



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 06:38 pm BST

PDB ID : 6Q9A / pdb_00006q9a
EMDB ID : EMD-4478
Title : Structure of tmRNA SmpB bound past E site of E. coli 70S ribosome
Authors : Rae, C.D.
Deposited on : 2018-12-17
Resolution : 3.70 Å (reported)
Based on initial model : 5MDZ

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:

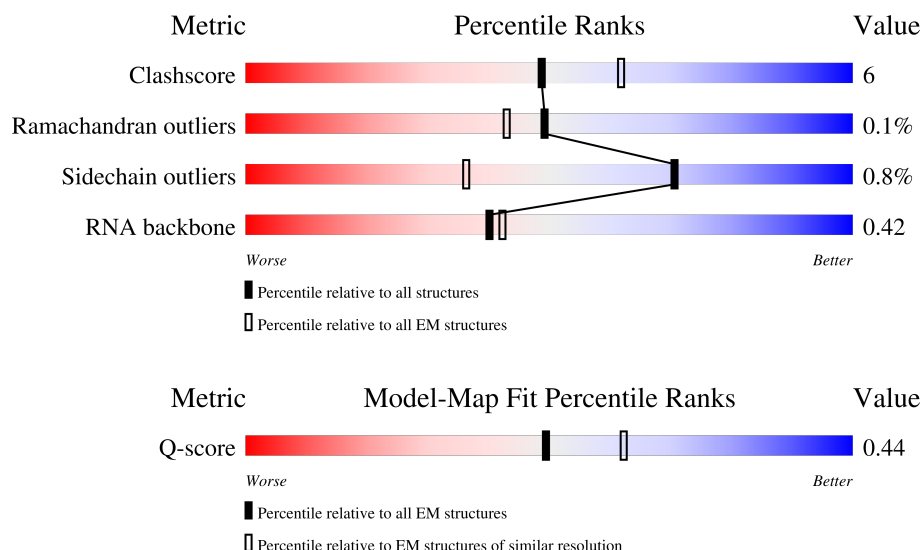
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1	2903	
2	2	1534	
3	3	120	

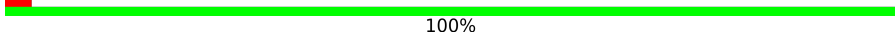
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Mol	Chain	Length	Quality of chain
4	6	23	
5	7	76	
6	B	271	
7	C	207	
8	D	201	
9	E	177	
10	F	175	
11	G	148	
12	H	130	
13	I	135	
14	J	142	
15	K	123	
16	L	143	
17	M	135	
18	N	119	
19	O	115	
20	P	113	
21	Q	117	
22	R	102	
23	S	109	
24	T	94	
25	U	101	
26	V	93	
27	W	75	
28	X	77	

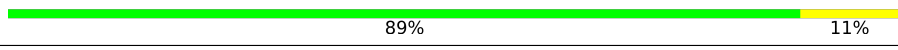
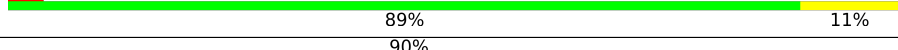
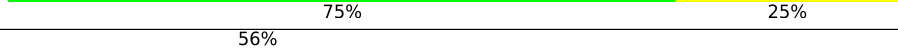
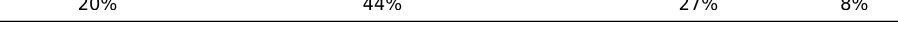
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Mol	Chain	Length	Quality of chain
29	Y	62	
30	Z	56	
31	a	66	
32	b	55	
33	c	51	
34	d	45	
35	e	64	
36	f	38	
37	g	225	
38	h	208	
39	i	205	
40	j	156	
41	k	104	
42	l	152	
43	m	129	
44	n	127	
45	o	99	
46	p	116	
47	q	122	
48	r	116	
49	s	100	
50	t	87	
51	u	82	
52	v	80	
53	w	66	

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Mol	Chain	Length	Quality of chain
54	x	83	
55	y	85	
56	z	70	
57	5	118	
58	4	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	1	1618	X	-	-	-
1	PSU	1	1911	X	-	-	-
1	3TD	1	1915	X	-	-	-
1	PSU	1	1917	X	-	-	-
1	5MU	1	1939	X	-	-	-
1	6MZ	1	2030	X	-	-	-
1	G7M	1	2069	X	-	-	-
1	OMG	1	2251	X	-	-	-
1	PSU	1	2457	X	-	-	-
1	OMC	1	2498	X	-	-	-
1	2MA	1	2503	X	-	-	-
1	PSU	1	2504	X	-	-	-
1	OMU	1	2552	X	-	-	-
1	PSU	1	2580	X	-	-	-
1	PSU	1	2605	X	-	-	-
1	1MG	1	745	X	-	-	-
1	PSU	1	746	X	-	-	-
1	5MU	1	747	X	-	-	-
1	PSU	1	955	X	-	-	-
2	4OC	2	1402	X	-	-	-
2	PSU	2	516	X	-	-	-
2	7MG	2	527	X	-	-	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 155169 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	6	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	76	Total	C	N	O	P	0	0
			1621	722	289	534	76		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	207	Total	C	N	O	S	0	0
			1551	971	286	291	3		

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1065	681	204	175	5		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	115	Total	C	N	O	0	0
			884	548	177	159		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 21 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	U	101	Total	C	N	O	0	0
			774	489	145	140		

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	93	Total	C	N	O	S	0	0
			747	476	136	132	3		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L31.

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

- Molecule 32 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	c	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 34 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 35 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 36 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 41 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	87	Total	C	N	O	S	0	0
			708	436	143	128	1		

- Molecule 51 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 52 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

- Molecule 56 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 57 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	118	Total	C	N	O	S	0	0
			940	601	168	168	3		

- Molecule 58 is a RNA chain called tmRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4	363	Total	C	N	O	P	0	0
			7758	3465	1410	2520	363		

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	1	292	Total	Mg	0
			292	292	
59	2	127	Total	Mg	0
			127	127	
59	3	8	Total	Mg	0
			8	8	
59	7	4	Total	Mg	0
			4	4	
59	O	1	Total	Mg	0
			1	1	
59	Q	1	Total	Mg	0
			1	1	
59	b	1	Total	Mg	0
			1	1	
59	f	1	Total	Mg	0
			1	1	
59	i	1	Total	Mg	0
			1	1	
59	s	1	Total	Mg	0
			1	1	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	a	1	Total 1	Zn 1	0
60	f	1	Total 1	Zn 1	0

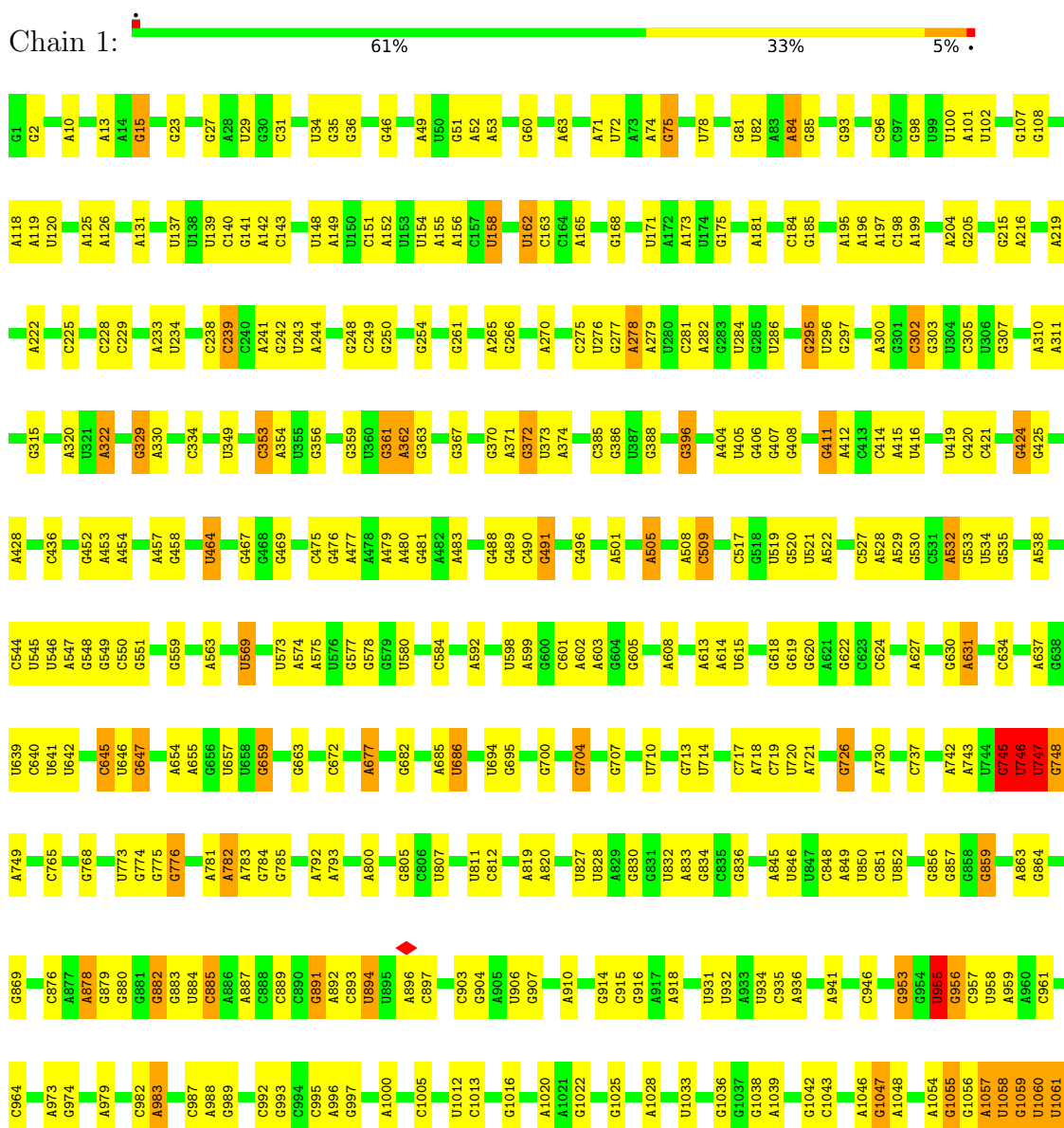
- Molecule 61 is water.

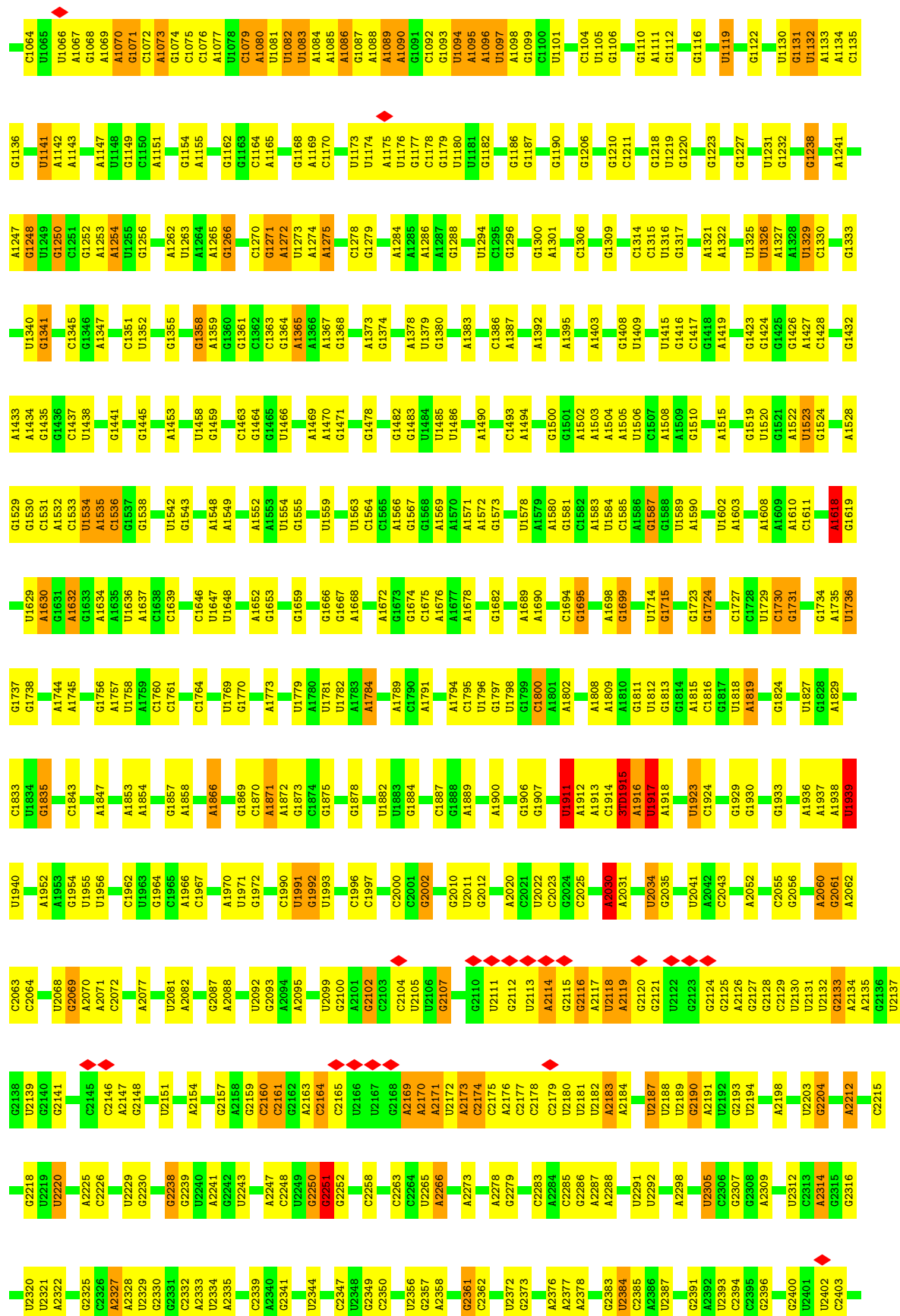
Mol	Chain	Residues	Atoms		AltConf
61	B	2	Total 2	O 2	0

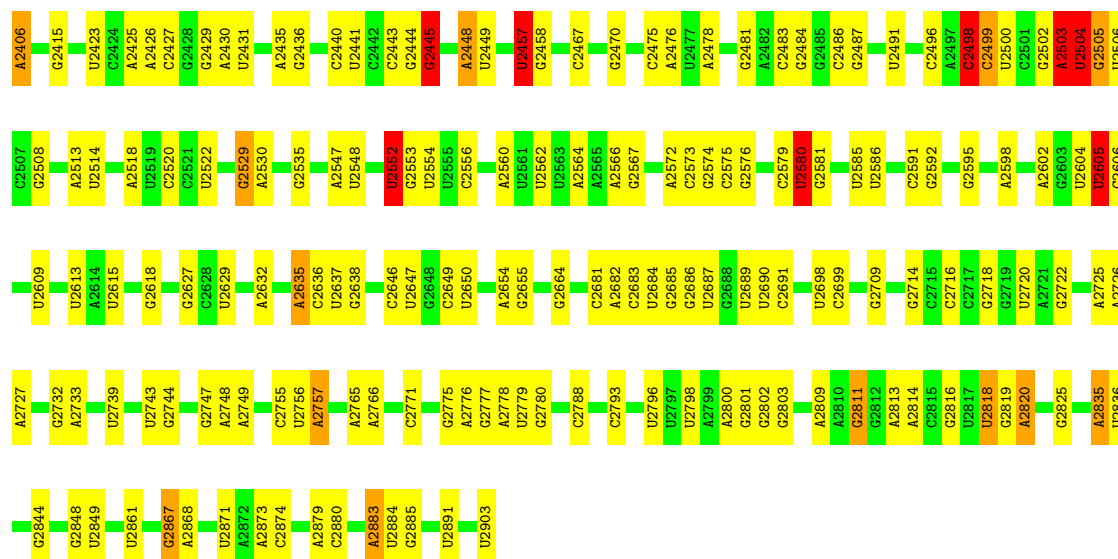
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA

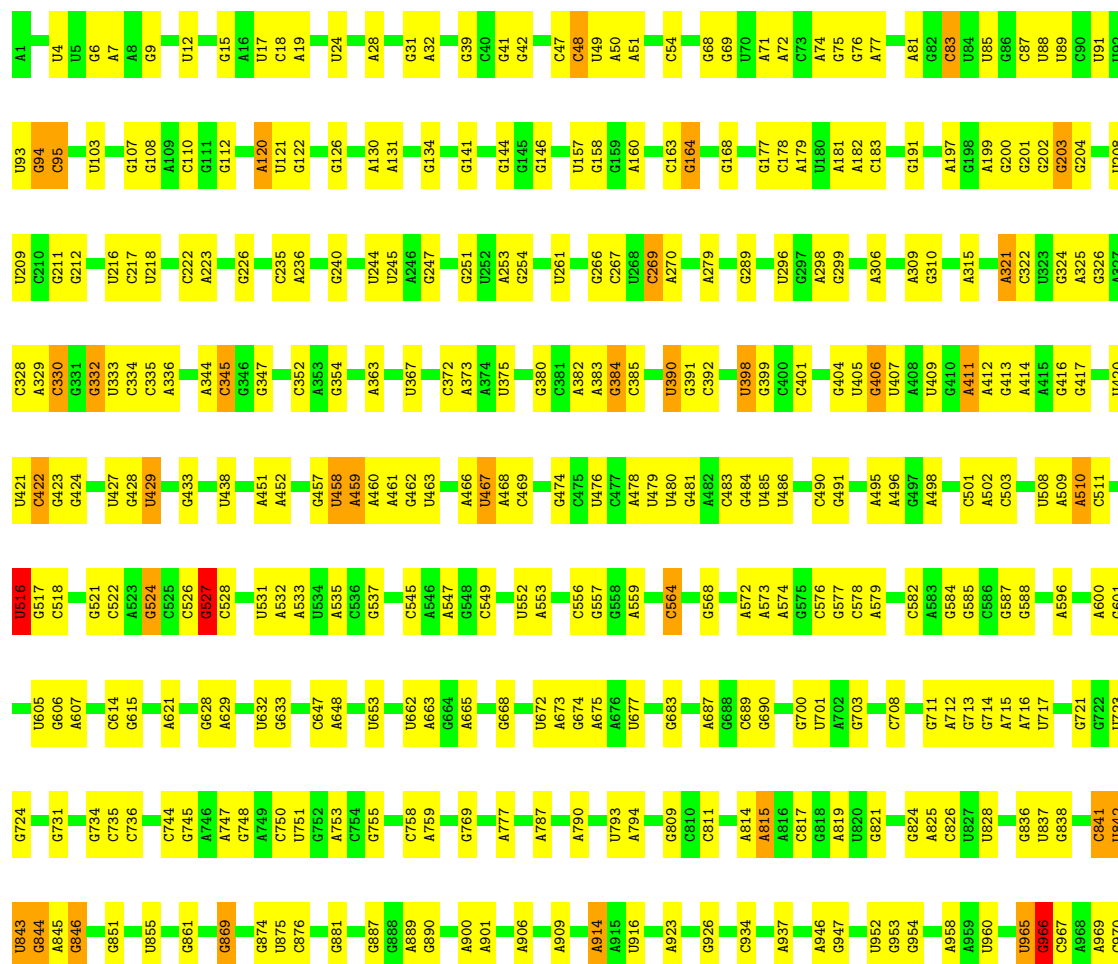


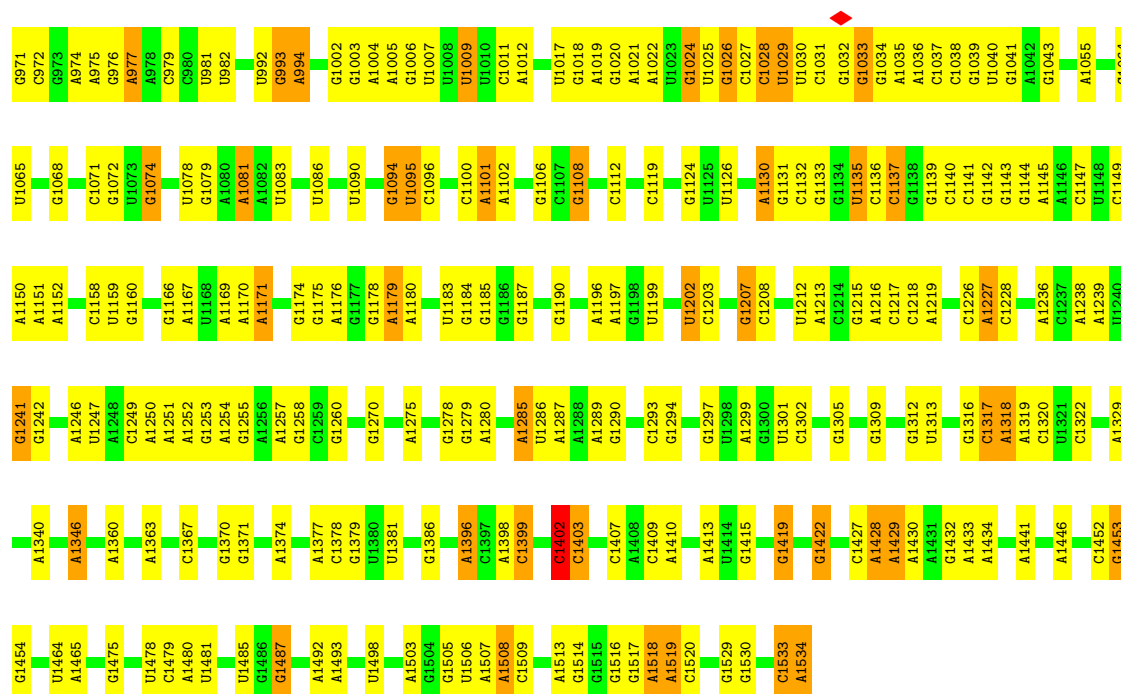




• Molecule 2: 16S ribosomal RNA

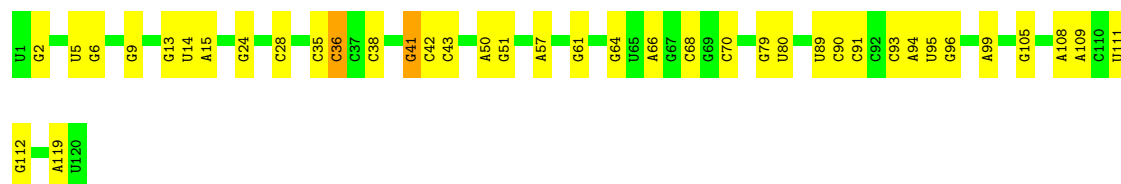
Chain 2: 62% 33% 5%





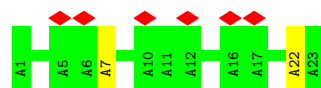
- Molecule 3: 5S ribosomal RNA

Chain 3: 68% 31%



- Molecule 4: Nascent peptide

Chain 6: 26% 91% 9%



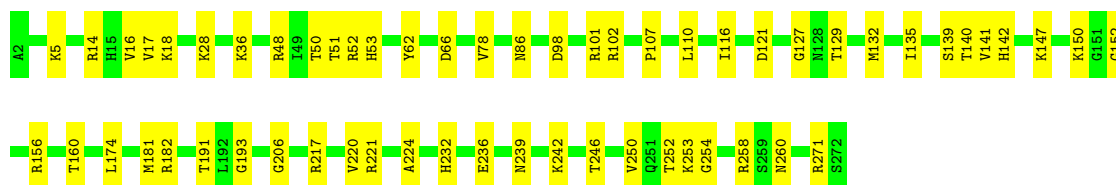
- Molecule 5: P-site tRNA

Chain 7: 50% 46%



- Molecule 6: 50S ribosomal protein L2

Chain B: 79% 21%



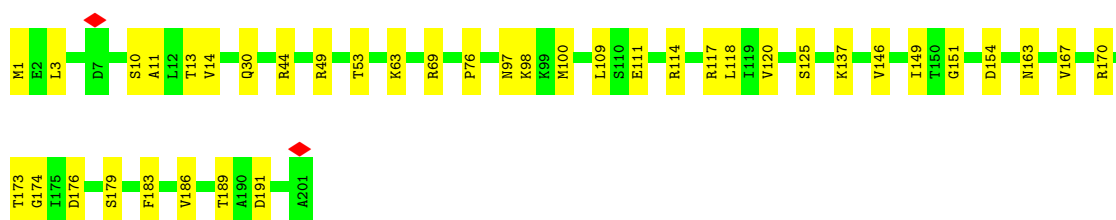
• Molecule 7: 50S ribosomal protein L3

Chain C: 88% 12%



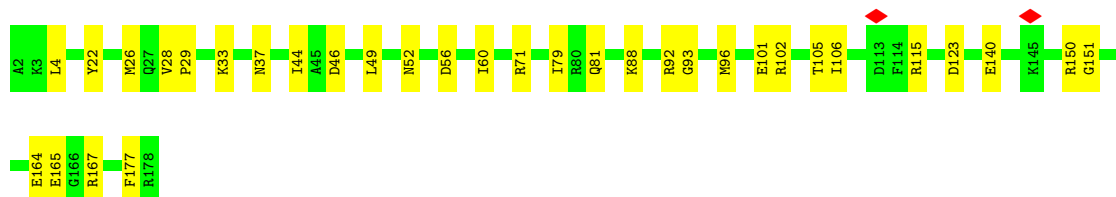
• Molecule 8: 50S ribosomal protein L4

Chain D: 81% 19%



• Molecule 9: 50S ribosomal protein L5

Chain E: 81% 19%



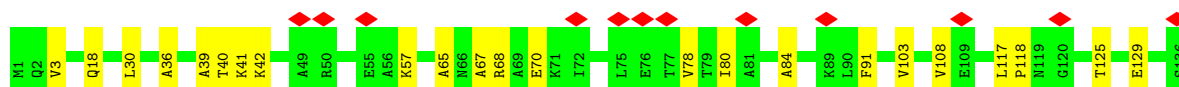
• Molecule 10: 50S ribosomal protein L6

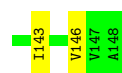
Chain F: 83% 17%



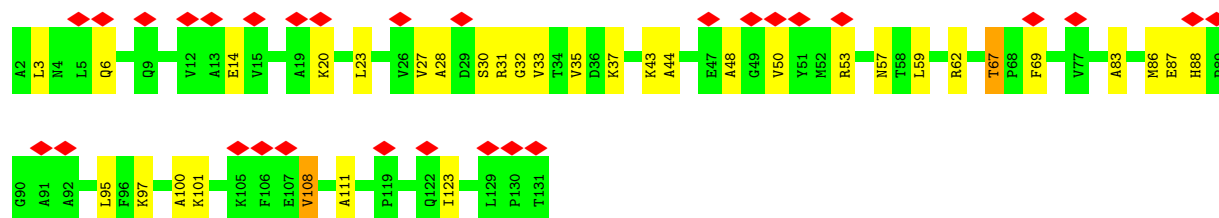
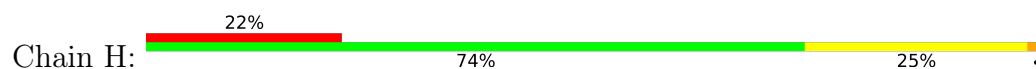
• Molecule 11: 50S ribosomal protein L9

Chain G: 8% 83% 17%

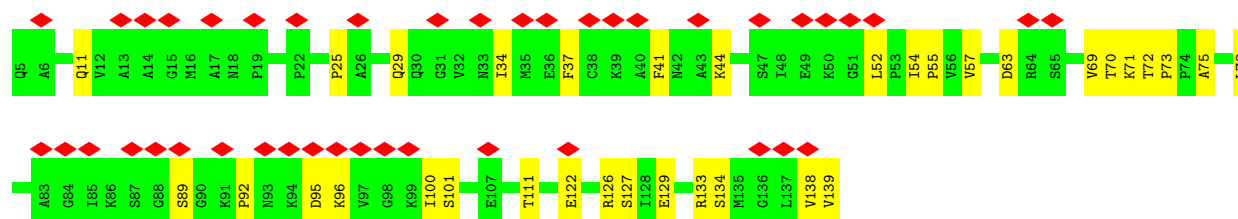
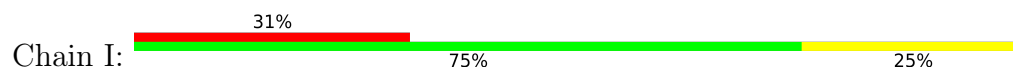




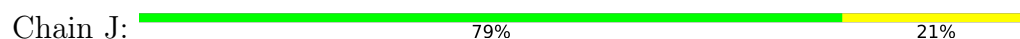
- Molecule 12: 50S ribosomal protein L10



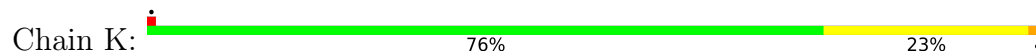
- Molecule 13: 50S ribosomal protein L11



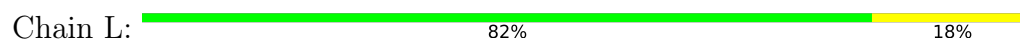
- Molecule 14: 50S ribosomal protein L13



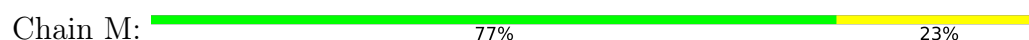
- Molecule 15: 50S ribosomal protein L14



- Molecule 16: 50S ribosomal protein L15

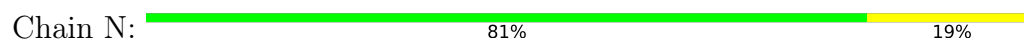


- Molecule 17: 50S ribosomal protein L16

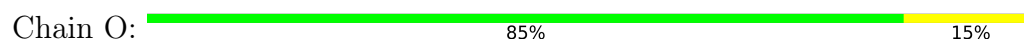




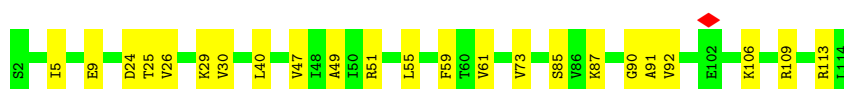
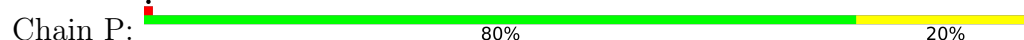
- Molecule 18: 50S ribosomal protein L17



