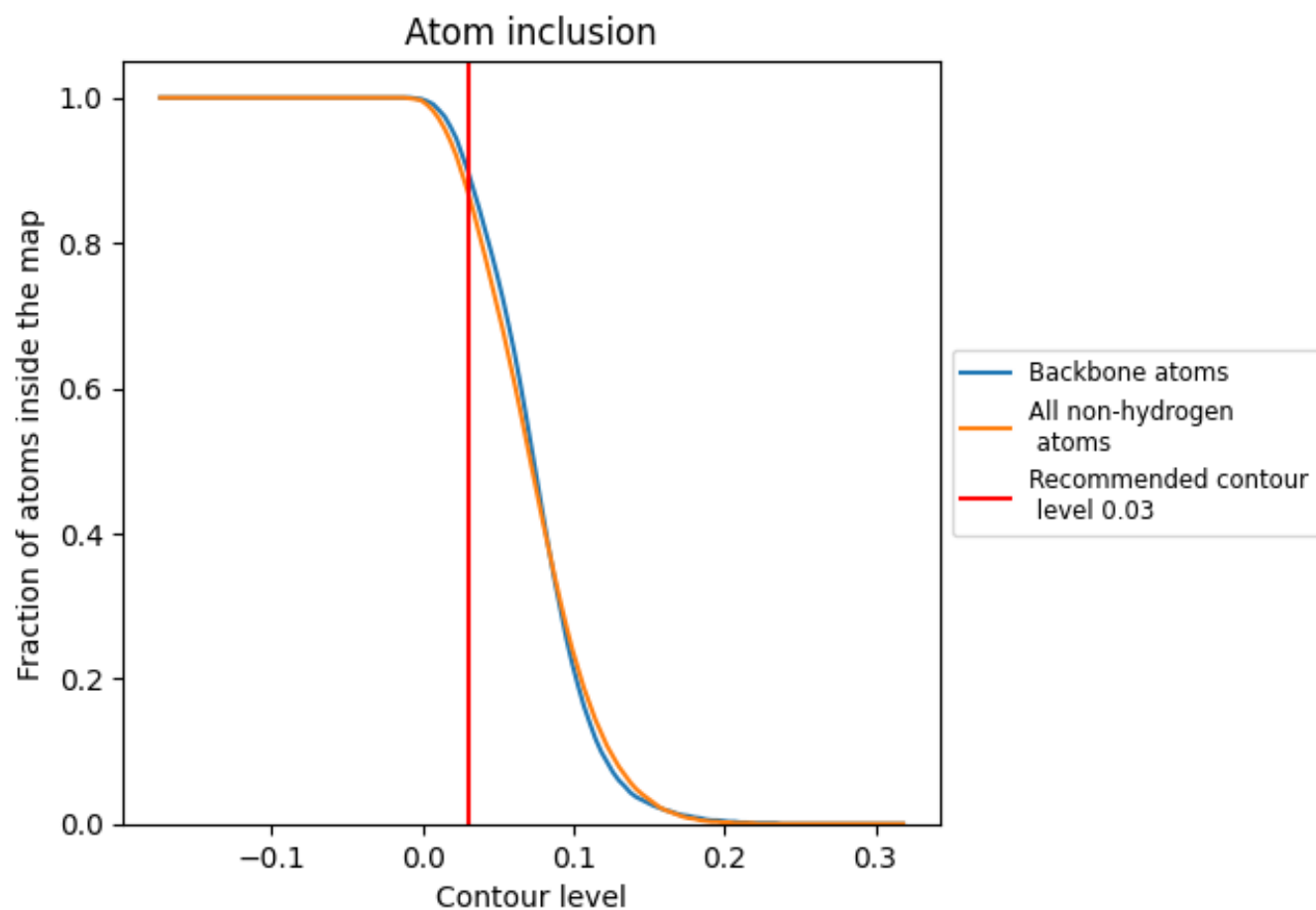
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.5580
0	 0.9260	 0.5680
1	 0.6770	 0.4790
2	 0.7490	 0.5300
3	 0.7430	 0.5250
4	 0.8200	 0.5570
5	 0.7300	 0.4990
6	 0.6570	 0.4860
7	 0.8110	 0.5570
8	 0.7380	 0.4890
9	 0.6350	 0.4720
A	 0.7680	 0.5310
B	 0.8060	 0.5630
C	 0.7390	 0.4970
D	 0.7880	 0.5180
E	 0.8010	 0.5410
F	 0.7870	 0.5270
G	 0.7500	 0.5280
H	 0.8140	 0.5480
I	 0.7540	 0.5100
J	 0.7640	 0.5280
K	 0.4680	 0.3800
L	 0.5520	 0.4100
M	 0.8000	 0.5240
N	 0.9140	 0.5700
O	 0.9450	 0.5730
P	 0.8810	 0.5940
Q	 0.8750	 0.5870
R	 0.7840	 0.5620
S	 0.7230	 0.5120
T	 0.7240	 0.5210
U	 0.6660	 0.4780
V	 0.0110	 0.1470
W	 0.8600	 0.5820
X	 0.8470	 0.5720



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Chain	Atom inclusion	Q-score
Y	 0.8440	 0.5730
Z	 0.8430	 0.5760
a	 0.8770	 0.5890
b	 0.8230	 0.5640
c	 0.8320	 0.5770
d	 0.8830	 0.6000
e	 0.8250	 0.5570
f	 0.8330	 0.5790
g	 0.7840	 0.5470
h	 0.7500	 0.5340
i	 0.7960	 0.5550
j	 0.8840	 0.5970
k	 0.8580	 0.5790
l	 0.7320	 0.5080
m	 0.8100	 0.5710
n	 0.8480	 0.5720
o	 0.7710	 0.5490
p	 0.8840	 0.6010
q	 0.9080	 0.6130
r	 0.8660	 0.5800
s	 0.6490	 0.5340
t	 0.8940	 0.5800