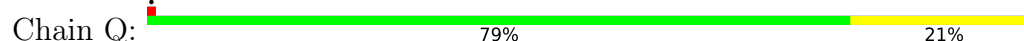
- Molecule 19: 50S ribosomal protein L18



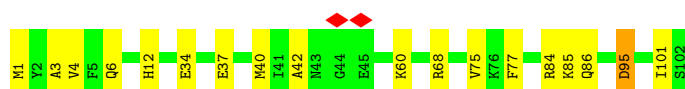
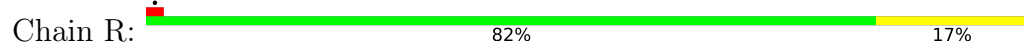
- Molecule 20: 50S ribosomal protein L19



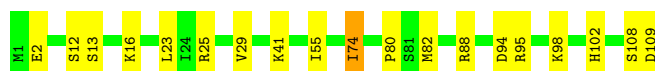
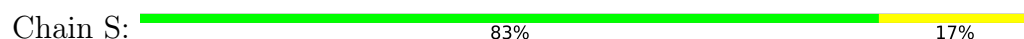
- Molecule 21: 50S ribosomal protein L20



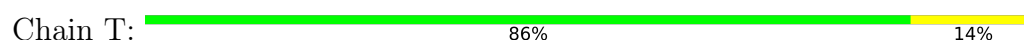
- Molecule 22: 50S ribosomal protein L21



- Molecule 23: 50S ribosomal protein L22

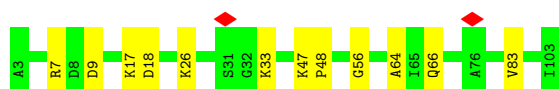
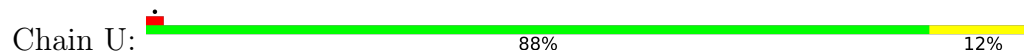


- Molecule 24: 50S ribosomal protein L23

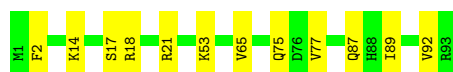
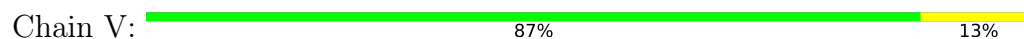




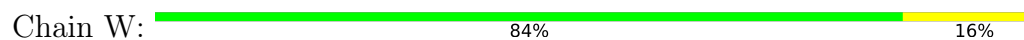
- Molecule 25: 50S ribosomal protein L24



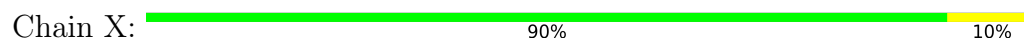
- Molecule 26: 50S ribosomal protein L25



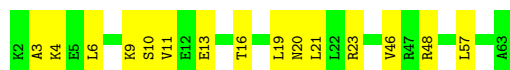
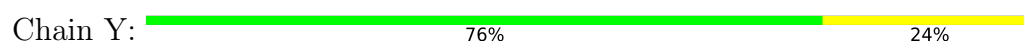
- Molecule 27: 50S ribosomal protein L27



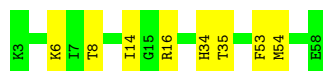
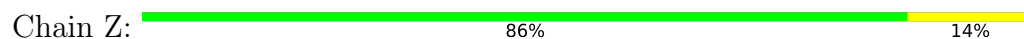
- Molecule 28: 50S ribosomal protein L28



- Molecule 29: 50S ribosomal protein L29



- Molecule 30: 50S ribosomal protein L30



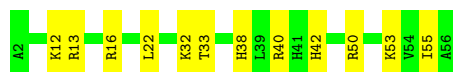
- Molecule 31: 50S ribosomal protein L31





- Molecule 32: 50S ribosomal protein L32

Chain b: 78% 22%



- Molecule 33: 50S ribosomal protein L33

Chain c: 80% 20%



- Molecule 34: 50S ribosomal protein L34

Chain d: 87% 13%



- Molecule 35: 50S ribosomal protein L35

Chain e: 81% 19%



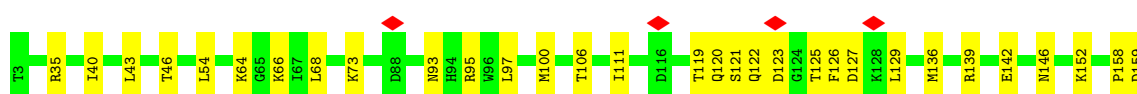
- Molecule 36: 50S ribosomal protein L36

Chain f: 100%



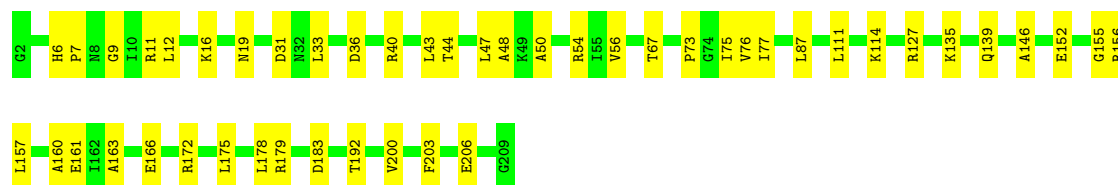
- Molecule 37: 30S ribosomal protein S2

Chain g: 82% 18%



- Molecule 38: 30S ribosomal protein S3

Chain h:  77% 23%



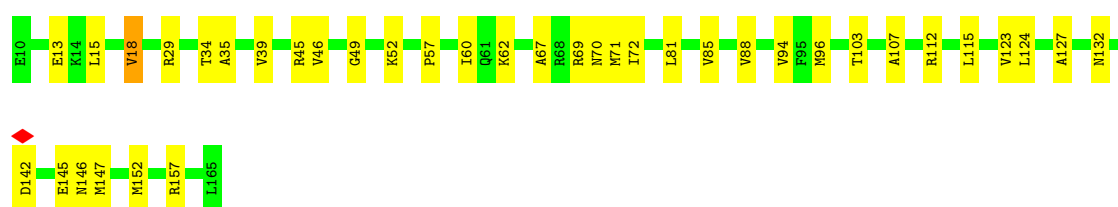
- Molecule 39: 30S ribosomal protein S4

Chain i:  80% 20%



- Molecule 40: 30S ribosomal protein S5

Chain j:  76% 24%



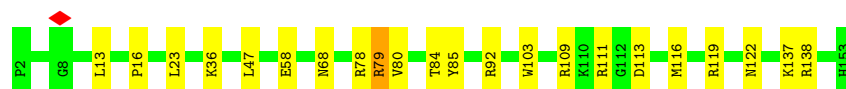
- Molecule 41: 30S ribosomal protein S6

Chain k:  85% 15%



- Molecule 42: 30S ribosomal protein S7

Chain l:  86% 14%



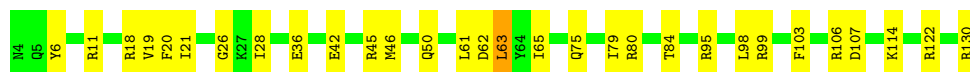
- Molecule 43: 30S ribosomal protein S8

Chain m:  82% 18%



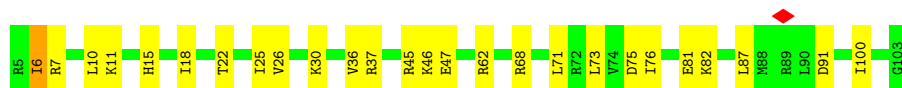
- Molecule 44: 30S ribosomal protein S9

Chain n: 76% 23%



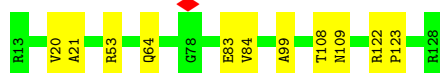
- Molecule 45: 30S ribosomal protein S10

Chain o: 74% 25%



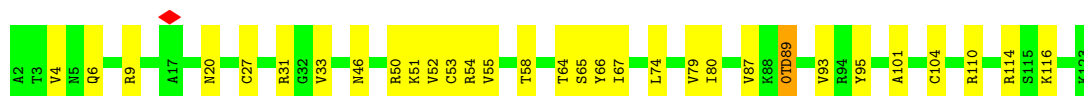
- Molecule 46: 30S ribosomal protein S11

Chain p: 91% 9%



- Molecule 47: 30S ribosomal protein S12

Chain q: 75% 25%



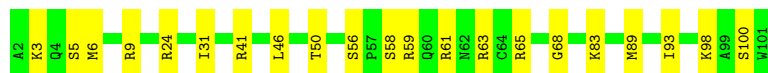
- Molecule 48: 30S ribosomal protein S13

Chain r: 81% 18%



- Molecule 49: 30S ribosomal protein S14

Chain s: 79% 21%



- Molecule 50: 30S ribosomal protein S15

Chain t:  82% 18%



- Molecule 51: 30S ribosomal protein S16

Chain u:  73% 26%



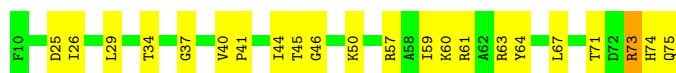
- Molecule 52: 30S ribosomal protein S17

Chain v:  89% 11%



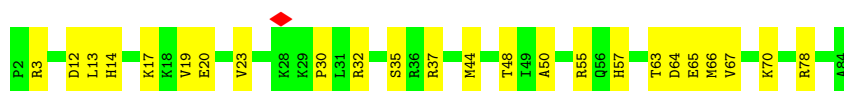
- Molecule 53: 30S ribosomal protein S18

Chain w:  67% 32%



- Molecule 54: 30S ribosomal protein S19

Chain x:  71% 29%



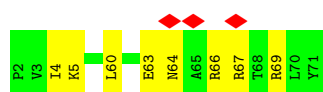
- Molecule 55: 30S ribosomal protein S20

Chain y:  89% 11%

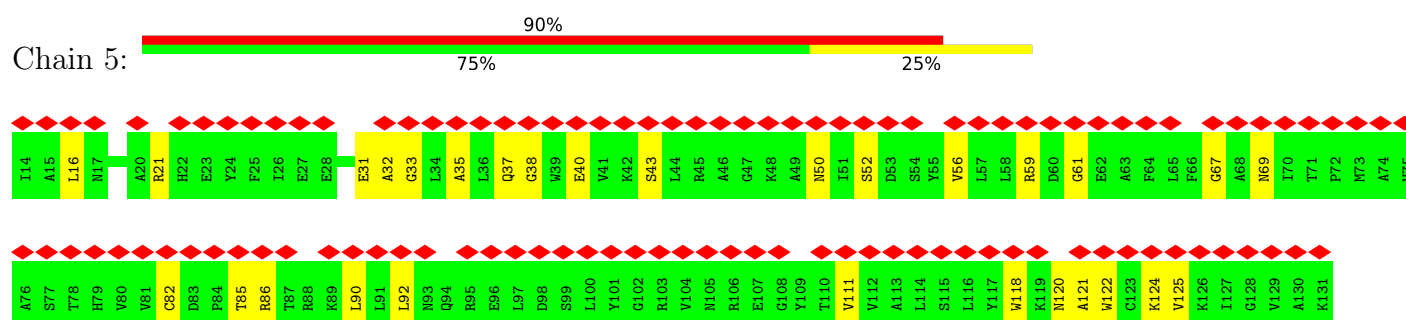


- Molecule 56: 30S ribosomal protein S21

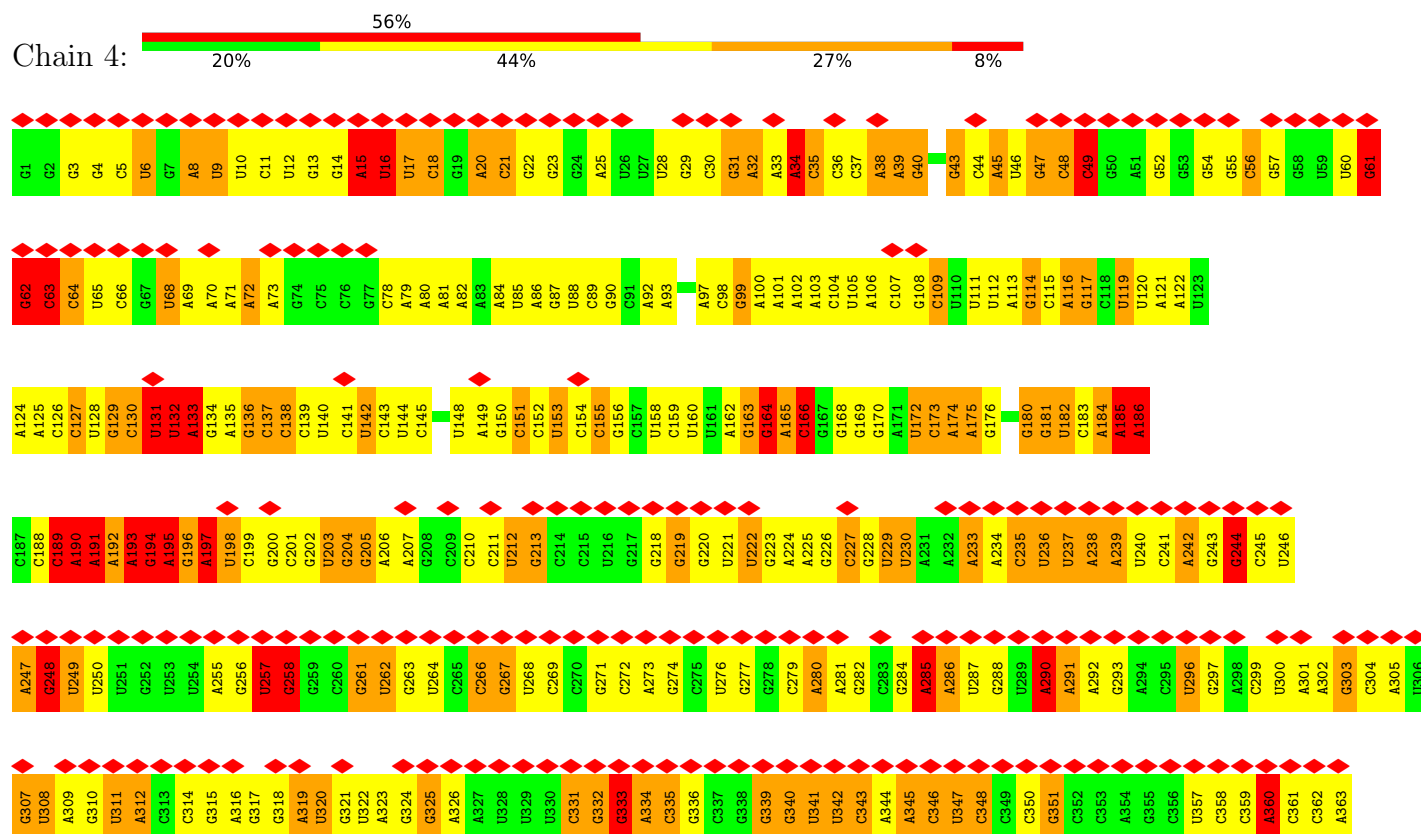
Chain z:  89% 11%



- Molecule 57: SsrA-binding protein



• Molecule 58: tmRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47115	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	0.517	Depositor
Minimum map value	-0.327	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	437.0, 437.0, 437.0	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMC, 6MZ, 2MA, MA6, UR3, 3TD, MG, G7M, 1MG, 7MG, 2MG, 5MU, OMU, 5MC, OMG, ZN, 4OC, 0TD

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	1	0.45	1/69285 (0.0%)	0.49	1/108083 (0.0%)
2	2	0.41	0/36587	0.46	0/57062
3	3	0.36	0/2872	0.43	0/4478
4	6	0.22	0/114	0.61	0/158
5	7	0.33	0/1810	0.52	0/2820
6	B	0.46	0/2122	0.59	0/2852
7	C	0.43	0/1572	0.58	0/2117
8	D	0.37	0/1571	0.56	0/2113
9	E	0.33	0/1435	0.61	0/1926
10	F	0.31	0/1333	0.57	0/1805
11	G	0.26	0/1112	0.60	0/1503
12	H	0.32	0/993	0.74	0/1340
13	I	0.28	0/998	0.64	0/1348
14	J	0.40	0/1152	0.54	0/1551
15	K	0.44	0/955	0.63	0/1279
16	L	0.40	0/1052	0.51	0/1401
17	M	0.41	0/1084	0.53	0/1450
18	N	0.40	0/964	0.61	0/1289
19	O	0.35	0/894	0.56	0/1198
20	P	0.40	0/920	0.54	0/1231
21	Q	0.47	0/960	0.58	0/1278
22	R	0.40	0/823	0.56	0/1100
23	S	0.40	0/852	0.60	0/1142
24	T	0.34	0/752	0.52	0/1005
25	U	0.31	0/782	0.59	0/1044
26	V	0.33	0/760	0.50	0/1018
27	W	0.41	0/579	0.55	0/767
28	X	0.39	0/635	0.52	0/848
29	Y	0.27	0/502	0.48	0/667
30	Z	0.38	0/438	0.60	0/586
31	a	0.24	0/531	0.56	0/709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.38	0/440	0.52	0/588
33	c	0.34	0/424	0.55	0/565
34	d	0.46	0/370	0.54	0/487
35	e	0.44	0/513	0.64	0/676
36	f	0.41	0/303	0.54	0/397
37	g	0.30	0/1791	0.58	0/2413
38	h	0.35	0/1663	0.55	0/2241
39	i	0.34	0/1665	0.53	0/2227
40	j	0.40	0/1165	0.70	0/1568
41	k	0.32	0/867	0.56	0/1171
42	l	0.30	0/1206	0.55	0/1617
43	m	0.34	0/989	0.54	0/1326
44	n	0.31	0/1034	0.58	0/1375
45	o	0.34	0/800	0.59	0/1082
46	p	0.35	0/885	0.53	0/1195
47	q	0.40	0/954	0.62	0/1279
48	r	0.31	0/909	0.59	0/1215
49	s	0.37	0/817	0.53	0/1088
50	t	0.35	0/716	0.54	0/956
51	u	0.36	0/659	0.57	0/884
52	v	0.31	0/658	0.59	0/881
53	w	0.36	0/553	0.58	0/743
54	x	0.33	0/680	0.51	0/915
55	y	0.33	0/670	0.51	0/888
56	z	0.31	0/597	0.60	0/792
57	5	0.26	0/958	0.73	0/1294
58	4	0.49	0/8681	1.20	109/13532 (0.8%)
All	All	0.42	1/167406 (0.0%)	0.57	110/250563 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	34	0
2	2	5	0
12	H	0	1
35	e	0	1
42	l	0	1
47	q	0	1
48	r	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	w	0	1
58	4	3	0
All	All	42	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2552	OMU	O3'-P	6.34	1.62	1.56

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	4	48	C	O3'-P-O5'	10.76	120.14	104.00
58	4	9	U	C4'-C3'-O3'	10.56	128.84	113.00
58	4	266	C	O3'-P-O5'	9.63	118.44	104.00
58	4	128	U	O3'-P-O5'	-8.87	90.70	104.00
58	4	137	C	O3'-P-O5'	8.17	116.25	104.00
58	4	239	A	O3'-P-O5'	8.17	116.25	104.00
58	4	137	C	P-O3'-C3'	8.06	132.29	120.20
58	4	191	A	O3'-P-O5'	7.99	115.98	104.00
58	4	8	A	P-O3'-C3'	7.76	131.84	120.20
58	4	188	C	O3'-P-O5'	7.74	115.61	104.00
58	4	197	A	P-O5'-C5'	7.57	132.25	120.90
58	4	182	U	O4'-C1'-N1	7.55	119.53	108.20
58	4	163	G	O3'-P-O5'	7.35	115.03	104.00
58	4	197	A	O5'-C5'-C4'	-7.33	100.51	111.50
58	4	155	C	O3'-P-O5'	7.30	114.94	104.00
58	4	290	A	P-O3'-C3'	7.23	131.04	120.20
58	4	190	A	O5'-C5'-C4'	7.20	122.31	111.50
58	4	9	U	P-O3'-C3'	7.15	130.92	120.20
58	4	34	A	O3'-P-O5'	7.10	114.66	104.00
58	4	164	G	P-O3'-C3'	6.94	130.61	120.20
58	4	180	G	O3'-P-O5'	6.93	114.39	104.00
58	4	133	A	C5'-C4'-O4'	-6.90	99.45	109.80
58	4	185	A	O4'-C1'-N9	6.83	118.75	108.50
58	4	166	C	P-O3'-C3'	6.81	130.41	120.20
58	4	16	U	O4'-C1'-N1	6.67	118.50	108.50
58	4	360	A	O3'-P-O5'	6.58	113.87	104.00
58	4	290	A	O3'-P-O5'	6.54	113.80	104.00
58	4	133	A	O5'-C5'-C4'	6.52	121.28	111.50
58	4	248	G	C5'-C4'-O4'	-6.52	100.02	109.80
58	4	182	U	N1-C1'-C2'	6.47	123.71	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	4	198	U	P-O5'-C5'	6.43	130.54	120.90
58	4	335	C	O5'-P-OP2	-6.42	88.75	108.00
58	4	185	A	C5'-C4'-O4'	-6.35	100.27	109.80
58	4	244	G	O3'-P-O5'	6.34	113.50	104.00
58	4	333	G	P-O3'-C3'	6.33	129.69	120.20
58	4	109	C	N1-C1'-C2'	6.30	121.46	112.00
58	4	272	C	P-O3'-C3'	6.29	129.63	120.20
58	4	266	C	P-O3'-C3'	6.22	129.53	120.20
58	4	62	G	C4'-C3'-O3'	-6.21	100.08	109.40
58	4	191	A	P-O3'-C3'	6.21	129.51	120.20
58	4	194	G	C5'-C4'-O4'	-6.17	100.55	109.80
58	4	131	U	O5'-C5'-C4'	6.15	120.93	111.70
58	4	166	C	N1-C1'-C2'	6.09	121.13	112.00
58	4	308	U	P-O3'-C3'	6.07	129.31	120.20
1	1	2552	OMU	P-O3'-C3'	6.02	126.92	119.70
58	4	8	A	O3'-P-O5'	5.99	112.99	104.00
58	4	189	C	O3'-P-O5'	5.90	112.85	104.00
58	4	48	C	P-O3'-C3'	5.87	129.01	120.20
58	4	6	U	O3'-P-O5'	5.86	112.80	104.00
58	4	258	G	P-O5'-C5'	5.82	129.63	120.90
58	4	63	C	O3'-P-O5'	5.79	112.68	104.00
58	4	132	U	O3'-P-O5'	5.76	112.65	104.00
58	4	257	U	O3'-P-O5'	5.76	112.65	104.00
58	4	239	A	P-O3'-C3'	5.74	128.81	120.20
58	4	203	U	P-O3'-C3'	5.71	128.77	120.20
58	4	331	C	O3'-P-O5'	5.68	112.53	104.00
58	4	62	G	C5'-C4'-C3'	5.68	123.72	115.20
58	4	257	U	OP1-P-O3'	5.66	124.99	108.00
58	4	184	A	P-O3'-C3'	5.66	128.69	120.20
58	4	229	U	P-O3'-C3'	5.66	128.69	120.20
58	4	311	U	C5'-C4'-C3'	5.65	124.48	116.00
58	4	16	U	N1-C1'-C2'	5.64	120.45	112.00
58	4	303	G	P-O5'-C5'	5.63	129.35	120.90
58	4	247	A	P-O5'-C5'	5.60	129.30	120.90
58	4	301	A	O3'-P-O5'	5.58	112.37	104.00
58	4	346	C	P-O3'-C3'	5.58	128.56	120.20
58	4	238	A	P-O3'-C3'	5.57	128.56	120.20
58	4	303	G	O5'-C5'-C4'	5.57	119.86	111.50
58	4	197	A	C5'-C4'-C3'	5.57	124.35	116.00
58	4	189	C	P-O3'-C3'	5.51	128.47	120.20
58	4	285	A	O3'-P-O5'	5.51	112.27	104.00
58	4	195	A	P-O3'-C3'	5.49	128.43	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	4	195	A	C5'-C4'-O4'	-5.48	101.57	109.80
58	4	285	A	P-O3'-C3'	5.48	128.43	120.20
58	4	197	A	C5'-C4'-O4'	-5.48	101.58	109.80
58	4	61	G	P-O3'-C3'	5.46	128.40	120.20
58	4	181	G	C5'-C4'-C3'	-5.46	107.81	116.00
58	4	5	C	O3'-P-O5'	5.45	112.17	104.00
58	4	129	G	O3'-P-O5'	5.45	112.17	104.00
58	4	130	C	C2'-C3'-O3'	5.43	117.65	109.50
58	4	15	A	C2'-C3'-O3'	5.43	117.64	109.50
58	4	267	G	P-O5'-C5'	5.43	129.04	120.90
58	4	185	A	O4'-C1'-C2'	-5.41	102.19	107.60
58	4	181	G	O5'-C5'-C4'	5.34	119.51	111.50
58	4	186	A	P-O5'-C5'	5.30	128.85	120.90
58	4	312	A	C5'-C4'-C3'	5.29	123.94	116.00
58	4	136	G	P-O3'-C3'	5.28	128.12	120.20
58	4	116	A	O3'-P-O5'	5.25	111.88	104.00
58	4	129	G	C5'-C4'-C3'	5.22	123.84	116.00
58	4	233	A	P-O3'-C3'	5.21	128.02	120.20
58	4	193	A	O3'-P-O5'	5.20	111.80	104.00
58	4	311	U	O5'-C5'-C4'	5.19	119.28	111.50
58	4	9	U	O3'-P-O5'	5.19	111.78	104.00
58	4	131	U	P-O3'-C3'	5.18	127.97	120.20
58	4	312	A	O5'-C5'-C4'	5.18	119.27	111.50
58	4	68	U	P-O3'-C3'	5.18	127.97	120.20
58	4	257	U	C2'-C3'-O3'	5.18	117.27	109.50
58	4	142	U	O3'-P-O5'	5.18	111.77	104.00
58	4	237	U	C2-N1-C1'	5.17	133.21	117.70
58	4	129	G	P-O3'-C3'	5.16	127.93	120.20
58	4	119	U	P-O3'-C3'	5.10	127.85	120.20
58	4	333	G	O5'-C5'-C4'	5.09	119.14	111.50
58	4	62	G	O5'-C5'-C4'	5.08	119.32	111.70
58	4	314	C	P-O5'-C5'	5.07	128.51	120.90
58	4	49	C	P-O5'-C5'	5.07	128.50	120.90
58	4	148	U	C4'-C3'-O3'	-5.05	105.43	113.00
58	4	6	U	P-O5'-C5'	5.04	128.47	120.90
58	4	18	C	N1-C1'-C2'	5.03	119.55	112.00
58	4	238	A	O3'-P-O5'	5.03	111.54	104.00
58	4	184	A	C4'-C3'-O3'	5.01	116.91	109.40

All (42) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
1	1	745	1MG	C4',C3'
1	1	746	PSU	C4',C3'
1	1	747	5MU	C2',C4'
1	1	955	PSU	C4',C3'
1	1	1618	6MZ	C2',C3'
1	1	1911	PSU	C4',C3'
1	1	1915	3TD	C3'
1	1	1917	PSU	C4',C3'
1	1	1939	5MU	C2',C4'
1	1	2030	6MZ	C2',C3'
1	1	2069	G7M	C2'
1	1	2251	OMG	C2'
1	1	2457	PSU	C4',C3'
1	1	2498	OMC	C4'
1	1	2503	2MA	C2',C3'
1	1	2504	PSU	C4',C3'
1	1	2552	OMU	C2',C3'
1	1	2580	PSU	C4',C3'
1	1	2605	PSU	C4',C3'
2	2	516	PSU	C4',C3'
2	2	527	7MG	C3'
2	2	1402	4OC	C1',C3'
58	4	9	U	C3'
58	4	181	G	C2'
58	4	182	U	C1'

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	H	67	THR	Peptide
35	e	31	HIS	Peptide
42	l	79	ARG	Peptide
47	q	101	ALA	Peptide
48	r	65	VAL	Peptide
53	w	73	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31371	432	0
2	2	32929	0	16590	254	0
3	3	2569	0	1301	14	0
4	6	115	0	117	2	0
5	7	1621	0	822	13	0
6	B	2083	0	2154	44	0
7	C	1551	0	1599	17	0
8	D	1552	0	1619	29	0
9	E	1411	0	1444	23	0
10	F	1313	0	1358	17	0
11	G	1101	0	1142	16	0
12	H	980	0	1013	22	0
13	I	984	0	1035	24	0
14	J	1129	0	1162	21	0
15	K	946	0	1023	21	0
16	L	1043	0	1123	18	0
17	M	1065	0	1148	23	0
18	N	951	0	994	17	0
19	O	884	0	919	13	0
20	P	908	0	956	15	0
21	Q	947	0	1019	21	0
22	R	810	0	834	14	0
23	S	845	0	909	14	0
24	T	746	0	811	8	0
25	U	774	0	825	7	0
26	V	747	0	775	7	0
27	W	572	0	593	11	0
28	X	625	0	652	6	0
29	Y	501	0	531	8	0
30	Z	434	0	477	7	0
31	a	522	0	521	12	0
32	b	434	0	445	10	0
33	c	417	0	451	7	0
34	d	367	0	404	6	0
35	e	504	0	572	10	0
36	f	302	0	340	0	0
37	g	1760	0	1787	26	0
38	h	1636	0	1710	28	0
39	i	1643	0	1707	29	0
40	j	1152	0	1196	30	0
41	k	848	0	846	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	l	1191	0	1245	13	0
43	m	979	0	1031	15	0
44	n	1022	0	1070	24	0
45	o	790	0	831	19	0
46	p	869	0	878	8	0
47	q	951	0	1012	21	0
48	r	900	0	965	17	0
49	s	805	0	844	18	0
50	t	708	0	729	10	0
51	u	649	0	666	14	0
52	v	649	0	691	7	0
53	w	544	0	560	15	0
54	x	663	0	688	20	0
55	y	664	0	714	8	0
56	z	589	0	629	7	0
57	5	940	0	953	17	0
58	4	7758	0	3919	121	0
59	1	292	0	0	0	0
59	2	127	0	0	0	0
59	3	8	0	0	0	0
59	7	4	0	0	0	0
59	O	1	0	0	0	0
59	Q	1	0	0	0	0
59	b	1	0	0	0	0
59	f	1	0	0	0	0
59	i	1	0	0	0	0
59	s	1	0	0	0	0
60	a	1	0	0	0	0
60	f	1	0	0	0	0
61	B	2	0	0	0	0
All	All	155169	0	103720	1422	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 6.

All (1422) 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)
12:H:27:VAL:O	12:H:83:ALA:HB3	1.66	0.95
1:1:1529:G:H1	1:1:1542:U:H3	1.04	0.93
1:1:78:U:H3	1:1:108:G:H1	1.10	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:641:U:H3	1:1:647:G:H1	1.18	0.88
58:4:343:C:H2'	58:4:343:C:O2	1.72	0.86
13:I:37:PHE:O	13:I:41:PHE:HB2	1.77	0.84
1:1:713:G:H21	1:1:718:A:H62	1.26	0.83
1:1:158:U:H3	1:1:168:G:H1	1.23	0.82
1:1:1483:G:H1	1:1:1506:U:H3	1.25	0.81
58:4:61:G:H4'	58:4:62:G:H5'	1.62	0.80
22:R:1:MET:HA	22:R:42:ALA:O	1.84	0.78
1:1:2747:G:H21	1:1:2757:A:H62	1.30	0.77
1:1:2687:U:H3	1:1:2722:G:H1	1.31	0.76
1:1:1415:U:H3	1:1:1587:G:H1	1.32	0.75
58:4:341:U:OP2	58:4:341:U:H3'	1.86	0.75
57:5:38:GLY:H	58:4:333:G:H1'	1.51	0.74
58:4:344:A:H2'	58:4:345:A:H4'	1.70	0.74
58:4:20:A:H62	58:4:332:G:H21	1.38	0.72
10:F:90:VAL:O	10:F:160:LYS:HA	1.89	0.72
53:w:41:PRO:HD2	53:w:44:ILE:HD12	1.73	0.70
38:h:155:GLY:HA2	38:h:163:ALA:HB1	1.73	0.70
1:1:2632:A:HO2'	1:1:2811:G:HO2'	1.36	0.70
8:D:1:MET:HB3	8:D:14:VAL:O	1.92	0.69
40:j:46:VAL:H	40:j:72:ILE:HG22	1.58	0.69
58:4:344:A:C2'	58:4:345:A:H4'	2.23	0.69
1:1:2848:G:N2	1:1:2868:A:H62	1.90	0.69
1:1:1252:G:H1	21:Q:37:GLN:HE21	1.40	0.69
1:1:2498:OMC:HM22	1:1:2499:C:H5'	1.75	0.68
58:4:341:U:H3'	58:4:341:U:P	2.33	0.68
2:2:409:U:H3	2:2:433:G:H1	1.41	0.67
1:1:1534:U:N3	1:1:1538:G:N1	2.43	0.67
2:2:1081:A:N7	40:j:52:LYS:NZ	2.41	0.67
1:1:1270:C:H5''	1:1:1271:G:H5'	1.76	0.67
21:Q:58:ARG:HE	21:Q:92:ARG:HD2	1.58	0.67
58:4:325:G:N2	58:4:326:A:N7	2.42	0.67
58:4:343:C:O2	58:4:343:C:C2'	2.43	0.67
1:1:475:C:O2	1:1:479:A:N6	2.28	0.67
1:1:1819:A:H5''	6:B:160:THR:HG21	1.78	0.66
2:2:76:G:H1	2:2:93:U:H3	1.44	0.66
1:1:2475:C:H42	1:1:2529:G:H22	1.42	0.65
17:M:50:ARG:HG3	17:M:65:ILE:HD11	1.78	0.65
58:4:40:G:N3	58:4:40:G:H2'	2.11	0.65
1:1:2475:C:H42	1:1:2529:G:N2	1.95	0.65
7:C:46:ARG:HH12	7:C:86:GLU:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:50:ALA:HB2	38:h:75:ILE:HB	1.78	0.64
1:1:2848:G:H21	1:1:2868:A:H62	1.43	0.64
7:C:148:GLN:HB2	7:C:152:PRO:HD2	1.80	0.64
39:i:44:ARG:NH2	58:4:102:A:N7	2.45	0.64
1:1:1036:G:H1	1:1:1119:U:H3	1.44	0.64
1:1:1070:A:N6	1:1:1096:A:N3	2.46	0.64
6:B:107:PRO:HD2	6:B:110:LEU:HD22	1.79	0.64
15:K:40:LYS:HE2	15:K:59:LYS:HZ2	1.63	0.64
13:I:57:VAL:HB	13:I:69:VAL:HB	1.80	0.63
12:H:59:LEU:HB2	12:H:62:ARG:HB2	1.78	0.63
58:4:152:C:O2	58:4:191:A:N6	2.31	0.63
51:u:5:ARG:NH2	51:u:27:ALA:O	2.31	0.63
1:1:2618:G:H21	7:C:155:VAL:HG21	1.64	0.63
39:i:12:SER:HA	39:i:19:LEU:HD13	1.80	0.63
58:4:43:G:H21	58:4:307:G:H21	1.47	0.63
13:I:25:PRO:O	13:I:29:GLN:HB2	1.99	0.62
58:4:331:C:H2'	58:4:332:G:H5'	1.80	0.62
1:1:244:A:OP2	35:e:8:ARG:NH2	2.31	0.62
10:F:137:ASP:HB3	10:F:140:VAL:HG22	1.80	0.62
2:2:363:A:N6	47:q:27:CYS:SG	2.73	0.62
58:4:48:C:H2'	58:4:49:C:H5''	1.81	0.62
12:H:44:ALA:O	12:H:48:ALA:HB3	1.99	0.62
38:h:156:ARG:NH1	38:h:160:ALA:O	2.32	0.62
1:1:677:A:HO2'	1:1:2070:A:HO2'	1.47	0.61
1:1:1695:G:N7	6:B:14:ARG:NH2	2.49	0.61
1:1:1069:A:O2'	1:1:1073:A:N6	2.33	0.61
41:k:85:ILE:HG22	41:k:86:ARG:HG2	1.83	0.61
10:F:24:ILE:HD11	10:F:43:VAL:HG11	1.83	0.61
39:i:8:LYS:HB3	39:i:21:LEU:HD13	1.81	0.61
48:r:101:ARG:HH21	48:r:103:LYS:HB3	1.65	0.61
1:1:569:U:O2'	1:1:983:A:N1	2.33	0.61
47:q:46:ASN:ND2	47:q:89:0TD:SB	2.74	0.61
1:1:1363:C:O2'	1:1:1809:A:N3	2.34	0.61
17:M:42:THR:HG22	17:M:93:VAL:HG12	1.82	0.61
1:1:1365:A:OP1	28:X:3:ARG:NH2	2.32	0.60
1:1:1800:C:OP2	6:B:182:ARG:NH1	2.33	0.60
1:1:1824:G:OP1	6:B:52:ARG:NH2	2.34	0.60
58:4:114:G:H1	58:4:132:U:H3	1.49	0.60
23:S:88:ARG:NH2	23:S:94:ASP:OD2	2.34	0.60
1:1:2107:G:H1'	1:1:2183:A:H61	1.65	0.60
1:1:2312:U:O2	9:E:37:ASN:ND2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:43:C:O2	9:E:92:ARG:NH2	2.35	0.60
48:r:106:ALA:HB3	48:r:110:LYS:HE2	1.83	0.60
1:1:1386:C:H2'	1:1:1387:A:H8	1.66	0.60
6:B:246:THR:HG22	6:B:250:VAL:H	1.67	0.60
53:w:73:ARG:O	53:w:75:GLN:NE2	2.35	0.60
1:1:243:U:OP2	35:e:8:ARG:NH1	2.35	0.60
1:1:848:C:H2'	1:1:849:A:H8	1.65	0.60
58:4:276:U:H2'	58:4:277:G:H8	1.65	0.60
1:1:2332:C:OP1	27:W:77:ARG:NH1	2.35	0.60
14:J:36:LEU:HD11	14:J:122:LEU:HB2	1.82	0.60
2:2:7:A:H2'	40:j:124:LEU:HD12	1.84	0.60
8:D:149:ILE:HG22	8:D:170:ARG:HB2	1.83	0.60
2:2:1319:A:OP1	54:x:70:LYS:NZ	2.35	0.60
1:1:2637:U:H3	1:1:2776:A:H62	1.48	0.60
1:1:372:G:H5'	28:X:58:VAL:HG23	1.85	0.59
1:1:807:U:OP2	16:L:41:ARG:NH1	2.35	0.59
1:1:1358:G:O2'	1:1:1373:A:N6	2.36	0.59
1:1:1798:U:OP2	6:B:271:ARG:NH2	2.35	0.59
38:h:33:LEU:HD11	49:s:93:ILE:HG12	1.85	0.59
57:5:33:GLY:HA2	57:5:125:VAL:HB	1.84	0.59
1:1:1187:G:OP1	22:R:85:LYS:NZ	2.35	0.59
2:2:1009:U:O2'	2:2:1020:G:N2	2.35	0.59
44:n:50:GLN:OE1	44:n:80:ARG:NH1	2.36	0.59
2:2:1071:C:H2'	2:2:1072:G:H8	1.67	0.59
6:B:132:MET:HG2	6:B:135:ILE:HD12	1.85	0.59
16:L:121:THR:HG23	16:L:141:LYS:HB2	1.85	0.59
1:1:2484:G:OP1	17:M:44:ARG:NH1	2.34	0.58
52:v:25:ILE:HD11	52:v:61:ILE:HD11	1.85	0.58
1:1:2475:C:N4	1:1:2529:G:H22	2.00	0.58
37:g:191:SER:OG	37:g:192:ASP:N	2.36	0.58
38:h:9:GLY:HA2	38:h:12:LEU:HG	1.85	0.58
57:5:82:CYS:SG	57:5:86:ARG:NH2	2.76	0.58
58:4:15:A:H1'	58:4:16:U:H3'	1.85	0.58
2:2:120:A:O2'	2:2:122:G:N7	2.34	0.58
6:B:16:VAL:HG22	6:B:206:GLY:HA3	1.86	0.58
20:P:29:LYS:HB3	20:P:40:LEU:HD22	1.85	0.58
1:1:162:U:O2'	1:1:165:A:N6	2.36	0.58
1:1:619:G:OP2	1:1:620:G:N2	2.36	0.58
10:F:60:ASP:OD1	10:F:60:ASP:N	2.31	0.58
44:n:6:TYR:O	44:n:20:PHE:HA	2.02	0.58
45:o:6:ILE:HG13	45:o:76:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:47:HIS:HB2	52:v:71:LYS:HD3	1.85	0.58
2:2:1029:U:H1'	2:2:1033:G:H22	1.68	0.58
58:4:339:G:H3'	58:4:340:G:C8	2.38	0.58
1:1:2362:C:OP1	35:e:40:ARG:NH1	2.36	0.58
1:1:2384:U:OP2	27:W:55:ARG:NH1	2.37	0.58
38:h:56:VAL:HB	38:h:67:THR:HB	1.85	0.58
1:1:2061:G:OP1	8:D:63:LYS:NZ	2.36	0.58
11:G:3:VAL:O	11:G:18:GLN:HA	2.04	0.58
41:k:86:ARG:NH1	53:w:64:TYR:O	2.36	0.58
2:2:993:G:O2'	2:2:994:A:N7	2.37	0.58
37:g:162:PHE:HA	37:g:184:PHE:O	2.03	0.58
53:w:29:LEU:HD12	53:w:59:ILE:HG13	1.85	0.58
1:1:1653:G:H3'	18:N:2:ARG:HB2	1.86	0.58
5:7:12:U:H3	5:7:22:G:H22	1.52	0.58
8:D:111:GLU:OE1	8:D:114:ARG:NH1	2.36	0.58
14:J:37:ARG:NH2	14:J:44:TYR:OH	2.37	0.58
1:1:782:A:O2'	6:B:224:ALA:O	2.22	0.57
1:1:2530:A:N7	10:F:172:LYS:NZ	2.51	0.57
2:2:1026:G:O6	2:2:1035:A:C6	2.57	0.57
42:l:13:LEU:HD22	44:n:50:GLN:HE22	1.69	0.57
2:2:126:G:OP1	2:2:605:U:O2'	2.21	0.57
4:6:7:ALA:O	23:S:95:ARG:NH2	2.37	0.57
17:M:17:ASN:O	17:M:38:ARG:NH1	2.37	0.57
30:Z:16:ARG:HE	30:Z:53:PHE:HE2	1.52	0.57
39:i:118:VAL:HG22	39:i:123:ILE:HG13	1.86	0.57
2:2:1317:C:OP1	49:s:24:ARG:NH2	2.38	0.57
1:1:2627:G:N2	1:1:2777:G:OP2	2.37	0.57
2:2:1126:U:OP1	45:o:7:ARG:NH2	2.37	0.57
17:M:66:ARG:NH1	17:M:104:GLU:OE2	2.35	0.57
19:O:24:THR:HG23	19:O:41:ALA:HA	1.86	0.57
1:1:682:G:O5'	34:d:26:ASN:ND2	2.36	0.57
1:1:2061:G:N2	4:6:22:ALA:O	2.37	0.57
8:D:170:ARG:NH2	8:D:176:ASP:OD1	2.37	0.57
37:g:142:GLU:OE1	37:g:146:ASN:ND2	2.38	0.57
43:m:11:LEU:HD22	43:m:75:ILE:HD11	1.87	0.57
44:n:106:ARG:NH1	44:n:107:ASP:O	2.37	0.57
19:O:15:ARG:NH2	19:O:95:SER:OG	2.37	0.57
31:a:11:GLU:HA	31:a:25:ARG:HA	1.84	0.57
32:b:38:HIS:ND1	32:b:42:HIS:O	2.37	0.57
1:1:2298:A:OP1	9:E:71:ARG:NH2	2.38	0.57
1:1:2522:U:O2'	1:1:2647:U:OP1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:53:VAL:HG11	24:T:93:LEU:HD22	1.87	0.57
47:q:55:VAL:HG11	47:q:80:ILE:HD11	1.87	0.57
54:x:32:ARG:HA	54:x:50:ALA:HB3	1.86	0.57
57:5:50:ASN:ND2	57:5:69:ASN:O	2.38	0.57
58:4:342:U:O5'	58:4:342:U:H6	1.88	0.57
2:2:201:G:H1	2:2:216:U:H3	1.53	0.57
2:2:1464:U:H2'	2:2:1465:A:H8	1.68	0.57
2:2:841:C:H2'	2:2:843:U:H5'	1.86	0.57
8:D:3:LEU:O	8:D:11:ALA:HA	2.05	0.57
1:1:592:A:O2'	35:e:64:TYR:OH	2.22	0.56
5:7:25:C:H2'	5:7:26:G:H8	1.70	0.56
14:J:32:LEU:HD22	14:J:54:ILE:HG21	1.87	0.56
9:E:164:GLU:OE2	9:E:167:ARG:NH1	2.38	0.56
53:w:25:ASP:OD1	53:w:25:ASP:N	2.34	0.56
1:1:746:PSU:O2'	1:1:748:G:N2	2.38	0.56
1:1:1131:G:N2	1:1:1132:U:O4	2.37	0.56
1:1:2263:C:N4	27:W:15:ASP:OD1	2.38	0.56
1:1:2387:U:OP1	27:W:55:ARG:NH2	2.37	0.56
2:2:401:C:O2'	2:2:621:A:N3	2.37	0.56
7:C:13:ARG:NE	7:C:21:SER:OG	2.37	0.56
23:S:108:SER:OG	23:S:109:ASP:N	2.37	0.56
58:4:46:U:H2'	58:4:47:G:C8	2.41	0.56
2:2:605:U:O2	2:2:633:G:O6	2.24	0.56
2:2:1096:C:O2	2:2:1170:A:O2'	2.23	0.56
8:D:176:ASP:OD1	8:D:176:ASP:N	2.38	0.56
37:g:43:LEU:HA	37:g:46:THR:HG22	1.88	0.56
58:4:339:G:H3'	58:4:340:G:H8	1.69	0.56
1:1:2064:C:O2'	1:1:2251:OMG:N2	2.34	0.56
2:2:826:C:O2	43:m:16:ASN:ND2	2.39	0.56
2:2:1340:A:HO2'	5:7:31:C:HO2'	1.46	0.56
1:1:284:U:H3	1:1:356:G:H1	1.53	0.56
1:1:906:U:O2'	17:M:66:ARG:NH2	2.39	0.56
1:1:2562:U:H4'	15:K:25:LEU:HD22	1.86	0.56
2:2:28:A:O2'	2:2:296:U:OP1	2.24	0.56
2:2:545:C:OP1	39:i:58:LYS:NZ	2.38	0.56
6:B:62:TYR:HA	6:B:86:ASN:HD21	1.70	0.56
18:N:20:MET:HE1	18:N:40:LYS:HD3	1.86	0.56
1:1:1250:G:OP2	16:L:21:ARG:NH2	2.39	0.56
2:2:405:U:OP2	39:i:3:ARG:NH1	2.39	0.56
7:C:46:ARG:NH2	7:C:88:GLU:O	2.39	0.56
38:h:19:ASN:OD1	38:h:54:ARG:NH2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:469:G:O6	34:d:39:ARG:NH1	2.36	0.56
40:j:15:LEU:HD21	40:j:18:VAL:HG13	1.88	0.56
2:2:689:C:OP2	46:p:53:ARG:NH2	2.35	0.56
11:G:125:THR:HA	11:G:146:VAL:HG13	1.87	0.56
51:u:5:ARG:O	51:u:19:VAL:HA	2.06	0.56
1:1:1843:C:O2'	6:B:254:GLY:O	2.24	0.55
2:2:663:A:H5''	53:w:50:LYS:HD2	1.88	0.55
37:g:127:ASP:HA	37:g:129:LEU:HD22	1.87	0.55
51:u:36:VAL:HG11	51:u:57:ILE:HG13	1.88	0.55
58:4:112:U:H2'	58:4:113:A:C8	2.41	0.55
1:1:411:G:OP2	1:1:2406:A:O2'	2.24	0.55
1:1:781:A:OP1	6:B:217:ARG:NH2	2.39	0.55
1:1:2099:U:O2	1:1:2190:G:O6	2.23	0.55
1:1:2505:G:H2'	1:1:2576:G:H1	1.72	0.55
2:2:508:U:O2	2:2:510:A:N6	2.39	0.55
2:2:958:A:OP1	54:x:55:ARG:NH1	2.37	0.55
2:2:1028:C:O2	2:2:1033:G:N1	2.36	0.55
57:5:52:SER:OG	57:5:69:ASN:ND2	2.38	0.55
58:4:189:C:H2'	58:4:190:A:H5''	1.88	0.55
1:1:279:A:H61	1:1:361:G:H1'	1.72	0.55
1:1:1812:U:H2'	1:1:1813:G:H8	1.72	0.55
1:1:2204:G:OP2	6:B:147:LYS:NZ	2.39	0.55
1:1:2683:C:OP1	20:P:51:ARG:NH2	2.38	0.55
2:2:19:A:OP2	40:j:132:ASN:ND2	2.40	0.55
2:2:677:U:H3	2:2:713:G:H22	1.55	0.55
2:2:1004:A:OP1	2:2:1024:G:N1	2.35	0.55
43:m:77:ARG:NH2	43:m:79:SER:O	2.40	0.55
1:1:476:G:N1	1:1:479:A:OP2	2.39	0.55
1:1:2394:C:H5''	16:L:63:LYS:HE2	1.88	0.55
2:2:1377:A:OP1	42:l:92:ARG:NH1	2.37	0.55
24:T:7:LEU:HD22	24:T:46:ALA:HB2	1.88	0.55
1:1:574:A:N6	1:1:2034:U:OP1	2.39	0.55
1:1:2000:C:OP1	18:N:5:LYS:NZ	2.36	0.55
1:1:2339:C:O2'	3:3:41:G:N2	2.40	0.55
18:N:28:LEU:HD23	18:N:48:VAL:HG21	1.87	0.55
45:o:37:ARG:HB2	45:o:75:ASP:HB3	1.88	0.55
1:1:1326:U:O2'	1:1:2010:G:O2'	2.21	0.55
2:2:522:C:H41	47:q:50:ARG:HH12	1.55	0.55
11:G:84:ALA:HA	11:G:91:PHE:H	1.71	0.55
20:P:106:LYS:O	20:P:109:ARG:NH2	2.32	0.55
2:2:673:A:H2'	2:2:674:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:674:G:H2'	2:2:675:A:H8	1.71	0.55
2:2:1074:G:OP1	40:j:69:ARG:NH1	2.38	0.55
17:M:75:GLU:HB2	17:M:90:GLU:HG3	1.87	0.55
1:1:992:C:H2'	1:1:993:G:H8	1.72	0.55
1:1:1364:G:N2	1:1:1367:A:OP2	2.40	0.55
2:2:1147:C:H1'	44:n:18:ARG:HH21	1.72	0.55
1:1:125:A:OP2	34:d:19:ARG:NH2	2.39	0.55
1:1:918:A:N3	3:3:80:U:O2'	2.39	0.55
1:1:1326:U:H2'	1:1:1327:A:H8	1.72	0.55
1:1:2848:G:O2'	1:1:2867:G:N2	2.40	0.55
2:2:537:G:OP1	47:q:110:ARG:NH2	2.35	0.55
40:j:34:THR:OG1	40:j:35:ALA:N	2.39	0.55
58:4:347:U:OP2	58:4:348:C:N4	2.39	0.55
1:1:2141:G:H22	1:1:2151:U:H3	1.52	0.55
2:2:334:C:HO2'	2:2:1434:A:HO2'	1.51	0.55
8:D:117:ARG:NH2	8:D:183:PHE:O	2.40	0.55
23:S:25:ARG:NH1	23:S:74:ILE:O	2.39	0.55
29:Y:16:THR:O	29:Y:20:ASN:ND2	2.40	0.55
53:w:37:GLY:O	53:w:63:ARG:NH2	2.40	0.55
12:H:23:LEU:O	12:H:86:MET:HA	2.08	0.54
1:1:1724:G:H22	1:1:1736:U:H3	1.55	0.54
1:1:2102:G:O6	1:1:2187:U:O2	2.25	0.54
16:L:123:ARG:NH2	16:L:143:GLU:OE2	2.38	0.54
12:H:43:LYS:HZ3	12:H:95:LEU:HB3	1.72	0.54
2:2:606:G:N2	2:2:633:G:N7	2.55	0.54
8:D:97:ASN:ND2	8:D:100:MET:SD	2.80	0.54
21:Q:92:ARG:HA	21:Q:95:LEU:HB2	1.88	0.54
1:1:1095:A:O2'	1:1:1096:A:N7	2.41	0.54
2:2:392:C:HO2'	2:2:483:C:HO2'	1.50	0.54
2:2:587:G:OP1	43:m:84:ARG:NH2	2.40	0.54
1:1:1263:U:OP1	32:b:13:ARG:NH1	2.41	0.54
2:2:861:G:HO2'	2:2:874:G:HO2'	1.56	0.54
3:3:79:G:N7	26:V:14:LYS:NZ	2.52	0.54
42:l:16:PRO:HB2	44:n:42:GLU:HG3	1.88	0.54
56:z:63:GLU:OE1	56:z:66:ARG:NH2	2.40	0.54
1:1:1020:A:N1	1:1:1141:U:O2'	2.40	0.54
1:1:1326:U:HO2'	1:1:2010:G:HO2'	1.48	0.54
1:1:2572:A:N6	7:C:150:GLN:OE1	2.40	0.54
6:B:116:ILE:HD12	6:B:127:GLY:HA3	1.89	0.54
37:g:73:LYS:NZ	37:g:165:ASP:OD2	2.39	0.54
54:x:12:ASP:OD1	54:x:12:ASP:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:882:G:O6	1:1:894:U:O2	2.26	0.54
1:1:1535:A:H5'	1:1:1536:C:H5	1.73	0.54
2:2:690:G:O6	46:p:53:ARG:NH1	2.41	0.54
21:Q:26:GLY:O	21:Q:30:ARG:NH1	2.41	0.54
54:x:64:ASP:OD1	54:x:64:ASP:N	2.41	0.54
1:1:630:G:OP2	35:e:23:LYS:NZ	2.41	0.54
1:1:885:C:H42	1:1:891:G:H22	1.56	0.54
1:1:1154:G:OP2	21:Q:58:ARG:NH1	2.40	0.54
1:1:1231:U:H2'	1:1:1232:G:H8	1.73	0.54
1:1:2635:A:O2'	7:C:49:GLN:NE2	2.41	0.54
6:B:174:LEU:O	6:B:181:MET:HA	2.07	0.54
11:G:129:GLU:HA	11:G:143:ILE:HG23	1.89	0.54
38:h:127:ARG:NH1	38:h:192:THR:OG1	2.41	0.54
1:1:2204:G:O6	1:1:2220:U:O2	2.26	0.53
2:2:736:C:OP1	53:w:61:ARG:NH1	2.42	0.53
13:I:44:LYS:NZ	13:I:54:ILE:O	2.42	0.53
58:4:62:G:H1'	58:4:63:C:H5	1.71	0.53
1:1:959:A:N3	1:1:2457:PSU:O2'	2.40	0.53
3:3:36:C:H5''	3:3:38:C:H41	1.73	0.53
1:1:370:G:O2'	1:1:424:G:OP1	2.24	0.53
5:7:14:A:OP2	5:7:15:G:N2	2.41	0.53
9:E:115:ARG:HA	31:a:47:LYS:HZ2	1.73	0.53
1:1:353:C:H2'	1:1:354:A:H8	1.72	0.53
1:1:2011:U:OP2	23:S:16:LYS:NZ	2.38	0.53
1:1:2356:U:O2	1:1:2361:G:O6	2.27	0.53
1:1:2743:U:OP2	1:1:2755:C:N4	2.41	0.53
6:B:139:SER:OG	6:B:140:THR:N	2.42	0.53
40:j:94:VAL:HG23	40:j:127:ALA:HA	1.89	0.53
6:B:258:ARG:NH1	6:B:260:ASN:OD1	2.41	0.53
28:X:2:SER:OG	28:X:3:ARG:N	2.40	0.53
1:1:1433:A:H2'	1:1:1434:A:C8	2.44	0.53
1:1:1666:G:H4'	15:K:6:THR:HG23	1.91	0.53
1:1:1779:U:OP2	1:1:1784:A:N6	2.39	0.53
1:1:2771:C:O2'	7:C:208:LYS:NZ	2.38	0.53
2:2:201:G:O2'	2:2:469:C:O2'	2.27	0.53
2:2:937:A:N3	2:2:1378:C:N4	2.57	0.53
1:1:239:C:HO2'	1:1:622:G:HO2'	1.54	0.53
2:2:461:A:H2'	2:2:462:G:H8	1.72	0.53
16:L:128:THR:O	16:L:132:ARG:HB3	2.09	0.53
26:V:21:ARG:NH2	26:V:87:GLN:O	2.42	0.53
44:n:36:GLU:OE1	44:n:45:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:o:45:ARG:NE	45:o:47:GLU:OE2	2.42	0.53
58:4:11:C:N4	58:4:348:C:O4'	2.42	0.53
10:F:22:GLN:NE2	10:F:38:ASN:O	2.42	0.53
28:X:53:ALA:HA	28:X:56:MET:HE3	1.91	0.53
38:h:31:ASP:OD1	49:s:65:ARG:NH1	2.40	0.53
1:1:1923:U:H4'	5:7:24:G:H21	1.74	0.53
2:2:981:U:OP1	49:s:9:ARG:NH1	2.42	0.53
58:4:196:G:O2'	58:4:197:A:N3	2.42	0.53
1:1:577:G:O2'	1:1:1254:A:OP1	2.27	0.53
2:2:24:U:HO2'	2:2:524:G:HO2'	1.56	0.53
14:J:73:VAL:HG12	14:J:88:THR:HG22	1.90	0.53
39:i:202:GLU:OE1	40:j:112:ARG:NH1	2.40	0.53
1:1:31:C:O2'	1:1:1238:G:OP1	2.26	0.52
2:2:1218:C:H2'	2:2:1219:A:H8	1.73	0.52
3:3:5:U:OP1	3:3:61:G:O2'	2.28	0.52
3:3:28:C:H5''	19:O:31:THR:HG21	1.91	0.52
7:C:179:ARG:NH2	7:C:181:ASP:OD2	2.41	0.52
21:Q:72:ASN:HB3	21:Q:110:VAL:HG11	1.90	0.52
2:2:107:G:H1	55:y:6:SER:HG	1.57	0.52
2:2:875:U:O2'	43:m:15:ARG:NH1	2.40	0.52
18:N:14:SER:OG	18:N:17:ARG:NH1	2.42	0.52
35:e:24:HIS:ND1	35:e:25:LYS:O	2.41	0.52
44:n:21:ILE:HD13	44:n:63:LEU:HB3	1.90	0.52
2:2:1226:C:O2'	48:r:110:LYS:NZ	2.42	0.52
2:2:1317:C:O2	54:x:37:ARG:NH2	2.43	0.52
23:S:2:GLU:HA	23:S:108:SER:HB2	1.92	0.52
50:t:82:ILE:HG13	50:t:87:LEU:HB3	1.91	0.52
58:4:32:A:O2'	58:4:35:C:OP2	2.28	0.52
1:1:859:G:O2'	1:1:916:G:O6	2.27	0.52
2:2:1119:C:OP2	44:n:11:ARG:NH1	2.42	0.52
8:D:1:MET:O	8:D:13:THR:HA	2.10	0.52
1:1:663:G:H5''	16:L:17:LYS:HD3	1.92	0.52
1:1:1528:A:N6	1:1:1543:G:O2'	2.42	0.52
1:1:2883:A:OP2	32:b:50:ARG:NH1	2.43	0.52
2:2:1218:C:H2'	2:2:1219:A:C8	2.44	0.52
1:1:1528:A:OP2	1:1:1543:G:N2	2.43	0.52
1:1:672:C:OP2	16:L:42:SER:OG	2.28	0.52
49:s:63:ARG:NH2	49:s:68:GLY:O	2.43	0.52
50:t:12:VAL:HG21	50:t:22:THR:HG22	1.91	0.52
58:4:120:U:H5	58:4:124:A:H62	1.57	0.52
1:1:1266:G:O2'	1:1:2012:G:O6	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:662:U:O2'	2:2:836:G:OP1	2.28	0.52
2:2:970:C:N4	44:n:130:ARG:OXT	2.42	0.52
2:2:1005:A:O2'	2:2:1037:C:O2'	2.25	0.52
2:2:1346:A:OP1	44:n:122:ARG:NH1	2.43	0.52
31:a:9:TYR:HD1	31:a:27:THR:HG23	1.75	0.52
1:1:1432:G:H2'	1:1:1433:A:C8	2.44	0.52
2:2:1422:G:H4'	15:K:48:PRO:HB3	1.92	0.52
18:N:90:ARG:NH2	18:N:117:ASP:OD1	2.43	0.52
1:1:464:U:O2'	34:d:12:ARG:NH1	2.37	0.52
1:1:1054:A:O2'	12:H:30:SER:O	2.23	0.52
1:1:1734:G:H2'	1:1:1735:A:H8	1.75	0.52
1:1:2377:A:O2'	19:O:117:PHE:O	2.27	0.52
1:1:2548:U:O2	15:K:23:LYS:NZ	2.36	0.52
2:2:1452:C:O2	2:2:1453:G:N2	2.43	0.52
47:q:31:ARG:O	47:q:58:THR:OG1	2.28	0.52
53:w:26:ILE:HD12	53:w:67:LEU:HB3	1.92	0.52
58:4:17:U:N3	58:4:333:G:O6	2.43	0.52
21:Q:100:VAL:O	21:Q:103:LYS:NZ	2.43	0.51
31:a:49:ARG:NH1	48:r:68:ASP:OD2	2.43	0.51
51:u:4:ILE:HG12	51:u:21:VAL:HG22	1.92	0.51
1:1:296:U:H2'	1:1:297:G:H8	1.74	0.51
1:1:1266:G:OP1	32:b:16:ARG:NE	2.44	0.51
2:2:1183:U:O2'	2:2:1185:G:OP2	2.28	0.51
2:2:1402:4OC:O2'	2:2:1402:4OC:O2	2.28	0.51
2:2:1419:G:O6	2:2:1481:U:O2	2.27	0.51
14:J:11:VAL:HG21	14:J:50:THR:HG22	1.91	0.51
25:U:33:LYS:HG2	25:U:66:GLN:HG2	1.93	0.51
37:g:119:THR:HG23	37:g:123:ASP:HB2	1.91	0.51
31:a:18:CYS:HB3	31:a:40:CYS:HB3	1.92	0.51
33:c:11:LEU:HD21	33:c:34:LEU:HD23	1.92	0.51
58:4:311:U:H2'	58:4:312:A:H8	1.75	0.51
1:1:284:U:O4	1:1:356:G:O6	2.29	0.51
2:2:1026:G:O6	2:2:1035:A:N1	2.43	0.51
2:2:1179:A:OP2	44:n:99:ARG:NH2	2.43	0.51
11:G:125:THR:OG1	11:G:146:VAL:O	2.26	0.51
40:j:57:PRO:HA	40:j:60:ILE:HG12	1.92	0.51
58:4:192:A:H2'	58:4:193:A:H8	1.75	0.51
1:1:2328:A:H2'	1:1:2329:U:C6	2.46	0.51
1:1:2747:G:N2	1:1:2757:A:H62	2.04	0.51
45:o:91:ASP:OD1	45:o:91:ASP:N	2.41	0.51
58:4:56:C:H2'	58:4:57:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1055:G:O2'	12:H:32:GLY:O	2.26	0.51
13:I:37:PHE:O	13:I:41:PHE:CB	2.55	0.51
16:L:110:VAL:HB	16:L:127:VAL:HG13	1.92	0.51
58:4:43:G:O6	58:4:312:A:N6	2.43	0.51
1:1:517:C:OP1	32:b:13:ARG:NH2	2.36	0.51
1:1:1039:A:H2	1:1:1116:G:H22	1.58	0.51
1:1:1272:A:O2'	1:1:1274:A:OP1	2.28	0.51
14:J:4:PHE:O	21:Q:64:ARG:NH2	2.43	0.51
18:N:13:ASN:OD1	18:N:13:ASN:N	2.42	0.51
38:h:11:ARG:NH2	38:h:175:LEU:O	2.43	0.51
40:j:157:ARG:NH2	43:m:99:LEU:O	2.44	0.51
51:u:50:THR:HG21	51:u:74:LEU:HD12	1.91	0.51
1:1:2278:A:OP2	27:W:12:ASN:ND2	2.44	0.51
3:3:14:U:OP2	3:3:70:C:O2'	2.28	0.51
12:H:28:ALA:HB3	12:H:111:ALA:HA	1.92	0.51
2:2:411:A:OP2	39:i:26:ARG:NH1	2.43	0.51
39:i:60:LYS:NZ	39:i:194:ASP:OD1	2.43	0.51
39:i:78:GLU:OE2	39:i:81:ARG:NH1	2.43	0.51
51:u:75:ILE:O	51:u:79:ASN:ND2	2.41	0.51
1:1:1500:G:O3'	6:B:101:ARG:NH2	2.44	0.51
12:H:33:VAL:HG12	12:H:35:VAL:H	1.75	0.51
16:L:76:GLU:OE2	16:L:78:ARG:NH1	2.43	0.51
23:S:82:MET:HG3	23:S:98:LYS:HB2	1.92	0.51
58:4:142:U:O2'	58:4:166:C:OP2	2.28	0.51
2:2:261:U:OP2	55:y:74:ARG:NH1	2.43	0.50
2:2:1135:U:H3'	2:2:1137:C:H42	1.76	0.50
1:1:713:G:N2	1:1:718:A:H62	2.03	0.50
1:1:2250:G:O2'	1:1:2496:C:OP1	2.28	0.50
6:B:98:ASP:OD1	6:B:98:ASP:N	2.41	0.50
14:J:60:ASP:OD1	14:J:60:ASP:N	2.43	0.50
39:i:126:ASN:ND2	39:i:141:ASP:OD1	2.44	0.50
43:m:18:GLN:HG2	43:m:63:LEU:HD13	1.93	0.50
56:z:60:LEU:HG	56:z:64:ASN:HD21	1.76	0.50
55:y:24:ARG:HH21	55:y:27:MET:HE1	1.75	0.50
1:1:538:A:H4'	14:J:7:LYS:HG2	1.93	0.50
1:1:641:U:O4	1:1:647:G:O6	2.29	0.50
1:1:1315:C:O2'	1:1:1392:A:N3	2.40	0.50
1:1:1415:U:O4	1:1:1587:G:O6	2.29	0.50
2:2:31:G:O2'	2:2:48:C:N4	2.45	0.50
2:2:407:U:O2'	39:i:113:GLU:OE1	2.30	0.50
2:2:1202:U:O2	49:s:83:LYS:NZ	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:54:ILE:HG12	13:I:73:PRO:HG3	1.91	0.50
38:h:44:THR:O	38:h:48:ALA:HB2	2.12	0.50
58:4:212:U:O2'	58:4:213:G:O5'	2.29	0.50
1:1:238:C:O2'	1:1:608:A:N3	2.43	0.50
22:R:77:PHE:HD1	22:R:84:ARG:HB3	1.76	0.50
27:W:37:ILE:HG22	27:W:38:VAL:HG23	1.94	0.50
38:h:7:PRO:O	38:h:11:ARG:NH1	2.44	0.50
1:1:774:G:H5''	6:B:48:ARG:HH12	1.77	0.50
9:E:44:ILE:HG21	9:E:79:ILE:HG22	1.94	0.50
9:E:49:LEU:HG	9:E:150:ARG:HH21	1.75	0.50
15:K:35:VAL:HG21	15:K:104:THR:HG21	1.92	0.50
50:t:64:ARG:NH1	50:t:89:ARG:OXT	2.44	0.50
1:1:396:G:OP2	28:X:10:LYS:NZ	2.44	0.50
1:1:1223:G:OP1	22:R:68:ARG:NH2	2.44	0.50
1:1:1445:G:O6	1:1:1466:U:O2	2.29	0.50
2:2:81:A:OP2	2:2:83:C:N4	2.44	0.50
8:D:10:SER:OG	8:D:11:ALA:N	2.44	0.50
15:K:71:ARG:NH2	15:K:104:THR:OG1	2.45	0.50
23:S:80:PRO:HD3	23:S:102:HIS:HE1	1.77	0.50
26:V:2:PHE:HZ	26:V:53:LYS:HD2	1.76	0.50
37:g:111:ILE:HD12	37:g:152:LYS:HA	1.94	0.50
54:x:14:HIS:NE2	54:x:35:SER:OG	2.45	0.50
58:4:319:A:H2'	58:4:320:U:H5''	1.93	0.50
1:1:1083:U:O2'	1:1:1085:A:OP2	2.29	0.50
1:1:2483:C:N3	17:M:123:LYS:NZ	2.55	0.50
2:2:1199:U:O2'	2:2:1202:U:OP2	2.30	0.50
19:O:31:THR:O	19:O:102:ARG:NH1	2.34	0.50
27:W:59:LEU:HD12	27:W:80:ILE:HD12	1.93	0.50
58:4:185:A:H8	58:4:186:A:N7	2.10	0.50
1:1:878:A:H3'	1:1:879:G:H8	1.76	0.50
1:1:1057:A:H2	1:1:1082:U:H3	1.59	0.50
2:2:1005:A:H3'	2:2:1006:G:H8	1.77	0.50
3:3:5:U:H2'	3:3:6:G:H8	1.76	0.50
12:H:50:VAL:HG22	12:H:53:ARG:HH22	1.77	0.50
30:Z:8:THR:HA	30:Z:34:HIS:O	2.12	0.50
42:l:78:ARG:HB3	42:l:85:TYR:HB2	1.94	0.50
48:r:90:ARG:HD2	48:r:95:LEU:HB2	1.93	0.50
1:1:997:G:OP1	21:Q:92:ARG:NH1	2.44	0.49
2:2:254:G:O3'	52:v:71:LYS:NZ	2.39	0.49
2:2:811:C:O2'	2:2:901:A:N1	2.45	0.49
2:2:890:G:O2'	2:2:906:A:N6	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1026:G:C6	2:2:1035:A:N1	2.80	0.49
20:P:24:ASP:OD1	20:P:90:GLY:N	2.44	0.49
24:T:19:LYS:NZ	24:T:84:TYR:OH	2.45	0.49
43:m:47:GLU:HG3	43:m:64:LYS:HG2	1.94	0.49
58:4:153:U:N3	58:4:163:G:N1	2.60	0.49
1:1:1296:G:OP1	1:1:2709:G:O2'	2.28	0.49
2:2:1032:G:N2	2:2:1033:G:O2'	2.45	0.49
6:B:135:ILE:HD13	6:B:141:VAL:HG11	1.94	0.49
6:B:232:HIS:HA	6:B:242:LYS:HD2	1.94	0.49
20:P:91:ALA:HB2	20:P:113:ARG:HB2	1.93	0.49
29:Y:3:ALA:HA	29:Y:6:LEU:HB2	1.94	0.49
39:i:85:ASN:HB3	39:i:88:GLU:HB3	1.93	0.49
56:z:63:GLU:HA	56:z:66:ARG:HG2	1.95	0.49
1:1:1534:U:O4	1:1:1538:G:O6	2.30	0.49
1:1:2258:C:O2'	1:1:2427:C:OP2	2.29	0.49
2:2:429:U:H3'	39:i:9:LEU:HD12	1.94	0.49
2:2:549:C:OP1	39:i:70:ARG:NH2	2.39	0.49
2:2:1249:C:O2'	44:n:75:GLN:NE2	2.46	0.49
9:E:33:LYS:HG3	9:E:157:THR:HB	1.94	0.49
11:G:30:LEU:HB3	11:G:36:ALA:HB3	1.95	0.49
54:x:63:THR:HG23	54:x:65:GLU:H	1.77	0.49
1:1:219:A:N3	1:1:234:U:O2'	2.42	0.49
2:2:1179:A:H5''	44:n:99:ARG:HH22	1.77	0.49
20:P:30:VAL:O	20:P:40:LEU:HA	2.12	0.49
21:Q:72:ASN:O	21:Q:114:LYS:NZ	2.46	0.49
23:S:41:LYS:HD2	32:b:22:LEU:HD11	1.93	0.49
57:5:118:TRP:HD1	57:5:120:ASN:H	1.59	0.49
58:4:31:G:OP1	58:4:318:G:N1	2.45	0.49
58:4:153:U:O2	58:4:163:G:C2	2.66	0.49
58:4:172:U:H2'	58:4:173:C:H6	1.77	0.49
1:1:773:U:O3'	6:B:48:ARG:NH1	2.46	0.49
1:1:2333:A:OP2	27:W:77:ARG:NH2	2.44	0.49
2:2:1329:A:H5''	48:r:26:GLY:H	1.78	0.49
37:g:120:GLN:HG2	37:g:126:PHE:HB3	1.94	0.49
57:5:121:ALA:HB3	57:5:122:TRP:HE3	1.76	0.49
1:1:265:A:O2'	1:1:428:A:N6	2.45	0.49
1:1:373:U:H2'	1:1:374:A:H8	1.78	0.49
1:1:1351:C:O2'	1:1:1571:A:N3	2.40	0.49
2:2:582:C:OP2	2:2:758:C:N4	2.41	0.49
1:1:75:G:H4'	29:Y:48:ARG:HH21	1.77	0.49
1:1:151:C:H2'	1:1:152:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:743:A:O2'	1:1:1659:G:OP1	2.28	0.49
2:2:157:U:O2	2:2:164:G:O6	2.30	0.49
2:2:672:U:H2'	2:2:673:A:C8	2.48	0.49
29:Y:9:LYS:HE3	29:Y:13:GLU:HB3	1.94	0.49
6:B:252:THR:OG1	6:B:253:LYS:N	2.45	0.49
14:J:49:ASP:OD1	14:J:121:LYS:NZ	2.44	0.49
20:P:9:GLU:OE2	20:P:55:LEU:N	2.45	0.49
45:o:26:VAL:HG23	45:o:36:VAL:HG11	1.94	0.49
48:r:16:VAL:O	48:r:20:THR:OG1	2.29	0.49
1:1:1827:U:OP2	6:B:221:ARG:NE	2.35	0.49
2:2:466:A:O2'	2:2:467:U:O2	2.25	0.49
2:2:1026:G:N1	2:2:1035:A:C2	2.81	0.49
15:K:34:GLY:N	15:K:37:ASP:OD2	2.41	0.49
38:h:179:ARG:NH2	38:h:206:GLU:OE1	2.46	0.49
44:n:84:THR:HG21	44:n:103:PHE:HB3	1.94	0.49
58:4:116:A:H2'	58:4:117:G:H5''	1.95	0.49
1:1:2835:A:OP1	7:C:56:LYS:NZ	2.44	0.48
2:2:501:C:OP1	47:q:114:ARG:NH2	2.29	0.48
1:1:278:A:N1	1:1:361:G:O2'	2.45	0.48
1:1:296:U:H2'	1:1:297:G:C8	2.48	0.48
1:1:1047:G:H4'	1:1:1048:A:H5'	1.95	0.48
2:2:406:G:H21	39:i:116:GLN:HE22	1.60	0.48
2:2:647:C:H2'	2:2:648:A:H8	1.77	0.48
2:2:1255:G:OP2	45:o:45:ARG:NH1	2.46	0.48
2:2:1513:A:H2'	2:2:1514:G:H8	1.78	0.48
27:W:23:VAL:HG13	27:W:38:VAL:HG22	1.95	0.48
42:l:79:ARG:HA	42:l:84:THR:HA	1.95	0.48
1:1:720:U:H2'	1:1:721:A:C8	2.48	0.48
1:1:1028:A:N3	1:1:2486:C:O2'	2.39	0.48
1:1:1636:U:O2'	1:1:1760:C:O2	2.27	0.48
2:2:41:G:H2'	2:2:42:G:H8	1.78	0.48
2:2:344:A:OP2	2:2:345:C:N4	2.46	0.48
2:2:490:C:H2'	2:2:491:G:H8	1.77	0.48
2:2:842:U:O2'	2:2:846:G:N7	2.44	0.48
2:2:946:A:H2'	2:2:947:G:C8	2.48	0.48
2:2:1226:C:H41	48:r:103:LYS:HE2	1.79	0.48
8:D:154:ASP:N	8:D:154:ASP:OD1	2.43	0.48
38:h:47:LEU:HD13	38:h:76:VAL:HG13	1.94	0.48
50:t:44:ALA:O	50:t:47:LYS:NZ	2.39	0.48
51:u:44:SER:N	51:u:47:GLU:OE2	2.45	0.48
58:4:168:G:H2'	58:4:169:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:407:U:OP1	39:i:3:ARG:NH2	2.46	0.48
2:2:1415:G:H1	2:2:1485:U:H3	1.59	0.48
3:3:93:C:OP2	26:V:18:ARG:NH1	2.46	0.48
46:p:64:GLN:HB2	46:p:99:ALA:HB2	1.96	0.48
1:1:505:A:HO2'	1:1:509:C:HO2'	1.59	0.48
1:1:793:A:OP2	1:1:2071:A:O2'	2.29	0.48
1:1:1529:G:O6	1:1:1542:U:O4	2.32	0.48
1:1:1678:A:N3	1:1:1990:C:O2'	2.45	0.48
1:1:2247:A:H2'	1:1:2248:C:H6	1.78	0.48
1:1:2333:A:H5'	1:1:2335:A:H1'	1.96	0.48
2:2:600:A:H2'	2:2:601:G:H8	1.78	0.48
10:F:135:GLY:HA3	10:F:141:ILE:HG21	1.94	0.48
18:N:58:ASP:OD1	18:N:63:ARG:NH1	2.46	0.48
1:1:713:G:H21	1:1:718:A:N6	2.04	0.48
1:1:2285:C:OP2	33:c:6:ARG:NH2	2.41	0.48
13:I:55:PRO:HD2	13:I:71:LYS:HG3	1.96	0.48
25:U:48:PRO:HG3	25:U:56:GLY:HA3	1.94	0.48
43:m:83:LEU:HD22	47:q:4:VAL:HG11	1.95	0.48
1:1:1386:C:H2'	1:1:1387:A:C8	2.47	0.48
2:2:309:A:H2'	2:2:310:G:H8	1.77	0.48
15:K:70:ARG:HG2	15:K:76:VAL:HG12	1.95	0.48
38:h:16:LYS:NZ	38:h:183:ASP:OD1	2.46	0.48
38:h:36:ASP:OD1	38:h:40:ARG:NH2	2.41	0.48
58:4:165:A:H5''	58:4:166:C:H3'	1.94	0.48
58:4:285:A:H2'	58:4:286:A:H5''	1.96	0.48
1:1:281:C:H2'	1:1:282:A:C8	2.49	0.48
1:1:2116:G:OP1	1:1:2165:C:N4	2.41	0.48
1:1:2788:C:O2'	1:1:2809:A:N3	2.39	0.48
1:1:2849:U:N3	1:1:2867:G:N3	2.62	0.48
21:Q:16:LYS:HB3	21:Q:16:LYS:HE2	1.72	0.48
40:j:147:MET:HB3	40:j:147:MET:HE3	1.79	0.48
45:o:87:LEU:HD13	45:o:100:ILE:HD13	1.94	0.48
53:w:57:ARG:HB3	53:w:61:ARG:HH22	1.79	0.48
1:1:29:U:H1'	21:Q:11:ARG:HH22	1.79	0.48
1:1:694:U:O2	1:1:768:G:O6	2.32	0.48
10:F:2:SER:OG	10:F:3:ARG:N	2.46	0.48
12:H:97:LYS:HD3	12:H:100:ALA:HB3	1.95	0.48
35:e:54:ASP:HA	35:e:57:LEU:HD12	1.95	0.48
1:1:1341:G:H21	24:T:59:ASN:HD22	1.61	0.48
2:2:315:A:O2'	2:2:330:C:O2'	2.31	0.48
25:U:9:ASP:OD1	25:U:9:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:29:SER:OG	43:m:30:SER:N	2.47	0.48
1:1:78:U:O4	1:1:108:G:O6	2.32	0.47
1:1:639:U:H2'	1:1:640:C:C6	2.49	0.47
1:1:2265:U:H4'	17:M:13:HIS:HE1	1.79	0.47
1:1:2655:G:O2'	1:1:2664:G:O6	2.26	0.47
1:1:2685:G:H2'	1:1:2686:G:H8	1.79	0.47
2:2:1252:A:H61	2:2:1285:A:H61	1.61	0.47
40:j:52:LYS:HB3	40:j:52:LYS:HE2	1.66	0.47
42:l:113:ASP:O	42:l:119:ARG:NH2	2.47	0.47
50:t:11:ILE:HG21	50:t:31:LEU:HG	1.95	0.47
1:1:464:U:H1'	1:1:686:U:H5	1.78	0.47
1:1:1079:C:H2'	1:1:1080:A:C8	2.49	0.47
2:2:427:U:OP1	39:i:13:ARG:NH2	2.46	0.47
2:2:1254:A:H2'	2:2:1255:G:H8	1.79	0.47
40:j:142:ASP:O	40:j:146:ASN:ND2	2.47	0.47
58:4:37:C:H6	58:4:37:C:O5'	1.97	0.47
1:1:158:U:O4	1:1:168:G:O6	2.32	0.47
1:1:686:U:O4	34:d:12:ARG:NH1	2.42	0.47
1:1:1529:G:N2	1:1:1542:U:O2	2.36	0.47
1:1:2378:A:HO2'	19:O:91:SER:HG	1.58	0.47
2:2:923:A:O2'	2:2:1399:C:OP2	2.31	0.47
31:a:57:VAL:HA	54:x:67:VAL:HG21	1.95	0.47
38:h:111:LEU:HD11	38:h:146:ALA:HB2	1.95	0.47
58:4:193:A:H2'	58:4:194:G:C8	2.50	0.47
58:4:281:A:O2'	58:4:286:A:N1	2.39	0.47
1:1:521:U:H2'	1:1:522:A:C8	2.50	0.47
1:1:2445:2MG:OP1	8:D:69:ARG:NH2	2.48	0.47
2:2:552:U:H2'	2:2:553:A:H8	1.80	0.47
2:2:837:U:H2'	2:2:838:G:H8	1.80	0.47
9:E:22:TYR:OH	9:E:165:GLU:OE2	2.30	0.47
12:H:31:ARG:HD3	12:H:108:VAL:HG21	1.97	0.47
1:1:2576:G:O2'	1:1:2579:C:OP2	2.25	0.47
1:1:2780:G:N1	14:J:102:GLU:OE2	2.45	0.47
11:G:18:GLN:HE21	11:G:39:ALA:HB1	1.79	0.47
13:I:122:GLU:HB3	13:I:126:ARG:HH12	1.78	0.47
40:j:107:ALA:O	40:j:112:ARG:NH2	2.48	0.47
51:u:19:VAL:HG22	51:u:37:GLY:H	1.78	0.47
1:1:883:G:O2'	1:1:885:C:N4	2.37	0.47
1:1:1143:A:N7	14:J:27:ARG:NH1	2.63	0.47
1:1:1915:3TD:O5'	1:1:1915:3TD:O4	2.32	0.47
1:1:1939:5MU:OP1	1:1:2604:U:O2'	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:522:C:H41	47:q:50:ARG:NH1	2.13	0.47
2:2:1270:G:O2'	2:2:1313:U:O2'	2.29	0.47
9:E:33:LYS:HE3	9:E:92:ARG:HE	1.80	0.47
14:J:60:ASP:HB3	14:J:97:PRO:HB2	1.97	0.47
16:L:49:GLY:HA3	16:L:58:TYR:HE1	1.80	0.47
22:R:4:VAL:HA	22:R:12:HIS:O	2.14	0.47
37:g:197:ASP:N	37:g:197:ASP:OD1	2.46	0.47
44:n:46:MET:HE3	44:n:50:GLN:HE21	1.79	0.47
47:q:33:VAL:HG22	47:q:79:VAL:HG12	1.95	0.47
49:s:50:THR:HG22	54:x:13:LEU:HD22	1.96	0.47
51:u:40:ASN:HB3	51:u:43:ALA:HB2	1.95	0.47
1:1:281:C:H2'	1:1:282:A:H8	1.78	0.47
1:1:1016:G:O6	1:1:1147:A:N6	2.48	0.47
1:1:2335:A:OP1	19:O:13:ARG:NH2	2.48	0.47
6:B:142:HIS:ND1	6:B:193:GLY:O	2.40	0.47
10:F:94:TYR:OH	10:F:152:ARG:NH1	2.48	0.47
1:1:154:U:H2'	1:1:155:A:H8	1.80	0.47
1:1:624:C:O2'	1:1:657:U:OP1	2.30	0.47
1:1:2164:C:OP1	1:1:2170:A:O2'	2.29	0.47
1:1:2305:U:N3	9:E:151:GLY:O	2.48	0.47
2:2:750:C:H2'	2:2:751:U:H6	1.79	0.47
2:2:759:A:O2'	47:q:9:ARG:NH1	2.48	0.47
2:2:1374:A:OP1	42:l:36:LYS:NZ	2.45	0.47
8:D:53:THR:O	8:D:53:THR:OG1	2.27	0.47
16:L:2:ARG:HD3	16:L:2:ARG:HA	1.78	0.47
38:h:203:PHE:HZ	38:h:206:GLU:HG3	1.80	0.47
45:o:46:LYS:HG2	45:o:68:ARG:HG3	1.96	0.47
1:1:195:A:H61	1:1:198:C:H3'	1.80	0.47
1:1:1190:G:H5''	16:L:32:GLY:HA2	1.97	0.47
1:1:1423:G:H2'	1:1:1424:G:H8	1.79	0.47
1:1:1954:G:O2'	1:1:1956:U:O4	2.31	0.47
1:1:2818:U:H2'	1:1:2819:G:H8	1.80	0.47
2:2:1038:C:N4	2:2:1039:G:O6	2.48	0.47
17:M:108:VAL:HG22	17:M:112:LEU:HB3	1.96	0.47
31:a:31:ASP:N	31:a:31:ASP:OD1	2.48	0.47
58:4:196:G:N1	58:4:230:U:OP2	2.48	0.47
2:2:324:G:O2'	2:2:326:G:O6	2.31	0.46
2:2:329:A:O2'	2:2:332:G:N7	2.45	0.46
2:2:769:G:H4'	2:2:1513:A:H4'	1.97	0.46
8:D:176:ASP:OD1	8:D:179:SER:OG	2.32	0.46
38:h:43:LEU:HD11	38:h:87:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:q:54:ARG:HA	47:q:64:THR:HA	1.96	0.46
53:w:45:THR:OG1	53:w:46:GLY:N	2.48	0.46
1:1:1218:G:H1	1:1:1231:U:H3	1.61	0.46
2:2:178:C:H2'	2:2:179:A:H8	1.80	0.46
8:D:189:THR:HG22	8:D:191:ASP:H	1.79	0.46
10:F:170:ARG:HD2	10:F:170:ARG:HA	1.72	0.46
22:R:95:ASP:OD1	22:R:95:ASP:N	2.48	0.46
33:c:33:LYS:NZ	33:c:51:GLU:O	2.41	0.46
37:g:66:LYS:O	37:g:159:ASP:N	2.46	0.46
40:j:13:GLU:HB3	40:j:39:VAL:HG23	1.97	0.46
1:1:2508:G:H1	1:1:2580:PSU:HN3	1.63	0.46
2:2:452:A:H62	2:2:480:U:H3	1.62	0.46
12:H:67:THR:O	12:H:69:PHE:N	2.49	0.46
37:g:122:GLN:O	37:g:125:THR:OG1	2.30	0.46
1:1:1853:A:H2'	1:1:1854:A:C8	2.51	0.46
1:1:1869:G:H21	1:1:1871:A:H3'	1.81	0.46
21:Q:86:ALA:HB2	21:Q:116:ALA:HB2	1.97	0.46
22:R:6:GLN:NE2	22:R:37:GLU:OE2	2.48	0.46
54:x:19:VAL:HG11	54:x:44:MET:HG2	1.97	0.46
54:x:63:THR:H	54:x:66:MET:HE3	1.81	0.46
58:4:137:C:H3'	58:4:138:C:H5''	1.97	0.46
1:1:592:A:HO2'	35:e:64:TYR:HH	1.62	0.46
1:1:659:G:N2	8:D:30:GLN:OE1	2.44	0.46
1:1:903:C:H2'	1:1:904:G:H8	1.81	0.46
1:1:1179:G:OP2	1:1:1179:G:N2	2.38	0.46
1:1:1227:G:OP2	21:Q:16:LYS:NZ	2.48	0.46
1:1:1309:G:O2'	1:1:1611:C:O2'	2.29	0.46
1:1:1915:3TD:H2'	1:1:1916:A:C8	2.51	0.46
2:2:1112:C:H42	38:h:178:LEU:HD23	1.81	0.46
5:7:63:G:O2'	17:M:10:ARG:NH1	2.48	0.46
10:F:44:LYS:HD3	10:F:44:LYS:HA	1.76	0.46
52:v:47:HIS:NE2	52:v:49:GLU:OE2	2.44	0.46
58:4:61:G:N3	58:4:62:G:N1	2.64	0.46
1:1:1744:A:H3'	1:1:1745:A:H8	1.80	0.46
18:N:12:ARG:O	18:N:17:ARG:NH2	2.48	0.46
35:e:15:LYS:HB2	35:e:23:LYS:HE2	1.97	0.46
49:s:3:LYS:HB2	49:s:6:MET:HG2	1.97	0.46
1:1:619:G:O6	8:D:98:LYS:NZ	2.42	0.46
1:1:2329:U:H2'	1:1:2330:G:C8	2.51	0.46
6:B:152:GLY:O	6:B:156:ARG:NH1	2.47	0.46
15:K:89:ASN:OD1	15:K:89:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:18:VAL:O	58:4:99:G:N2	2.48	0.46
42:l:109:ARG:HG3	42:l:116:MET:HE1	1.97	0.46
57:5:16:LEU:HD21	57:5:21:ARG:HE	1.78	0.46
58:4:340:G:N2	58:4:345:A:N7	2.64	0.46
1:1:534:U:H2'	1:1:535:G:H8	1.80	0.46
2:2:600:A:H2'	2:2:601:G:C8	2.51	0.46
2:2:715:A:H2'	2:2:716:A:C8	2.50	0.46
9:E:4:LEU:HD12	9:E:101:GLU:HG2	1.98	0.46
17:M:56:ALA:HB2	17:M:119:LEU:HD23	1.98	0.46
58:4:63:C:H2'	58:4:64:C:H5'	1.98	0.46
1:1:385:C:O2'	1:1:388:G:N2	2.43	0.46
1:1:1667:G:O2'	1:1:1991:U:O4	2.33	0.46
1:1:2780:G:O6	14:J:99:ARG:NH1	2.48	0.46
2:2:1090:U:HO2'	2:2:1171:A:HO2'	1.59	0.46
6:B:53:HIS:HA	6:B:217:ARG:HB2	1.96	0.46
40:j:152:MET:HE2	40:j:152:MET:HB3	1.81	0.46
42:l:68:ASN:O	42:l:138:ARG:NH2	2.49	0.46
1:1:717:C:H3'	1:1:718:A:H8	1.80	0.46
1:1:1077:A:N3	13:I:134:SER:OG	2.48	0.46
1:1:1668:A:H61	1:1:1676:A:H61	1.63	0.46
1:1:2575:C:H5'	7:C:149:ASN:HB2	1.97	0.46
2:2:1429:A:H2'	2:2:1430:A:H8	1.80	0.46
6:B:236:GLU:O	6:B:239:ASN:ND2	2.49	0.46
10:F:89:LEU:HD23	10:F:107:LEU:HD21	1.98	0.46
12:H:101:LYS:HB2	12:H:101:LYS:HE2	1.81	0.46
20:P:49:ALA:O	20:P:59:PHE:HA	2.16	0.46
41:k:91:ARG:HH12	41:k:93:LYS:HA	1.80	0.46
48:r:89:LEU:HD23	48:r:92:ARG:HE	1.79	0.46
58:4:162:A:H1'	58:4:193:A:H1'	1.98	0.46
1:1:807:U:O2'	1:1:2060:A:N1	2.49	0.45
1:1:1629:U:O4	1:1:1630:A:N6	2.49	0.45
1:1:1796:U:H2'	1:1:1797:G:H8	1.81	0.45
1:1:2595:G:N2	1:1:2598:A:OP2	2.44	0.45
1:1:2681:C:N4	1:1:2727:A:N1	2.64	0.45
3:3:95:U:H2'	3:3:96:G:H8	1.80	0.45
7:C:179:ARG:HB2	7:C:188:LEU:HD12	1.97	0.45
13:I:129:GLU:HG2	13:I:139:VAL:HG21	1.98	0.45
19:O:67:ASN:OD1	19:O:67:ASN:N	2.47	0.45
21:Q:84:LYS:HA	21:Q:84:LYS:HD3	1.75	0.45
25:U:7:ARG:NE	25:U:26:LYS:O	2.47	0.45
30:Z:8:THR:HG23	30:Z:35:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:198:HIS:HA	39:i:201:VAL:HG12	1.98	0.45
47:q:20:ASN:OD1	47:q:20:ASN:N	2.41	0.45
55:y:67:ILE:HB	55:y:71:LYS:HD3	1.97	0.45
58:4:52:G:H21	58:4:72:A:H61	1.64	0.45
58:4:140:U:H2'	58:4:141:C:H6	1.82	0.45
58:4:261:G:H2'	58:4:262:U:H5	1.80	0.45
1:1:1275:A:OP2	1:1:1646:C:N4	2.47	0.45
2:2:668:G:H21	50:t:46:HIS:CE1	2.34	0.45
2:2:977:A:O2'	2:2:979:C:OP2	2.24	0.45
2:2:1247:U:H3	2:2:1290:G:H1	1.64	0.45
2:2:1409:C:H2'	2:2:1410:A:H8	1.81	0.45
40:j:81:LEU:HD21	40:j:96:MET:HE2	1.99	0.45
44:n:21:ILE:HD12	44:n:61:LEU:HD13	1.99	0.45
49:s:31:ILE:O	49:s:41:ARG:NH2	2.40	0.45
58:4:248:G:O2'	58:4:249:U:H5'	2.16	0.45
1:1:307:G:N1	1:1:310:A:OP2	2.44	0.45
1:1:887:A:O2'	1:1:889:C:OP2	2.21	0.45
1:1:2377:A:H2'	1:1:2378:A:H8	1.81	0.45
2:2:628:G:H2'	2:2:629:A:C8	2.50	0.45
6:B:5:LYS:HG3	6:B:17:VAL:HG22	1.97	0.45
15:K:8:LEU:HD13	15:K:84:CYS:HB3	1.98	0.45
30:Z:16:ARG:HG3	30:Z:54:MET:HE1	1.98	0.45
58:4:235:C:H2'	58:4:236:U:C6	2.52	0.45
58:4:360:A:H2'	58:4:361:C:O4'	2.15	0.45
1:1:1471:G:O6	1:1:1520:U:O2	2.34	0.45
1:1:2378:A:O2'	19:O:91:SER:OG	2.32	0.45
2:2:672:U:H2'	2:2:673:A:H8	1.81	0.45
2:2:1318:A:H5''	54:x:3:ARG:HH12	1.79	0.45
11:G:40:THR:HG22	11:G:42:LYS:H	1.81	0.45
26:V:77:VAL:HG22	26:V:89:ILE:HG12	1.99	0.45
44:n:26:GLY:N	44:n:62:ASP:OD1	2.35	0.45
45:o:22:THR:HA	45:o:25:ILE:HG22	1.99	0.45
49:s:5:SER:O	49:s:9:ARG:HB2	2.17	0.45
58:4:221:U:H2'	58:4:222:U:H6	1.81	0.45
1:1:81:G:O2'	1:1:295:G:O2'	2.34	0.45
1:1:2820:A:O2'	7:C:114:LYS:NZ	2.50	0.45
28:X:16:ASN:HD22	28:X:24:ALA:HB1	1.81	0.45
1:1:1278:C:H2'	1:1:1279:G:C8	2.52	0.45
1:1:1361:G:O2'	1:1:2215:C:O2'	2.30	0.45
1:1:2229:U:H2'	1:1:2230:G:H8	1.82	0.45
11:G:80:ILE:O	11:G:146:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:25:PRO:O	13:I:29:GLN:CB	2.63	0.45
51:u:56:ARG:HD2	51:u:56:ARG:HA	1.82	0.45
52:v:68:SER:OG	52:v:69:LYS:N	2.44	0.45
1:1:1094:U:N3	1:1:1097:U:OP1	2.50	0.45
1:1:1652:A:OP1	18:N:8:ARG:NH2	2.42	0.45
2:2:522:C:OP2	47:q:66:TYR:OH	2.28	0.45
2:2:1402:4OC:H2'	2:2:1403:C:O5'	2.17	0.45
6:B:36:LYS:HE3	6:B:36:LYS:HB3	1.78	0.45
9:E:102:ARG:NH2	9:E:140:GLU:OE2	2.49	0.45
24:T:47:VAL:HG13	24:T:55:VAL:HG21	1.98	0.45
40:j:72:ILE:HD11	40:j:145:GLU:HG2	1.99	0.45
46:p:20:VAL:HG13	46:p:83:GLU:HG3	1.99	0.45
47:q:51:LYS:HB3	47:q:67:ILE:HD12	1.98	0.45
58:4:38:A:H2'	58:4:39:A:H4'	1.99	0.45
10:F:17:VAL:HG21	10:F:50:LEU:HD21	1.98	0.45
14:J:65:THR:OG1	14:J:66:GLY:N	2.42	0.45
20:P:5:ILE:O	20:P:9:GLU:HB2	2.17	0.45
39:i:150:LYS:NZ	39:i:177:LYS:O	2.50	0.45
1:1:704:G:H1'	1:1:726:G:H22	1.82	0.45
1:1:2844:G:N2	1:1:2874:C:N3	2.65	0.45
2:2:222:C:H2'	2:2:223:A:C8	2.52	0.45
2:2:674:G:H2'	2:2:675:A:C8	2.52	0.45
2:2:1106:G:H5''	38:h:172:ARG:HB3	1.99	0.45
2:2:1513:A:H2'	2:2:1514:G:C8	2.51	0.45
8:D:49:ARG:HD2	8:D:76:PRO:HD3	1.99	0.45
45:o:81:GLU:HB3	45:o:82:LYS:HD3	1.98	0.45
53:w:71:THR:O	53:w:74:HIS:ND1	2.43	0.45
54:x:63:THR:OG1	54:x:64:ASP:OD1	2.35	0.45
1:1:1469:A:H2'	1:1:1470:A:H8	1.82	0.45
10:F:52:PHE:HZ	10:F:72:LEU:HD22	1.82	0.45
12:H:20:LYS:HB3	12:H:88:HIS:CD2	2.52	0.45
29:Y:21:LEU:HD22	29:Y:46:VAL:HG13	1.98	0.45
39:i:101:VAL:HG21	39:i:137:VAL:HG11	1.99	0.45
40:j:46:VAL:O	40:j:72:ILE:N	2.50	0.45
53:w:34:THR:HB	53:w:40:VAL:HG13	1.98	0.45
58:4:173:C:O2'	58:4:174:A:H5'	2.16	0.45
58:4:195:A:H2'	58:4:196:G:H8	1.82	0.45
1:1:776:G:N2	1:1:2241:A:OP1	2.41	0.44
1:1:820:A:H4'	1:1:836:G:H22	1.82	0.44
1:1:1278:C:H2'	1:1:1279:G:H8	1.81	0.44
1:1:2698:U:H2'	1:1:2699:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:713:G:H2'	2:2:714:G:C8	2.52	0.44
8:D:173:THR:OG1	8:D:174:GLY:N	2.49	0.44
11:G:67:ALA:HA	11:G:70:GLU:HG2	1.99	0.44
12:H:3:LEU:HD23	12:H:6:GLN:H	1.82	0.44
12:H:14:GLU:HG3	12:H:57:ASN:HD21	1.82	0.44
1:1:1092:C:H2'	1:1:1093:G:C4	2.53	0.44
1:1:1105:U:H2'	1:1:1106:G:H8	1.83	0.44
1:1:1534:U:N3	1:1:1538:G:C6	2.80	0.44
1:1:2266:A:N6	1:1:2273:A:OP2	2.42	0.44
1:1:2816:G:N3	1:1:2883:A:O2'	2.46	0.44
2:2:1025:U:O2'	2:2:1026:G:N7	2.44	0.44
37:g:54:LEU:HB3	37:g:220:THR:HG21	1.99	0.44
37:g:93:ASN:OD1	37:g:93:ASN:N	2.44	0.44
43:m:40:LEU:HD21	43:m:129:VAL:HG21	1.99	0.44
45:o:15:HIS:HA	45:o:18:ILE:HG22	1.99	0.44
58:4:15:A:H61	58:4:334:A:H61	1.64	0.44
1:1:1286:A:N6	1:1:1329:U:O2	2.51	0.44
2:2:1011:C:H2'	2:2:1012:A:H8	1.83	0.44
2:2:1187:G:N2	49:s:100:SER:OG	2.43	0.44
2:2:1422:G:O2'	15:K:49:ARG:NH1	2.50	0.44
6:B:50:THR:OG1	6:B:51:THR:N	2.49	0.44
17:M:78:LEU:HD13	17:M:78:LEU:HA	1.82	0.44
30:Z:6:LYS:HB3	30:Z:6:LYS:HE2	1.80	0.44
33:c:44:ARG:HE	33:c:44:ARG:HB2	1.60	0.44
58:4:133:A:H2'	58:4:134:G:C8	2.52	0.44
1:1:302:C:H2'	1:1:303:G:H8	1.83	0.44
2:2:103:U:OP2	55:y:9:LYS:NZ	2.49	0.44
2:2:1004:A:H8	2:2:1024:G:H21	1.65	0.44
7:C:79:LEU:HD23	7:C:79:LEU:HA	1.87	0.44
9:E:93:GLY:H	9:E:96:MET:HE2	1.83	0.44
17:M:70:ASP:OD1	17:M:70:ASP:N	2.49	0.44
37:g:136:MET:HG2	37:g:139:ARG:HH12	1.82	0.44
38:h:135:LYS:HD2	38:h:139:GLN:HE21	1.81	0.44
46:p:109:ASN:HD21	56:z:5:LYS:HG2	1.82	0.44
52:v:72:SER:O	52:v:72:SER:OG	2.33	0.44
1:1:414:C:H2'	1:1:415:A:C8	2.53	0.44
1:1:956:G:O6	17:M:14:LYS:NZ	2.51	0.44
2:2:269:C:H2'	2:2:270:A:H8	1.82	0.44
2:2:380:G:N2	2:2:383:A:OP2	2.39	0.44
2:2:824:G:H2'	2:2:825:A:H8	1.82	0.44
2:2:861:G:O6	2:2:869:G:N2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1166:G:O2'	2:2:1169:A:N6	2.50	0.44
6:B:121:ASP:OD1	6:B:121:ASP:N	2.47	0.44
6:B:129:THR:OG1	6:B:191:THR:OG1	2.32	0.44
8:D:146:VAL:HG13	8:D:167:VAL:HG13	1.98	0.44
13:I:44:LYS:HD2	13:I:70:THR:HG22	1.99	0.44
37:g:100:MET:HE3	37:g:100:MET:HB2	1.77	0.44
39:i:9:LEU:HD23	39:i:9:LEU:HA	1.77	0.44
1:1:320:A:O2'	8:D:163:ASN:ND2	2.41	0.44
1:1:2107:G:H21	1:1:2183:A:H62	1.65	0.44
2:2:1072:G:H21	37:g:106:THR:HG21	1.81	0.44
25:U:33:LYS:HB3	25:U:64:ALA:HB1	2.00	0.44
58:4:211:C:N4	58:4:242:A:OP2	2.50	0.44
58:4:249:U:H2'	58:4:250:U:C6	2.53	0.44
1:1:519:U:H2'	1:1:520:G:H8	1.83	0.44
1:1:714:U:OP2	50:t:88:ARG:NH2	2.48	0.44
1:1:1288:G:OP2	1:1:1288:G:N2	2.47	0.44
1:1:1340:U:OP1	24:T:84:TYR:OH	2.25	0.44
1:1:1438:U:OP2	1:1:1552:A:N6	2.47	0.44
2:2:390:U:H2'	2:2:391:G:C8	2.53	0.44
5:7:64:C:H2'	5:7:65:A:C8	2.52	0.44
8:D:125:SER:O	8:D:137:LYS:NZ	2.46	0.44
32:b:40:ARG:HD2	32:b:40:ARG:HA	1.87	0.44
39:i:76:TYR:OH	39:i:205:SER:OG	2.35	0.44
41:k:12:PRO:HD2	41:k:54:LEU:HD21	1.99	0.44
57:5:35:ALA:O	57:5:37:GLN:NE2	2.51	0.44
1:1:302:C:H2'	1:1:303:G:C8	2.53	0.44
1:1:407:G:H2'	1:1:408:G:H8	1.83	0.44
1:1:598:U:H2'	1:1:599:A:H8	1.83	0.44
1:1:2077:A:OP1	1:1:2238:G:N2	2.43	0.44
1:1:2813:A:H2'	1:1:2814:A:H8	1.82	0.44
2:2:979:C:O2	49:s:59:ARG:NH2	2.50	0.44
2:2:1396:A:O2'	40:j:29:ARG:NH2	2.44	0.44
9:E:71:ARG:O	9:E:81:GLN:NE2	2.41	0.44
23:S:109:ASP:N	23:S:109:ASP:OD1	2.38	0.44
37:g:73:LYS:HE2	37:g:165:ASP:HB2	2.00	0.44
37:g:161:LEU:HD13	37:g:176:ALA:HB2	2.00	0.44
40:j:69:ARG:HG3	40:j:70:ASN:HD22	1.82	0.44
58:4:36:C:H2'	58:4:37:C:H5'	1.98	0.44
1:1:1548:A:H2'	1:1:1549:A:C8	2.52	0.44
1:1:2691:C:HO2'	1:1:2871:U:HO2'	1.54	0.44
2:2:390:U:H2'	2:2:391:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:404:G:O2'	2:2:498:A:N1	2.47	0.44
2:2:438:U:OP1	39:i:148:LYS:NZ	2.50	0.44
2:2:1479:C:H2'	2:2:1480:A:H8	1.82	0.44
6:B:66:ASP:OD2	6:B:102:ARG:NH1	2.49	0.44
42:l:47:LEU:HB3	42:l:58:GLU:HG2	2.00	0.44
47:q:74:LEU:HD21	47:q:104:CYS:HB3	2.00	0.44
49:s:58:SER:O	49:s:58:SER:OG	2.35	0.44
58:4:174:A:O2'	58:4:175:A:H5'	2.18	0.44
1:1:1715:G:N2	1:1:1744:A:OP2	2.40	0.43
1:1:2684:U:O4'	15:K:70:ARG:NH1	2.50	0.43
2:2:335:C:H2'	2:2:336:A:H8	1.82	0.43
2:2:1241:G:H2'	2:2:1242:G:H8	1.83	0.43
5:7:62:C:H2'	5:7:63:G:C8	2.53	0.43
9:E:52:ASN:HB2	9:E:150:ARG:HH22	1.82	0.43
11:G:65:ALA:HA	11:G:68:ARG:HD3	2.00	0.43
15:K:10:VAL:HG21	15:K:16:ALA:HB3	2.00	0.43
21:Q:66:ASN:OD1	21:Q:70:ARG:NE	2.38	0.43
58:4:243:G:H2'	58:4:244:G:C8	2.53	0.43
1:1:964:C:O2'	1:1:2273:A:N3	2.42	0.43
2:2:459:A:H2'	2:2:460:A:C8	2.53	0.43
2:2:1254:A:H2'	2:2:1255:G:C8	2.53	0.43
11:G:41:LYS:H	11:G:41:LYS:HD2	1.83	0.43
31:a:16:CYS:SG	31:a:17:SER:N	2.91	0.43
32:b:32:LYS:HG3	32:b:33:THR:HG23	2.00	0.43
1:1:414:C:H2'	1:1:415:A:H8	1.83	0.43
1:1:1085:A:H2'	1:1:1086:A:H4'	2.00	0.43
1:1:2002:G:H5''	18:N:9:GLN:HE21	1.84	0.43
2:2:203:G:N2	2:2:204:G:O6	2.44	0.43
2:2:261:U:OP2	55:y:71:LYS:NZ	2.51	0.43
2:2:1478:U:H2'	2:2:1479:C:C6	2.54	0.43
13:I:96:LYS:HD2	13:I:96:LYS:HA	1.74	0.43
40:j:45:ARG:HH11	40:j:71:MET:HE3	1.83	0.43
58:4:38:A:C5'	58:4:38:A:N3	2.81	0.43
58:4:190:A:H2'	58:4:191:A:C4	2.52	0.43
1:1:488:G:O2'	1:1:491:G:O6	2.32	0.43
1:1:559:G:N3	21:Q:56:GLN:NE2	2.65	0.43
1:1:1248:G:OP2	8:D:44:ARG:NH1	2.51	0.43
1:1:1426:G:O2'	1:1:1572:A:N6	2.51	0.43
1:1:1534:U:O2	1:1:1538:G:N2	2.51	0.43
1:1:2638:G:O2'	1:1:2775:G:N2	2.35	0.43
2:2:222:C:H2'	2:2:223:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:420:U:N3	2:2:422:C:O2	2.52	0.43
2:2:503:C:OP1	47:q:116:LYS:NZ	2.43	0.43
5:7:63:G:H2'	5:7:64:C:C6	2.53	0.43
8:D:118:LEU:HA	8:D:186:VAL:O	2.18	0.43
17:M:103:TYR:HB2	17:M:117:PHE:HE1	1.82	0.43
18:N:65:LEU:HA	18:N:65:LEU:HD12	1.83	0.43
19:O:45:SER:O	19:O:45:SER:OG	2.35	0.43
20:P:25:THR:HG23	20:P:87:LYS:HB2	2.00	0.43
25:U:47:LYS:HA	25:U:48:PRO:HD3	1.87	0.43
29:Y:4:LYS:HD3	29:Y:4:LYS:HA	1.75	0.43
39:i:98:LEU:HB2	39:i:135:TYR:HB3	2.00	0.43
40:j:85:VAL:HG23	40:j:96:MET:HG3	2.00	0.43
1:1:151:C:H2'	1:1:152:A:C8	2.54	0.43
1:1:242:G:O2'	1:1:254:G:O6	2.36	0.43
1:1:320:A:O2'	1:1:322:A:OP2	2.28	0.43
1:1:832:U:H2'	1:1:833:A:C8	2.54	0.43
1:1:1818:U:H2'	6:B:156:ARG:HG2	2.00	0.43
1:1:1952:A:N3	1:1:2560:A:O2'	2.42	0.43
2:2:416:G:H2'	2:2:417:G:H8	1.83	0.43
15:K:104:THR:OG1	15:K:105:ARG:N	2.51	0.43
37:g:95:ARG:HH11	37:g:97:LEU:HD23	1.84	0.43
42:l:103:TRP:CD1	42:l:137:LYS:HZ3	2.35	0.43
1:1:935:C:H2'	1:1:936:A:C8	2.53	0.43
1:1:1769:U:H2'	1:1:1770:G:H8	1.84	0.43
1:1:1866:A:N6	1:1:1875:G:O2'	2.52	0.43
1:1:2801:G:H2'	1:1:2802:G:H8	1.84	0.43
2:2:235:C:H2'	2:2:236:A:H8	1.83	0.43
2:2:501:C:H2'	2:2:502:A:H8	1.84	0.43
2:2:584:G:H2'	2:2:585:G:H8	1.83	0.43
5:7:67:A:H2'	5:7:68:G:C8	2.53	0.43
13:I:75:ALA:HA	13:I:78:LEU:HD12	2.00	0.43
14:J:99:ARG:HA	14:J:99:ARG:HD2	1.82	0.43
32:b:12:LYS:HA	32:b:12:LYS:HD3	1.82	0.43
47:q:53:CYS:HB3	47:q:67:ILE:HD11	1.99	0.43
58:4:151:C:H2'	58:4:152:C:C6	2.52	0.43
1:1:1038:G:H2'	1:1:1039:A:C8	2.54	0.43
1:1:2087:G:H2'	1:1:2088:A:H8	1.83	0.43
2:2:1149:C:H2'	2:2:1150:A:H8	1.84	0.43
5:7:64:C:H2'	5:7:65:A:H8	1.82	0.43
12:H:50:VAL:O	12:H:53:ARG:NH1	2.52	0.43
20:P:47:VAL:HG22	20:P:61:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:U:O2'	2:2:914:A:OP2	2.31	0.43
2:2:384:G:H2'	2:2:385:C:C6	2.53	0.43
8:D:1:MET:CB	8:D:14:VAL:O	2.65	0.43
11:G:117:LEU:HD23	11:G:118:PRO:HD2	2.00	0.43
21:Q:94:ILE:HG21	22:R:4:VAL:HG11	2.01	0.43
32:b:53:LYS:NZ	32:b:55:ILE:O	2.43	0.43
39:i:83:LYS:O	39:i:89:ASN:ND2	2.45	0.43
41:k:22:ILE:HG23	41:k:39:LEU:HD21	2.01	0.43
49:s:24:ARG:HH22	49:s:56:SER:HB2	1.84	0.43
1:1:329:G:O6	25:U:17:LYS:N	2.51	0.43
1:1:987:C:O2'	1:1:1000:A:N3	2.39	0.43
1:1:1534:U:O2	1:1:1538:G:C2	2.72	0.43
1:1:2291:U:H2'	1:1:2292:U:C6	2.53	0.43
2:2:1178:G:OP1	44:n:95:ARG:NH1	2.51	0.43
2:2:1464:U:OP1	20:P:109:ARG:NH1	2.52	0.43
2:2:1533:C:H4'	2:2:1534:A:C8	2.54	0.43
9:E:26:MET:HB3	9:E:26:MET:HE2	1.80	0.43
13:I:133:ARG:HG3	13:I:138:VAL:HG13	2.00	0.43
14:J:98:GLU:HB2	14:J:124:VAL:HG23	2.01	0.43
17:M:38:ARG:HB2	17:M:98:PRO:HD3	2.01	0.43
33:c:29:THR:HG23	33:c:30:LYS:HG2	2.00	0.43
45:o:10:LEU:HD13	45:o:22:THR:HG22	2.01	0.43
48:r:48:LEU:HD23	48:r:48:LEU:HA	1.93	0.43
58:4:31:G:H3'	58:4:35:C:H41	1.84	0.43
2:2:683:G:O6	2:2:708:C:N4	2.52	0.43
2:2:909:A:N3	2:2:1413:A:O2'	2.49	0.43
2:2:946:A:H2'	2:2:947:G:H8	1.83	0.43
18:N:90:ARG:HH12	18:N:116:VAL:HB	1.83	0.43
29:Y:10:SER:OG	29:Y:11:VAL:N	2.52	0.43
42:l:111:ARG:HH21	42:l:122:ASN:HD22	1.67	0.43
54:x:50:ALA:HB1	54:x:57:HIS:HB3	1.99	0.43
58:4:129:G:H2'	58:4:131:U:OP2	2.19	0.43
1:1:300:A:H2'	1:1:334:C:H1'	2.00	0.42
1:1:452:G:H2'	1:1:453:A:H8	1.84	0.42
1:1:1074:G:H2'	1:1:1075:C:C6	2.54	0.42
1:1:1086:A:H2	12:H:37:LYS:HZ2	1.67	0.42
1:1:1992:G:N1	1:1:1996:C:O2	2.52	0.42
2:2:110:C:O2'	51:u:25:ARG:O	2.32	0.42
8:D:151:GLY:HA3	8:D:191:ASP:HB2	2.01	0.42
15:K:35:VAL:HG22	15:K:69:VAL:HG11	2.00	0.42
15:K:38:ILE:HD11	15:K:112:PHE:HZ	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:6:ILE:HG12	41:k:89:VAL:HG22	2.01	0.42
54:x:12:ASP:OD2	54:x:35:SER:OG	2.34	0.42
55:y:54:MET:HE3	55:y:54:MET:HB3	1.94	0.42
58:4:153:U:C2	58:4:163:G:N1	2.86	0.42
1:1:13:A:O2'	1:1:15:G:N7	2.42	0.42
1:1:373:U:H2'	1:1:374:A:C8	2.54	0.42
2:2:269:C:H2'	2:2:270:A:C8	2.54	0.42
2:2:321:A:H2'	2:2:322:C:C6	2.54	0.42
2:2:375:U:OP1	51:u:70:ARG:NH1	2.52	0.42
5:7:7:A:O2'	5:7:21:A:N1	2.46	0.42
22:R:85:LYS:HB2	22:R:85:LYS:HE3	1.74	0.42
39:i:100:ASN:OD1	39:i:111:ARG:NH1	2.33	0.42
49:s:89:MET:HE1	49:s:98:LYS:HD2	1.99	0.42
56:z:63:GLU:HG2	56:z:67:ARG:HE	1.84	0.42
1:1:1060:U:P	13:I:75:ALA:H	2.42	0.42
1:1:1085:A:HO2'	1:1:1104:C:HO2'	1.67	0.42
1:1:1523:U:H3'	1:1:1524:G:H8	1.85	0.42
1:1:2250:G:H8	1:1:2496:C:H5''	1.84	0.42
2:2:217:C:H2'	2:2:218:U:C6	2.54	0.42
2:2:1309:G:OP1	48:r:87:ARG:NH1	2.53	0.42
2:2:1367:C:OP2	44:n:114:LYS:NZ	2.52	0.42
33:c:10:LYS:HB2	33:c:10:LYS:HE3	1.85	0.42
45:o:25:ILE:HD12	45:o:25:ILE:HA	1.89	0.42
57:5:56:VAL:H	57:5:111:VAL:HG22	1.84	0.42
58:4:164:G:O2'	58:4:165:A:OP2	2.35	0.42
58:4:243:G:H2'	58:4:244:G:H8	1.84	0.42
1:1:527:C:HO2'	1:1:2779:U:HO2'	1.58	0.42
1:1:532:A:N1	1:1:2035:G:N2	2.68	0.42
1:1:747:5MU:O2'	23:S:88:ARG:NH1	2.52	0.42
1:1:851:C:H2'	1:1:852:U:C6	2.54	0.42
1:1:1089:A:O2'	1:1:1090:A:N7	2.47	0.42
1:1:2247:A:H2'	1:1:2248:C:C6	2.53	0.42
1:1:2328:A:H2'	1:1:2329:U:H6	1.84	0.42
6:B:78:VAL:HG21	6:B:110:LEU:HD21	2.00	0.42
11:G:78:VAL:HG21	11:G:103:VAL:HG12	2.01	0.42
22:R:101:ILE:HD13	22:R:101:ILE:HA	1.92	0.42
39:i:152:GLN:HB2	39:i:155:VAL:HG23	2.01	0.42
40:j:103:THR:O	40:j:103:THR:OG1	2.36	0.42
41:k:12:PRO:O	41:k:44:ARG:NH2	2.43	0.42
58:4:65:U:H2'	58:4:66:C:C6	2.54	0.42
58:4:227:C:H2'	58:4:228:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:385:C:HO2'	1:1:388:G:H22	1.66	0.42
1:1:2848:G:HO2'	1:1:2867:G:H22	1.67	0.42
2:2:647:C:H2'	2:2:648:A:C8	2.54	0.42
3:3:111:U:H2'	3:3:112:G:H8	1.83	0.42
11:G:57:LYS:HB3	11:G:57:LYS:HE3	1.83	0.42
12:H:23:LEU:HD13	12:H:87:GLU:HG3	2.02	0.42
17:M:5:LYS:HB2	17:M:5:LYS:HE3	1.83	0.42
18:N:71:ARG:HA	18:N:71:ARG:HD2	1.79	0.42
43:m:77:ARG:HD2	43:m:77:ARG:HA	1.68	0.42
45:o:26:VAL:HG22	45:o:30:LYS:HE2	2.02	0.42
48:r:26:GLY:O	48:r:30:SER:HB3	2.19	0.42
58:4:163:G:H2'	58:4:164:G:H5'	2.02	0.42
58:4:219:G:H2'	58:4:220:G:H8	1.84	0.42
1:1:1463:C:H2'	1:1:1464:G:C8	2.54	0.42
2:2:1289:A:N1	2:2:1371:G:O2'	2.49	0.42
2:2:1293:C:H2'	2:2:1294:G:H8	1.84	0.42
5:7:63:G:H5''	27:W:11:ARG:HH12	1.85	0.42
40:j:49:GLY:HA3	40:j:67:ALA:HB2	2.02	0.42
50:t:50:HIS:HA	50:t:53:ARG:HB3	2.01	0.42
53:w:71:THR:H	53:w:74:HIS:CE1	2.37	0.42
56:z:4:ILE:HD13	56:z:4:ILE:HA	1.91	0.42
58:4:192:A:H2'	58:4:193:A:C8	2.54	0.42
58:4:219:G:H2'	58:4:220:G:C8	2.55	0.42
1:1:278:A:N6	1:1:362:A:N7	2.67	0.42
1:1:1315:C:H2'	1:1:1316:U:H6	1.84	0.42
1:1:1316:U:H2'	1:1:1317:G:H8	1.85	0.42
1:1:2204:G:H4'	6:B:150:LYS:HE2	2.02	0.42
2:2:398:U:H2'	2:2:399:G:C8	2.55	0.42
2:2:461:A:H2'	2:2:462:G:C8	2.53	0.42
2:2:952:U:H2'	2:2:953:G:H8	1.84	0.42
2:2:1083:U:O2'	2:2:1102:A:OP2	2.31	0.42
2:2:1402:4OC:H2'	2:2:1403:C:O4'	2.20	0.42
19:O:35:ILE:H	19:O:53:THR:HG22	1.83	0.42
48:r:90:ARG:HG2	48:r:97:VAL:HA	2.01	0.42
58:4:165:A:H3'	58:4:166:C:C6	2.55	0.42
1:1:475:C:N3	1:1:479:A:N7	2.67	0.42
1:1:742:A:H2'	1:1:743:A:C8	2.55	0.42
1:1:1730:C:O2	1:1:1731:G:N1	2.53	0.42
2:2:501:C:H2'	2:2:502:A:C8	2.55	0.42
2:2:714:G:H2'	2:2:715:A:C8	2.54	0.42
2:2:965:U:H4'	2:2:966:2MG:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1040:U:H2'	2:2:1041:G:H8	1.85	0.42
7:C:38:LYS:HD3	7:C:45:TYR:HE1	1.85	0.42
13:I:71:LYS:NZ	13:I:72:THR:O	2.53	0.42
16:L:4:ASN:OD1	16:L:4:ASN:N	2.52	0.42
24:T:67:VAL:HG22	24:T:76:ARG:HD3	2.02	0.42
41:k:39:LEU:HD13	41:k:62:MET:HB3	2.00	0.42
58:4:34:A:H2'	58:4:35:C:H5'	2.02	0.42
1:1:642:U:N3	1:1:645:C:OP2	2.49	0.42
1:1:1079:C:H2'	1:1:1080:A:H8	1.85	0.42
1:1:1434:A:H2'	1:1:1435:G:C8	2.55	0.42
1:1:2133:G:N1	1:1:2157:G:N7	2.68	0.42
1:1:2547:A:H2'	1:1:2548:U:C6	2.54	0.42
2:2:335:C:H2'	2:2:336:A:C8	2.55	0.42
6:B:18:LYS:HE3	6:B:18:LYS:HB2	1.84	0.42
9:E:56:ASP:O	9:E:60:ILE:HG12	2.20	0.42
10:F:152:ARG:HB2	10:F:162:VAL:HG23	2.02	0.42
26:V:17:SER:HB2	26:V:21:ARG:HH12	1.84	0.42
45:o:7:ARG:O	45:o:100:ILE:HA	2.20	0.42
51:u:45:GLU:H	51:u:45:GLU:HG3	1.69	0.42
57:5:32:ALA:HB1	57:5:90:LEU:HB3	2.02	0.42
57:5:40:GLU:HG2	57:5:43:SER:HB2	2.02	0.42
58:4:341:U:C3'	58:4:341:U:C6	3.03	0.42
1:1:184:C:H2'	1:1:185:G:C8	2.55	0.42
1:1:1309:G:HO2'	1:1:1611:C:HO2'	1.62	0.42
1:1:1373:A:H4'	1:1:2212:A:C8	2.54	0.42
1:1:2372:U:H2'	1:1:2373:G:H8	1.85	0.42
1:1:2500:U:O2'	1:1:2504:PSU:OP1	2.37	0.42
2:2:17:U:H2'	2:2:18:C:C6	2.54	0.42
2:2:41:G:H2'	2:2:42:G:C8	2.55	0.42
2:2:533:A:O2'	2:2:535:A:OP2	2.30	0.42
2:2:1095:U:P	2:2:1108:G:H1	2.43	0.42
6:B:28:LYS:HD3	6:B:28:LYS:HA	1.82	0.42
15:K:64:ARG:HB2	15:K:83:ALA:HB3	2.02	0.42
24:T:29:THR:HA	24:T:86:THR:HA	2.02	0.42
37:g:121:SER:OG	37:g:122:GLN:N	2.53	0.42
58:4:296:U:H2'	58:4:297:G:H8	1.85	0.42
58:4:342:U:O5'	58:4:342:U:C6	2.69	0.42
1:1:601:C:O2'	1:1:605:G:OP1	2.38	0.41
1:1:863:A:H2'	1:1:864:G:C8	2.54	0.41
1:1:1548:A:H2'	1:1:1549:A:H8	1.85	0.41
2:2:235:C:H2'	2:2:236:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1064:G:O2'	2:2:1190:G:N2	2.53	0.41
12:H:97:LYS:HD3	12:H:97:LYS:HA	1.87	0.41
15:K:108:ARG:HA	15:K:116:ILE:HD13	2.02	0.41
34:d:34:ARG:NE	34:d:42:LEU:O	2.53	0.41
45:o:11:LYS:HG2	45:o:71:LEU:HG	2.02	0.41
47:q:52:VAL:HG11	47:q:93:VAL:HG21	2.02	0.41
51:u:15:PRO:HG2	51:u:41:PRO:HG3	2.02	0.41
54:x:17:LYS:HA	54:x:17:LYS:HD2	1.81	0.41
57:5:37:GLN:HG3	58:4:333:G:C8	2.55	0.41
58:4:126:C:H2'	58:4:127:C:C6	2.55	0.41
1:1:1059:G:N3	13:I:127:SER:HB3	2.35	0.41
1:1:2102:G:O6	1:1:2187:U:C2	2.72	0.41
1:1:2173:A:H2'	1:1:2174:C:C6	2.55	0.41
1:1:2349:G:OP1	35:e:45:ARG:NH2	2.37	0.41
2:2:321:A:H2'	2:2:322:C:H6	1.85	0.41
3:3:95:U:H2'	3:3:96:G:C8	2.55	0.41
16:L:14:LYS:HB3	16:L:14:LYS:HE3	1.83	0.41
16:L:85:VAL:HG11	16:L:90:VAL:HG22	2.02	0.41
38:h:157:LEU:HA	38:h:157:LEU:HD23	1.84	0.41
45:o:62:ARG:HH11	45:o:62:ARG:HD2	1.73	0.41
1:1:1322:A:N1	1:1:1333:G:O2'	2.44	0.41
9:E:28:VAL:HA	9:E:29:PRO:HD3	1.95	0.41
10:F:11:VAL:HA	10:F:12:PRO:HD3	1.93	0.41
14:J:78:THR:OG1	14:J:79:GLY:N	2.53	0.41
58:4:257:U:H4'	58:4:258:G:OP1	2.19	0.41
1:1:534:U:O2'	21:Q:49:ASP:OD2	2.33	0.41
1:1:782:A:C8	6:B:220:VAL:HG21	2.55	0.41
1:1:1445:G:O6	1:1:1466:U:C2	2.73	0.41
1:1:1794:A:H2'	1:1:1795:C:C6	2.55	0.41
1:1:2443:C:H2'	1:1:2444:G:H8	1.84	0.41
2:2:333:U:OP1	55:y:2:ALA:N	2.53	0.41
2:2:881:G:N7	47:q:6:GLN:NE2	2.66	0.41
2:2:1068:G:N7	2:2:1094:G:O2'	2.44	0.41
2:2:1179:A:H2'	2:2:1180:A:C8	2.56	0.41
9:E:105:THR:HG23	9:E:106:ILE:HG13	2.02	0.41
16:L:100:ILE:HD13	16:L:100:ILE:HA	1.94	0.41
17:M:112:LEU:HA	17:M:112:LEU:HD12	1.83	0.41
23:S:12:SER:OG	23:S:13:SER:N	2.53	0.41
38:h:114:LYS:HA	38:h:114:LYS:HD2	1.86	0.41
40:j:115:LEU:HD23	40:j:115:LEU:HA	1.90	0.41
58:4:194:G:C2'	58:4:195:A:H5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:52:A:H2'	1:1:53:A:C8	2.56	0.41
1:1:578:G:O2'	1:1:580:U:OP2	2.37	0.41
1:1:1682:G:OP2	1:1:1699:G:N2	2.43	0.41
1:1:1734:G:H2'	1:1:1735:A:C8	2.55	0.41
1:1:1789:A:H5'	6:B:220:VAL:HG22	2.02	0.41
1:1:2114:A:H61	1:1:2171:A:H61	1.68	0.41
1:1:2285:C:OP1	33:c:26:ASN:ND2	2.48	0.41
1:1:2291:U:H3	1:1:2341:G:H1	1.67	0.41
2:2:409:U:O2	2:2:433:G:N2	2.48	0.41
2:2:735:C:H5'	53:w:60:LYS:HD3	2.02	0.41
2:2:1227:A:H2'	48:r:116:ILE:HD11	2.01	0.41
2:2:1507:A:H2'	2:2:1508:A:C8	2.56	0.41
17:M:26:VAL:HG13	17:M:104:GLU:HG2	2.02	0.41
26:V:75:GLN:HB2	26:V:92:VAL:HG23	2.02	0.41
30:Z:35:THR:O	30:Z:35:THR:OG1	2.38	0.41
41:k:41:ASP:OD1	41:k:58:HIS:NE2	2.53	0.41
58:4:279:C:H2'	58:4:280:A:H5''	2.02	0.41
1:1:598:U:H2'	1:1:599:A:C8	2.55	0.41
1:1:1057:A:H2'	1:1:1058:U:C6	2.56	0.41
1:1:2802:G:H2'	1:1:2803:G:H8	1.85	0.41
2:2:335:C:O2'	2:2:1433:A:N3	2.40	0.41
2:2:458:U:H2'	2:2:459:A:C8	2.55	0.41
2:2:844:G:H1	2:2:846:G:H1'	1.86	0.41
2:2:1130:A:H61	2:2:1144:G:H1'	1.86	0.41
22:R:34:GLU:OE2	22:R:60:LYS:NZ	2.51	0.41
29:Y:19:LEU:HD21	29:Y:23:ARG:HH21	1.86	0.41
42:l:23:LEU:HD12	42:l:23:LEU:HA	1.86	0.41
44:n:75:GLN:O	44:n:79:ILE:HG12	2.20	0.41
45:o:7:ARG:HD3	45:o:73:LEU:HD11	2.01	0.41
48:r:65:VAL:HG12	48:r:66:GLU:H	1.84	0.41
57:5:118:TRP:CD1	57:5:120:ASN:H	2.38	0.41
58:4:38:A:C3'	58:4:39:A:H4'	2.51	0.41
58:4:40:G:N3	58:4:40:G:C2'	2.83	0.41
58:4:133:A:H2'	58:4:134:G:H8	1.86	0.41
58:4:227:C:H2'	58:4:228:G:H8	1.85	0.41
1:1:78:U:O2	1:1:108:G:N2	2.42	0.41
1:1:419:U:H2'	1:1:420:C:C6	2.55	0.41
1:1:979:A:H2'	1:1:982:C:H42	1.86	0.41
1:1:1061:U:O4	13:I:11:GLN:N	2.45	0.41
1:1:1076:C:H1'	13:I:92:PRO:HD2	2.03	0.41
1:1:1219:U:H2'	1:1:1220:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1636:U:H2'	1:1:1637:A:C8	2.55	0.41
1:1:1689:A:H2'	1:1:1690:A:C8	2.56	0.41
2:2:1101:A:N6	37:g:175:GLU:OE1	2.53	0.41
2:2:1250:A:H2'	2:2:1251:A:C8	2.56	0.41
2:2:1322:C:OP1	54:x:78:ARG:NH2	2.54	0.41
6:B:121:ASP:HB3	11:G:91:PHE:CZ	2.56	0.41
20:P:26:VAL:HA	20:P:85:SER:O	2.20	0.41
37:g:64:LYS:HA	37:g:64:LYS:HD3	1.94	0.41
43:m:22:LYS:HA	43:m:22:LYS:HD2	1.82	0.41
58:4:15:A:O2'	58:4:16:U:OP2	2.32	0.41
58:4:204:G:O2'	58:4:205:G:OP2	2.37	0.41
58:4:304:C:H2'	58:4:305:A:C8	2.56	0.41
1:1:833:A:H2'	1:1:834:G:C8	2.56	0.41
1:1:2160:C:N4	1:1:2161:C:O2	2.54	0.41
1:1:2467:C:O2	17:M:123:LYS:NZ	2.46	0.41
2:2:556:C:H2'	2:2:557:G:H8	1.86	0.41
2:2:1100:C:P	56:z:69:ARG:HH11	2.44	0.41
7:C:24:VAL:HA	7:C:189:VAL:O	2.20	0.41
8:D:109:LEU:HD23	8:D:109:LEU:HA	1.91	0.41
13:I:100:ILE:HG13	13:I:101:SER:H	1.86	0.41
14:J:2:LYS:HE3	14:J:2:LYS:HB2	1.85	0.41
18:N:79:LEU:HD23	18:N:83:LEU:HB2	2.01	0.41
21:Q:49:ASP:HA	21:Q:52:GLN:HB2	2.02	0.41
31:a:8:LYS:HB3	31:a:8:LYS:HE3	1.75	0.41
38:h:6:HIS:HA	38:h:7:PRO:HD3	1.96	0.41
40:j:115:LEU:HD13	40:j:123:VAL:HG21	2.03	0.41
48:r:16:VAL:HG13	48:r:34:LEU:HD12	2.02	0.41
57:5:59:ARG:HG3	57:5:61:GLY:H	1.85	0.41
58:4:139:C:H2'	58:4:140:U:C6	2.55	0.41
58:4:284:G:H4'	58:4:285:A:O5'	2.21	0.41
58:4:311:U:O2'	58:4:312:A:H5'	2.21	0.41
1:1:84:A:N1	1:1:98:G:O2'	2.48	0.41
1:1:953:G:O2'	1:1:2266:A:OP1	2.37	0.41
1:1:1071:G:H2'	1:1:1072:C:C6	2.55	0.41
1:1:1131:G:O2'	1:1:2025:C:O2'	2.33	0.41
1:1:1534:U:C2	1:1:1538:G:N1	2.89	0.41
1:1:2327:A:H2'	1:1:2328:A:C8	2.55	0.41
2:2:112:G:N2	2:2:330:C:N3	2.69	0.41
2:2:199:A:H2'	2:2:200:G:H8	1.85	0.41
2:2:1100:C:H3'	37:g:95:ARG:HH21	1.86	0.41
7:C:125:TRP:CD1	7:C:160:LYS:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:52:LEU:HD13	13:I:73:PRO:HG2	2.03	0.41
18:N:59:SER:O	18:N:63:ARG:HB2	2.21	0.41
19:O:30:ARG:HH21	19:O:97:PHE:HB3	1.85	0.41
21:Q:105:ALA:HB1	22:R:40:MET:HE1	2.03	0.41
22:R:3:ALA:HA	22:R:40:MET:O	2.20	0.41
22:R:75:VAL:HG22	22:R:86:GLN:HG3	2.02	0.41
31:a:15:SER:O	31:a:33:ASN:HA	2.20	0.41
31:a:22:MET:HE3	31:a:22:MET:HB2	1.91	0.41
39:i:177:LYS:HB2	39:i:177:LYS:HE2	1.85	0.41
44:n:28:ILE:HG23	44:n:63:LEU:HD11	2.02	0.41
44:n:98:LEU:HD23	44:n:98:LEU:HA	1.93	0.41
49:s:6:MET:SD	49:s:9:ARG:NH2	2.93	0.41
50:t:23:GLY:O	50:t:28:GLN:NE2	2.54	0.41
54:x:20:GLU:HA	54:x:23:VAL:HG12	2.03	0.41
57:5:67:GLY:HA2	57:5:85:THR:HB	2.03	0.41
58:4:45:A:O2'	58:4:46:U:H5'	2.21	0.41
58:4:159:C:H2'	58:4:160:U:C6	2.56	0.41
1:1:631:A:N3	1:1:2415:G:O2'	2.46	0.41
1:1:1434:A:H2'	1:1:1435:G:H8	1.85	0.41
1:1:1504:A:H2'	1:1:1505:A:C8	2.56	0.41
1:1:1915:3TD:H2'	1:1:1916:A:H8	1.85	0.41
1:1:2081:U:H2'	1:1:2082:A:H8	1.86	0.41
1:1:2314:A:OP1	9:E:88:LYS:NZ	2.53	0.41
2:2:815:A:N7	2:2:1509:C:O2'	2.47	0.41
2:2:900:A:H2'	2:2:901:A:C8	2.56	0.41
2:2:977:A:OP1	49:s:61:ARG:NH2	2.43	0.41
13:I:63:ASP:OD1	13:I:63:ASP:N	2.54	0.41
15:K:76:VAL:HG22	20:P:73:VAL:HG12	2.03	0.41
17:M:1:MET:HB2	17:M:2:LEU:H	1.69	0.41
46:p:108:THR:OG1	46:p:109:ASN:N	2.54	0.41
50:t:11:ILE:HD13	50:t:11:ILE:HA	1.94	0.41
58:4:140:U:H2'	58:4:141:C:C6	2.55	0.41
1:1:107:G:H2'	1:1:108:G:H8	1.85	0.40
1:1:1563:U:H2'	1:1:1564:C:C6	2.56	0.40
1:1:2393:U:H5''	16:L:62:PRO:HB3	2.02	0.40
2:2:94:G:H4'	2:2:95:C:H5'	2.02	0.40
2:2:411:A:H4'	2:2:412:A:H5'	2.04	0.40
2:2:578:C:H2'	2:2:579:A:H8	1.86	0.40
2:2:744:C:H2'	2:2:745:G:C8	2.56	0.40
2:2:1149:C:H2'	2:2:1150:A:C8	2.56	0.40
2:2:1207:2MG:H2'	2:2:1208:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:118:LEU:HD23	8:D:120:VAL:HG22	2.02	0.40
13:I:89:SER:OG	13:I:95:ASP:OD1	2.28	0.40
14:J:17:VAL:HG23	14:J:137:PRO:HB2	2.03	0.40
15:K:1:MET:HE3	15:K:67:LYS:HG2	2.02	0.40
18:N:2:ARG:HE	18:N:2:ARG:HB3	1.78	0.40
23:S:29:VAL:HB	23:S:55:ILE:HD11	2.02	0.40
38:h:152:GLU:HA	38:h:166:GLU:O	2.21	0.40
40:j:62:LYS:HB2	40:j:62:LYS:HE3	1.89	0.40
57:5:31:GLU:HG3	57:5:124:LYS:HE2	2.03	0.40
58:4:290:A:H4'	58:4:291:A:H5'	2.03	0.40
1:1:414:C:O3'	1:1:1878:G:N2	2.53	0.40
1:1:1219:U:H2'	1:1:1220:G:C8	2.56	0.40
1:1:2448:A:H3'	1:1:2449:U:H2'	2.03	0.40
2:2:526:C:H2'	2:2:527:7MG:H4'	2.03	0.40
2:2:1055:A:O2'	38:h:161:GLU:O	2.35	0.40
3:3:93:C:H2'	3:3:94:A:H8	1.86	0.40
38:h:73:PRO:O	38:h:77:ILE:HG13	2.21	0.40
43:m:48:ASP:O	43:m:62:THR:OG1	2.34	0.40
46:p:122:ARG:HA	46:p:123:PRO:HD3	1.94	0.40
47:q:65:SER:HB2	47:q:95:TYR:HB2	2.03	0.40
58:4:21:C:H2'	58:4:22:G:H8	1.86	0.40
58:4:168:G:H2'	58:4:169:G:C8	2.55	0.40
58:4:350:C:H2'	58:4:351:G:C8	2.57	0.40
1:1:2250:G:N3	1:1:2250:G:H5'	2.36	0.40
1:1:2684:U:OP2	20:P:51:ARG:NH1	2.54	0.40
2:2:564:C:C4	52:v:33:ILE:HD11	2.56	0.40
9:E:4:LEU:HD23	9:E:4:LEU:HA	1.95	0.40
9:E:46:ASP:OD1	9:E:46:ASP:N	2.55	0.40
10:F:99:LYS:HA	10:F:99:LYS:HD3	1.79	0.40
19:O:62:LEU:HD23	19:O:70:ALA:HB2	2.03	0.40
31:a:30:HIS:ND1	31:a:31:ASP:O	2.40	0.40
48:r:117:LYS:HB2	48:r:117:LYS:HE2	1.90	0.40
49:s:46:LEU:O	49:s:50:THR:HG23	2.21	0.40
58:4:63:C:C2'	58:4:64:C:H5'	2.52	0.40
58:4:311:U:H2'	58:4:312:A:C8	2.53	0.40
58:4:331:C:C2'	58:4:332:G:H5'	2.50	0.40
1:1:155:A:H2'	1:1:156:A:C8	2.56	0.40
1:1:700:G:O2'	1:1:1632:A:N3	2.53	0.40
1:1:704:G:O2'	1:1:726:G:N1	2.50	0.40
1:1:988:A:C8	30:Z:14:ILE:HD12	2.57	0.40
1:1:1164:C:H2'	1:1:1165:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1485:U:H2'	1:1:1486:U:C6	2.56	0.40
1:1:2637:U:O4	1:1:2776:A:N7	2.54	0.40
1:1:2649:C:H2'	1:1:2650:U:C6	2.56	0.40
2:2:1130:A:H2'	2:2:1131:G:C8	2.57	0.40
2:2:1427:C:H2'	2:2:1428:A:C8	2.56	0.40
17:M:118:LYS:HE3	17:M:118:LYS:HB2	1.90	0.40
23:S:23:LEU:HD23	23:S:23:LEU:HA	1.89	0.40
37:g:68:LEU:HD22	37:g:158:PRO:HG3	2.03	0.40
44:n:19:VAL:HG22	44:n:65:ILE:HG12	2.03	0.40
54:x:30:PRO:HA	54:x:48:THR:HG23	2.04	0.40
58:4:3:G:H2'	58:4:4:G:H8	1.87	0.40
58:4:255:A:H2'	58:4:256:G:C8	2.57	0.40
1:1:1054:A:O3'	12:H:31:ARG:HG3	2.21	0.40
1:1:2118:U:H5	1:1:2147:A:H2	1.70	0.40
1:1:2119:A:N6	1:1:2169:A:O2'	2.55	0.40
1:1:2514:U:H4'	14:J:81:ILE:HG12	2.02	0.40
1:1:2591:C:H2'	1:1:2592:G:C8	2.56	0.40
2:2:568:G:O2'	2:2:574:A:N1	2.46	0.40
2:2:826:C:H5'	43:m:13:ARG:HH21	1.86	0.40
2:2:1316:G:N1	2:2:1319:A:OP2	2.55	0.40
2:2:1413:A:H2	2:2:1487:G:H22	1.69	0.40
14:J:114:LEU:HD12	14:J:114:LEU:HA	1.88	0.40
27:W:70:GLU:HG3	27:W:79:PHE:HB2	2.03	0.40
37:g:35:ARG:HB2	37:g:40:ILE:HD13	2.04	0.40
46:p:21:ALA:HB3	46:p:84:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	6	21/23 (91%)	16 (76%)	5 (24%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	269/271 (99%)	240 (89%)	29 (11%)	0	100	100
7	C	205/207 (99%)	182 (89%)	23 (11%)	0	100	100
8	D	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
9	E	175/177 (99%)	156 (89%)	17 (10%)	2 (1%)	11	42
10	F	173/175 (99%)	153 (88%)	20 (12%)	0	100	100
11	G	146/148 (99%)	131 (90%)	15 (10%)	0	100	100
12	H	128/130 (98%)	104 (81%)	24 (19%)	0	100	100
13	I	133/135 (98%)	113 (85%)	20 (15%)	0	100	100
14	J	140/142 (99%)	126 (90%)	14 (10%)	0	100	100
15	K	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
16	L	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
17	M	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
18	N	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
19	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
20	P	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
21	Q	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
22	R	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
23	S	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
24	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
25	U	99/101 (98%)	81 (82%)	18 (18%)	0	100	100
26	V	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
27	W	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
28	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
29	Y	60/62 (97%)	60 (100%)	0	0	100	100
30	Z	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
31	a	64/66 (97%)	58 (91%)	6 (9%)	0	100	100
32	b	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
33	c	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
34	d	43/45 (96%)	38 (88%)	5 (12%)	0	100	100
35	e	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	7	35
36	f	36/38 (95%)	33 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	g	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
38	h	206/208 (99%)	190 (92%)	16 (8%)	0	100	100
39	i	203/205 (99%)	190 (94%)	13 (6%)	0	100	100
40	j	154/156 (99%)	140 (91%)	14 (9%)	0	100	100
41	k	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
42	l	150/152 (99%)	137 (91%)	13 (9%)	0	100	100
43	m	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
44	n	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
45	o	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
46	p	114/116 (98%)	101 (89%)	13 (11%)	0	100	100
47	q	119/122 (98%)	111 (93%)	8 (7%)	0	100	100
48	r	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
49	s	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
50	t	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
51	u	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
52	v	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
53	w	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
54	x	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
55	y	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
56	z	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
57	5	116/118 (98%)	89 (77%)	27 (23%)	0	100	100
All	All	5985/6092 (98%)	5440 (91%)	542 (9%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	E	123	ASP
35	e	32	ILE
9	E	177	PHE

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	
6	B	216/216 (100%)	216 (100%)	0	100	100
7	C	163/163 (100%)	162 (99%)	1 (1%)	78	79
8	D	165/165 (100%)	165 (100%)	0	100	100
9	E	148/148 (100%)	148 (100%)	0	100	100
10	F	136/136 (100%)	133 (98%)	3 (2%)	45	63
11	G	113/113 (100%)	112 (99%)	1 (1%)	70	75
12	H	99/99 (100%)	97 (98%)	2 (2%)	48	64
13	I	104/104 (100%)	102 (98%)	2 (2%)	50	65
14	J	116/116 (100%)	116 (100%)	0	100	100
15	K	104/104 (100%)	101 (97%)	3 (3%)	37	57
16	L	102/102 (100%)	101 (99%)	1 (1%)	68	74
17	M	108/108 (100%)	106 (98%)	2 (2%)	50	65
18	N	99/99 (100%)	98 (99%)	1 (1%)	68	74
19	O	85/85 (100%)	85 (100%)	0	100	100
20	P	98/98 (100%)	97 (99%)	1 (1%)	68	74
21	Q	89/89 (100%)	89 (100%)	0	100	100
22	R	84/84 (100%)	83 (99%)	1 (1%)	63	72
23	S	92/92 (100%)	91 (99%)	1 (1%)	65	73
24	T	81/81 (100%)	81 (100%)	0	100	100
25	U	83/83 (100%)	81 (98%)	2 (2%)	43	61
26	V	78/78 (100%)	77 (99%)	1 (1%)	61	71
27	W	57/57 (100%)	57 (100%)	0	100	100
28	X	67/67 (100%)	67 (100%)	0	100	100
29	Y	54/54 (100%)	53 (98%)	1 (2%)	50	65
30	Z	47/47 (100%)	47 (100%)	0	100	100
31	a	59/59 (100%)	59 (100%)	0	100	100
32	b	46/46 (100%)	46 (100%)	0	100	100
33	c	46/46 (100%)	46 (100%)	0	100	100
34	d	37/37 (100%)	37 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	e	51/51 (100%)	51 (100%)	0	100	100
36	f	34/34 (100%)	34 (100%)	0	100	100
37	g	187/187 (100%)	186 (100%)	1 (0%)	81	80
38	h	171/171 (100%)	170 (99%)	1 (1%)	78	79
39	i	172/172 (100%)	171 (99%)	1 (1%)	78	79
40	j	119/119 (100%)	117 (98%)	2 (2%)	53	67
41	k	91/91 (100%)	89 (98%)	2 (2%)	45	63
42	l	125/125 (100%)	124 (99%)	1 (1%)	73	76
43	m	104/104 (100%)	102 (98%)	2 (2%)	50	65
44	n	105/105 (100%)	104 (99%)	1 (1%)	68	74
45	o	86/86 (100%)	85 (99%)	1 (1%)	63	72
46	p	89/89 (100%)	89 (100%)	0	100	100
47	q	102/102 (100%)	101 (99%)	1 (1%)	68	74
48	r	94/94 (100%)	93 (99%)	1 (1%)	65	73
49	s	83/83 (100%)	83 (100%)	0	100	100
50	t	75/75 (100%)	75 (100%)	0	100	100
51	u	65/65 (100%)	64 (98%)	1 (2%)	57	68
52	v	74/74 (100%)	74 (100%)	0	100	100
53	w	57/57 (100%)	57 (100%)	0	100	100
54	x	72/72 (100%)	72 (100%)	0	100	100
55	y	65/65 (100%)	65 (100%)	0	100	100
56	z	60/60 (100%)	60 (100%)	0	100	100
57	5	97/97 (100%)	96 (99%)	1 (1%)	68	74
All	All	4954/4954 (100%)	4915 (99%)	39 (1%)	70	76

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	151	THR
10	F	47	ASP
10	F	60	ASP
10	F	92	VAL
11	G	108	VAL
12	H	108	VAL

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Mol	Chain	Res	Type
12	H	123	ILE
13	I	34	ILE
13	I	111	THR
15	K	76	VAL
15	K	89	ASN
15	K	99	ILE
16	L	120	VAL
17	M	7	THR
17	M	89	VAL
18	N	113	ILE
20	P	92	VAL
22	R	95	ASP
23	S	74	ILE
25	U	18	ASP
25	U	83	VAL
26	V	65	VAL
29	Y	57	LEU
37	g	161	LEU
38	h	200	VAL
39	i	143	VAL
40	j	18	VAL
40	j	88	VAL
41	k	7	VAL
41	k	84	VAL
42	l	80	VAL
43	m	12	THR
43	m	51	VAL
44	n	63	LEU
45	o	6	ILE
47	q	87	VAL
48	r	64	VAL
51	u	19	VAL
57	5	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
6	B	25	HIS
6	B	53	HIS
6	B	58	HIS
6	B	86	ASN
6	B	239	ASN

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Mol	Chain	Res	Type
7	C	49	GLN
7	C	136	ASN
8	D	41	GLN
8	D	62	GLN
8	D	136	GLN
9	E	21	ASN
9	E	27	GLN
9	E	63	GLN
10	F	38	ASN
11	G	18	GLN
11	G	133	GLN
13	I	11	GLN
13	I	18	ASN
13	I	42	ASN
14	J	47	HIS
14	J	76	HIS
14	J	128	ASN
14	J	135	GLN
15	K	90	ASN
16	L	54	GLN
17	M	13	HIS
18	N	73	ASN
20	P	3	ASN
20	P	10	GLN
20	P	52	ASN
20	P	56	HIS
21	Q	37	GLN
22	R	12	HIS
23	S	60	HIS
23	S	102	HIS
24	T	59	ASN
24	T	72	GLN
24	T	91	GLN
25	U	27	ASN
25	U	54	GLN
25	U	69	ASN
26	V	78	GLN
27	W	46	HIS
27	W	57	HIS
28	X	16	ASN
28	X	23	ASN
29	Y	25	GLN

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Mol	Chain	Res	Type
30	Z	9	GLN
32	b	5	GLN
33	c	19	HIS
34	d	26	ASN
35	e	43	HIS
37	g	58	ASN
37	g	170	HIS
38	h	8	ASN
38	h	139	GLN
39	i	116	GLN
40	j	122	ASN
40	j	146	ASN
41	k	37	HIS
42	l	86	GLN
44	n	25	ASN
44	n	75	GLN
44	n	110	GLN
44	n	126	GLN
45	o	64	GLN
46	p	40	ASN
46	p	109	ASN
47	q	46	ASN
47	q	75	GLN
47	q	112	GLN
48	r	105	ASN
49	s	4	GLN
50	t	50	HIS
51	u	29	ASN
53	w	19	GLN
53	w	54	GLN
53	w	75	GLN
54	x	52	HIS
54	x	57	HIS
56	z	64	ASN
57	5	37	GLN
57	5	69	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2901/2903 (99%)	707 (24%)	18 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1530/1534 (99%)	325 (21%)	2 (0%)
3	3	119/120 (99%)	23 (19%)	0
5	7	75/76 (98%)	25 (33%)	1 (1%)
58	4	362/363 (99%)	220 (60%)	32 (8%)
All	All	4987/4996 (99%)	1300 (26%)	53 (1%)

All (1300) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	G
1	1	10	A
1	1	15	G
1	1	23	G
1	1	27	G
1	1	34	U
1	1	35	G
1	1	36	G
1	1	46	G
1	1	49	A
1	1	51	G
1	1	60	G
1	1	63	A
1	1	71	A
1	1	72	U
1	1	74	A
1	1	75	G
1	1	82	U
1	1	84	A
1	1	85	G
1	1	93	G
1	1	96	C
1	1	100	U
1	1	101	A
1	1	102	U
1	1	118	A
1	1	119	A
1	1	120	U
1	1	126	A
1	1	131	A
1	1	137	U
1	1	139	U
1	1	140	C

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Mol	Chain	Res	Type
1	1	141	G
1	1	142	A
1	1	143	C
1	1	148	U
1	1	149	A
1	1	158	U
1	1	162	U
1	1	163	C
1	1	171	U
1	1	173	A
1	1	175	G
1	1	181	A
1	1	196	A
1	1	197	A
1	1	199	A
1	1	204	A
1	1	205	G
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	228	C
1	1	229	C
1	1	233	A
1	1	239	C
1	1	241	A
1	1	248	G
1	1	249	C
1	1	250	G
1	1	261	G
1	1	266	G
1	1	270	A
1	1	275	C
1	1	276	U
1	1	277	G
1	1	278	A
1	1	286	U
1	1	295	G
1	1	302	C
1	1	305	C
1	1	311	A
1	1	315	G

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Mol	Chain	Res	Type
1	1	322	A
1	1	329	G
1	1	330	A
1	1	349	U
1	1	353	C
1	1	359	G
1	1	361	G
1	1	362	A
1	1	363	G
1	1	367	G
1	1	371	A
1	1	372	G
1	1	386	G
1	1	396	G
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	416	U
1	1	421	C
1	1	424	G
1	1	425	G
1	1	436	C
1	1	454	A
1	1	457	A
1	1	458	G
1	1	464	U
1	1	467	G
1	1	477	A
1	1	480	A
1	1	481	G
1	1	483	A
1	1	489	G
1	1	490	C
1	1	491	G
1	1	496	G
1	1	501	A
1	1	505	A
1	1	508	A
1	1	509	C
1	1	528	A

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Mol	Chain	Res	Type
1	1	529	A
1	1	530	G
1	1	532	A
1	1	533	G
1	1	544	C
1	1	545	U
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	550	C
1	1	551	G
1	1	563	A
1	1	569	U
1	1	573	U
1	1	575	A
1	1	584	C
1	1	602	A
1	1	603	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	618	G
1	1	627	A
1	1	631	A
1	1	634	C
1	1	637	A
1	1	645	C
1	1	646	U
1	1	647	G
1	1	654	A
1	1	655	A
1	1	659	G
1	1	677	A
1	1	685	A
1	1	686	U
1	1	695	G
1	1	704	G
1	1	707	G
1	1	710	U
1	1	719	C
1	1	726	G

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Mol	Chain	Res	Type
1	1	730	A
1	1	737	C
1	1	745	1MG
1	1	746	PSU
1	1	747	5MU
1	1	748	G
1	1	749	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	783	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	811	U
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	830	G
1	1	845	A
1	1	846	U
1	1	850	U
1	1	856	G
1	1	857	G
1	1	859	G
1	1	869	G
1	1	876	C
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	894	U
1	1	896	A
1	1	897	C

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Mol	Chain	Res	Type
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	932	U
1	1	934	U
1	1	941	A
1	1	946	C
1	1	953	G
1	1	955	PSU
1	1	956	G
1	1	957	C
1	1	958	U
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1025	G
1	1	1033	U
1	1	1042	G
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1055	G
1	1	1056	G
1	1	1057	A
1	1	1058	U
1	1	1059	G
1	1	1060	U
1	1	1061	U
1	1	1064	C
1	1	1066	U
1	1	1067	A
1	1	1068	G

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Mol	Chain	Res	Type
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1079	C
1	1	1080	A
1	1	1081	U
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1086	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1090	A
1	1	1094	U
1	1	1095	A
1	1	1096	A
1	1	1097	U
1	1	1098	A
1	1	1099	G
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1141	U
1	1	1142	A
1	1	1149	G
1	1	1151	A
1	1	1155	A
1	1	1162	G
1	1	1168	G
1	1	1169	A
1	1	1170	C

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Mol	Chain	Res	Type
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1180	U
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1210	G
1	1	1211	C
1	1	1238	G
1	1	1241	A
1	1	1247	A
1	1	1248	G
1	1	1250	G
1	1	1253	A
1	1	1254	A
1	1	1256	G
1	1	1262	A
1	1	1265	A
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1275	A
1	1	1284	A
1	1	1294	U
1	1	1300	G
1	1	1301	A
1	1	1306	C
1	1	1314	C
1	1	1321	A
1	1	1325	U
1	1	1326	U
1	1	1329	U
1	1	1330	C
1	1	1341	G
1	1	1345	C
1	1	1347	A
1	1	1352	U

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Mol	Chain	Res	Type
1	1	1355	G
1	1	1358	G
1	1	1359	A
1	1	1365	A
1	1	1368	G
1	1	1374	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1395	A
1	1	1403	A
1	1	1408	G
1	1	1409	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1441	G
1	1	1453	A
1	1	1458	U
1	1	1459	G
1	1	1478	G
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1502	A
1	1	1503	A
1	1	1508	A
1	1	1510	G
1	1	1515	A
1	1	1519	G
1	1	1522	A
1	1	1523	U
1	1	1530	G
1	1	1531	C
1	1	1532	A
1	1	1533	C
1	1	1534	U

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Mol	Chain	Res	Type
1	1	1535	A
1	1	1536	C
1	1	1554	U
1	1	1555	G
1	1	1559	U
1	1	1566	A
1	1	1567	G
1	1	1569	A
1	1	1573	G
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1583	A
1	1	1584	U
1	1	1585	C
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1602	U
1	1	1603	A
1	1	1608	A
1	1	1610	A
1	1	1618	6MZ
1	1	1619	G
1	1	1630	A
1	1	1632	A
1	1	1634	A
1	1	1639	C
1	1	1647	U
1	1	1648	U
1	1	1672	A
1	1	1674	G
1	1	1675	C
1	1	1694	C
1	1	1695	G
1	1	1698	A
1	1	1699	G
1	1	1714	U
1	1	1715	G
1	1	1723	G
1	1	1724	G
1	1	1727	C

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Mol	Chain	Res	Type
1	1	1729	U
1	1	1730	C
1	1	1731	G
1	1	1736	U
1	1	1737	G
1	1	1738	G
1	1	1756	G
1	1	1757	A
1	1	1758	U
1	1	1761	C
1	1	1764	C
1	1	1773	A
1	1	1781	U
1	1	1782	U
1	1	1784	A
1	1	1791	A
1	1	1800	C
1	1	1802	A
1	1	1808	A
1	1	1811	G
1	1	1815	A
1	1	1816	C
1	1	1819	A
1	1	1829	A
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1857	G
1	1	1858	A
1	1	1866	A
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1882	U
1	1	1884	G
1	1	1887	C
1	1	1889	A
1	1	1900	A
1	1	1906	G
1	1	1907	G
1	1	1911	PSU

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Mol	Chain	Res	Type
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1915	3TD
1	1	1916	A
1	1	1917	PSU
1	1	1918	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1933	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1939	5MU
1	1	1940	U
1	1	1955	U
1	1	1964	G
1	1	1966	A
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2020	A
1	1	2022	U
1	1	2023	C
1	1	2030	6MZ
1	1	2031	A
1	1	2034	U
1	1	2041	U
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G

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Mol	Chain	Res	Type
1	1	2062	A
1	1	2063	C
1	1	2068	U
1	1	2069	G7M
1	1	2072	C
1	1	2092	U
1	1	2093	G
1	1	2095	A
1	1	2100	G
1	1	2102	G
1	1	2104	C
1	1	2105	U
1	1	2107	G
1	1	2111	U
1	1	2112	G
1	1	2113	U
1	1	2114	A
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2120	G
1	1	2121	G
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2129	C
1	1	2130	U
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2135	A
1	1	2137	U
1	1	2139	U
1	1	2146	C
1	1	2148	G
1	1	2154	A
1	1	2159	G

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Mol	Chain	Res	Type
1	1	2160	C
1	1	2161	C
1	1	2163	A
1	1	2164	C
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2174	C
1	1	2175	C
1	1	2176	A
1	1	2177	C
1	1	2178	C
1	1	2179	C
1	1	2180	U
1	1	2181	U
1	1	2182	U
1	1	2183	A
1	1	2184	A
1	1	2187	U
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2203	U
1	1	2204	G
1	1	2212	A
1	1	2218	G
1	1	2220	U
1	1	2225	A
1	1	2226	C
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2251	OMG
1	1	2252	G
1	1	2266	A

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Mol	Chain	Res	Type
1	1	2279	G
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2307	G
1	1	2309	A
1	1	2314	A
1	1	2316	G
1	1	2320	U
1	1	2321	U
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2334	U
1	1	2344	U
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2358	A
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2384	U
1	1	2385	C
1	1	2391	G
1	1	2396	G
1	1	2400	G
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2436	G
1	1	2440	C
1	1	2441	U

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Mol	Chain	Res	Type
1	1	2445	2MG
1	1	2448	A
1	1	2457	PSU
1	1	2458	G
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2481	G
1	1	2487	G
1	1	2491	U
1	1	2498	OMC
1	1	2499	C
1	1	2502	G
1	1	2503	2MA
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2552	OMU
1	1	2553	G
1	1	2554	U
1	1	2556	C
1	1	2564	A
1	1	2566	A
1	1	2567	G
1	1	2573	C
1	1	2574	G
1	1	2580	PSU
1	1	2581	G
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2605	PSU
1	1	2606	C
1	1	2609	U
1	1	2613	U
1	1	2615	U
1	1	2629	U

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Mol	Chain	Res	Type
1	1	2635	A
1	1	2636	C
1	1	2646	C
1	1	2654	A
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2720	U
1	1	2725	A
1	1	2726	A
1	1	2732	G
1	1	2733	A
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2749	A
1	1	2756	U
1	1	2757	A
1	1	2765	A
1	1	2766	A
1	1	2778	A
1	1	2793	C
1	1	2796	U
1	1	2798	U
1	1	2800	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2825	G
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G

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Mol	Chain	Res	Type
1	1	2891	U
1	1	2903	U
2	2	4	U
2	2	6	G
2	2	9	G
2	2	15	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	49	U
2	2	50	A
2	2	51	A
2	2	54	C
2	2	68	G
2	2	69	G
2	2	71	A
2	2	72	A
2	2	74	A
2	2	75	G
2	2	77	A
2	2	83	C
2	2	85	U
2	2	87	C
2	2	88	U
2	2	89	U
2	2	91	U
2	2	94	G
2	2	95	C
2	2	108	G
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	134	G
2	2	141	G
2	2	144	G
2	2	146	G
2	2	158	G
2	2	160	A
2	2	163	C
2	2	164	G

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Mol	Chain	Res	Type
2	2	168	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	183	C
2	2	191	G
2	2	197	A
2	2	202	G
2	2	203	G
2	2	208	U
2	2	209	U
2	2	211	G
2	2	212	G
2	2	226	G
2	2	240	G
2	2	244	U
2	2	245	U
2	2	247	G
2	2	251	G
2	2	253	A
2	2	266	G
2	2	267	C
2	2	269	C
2	2	279	A
2	2	289	G
2	2	298	A
2	2	299	G
2	2	306	A
2	2	321	A
2	2	325	A
2	2	328	C
2	2	330	C
2	2	332	G
2	2	345	C
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
2	2	373	A
2	2	382	A
2	2	384	G

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Mol	Chain	Res	Type
2	2	390	U
2	2	398	U
2	2	406	G
2	2	411	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	423	G
2	2	424	G
2	2	428	G
2	2	429	U
2	2	451	A
2	2	457	G
2	2	458	U
2	2	459	A
2	2	463	U
2	2	467	U
2	2	468	A
2	2	474	G
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	495	A
2	2	496	A
2	2	509	A
2	2	510	A
2	2	511	C
2	2	516	PSU
2	2	517	G
2	2	518	C
2	2	521	G
2	2	524	G
2	2	527	7MG
2	2	528	C
2	2	531	U
2	2	532	A
2	2	547	A

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Mol	Chain	Res	Type
2	2	559	A
2	2	564	C
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	588	G
2	2	596	A
2	2	607	A
2	2	614	C
2	2	615	G
2	2	632	U
2	2	653	U
2	2	665	A
2	2	687	A
2	2	700	G
2	2	701	U
2	2	703	G
2	2	711	G
2	2	712	A
2	2	717	U
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	790	A
2	2	793	U
2	2	794	A
2	2	809	G
2	2	814	A
2	2	815	A
2	2	817	C
2	2	819	A
2	2	821	G
2	2	828	U

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Mol	Chain	Res	Type
2	2	841	C
2	2	842	U
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	851	G
2	2	855	U
2	2	869	G
2	2	876	C
2	2	887	G
2	2	889	A
2	2	914	A
2	2	916	U
2	2	926	G
2	2	934	C
2	2	954	G
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	992	U
2	2	993	G
2	2	994	A
2	2	1002	G
2	2	1003	G
2	2	1007	U
2	2	1009	U
2	2	1017	U
2	2	1018	G
2	2	1019	A
2	2	1021	A
2	2	1022	A
2	2	1024	G
2	2	1026	G

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Mol	Chain	Res	Type
2	2	1027	C
2	2	1028	C
2	2	1029	U
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1034	G
2	2	1036	A
2	2	1043	G
2	2	1065	U
2	2	1074	G
2	2	1078	U
2	2	1079	G
2	2	1081	A
2	2	1086	U
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1108	G
2	2	1124	G
2	2	1130	A
2	2	1132	C
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1143	G
2	2	1145	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1171	A
2	2	1174	G
2	2	1175	G
2	2	1176	A

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Mol	Chain	Res	Type
2	2	1179	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1202	U
2	2	1203	C
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1216	A
2	2	1217	C
2	2	1227	A
2	2	1228	C
2	2	1236	A
2	2	1238	A
2	2	1239	A
2	2	1241	G
2	2	1246	A
2	2	1253	G
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1275	A
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1301	U
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1318	A
2	2	1320	C
2	2	1346	A
2	2	1360	A
2	2	1363	A
2	2	1370	G

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Mol	Chain	Res	Type
2	2	1379	G
2	2	1381	U
2	2	1386	G
2	2	1396	A
2	2	1398	A
2	2	1399	C
2	2	1402	4OC
2	2	1403	C
2	2	1419	G
2	2	1422	G
2	2	1428	A
2	2	1429	A
2	2	1432	G
2	2	1441	A
2	2	1446	A
2	2	1453	G
2	2	1454	G
2	2	1475	G
2	2	1487	G
2	2	1492	A
2	2	1493	A
2	2	1503	A
2	2	1505	G
2	2	1506	U
2	2	1508	A
2	2	1517	G
2	2	1518	MA6
2	2	1519	MA6
2	2	1520	C
2	2	1529	G
2	2	1530	G
2	2	1533	C
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	15	A
3	3	24	G
3	3	35	C
3	3	36	C
3	3	41	G
3	3	42	C

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Mol	Chain	Res	Type
3	3	50	A
3	3	51	G
3	3	57	A
3	3	64	G
3	3	66	A
3	3	68	C
3	3	89	U
3	3	90	C
3	3	91	C
3	3	99	A
3	3	105	G
3	3	108	A
3	3	109	A
3	3	119	A
5	7	8	U
5	7	10	G
5	7	13	C
5	7	14	A
5	7	15	G
5	7	16	C
5	7	17	U
5	7	18	G
5	7	19	G
5	7	20	G
5	7	22	G
5	7	23	A
5	7	30	G
5	7	35	G
5	7	36	C
5	7	47	U
5	7	48	C
5	7	53	G
5	7	55	U
5	7	56	C
5	7	60	C
5	7	73	A
5	7	74	C
5	7	75	C
5	7	76	A
58	4	6	U
58	4	8	A
58	4	9	U

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Mol	Chain	Res	Type
58	4	10	U
58	4	12	U
58	4	13	G
58	4	14	G
58	4	15	A
58	4	16	U
58	4	17	U
58	4	18	C
58	4	21	C
58	4	23	G
58	4	25	A
58	4	28	U
58	4	29	G
58	4	30	C
58	4	31	G
58	4	32	A
58	4	33	A
58	4	34	A
58	4	35	C
58	4	38	A
58	4	39	A
58	4	40	G
58	4	43	G
58	4	44	C
58	4	45	A
58	4	47	G
58	4	49	C
58	4	54	G
58	4	55	G
58	4	56	C
58	4	60	U
58	4	61	G
58	4	62	G
58	4	63	C
58	4	64	C
58	4	68	U
58	4	69	A
58	4	70	A
58	4	71	A
58	4	72	A
58	4	73	A
58	4	78	C

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Mol	Chain	Res	Type
58	4	79	A
58	4	80	A
58	4	81	A
58	4	82	A
58	4	84	A
58	4	85	U
58	4	86	A
58	4	87	G
58	4	88	U
58	4	89	C
58	4	90	G
58	4	92	A
58	4	93	A
58	4	97	A
58	4	98	C
58	4	99	G
58	4	100	A
58	4	101	A
58	4	103	A
58	4	104	C
58	4	105	U
58	4	106	A
58	4	107	C
58	4	108	G
58	4	109	C
58	4	111	U
58	4	114	G
58	4	115	C
58	4	117	G
58	4	119	U
58	4	121	A
58	4	122	A
58	4	125	A
58	4	127	C
58	4	130	C
58	4	131	U
58	4	132	U
58	4	133	A
58	4	135	A
58	4	136	G
58	4	138	C
58	4	143	C

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Mol	Chain	Res	Type
58	4	144	U
58	4	145	C
58	4	149	A
58	4	150	G
58	4	151	C
58	4	154	C
58	4	155	C
58	4	156	G
58	4	158	U
58	4	164	G
58	4	165	A
58	4	166	C
58	4	170	G
58	4	172	U
58	4	173	C
58	4	174	A
58	4	175	A
58	4	176	G
58	4	180	G
58	4	181	G
58	4	182	U
58	4	183	C
58	4	184	A
58	4	185	A
58	4	186	A
58	4	189	C
58	4	190	A
58	4	191	A
58	4	192	A
58	4	193	A
58	4	194	G
58	4	196	G
58	4	197	A
58	4	198	U
58	4	199	C
58	4	200	G
58	4	201	C
58	4	202	G
58	4	203	U
58	4	204	G
58	4	205	G
58	4	206	A

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Mol	Chain	Res	Type
58	4	207	A
58	4	210	C
58	4	213	G
58	4	218	G
58	4	219	G
58	4	222	U
58	4	223	G
58	4	224	A
58	4	225	A
58	4	226	G
58	4	227	C
58	4	229	U
58	4	230	U
58	4	233	A
58	4	234	A
58	4	235	C
58	4	236	U
58	4	237	U
58	4	238	A
58	4	239	A
58	4	240	U
58	4	241	C
58	4	242	A
58	4	244	G
58	4	245	C
58	4	246	U
58	4	247	A
58	4	248	G
58	4	249	U
58	4	257	U
58	4	258	G
58	4	261	G
58	4	262	U
58	4	263	G
58	4	264	U
58	4	266	C
58	4	267	G
58	4	268	U
58	4	269	C
58	4	271	G
58	4	273	A
58	4	274	G

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Mol	Chain	Res	Type
58	4	280	A
58	4	282	G
58	4	285	A
58	4	286	A
58	4	287	U
58	4	288	G
58	4	290	A
58	4	291	A
58	4	292	A
58	4	293	G
58	4	296	U
58	4	299	C
58	4	300	U
58	4	302	A
58	4	303	G
58	4	307	G
58	4	308	U
58	4	309	A
58	4	310	G
58	4	315	G
58	4	316	A
58	4	317	G
58	4	319	A
58	4	320	U
58	4	321	G
58	4	322	U
58	4	323	A
58	4	324	G
58	4	325	G
58	4	332	G
58	4	333	G
58	4	334	A
58	4	335	C
58	4	336	G
58	4	339	G
58	4	340	G
58	4	341	U
58	4	342	U
58	4	343	C
58	4	345	A
58	4	347	U
58	4	348	C

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Mol	Chain	Res	Type
58	4	351	G
58	4	357	U
58	4	358	C
58	4	359	C
58	4	360	A
58	4	362	C
58	4	363	A

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	546	U
1	1	747	5MU
1	1	784	G
1	1	955	PSU
1	1	1379	U
1	1	1911	PSU
1	1	1917	PSU
1	1	1929	G
1	1	1939	5MU
1	1	2127	G
1	1	2193	G
1	1	2425	A
1	1	2457	PSU
1	1	2498	OMC
1	1	2504	PSU
1	1	2580	PSU
1	1	2605	PSU
2	2	516	PSU
2	2	527	7MG
5	7	17	U
58	4	9	U
58	4	13	G
58	4	14	G
58	4	17	U
58	4	20	A
58	4	31	G
58	4	32	A
58	4	33	A
58	4	68	U
58	4	130	C

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Mol	Chain	Res	Type
58	4	131	U
58	4	153	U
58	4	164	G
58	4	182	U
58	4	183	C
58	4	184	A
58	4	185	A
58	4	195	A
58	4	202	G
58	4	212	U
58	4	223	G
58	4	229	U
58	4	233	A
58	4	257	U
58	4	261	G
58	4	290	A
58	4	308	U
58	4	320	U
58	4	333	G
58	4	335	C
58	4	341	U
58	4	346	C

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

34 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	5MC	2	1407	2	18,22,23	2.08	3 (16%)	26,32,35	1.33	4 (15%)
1	PSU	1	746	1,59	18,21,22	2.15	6 (33%)	22,30,33	1.90	5 (22%)
1	2MG	1	2445	1	23,26,27	2.73	6 (26%)	32,38,41	2.08	9 (28%)
1	PSU	1	955	1	18,21,22	2.27	6 (33%)	22,30,33	2.45	5 (22%)
1	PSU	1	2605	1	18,21,22	2.09	6 (33%)	22,30,33	2.22	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	3TD	1	1915	1	18,22,23	2.75	7 (38%)	22,32,35	1.80	4 (18%)
1	OMU	1	2552	1	19,22,23	2.71	7 (36%)	26,31,34	2.12	9 (34%)
47	0TD	q	89	47	7,9,10	1.48	0	6,11,13	2.20	2 (33%)
2	MA6	2	1519	2	23,26,27	1.44	3 (13%)	34,38,41	2.12	10 (29%)
2	MA6	2	1518	2	23,26,27	1.36	4 (17%)	34,38,41	2.03	9 (26%)
2	UR3	2	1498	2	19,22,23	2.94	7 (36%)	26,32,35	1.41	2 (7%)
2	2MG	2	966	2	23,26,27	2.62	6 (26%)	32,38,41	2.56	9 (28%)
2	7MG	2	527	2	22,26,27	6.22	6 (27%)	29,39,42	2.47	8 (27%)
1	OMC	1	2498	1,59	19,22,23	1.90	6 (31%)	26,31,34	2.20	7 (26%)
1	2MA	1	2503	1,59	22,25,26	1.53	3 (13%)	33,37,40	2.42	11 (33%)
1	6MZ	1	1618	1	22,25,26	2.78	3 (13%)	30,36,39	2.21	11 (36%)
1	1MG	1	745	1	22,26,27	2.66	6 (27%)	33,39,42	2.43	14 (42%)
1	5MU	1	1939	1	19,22,23	2.63	7 (36%)	28,32,35	3.51	10 (35%)
2	2MG	2	1516	2	23,26,27	2.60	6 (26%)	32,38,41	2.31	11 (34%)
1	PSU	1	1917	1	18,21,22	2.05	6 (33%)	22,30,33	2.12	5 (22%)
1	5MC	1	1962	1	18,22,23	2.04	3 (16%)	26,32,35	1.52	4 (15%)
1	PSU	1	2504	1	18,21,22	2.17	5 (27%)	22,30,33	2.26	5 (22%)
1	PSU	1	2457	1	18,21,22	2.03	5 (27%)	22,30,33	2.25	5 (22%)
2	2MG	2	1207	2	23,26,27	2.61	6 (26%)	32,38,41	2.35	10 (31%)
1	5MU	1	747	1	19,22,23	2.50	8 (42%)	28,32,35	3.59	11 (39%)
1	PSU	1	1911	1	18,21,22	2.01	5 (27%)	22,30,33	2.35	4 (18%)
2	PSU	2	516	2,59	18,21,22	2.25	6 (33%)	22,30,33	2.24	5 (22%)
1	PSU	1	2580	1	18,21,22	2.13	5 (27%)	22,30,33	2.24	6 (27%)
1	2MG	1	1835	1	23,26,27	2.61	6 (26%)	32,38,41	2.52	11 (34%)
1	OMG	1	2251	1,5	23,26,27	2.71	7 (30%)	33,38,41	2.36	9 (27%)
2	5MC	2	967	2	18,22,23	2.15	3 (16%)	26,32,35	1.46	2 (7%)
1	6MZ	1	2030	1	22,25,26	2.74	4 (18%)	30,36,39	2.67	10 (33%)
1	G7M	1	2069	1	23,26,27	2.78	5 (21%)	35,39,42	1.81	7 (20%)
2	4OC	2	1402	2	20,23,24	2.45	5 (25%)	26,32,35	2.28	6 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	746	1,59	2/2/5/5	4/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	1	955	1	2/2/5/5	4/7/25/26	0/2/2/2
1	PSU	1	2605	1	2/2/5/5	3/7/25/26	0/2/2/2
1	3TD	1	1915	1	1/1/5/5	5/7/25/26	0/2/2/2
1	OMU	1	2552	1	2/2/5/5	3/9/27/28	0/2/2/2
47	0TD	q	89	47	-	1/7/12/14	-
2	MA6	2	1519	2	-	6/11/29/30	0/3/3/3
2	MA6	2	1518	2	-	5/11/29/30	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
2	2MG	2	966	2	-	4/9/27/28	0/3/3/3
2	7MG	2	527	2	1/1/7/7	3/7/37/38	0/3/3/3
1	OMC	1	2498	1,59	1/1/5/5	6/9/27/28	0/2/2/2
1	6MZ	1	1618	1	2/2/5/6	5/9/27/28	0/3/3/3
1	5MU	1	1939	1	2/2/5/5	1/7/25/26	0/2/2/2
1	1MG	1	745	1	2/2/5/5	2/7/25/26	0/3/3/3
1	2MA	1	2503	1,59	2/2/5/5	4/7/25/26	0/3/3/3
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
1	PSU	1	1917	1	2/2/5/5	3/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	4/7/25/26	0/2/2/2
1	PSU	1	2504	1	2/2/5/5	3/7/25/26	0/2/2/2
1	PSU	1	2457	1	2/2/5/5	1/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	2/9/27/28	0/3/3/3
1	5MU	1	747	1	2/2/5/5	3/7/25/26	0/2/2/2
1	PSU	1	1911	1	2/2/5/5	3/7/25/26	0/2/2/2
2	PSU	2	516	2,59	2/2/5/5	3/7/25/26	0/2/2/2
1	PSU	1	2580	1	2/2/5/5	3/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
1	OMG	1	2251	1,5	1/1/5/5	3/9/27/28	0/3/3/3
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	2/2/5/6	2/9/27/28	0/3/3/3
1	G7M	1	2069	1	1/1/5/5	2/7/25/26	0/3/3/3
2	4OC	2	1402	2	2/2/5/6	6/9/29/30	0/2/2/2

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	527	7MG	C8-N9	-26.70	1.31	1.46
1	1	1618	6MZ	C6-N6	11.85	1.47	1.34
1	1	2030	6MZ	C6-N6	11.25	1.46	1.34
1	1	2069	G7M	O6-C6	10.52	1.43	1.23
1	1	2251	OMG	O6-C6	9.70	1.42	1.23
2	2	1516	2MG	O6-C6	9.35	1.41	1.23
2	2	1207	2MG	O6-C6	9.25	1.41	1.23
2	2	966	2MG	O6-C6	9.23	1.41	1.23
1	1	2445	2MG	O6-C6	9.14	1.41	1.23
1	1	1835	2MG	O6-C6	9.06	1.40	1.23
2	2	1402	4OC	O2-C2	8.35	1.39	1.23
2	2	1498	UR3	O4-C4	8.15	1.41	1.23
1	1	2552	OMU	O4-C4	7.92	1.39	1.24
1	1	1915	3TD	O4-C4	7.72	1.39	1.23
1	1	745	1MG	O6-C6	7.67	1.39	1.23
2	2	527	7MG	O6-C6	7.52	1.37	1.23
2	2	527	7MG	C2-N2	6.42	1.49	1.34
2	2	967	5MC	C4-N4	6.41	1.50	1.34
1	1	1939	5MU	C2-N1	-6.36	1.28	1.38
2	2	1407	5MC	C4-N4	6.28	1.50	1.34
1	1	1962	5MC	C4-N4	6.26	1.50	1.34
1	1	745	1MG	C2-N2	5.97	1.45	1.34
2	2	966	2MG	C2-N2	5.67	1.46	1.33
2	2	516	PSU	C4-N3	-5.54	1.28	1.38
2	2	1207	2MG	C2-N2	5.54	1.45	1.33
1	1	2445	2MG	C2-N2	5.52	1.45	1.33
2	2	1516	2MG	C2-N2	5.40	1.45	1.33
1	1	747	5MU	C2-N1	-5.35	1.29	1.38
1	1	1835	2MG	C2-N2	5.33	1.45	1.33
2	2	1498	UR3	C2-N1	-5.23	1.31	1.38
2	2	967	5MC	C2-N1	-5.21	1.28	1.40
1	1	955	PSU	C2-N1	-5.05	1.29	1.36
2	2	1407	5MC	C2-N1	-4.95	1.29	1.40
1	1	1962	5MC	C2-N1	-4.93	1.29	1.40
1	1	2504	PSU	C4-N3	-4.80	1.29	1.38
1	1	2605	PSU	C4-N3	-4.80	1.29	1.38
1	1	955	PSU	C4-N3	-4.79	1.30	1.38
1	1	2251	OMG	C2-N2	4.75	1.45	1.34
1	1	1939	5MU	C2-N3	-4.75	1.29	1.38
1	1	2580	PSU	C4-N3	-4.69	1.30	1.38
1	1	746	PSU	C4-N3	-4.57	1.30	1.38
1	1	745	1MG	C6-N1	-4.54	1.30	1.40
1	1	1917	PSU	C4-N3	-4.51	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2498	OMC	C4-N4	4.51	1.44	1.33
1	1	1911	PSU	C4-N3	-4.50	1.30	1.38
1	1	747	5MU	C2-N3	-4.50	1.30	1.38
1	1	2552	OMU	C2-N1	-4.49	1.31	1.38
2	2	1498	UR3	C4-N3	-4.43	1.30	1.40
1	1	2503	2MA	C6-N6	4.41	1.45	1.34
1	1	2457	PSU	C4-N3	-4.29	1.30	1.38
1	1	2069	G7M	C2-N2	4.28	1.44	1.34
1	1	2504	PSU	C6-C5	4.26	1.40	1.35
2	2	1402	4OC	C4-N4	4.24	1.44	1.35
1	1	1915	3TD	C4-N3	-4.18	1.31	1.40
1	1	2580	PSU	C2-N1	-4.18	1.31	1.36
1	1	1915	3TD	C2-N1	-4.16	1.31	1.37
1	1	1917	PSU	C6-C5	4.12	1.40	1.35
1	1	2504	PSU	C2-N1	-4.11	1.31	1.36
1	1	2069	G7M	C6-N1	-4.10	1.31	1.38
1	1	2580	PSU	C6-N1	-4.07	1.29	1.36
1	1	1939	5MU	C6-N1	-4.02	1.31	1.38
1	1	2605	PSU	C2-N1	-3.95	1.31	1.36
1	1	2445	2MG	C6-N1	-3.91	1.31	1.38
2	2	1498	UR3	C2-N3	-3.90	1.31	1.39
1	1	2251	OMG	C6-N1	-3.86	1.31	1.38
1	1	2030	6MZ	C8-N9	-3.83	1.30	1.37
1	1	2457	PSU	C2-N1	-3.81	1.31	1.36
1	1	747	5MU	C6-N1	-3.79	1.31	1.38
1	1	955	PSU	C6-N1	-3.78	1.29	1.36
2	2	527	7MG	C4-N9	-3.76	1.33	1.37
1	1	1911	PSU	C6-C5	3.74	1.39	1.35
1	1	2457	PSU	C6-C5	3.73	1.39	1.35
1	1	2069	G7M	C5-N7	-3.73	1.34	1.39
1	1	1917	PSU	C2-N1	-3.73	1.31	1.36
1	1	2457	PSU	C6-N1	-3.72	1.30	1.36
1	1	1939	5MU	C4-N3	-3.68	1.32	1.38
1	1	746	PSU	C6-C5	3.68	1.39	1.35
1	1	2552	OMU	C4-N3	-3.67	1.32	1.38
1	1	747	5MU	C4-N3	-3.66	1.32	1.38
2	2	516	PSU	O4'-C1'	-3.66	1.38	1.43
2	2	1519	MA6	C5-N7	-3.65	1.32	1.39
1	1	747	5MU	O4-C4	-3.65	1.16	1.23
1	1	746	PSU	C2-N1	-3.64	1.31	1.36
1	1	1917	PSU	C6-N1	-3.62	1.30	1.36
2	2	516	PSU	C2-N3	-3.61	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1519	MA6	C8-N9	-3.55	1.31	1.37
1	1	2504	PSU	C6-N1	-3.53	1.30	1.36
2	2	966	2MG	C6-N1	-3.51	1.32	1.38
1	1	746	PSU	O4'-C1'	-3.50	1.39	1.43
1	1	746	PSU	C6-N1	-3.49	1.30	1.36
1	1	2503	2MA	C8-N9	-3.45	1.31	1.37
1	1	1939	5MU	O2-C2	-3.45	1.16	1.23
1	1	2552	OMU	C2-N3	-3.44	1.31	1.38
2	2	1518	MA6	C8-N9	-3.43	1.31	1.37
1	1	1939	5MU	C6-C5	3.42	1.40	1.34
1	1	1911	PSU	C6-N1	-3.41	1.30	1.36
1	1	2605	PSU	C6-C5	3.41	1.39	1.35
2	2	1402	4OC	C2-N1	-3.40	1.32	1.40
1	1	745	1MG	C5-N7	-3.39	1.32	1.39
1	1	1835	2MG	C6-N1	-3.39	1.32	1.38
1	1	1618	6MZ	C8-N9	-3.39	1.31	1.37
1	1	2445	2MG	C5-N7	-3.37	1.32	1.39
1	1	2580	PSU	C6-C5	3.37	1.39	1.35
2	2	1498	UR3	O2-C2	-3.35	1.16	1.22
2	2	1207	2MG	C6-N1	-3.33	1.32	1.38
1	1	1911	PSU	C2-N1	-3.32	1.32	1.36
1	1	955	PSU	C6-C5	3.32	1.39	1.35
1	1	1915	3TD	C2-N3	-3.29	1.31	1.38
2	2	1498	UR3	C6-N1	-3.28	1.30	1.38
2	2	527	7MG	C6-N1	-3.23	1.32	1.38
1	1	2498	OMC	C5-C4	-3.22	1.35	1.42
1	1	747	5MU	C6-C5	3.22	1.39	1.34
1	1	2605	PSU	C6-N1	-3.21	1.30	1.36
2	2	1516	2MG	C6-N1	-3.20	1.32	1.38
2	2	516	PSU	C6-N1	-3.18	1.30	1.36
1	1	1835	2MG	C2-N1	-3.16	1.31	1.36
1	1	2445	2MG	C8-N9	-3.15	1.30	1.37
1	1	2498	OMC	C2-N1	-3.11	1.33	1.40
2	2	516	PSU	C2-N1	-3.02	1.32	1.36
1	1	1939	5MU	O4-C4	-3.00	1.17	1.23
1	1	2030	6MZ	C5-N7	-2.98	1.33	1.39
1	1	2445	2MG	C2-N1	-2.97	1.32	1.36
1	1	747	5MU	O2-C2	-2.97	1.17	1.23
1	1	2251	OMG	C2-N1	-2.95	1.30	1.37
1	1	1835	2MG	C8-N9	-2.95	1.31	1.37
1	1	955	PSU	C2-N3	-2.93	1.32	1.37
1	1	1915	3TD	C6-C5	2.90	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2251	OMG	C8-N9	-2.88	1.31	1.37
1	1	1835	2MG	C5-N7	-2.86	1.33	1.39
1	1	745	1MG	C5-C6	-2.86	1.38	1.45
1	1	2251	OMG	C5-N7	-2.81	1.33	1.39
1	1	2552	OMU	C5-C4	-2.80	1.37	1.43
2	2	966	2MG	C2-N1	-2.80	1.32	1.36
2	2	1207	2MG	C5-N7	-2.79	1.33	1.39
1	1	1618	6MZ	C5-N7	-2.79	1.33	1.39
2	2	1518	MA6	C5-N7	-2.78	1.33	1.39
1	1	745	1MG	C8-N9	-2.78	1.31	1.37
2	2	1207	2MG	C8-N9	-2.77	1.31	1.37
1	1	2498	OMC	C2-N3	-2.77	1.30	1.36
2	2	1516	2MG	C2-N1	-2.77	1.32	1.36
2	2	1519	MA6	C6-N6	2.75	1.45	1.36
1	1	2498	OMC	O2-C2	-2.74	1.18	1.23
1	1	2605	PSU	C2-N3	-2.73	1.32	1.37
2	2	516	PSU	C6-C5	2.72	1.38	1.35
2	2	1518	MA6	C6-N6	2.70	1.44	1.36
2	2	527	7MG	C2-N1	-2.68	1.31	1.37
1	1	2552	OMU	O2-C2	-2.68	1.18	1.23
1	1	2503	2MA	C5-N7	-2.67	1.34	1.39
2	2	966	2MG	C8-N9	-2.66	1.31	1.37
1	1	2552	OMU	C6-N1	-2.65	1.31	1.38
1	1	1915	3TD	O2-C2	-2.64	1.18	1.23
1	1	2504	PSU	C2-N3	-2.64	1.33	1.37
1	1	2069	G7M	C2-N1	-2.62	1.31	1.37
2	2	1207	2MG	C2-N1	-2.61	1.32	1.36
2	2	1516	2MG	C8-N9	-2.59	1.31	1.37
1	1	2251	OMG	O2'-CM2	-2.54	1.33	1.42
2	2	1402	4OC	C6-N1	-2.50	1.31	1.38
1	1	747	5MU	C4-C5	-2.46	1.40	1.44
2	2	1407	5MC	C2-N3	-2.43	1.31	1.36
2	2	1516	2MG	C5-N7	-2.42	1.34	1.39
2	2	966	2MG	C5-N7	-2.41	1.34	1.39
2	2	967	5MC	C2-N3	-2.39	1.31	1.36
1	1	2580	PSU	C2-N3	-2.37	1.33	1.37
1	1	1915	3TD	C6-N1	-2.37	1.32	1.36
1	1	1962	5MC	C2-N3	-2.37	1.31	1.36
2	2	1498	UR3	C5-C4	-2.35	1.37	1.43
1	1	1911	PSU	O4'-C1'	-2.32	1.40	1.43
1	1	2030	6MZ	C6-N1	-2.21	1.31	1.35
1	1	2457	PSU	C2-N3	-2.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	955	PSU	O4'-C1'	-2.15	1.40	1.43
1	1	746	PSU	C2-N3	-2.13	1.33	1.37
2	2	1402	4OC	C2-N3	-2.12	1.32	1.36
2	2	1518	MA6	C4-N9	-2.11	1.33	1.37
1	1	2498	OMC	C4-N3	-2.11	1.30	1.34
1	1	1917	PSU	C2-N3	-2.05	1.34	1.37
1	1	2605	PSU	O4'-C1'	-2.03	1.41	1.43
1	1	1917	PSU	O4'-C1'	-2.02	1.41	1.43

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1939	5MU	N3-C2-N1	8.55	126.24	114.89
1	1	747	5MU	N3-C2-N1	8.44	126.09	114.89
1	1	2503	2MA	C5-C4-N3	-8.34	117.81	127.19
1	1	1835	2MG	C2-N3-C4	8.12	122.11	112.04
1	1	747	5MU	C4-N3-C2	-8.06	116.92	127.35
2	2	966	2MG	C2-N3-C4	8.02	121.98	112.04
1	1	1939	5MU	C5M-C5-C4	8.01	127.59	118.77
1	1	747	5MU	C5M-C5-C4	7.64	127.18	118.77
2	2	1207	2MG	C2-N3-C4	7.56	121.41	112.04
1	1	1939	5MU	C4-N3-C2	-7.53	117.60	127.35
2	2	1516	2MG	C2-N3-C4	7.46	121.29	112.04
2	2	966	2MG	C5-C4-N3	-7.19	116.79	128.46
1	1	2251	OMG	C5-C4-N3	-7.10	116.94	128.46
1	1	1911	PSU	N1-C2-N3	7.03	123.09	115.13
1	1	2445	2MG	C2-N3-C4	6.84	120.52	112.04
1	1	1835	2MG	C5-C4-N3	-6.70	117.59	128.46
1	1	2498	OMC	O2-C2-N3	-6.68	111.46	122.33
2	2	1402	4OC	C1'-N1-C2	6.64	133.24	118.42
1	1	747	5MU	C5-C4-N3	6.63	120.97	115.31
1	1	2503	2MA	N3-C4-N9	6.55	136.07	126.99
2	2	1207	2MG	C5-C4-N3	-6.46	117.99	128.46
1	1	2605	PSU	N1-C2-N3	6.40	122.38	115.13
2	2	516	PSU	N1-C2-N3	6.19	122.14	115.13
1	1	955	PSU	C6-C5-C4	-6.13	113.91	118.20
1	1	2504	PSU	N1-C2-N3	6.07	122.01	115.13
1	1	1917	PSU	N1-C2-N3	6.07	122.01	115.13
2	2	1519	MA6	C5-C4-N3	-6.06	118.84	126.75
1	1	2580	PSU	N1-C2-N3	6.05	121.99	115.13
2	2	1516	2MG	C5-C4-N3	-5.90	118.88	128.46
1	1	955	PSU	N1-C2-N3	5.89	121.81	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	527	7MG	N9-C4-N3	5.87	134.25	125.47
1	1	2457	PSU	N1-C2-N3	5.87	121.78	115.13
1	1	745	1MG	C5-C4-N3	-5.82	119.01	128.46
1	1	1915	3TD	N1-C2-N3	5.82	120.73	116.14
1	1	1939	5MU	C5M-C5-C6	-5.74	115.19	122.85
1	1	2251	OMG	C2-N3-C4	5.67	122.40	112.30
2	2	527	7MG	C5-C6-N1	5.64	120.93	110.99
2	2	516	PSU	C4-N3-C2	-5.62	118.25	126.34
1	1	747	5MU	C5M-C5-C6	-5.62	115.35	122.85
2	2	967	5MC	C5-C6-N1	-5.61	117.56	123.34
1	1	2030	6MZ	C5-C4-N3	-5.60	119.44	126.75
1	1	2030	6MZ	C9-N6-C6	-5.60	118.05	122.87
1	1	1939	5MU	C5-C4-N3	5.56	120.05	115.31
1	1	2445	2MG	C5-C4-N3	-5.54	119.48	128.46
1	1	746	PSU	N1-C2-N3	5.49	121.36	115.13
2	2	966	2MG	N9-C4-N3	5.46	136.90	125.94
1	1	2251	OMG	N9-C4-N3	5.29	136.56	125.94
2	2	1402	4OC	C1'-N1-C6	-5.28	109.33	120.84
2	2	527	7MG	C2-N3-C4	5.28	121.71	112.30
1	1	747	5MU	C5-C6-N1	-5.27	117.92	123.34
1	1	1618	6MZ	C5-C4-N3	-5.26	119.89	126.75
1	1	1939	5MU	C5-C6-N1	-5.25	117.94	123.34
1	1	1962	5MC	C5-C6-N1	-5.15	118.04	123.34
1	1	2030	6MZ	N1-C2-N3	-5.05	120.70	128.60
2	2	1498	UR3	C4-N3-C2	-5.01	119.85	124.56
2	2	527	7MG	C5-C4-N3	-5.00	118.60	128.13
2	2	1518	MA6	C5-C4-N3	-4.90	120.36	126.75
1	1	1911	PSU	O2-C2-N1	-4.83	117.47	122.79
1	1	2504	PSU	C6-C5-C4	-4.77	114.86	118.20
1	1	2069	G7M	C2-N3-C4	4.73	120.73	112.30
2	2	1518	MA6	N1-C2-N3	-4.71	121.23	128.60
1	1	1835	2MG	N9-C4-N3	4.70	135.38	125.94
2	2	1518	MA6	C2-N1-C6	4.67	122.78	111.75
2	2	1207	2MG	N9-C4-N3	4.62	135.22	125.94
1	1	1911	PSU	C4-N3-C2	-4.60	119.71	126.34
1	1	2030	6MZ	C5-N7-C8	4.57	110.00	103.51
1	1	2580	PSU	O2-C2-N1	-4.50	117.84	122.79
1	1	2457	PSU	O2-C2-N1	-4.48	117.86	122.79
1	1	1939	5MU	O2-C2-N3	-4.47	113.17	121.50
1	1	2069	G7M	C5-C6-N1	4.46	121.11	111.79
1	1	2605	PSU	C4-N3-C2	-4.46	119.91	126.34
2	2	1407	5MC	C5-C6-N1	-4.43	118.78	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2552	OMU	N3-C2-N1	4.43	120.77	114.89
1	1	2552	OMU	C4-N3-C2	-4.43	120.74	126.58
1	1	955	PSU	O2-C2-N1	-4.40	117.94	122.79
1	1	1835	2MG	C2-N1-C6	-4.40	119.42	124.48
1	1	745	1MG	C2'-C1'-N9	4.38	125.62	113.22
2	2	1519	MA6	N3-C4-N9	4.37	134.29	127.08
1	1	2498	OMC	O2-C2-N1	4.36	127.89	118.89
1	1	1917	PSU	O2-C2-N1	-4.34	118.01	122.79
2	2	966	2MG	C2-N1-C6	-4.34	119.49	124.48
1	1	2030	6MZ	N9-C8-N7	-4.30	108.03	113.91
1	1	1618	6MZ	N1-C2-N3	-4.28	121.91	128.60
1	1	2498	OMC	C1'-N1-C2	4.22	127.84	118.42
1	1	2030	6MZ	C4-C5-N7	-4.21	105.50	110.62
1	1	2605	PSU	O2-C2-N1	-4.15	118.22	122.79
2	2	1519	MA6	N1-C2-N3	-4.14	122.13	128.60
1	1	2069	G7M	C6-C5-N7	4.09	137.20	132.25
47	q	89	0TD	OD2-CG-CB	4.09	121.99	113.15
1	1	2030	6MZ	C6-C5-N7	4.08	136.80	132.39
1	1	2030	6MZ	C2-N3-C4	4.07	121.37	111.75
1	1	2457	PSU	C6-C5-C4	-4.06	115.36	118.20
1	1	1618	6MZ	N3-C4-N9	4.04	133.74	127.08
2	2	1519	MA6	C2-N1-C6	3.97	121.14	111.75
1	1	745	1MG	N9-C4-N3	3.97	133.91	125.94
1	1	2457	PSU	C4-N3-C2	-3.97	120.62	126.34
1	1	2069	G7M	C5-C4-N3	-3.93	120.61	128.15
2	2	1207	2MG	C2-N1-C6	-3.77	120.14	124.48
1	1	2251	OMG	C1'-N9-C8	-3.76	115.98	126.70
2	2	1402	4OC	O2-C2-N3	-3.74	116.24	122.33
1	1	1939	5MU	O4-C4-N3	-3.71	113.01	120.12
2	2	1518	MA6	C4-C5-N7	-3.70	106.11	110.62
2	2	1516	2MG	C2-N1-C6	-3.70	120.22	124.48
1	1	2445	2MG	N9-C4-N3	3.69	133.34	125.94
2	2	1516	2MG	N9-C4-N3	3.68	133.32	125.94
1	1	747	5MU	O2-C2-N3	-3.67	114.67	121.50
1	1	745	1MG	O2'-C2'-C3'	3.67	123.68	111.82
2	2	527	7MG	N9-C8-N7	3.66	108.62	103.38
1	1	2251	OMG	C1'-N9-C4	3.64	137.31	126.50
1	1	746	PSU	O2-C2-N1	-3.60	118.83	122.79
1	1	2504	PSU	C4-N3-C2	-3.60	121.16	126.34
1	1	2580	PSU	C4-N3-C2	-3.59	121.17	126.34
1	1	2552	OMU	C5-C4-N3	3.58	120.20	114.84
1	1	745	1MG	O4'-C1'-N9	3.58	116.55	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1518	MA6	C2-N3-C4	3.57	120.18	111.75
1	1	747	5MU	C1'-N1-C2	3.57	124.03	117.57
1	1	2504	PSU	O2-C2-N1	-3.55	118.88	122.79
2	2	1519	MA6	C2-N3-C4	3.54	120.12	111.75
1	1	747	5MU	C1'-N1-C6	-3.53	115.24	121.12
2	2	1519	MA6	N1-C6-N6	3.53	120.94	117.08
1	1	2030	6MZ	N3-C4-N9	3.47	132.80	127.08
1	1	2552	OMU	O4-C4-C5	-3.47	119.06	125.16
1	1	2552	OMU	O3'-C3'-C4'	3.46	121.06	111.05
2	2	1516	2MG	CM2-N2-C2	-3.43	116.28	123.86
1	1	1917	PSU	C4-N3-C2	-3.43	121.39	126.34
1	1	1618	6MZ	C5-N7-C8	3.42	108.37	103.51
2	2	527	7MG	C6-C5-N7	3.42	137.29	131.91
1	1	745	1MG	C2-N3-C4	3.41	119.65	111.98
2	2	1519	MA6	C4-C5-C6	3.40	119.69	115.88
1	1	1618	6MZ	C2-N3-C4	3.39	119.77	111.75
1	1	955	PSU	C4-N3-C2	-3.35	121.51	126.34
1	1	2503	2MA	C5-N7-C8	3.30	108.20	103.51
1	1	955	PSU	C6-N1-C2	-3.29	119.32	122.68
2	2	1402	4OC	C2'-C1'-N1	3.29	120.61	114.22
1	1	745	1MG	O2'-C2'-C1'	3.28	121.00	110.02
1	1	2503	2MA	N9-C8-N7	-3.28	109.43	113.91
1	1	2580	PSU	C6-N1-C2	-3.26	119.35	122.68
1	1	1618	6MZ	C9-N6-C6	-3.23	120.09	122.87
1	1	746	PSU	C4-N3-C2	-3.23	121.69	126.34
1	1	747	5MU	O4-C4-N3	-3.21	113.97	120.12
1	1	745	1MG	O4'-C4'-C5'	3.20	119.90	109.37
1	1	745	1MG	C5'-C4'-C3'	3.16	127.03	115.18
1	1	745	1MG	O3'-C3'-C4'	3.16	120.17	111.05
1	1	1618	6MZ	N9-C8-N7	-3.16	109.60	113.91
1	1	2498	OMC	C6-N1-C2	-3.15	115.03	120.49
1	1	1835	2MG	CM2-N2-C2	-3.13	116.94	123.86
1	1	2251	OMG	C2-N1-C6	-3.12	119.42	125.10
2	2	516	PSU	O2-C2-N3	-3.08	116.01	121.82
2	2	516	PSU	C5-C6-N1	-3.08	117.49	122.11
2	2	1518	MA6	C5-N7-C8	3.07	107.87	103.51
1	1	745	1MG	O3'-C3'-C2'	3.07	121.74	111.82
1	1	746	PSU	C6-C5-C4	-3.04	116.07	118.20
1	1	1917	PSU	C6-N1-C2	-3.03	119.59	122.68
2	2	1207	2MG	CM2-N2-C2	-3.03	117.18	123.86
1	1	1915	3TD	C4-N3-C2	-3.02	121.33	124.61
1	1	2504	PSU	C6-N1-C2	-3.01	119.61	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1407	5MC	O2-C2-N3	-2.97	117.50	122.33
1	1	1618	6MZ	C4-C5-N7	-2.94	107.04	110.62
2	2	527	7MG	C2-N1-C6	-2.93	119.77	125.10
1	1	2069	G7M	O6-C6-C5	-2.92	121.47	128.06
1	1	2445	2MG	CM2-N2-C2	-2.90	117.47	123.86
1	1	2069	G7M	N9-C4-N3	2.85	131.66	125.94
1	1	2580	PSU	C6-C5-C4	-2.84	116.21	118.20
1	1	2503	2MA	N3-C2-N1	-2.81	120.56	125.72
1	1	2552	OMU	C1'-N1-C2	2.81	122.65	117.57
1	1	2069	G7M	C2-N1-C6	-2.80	119.99	125.10
1	1	1911	PSU	C6-N1-C2	-2.79	119.83	122.68
1	1	1835	2MG	C5-C6-N1	2.77	120.23	113.19
1	1	2030	6MZ	C4-N9-C8	2.76	108.72	105.73
1	1	747	5MU	O2-C2-N1	-2.74	119.15	122.79
1	1	2251	OMG	C5-C6-N1	2.73	120.13	113.19
2	2	1516	2MG	C6-C5-N7	2.72	135.31	130.25
1	1	1939	5MU	C1'-N1-C6	-2.72	116.61	121.12
2	2	966	2MG	C5-C6-N1	2.70	120.05	113.19
1	1	1917	PSU	C6-C5-C4	-2.70	116.31	118.20
1	1	2503	2MA	C4-N9-C8	2.70	108.65	105.73
2	2	516	PSU	C5-C4-N3	2.69	122.66	116.58
1	1	2498	OMC	C5-C6-N1	2.67	126.27	121.81
2	2	1518	MA6	N3-C4-N9	2.66	131.47	127.08
1	1	1939	5MU	C1'-N1-C2	2.66	122.38	117.57
1	1	1618	6MZ	C4-N9-C8	2.66	108.61	105.73
2	2	527	7MG	C6-C5-C4	-2.65	117.15	122.62
1	1	2457	PSU	C6-N1-C2	-2.60	120.02	122.68
1	1	746	PSU	C6-N1-C2	-2.59	120.04	122.68
2	2	1516	2MG	C4-C5-N7	-2.58	106.64	110.72
47	q	89	0TD	OD1-CG-CB	-2.55	117.11	122.44
1	1	1835	2MG	O6-C6-C5	-2.53	119.88	126.60
1	1	1962	5MC	O2-C2-N3	-2.53	118.22	122.33
2	2	1519	MA6	C5-C6-N6	-2.49	120.96	125.30
1	1	2445	2MG	C2-N1-C6	-2.49	121.61	124.48
1	1	2503	2MA	C4-C5-N7	-2.48	107.60	110.62
1	1	1915	3TD	O3'-C3'-C4'	2.46	118.17	111.05
1	1	1618	6MZ	C1'-N9-C8	-2.41	121.70	127.14
1	1	2503	2MA	N6-C6-N1	2.40	120.43	117.03
2	2	1207	2MG	C5-C6-N1	2.40	119.28	113.19
1	1	2498	OMC	C4-N3-C2	2.38	124.09	120.25
2	2	1518	MA6	N9-C8-N7	-2.37	110.67	113.91
1	1	2503	2MA	C2-N3-C4	2.37	122.81	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2251	OMG	C2'-C1'-N9	2.37	118.82	114.22
2	2	1516	2MG	C5-C6-N1	2.37	119.20	113.19
1	1	2251	OMG	O6-C6-C5	-2.36	120.33	126.60
2	2	1207	2MG	O6-C6-C5	-2.35	120.38	126.60
1	1	2552	OMU	C1'-N1-C6	-2.34	115.74	120.84
2	2	966	2MG	O6-C6-C5	-2.32	120.43	126.60
1	1	745	1MG	C4-C5-N7	-2.32	107.05	110.72
1	1	2580	PSU	O3'-C3'-C4'	2.31	117.74	111.05
2	2	966	2MG	CM2-N2-C2	-2.30	118.78	123.86
1	1	2605	PSU	C6-N1-C2	-2.29	120.35	122.68
1	1	2503	2MA	C1'-N9-C8	-2.28	121.98	127.14
1	1	2552	OMU	CM2-O2'-C2'	-2.27	108.57	114.52
1	1	745	1MG	C1'-N9-C8	-2.26	120.25	126.70
1	1	1835	2MG	C4-C5-N7	-2.25	107.15	110.72
2	2	1402	4OC	CM4-N4-C4	-2.22	118.12	122.45
1	1	745	1MG	C8-N7-C5	2.21	108.24	104.24
2	2	1498	UR3	C5-C6-N1	-2.20	118.12	121.81
1	1	2605	PSU	C6-C5-C4	-2.20	116.66	118.20
2	2	1407	5MC	C5-C4-N3	-2.19	119.31	121.67
2	2	1402	4OC	C5-C4-N3	-2.19	119.07	122.59
1	1	1962	5MC	C5-C4-N4	-2.19	118.21	121.48
1	1	2445	2MG	O6-C6-C5	-2.18	120.81	126.60
2	2	967	5MC	O2-C2-N3	-2.18	118.78	122.33
1	1	1835	2MG	N9-C8-N7	-2.17	109.30	113.39
1	1	1962	5MC	C1'-N1-C6	-2.17	117.51	121.12
1	1	1835	2MG	C6-C5-N7	2.16	134.27	130.25
2	2	966	2MG	C8-N7-C5	2.15	108.14	104.24
1	1	1835	2MG	C8-N7-C5	2.14	108.12	104.24
1	1	2552	OMU	O3'-C3'-C2'	2.14	117.24	111.17
2	2	1207	2MG	C4-C5-N7	-2.13	107.34	110.72
1	1	2503	2MA	C5-C6-N6	-2.13	118.79	123.43
2	2	966	2MG	C4-C5-N7	-2.12	107.36	110.72
1	1	1618	6MZ	C6-C5-N7	2.11	134.68	132.39
2	2	1516	2MG	C8-N7-C5	2.11	108.06	104.24
2	2	1516	2MG	N9-C8-N7	-2.11	109.42	113.39
1	1	2445	2MG	C5-C6-N1	2.10	118.52	113.19
2	2	1519	MA6	C4-C5-N7	-2.09	108.07	110.62
2	2	1407	5MC	N1-C2-N3	2.07	122.58	118.81
2	2	1516	2MG	O6-C6-C5	-2.07	121.11	126.60
2	2	1207	2MG	C8-N7-C5	2.07	107.98	104.24
2	2	1518	MA6	C5-C4-N9	2.06	108.17	105.78
1	1	2498	OMC	C6-C5-C4	-2.05	114.20	117.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1915	3TD	O3'-C3'-C2'	2.05	118.44	111.82
1	1	2445	2MG	C4-C5-N7	-2.02	107.52	110.72
1	1	2445	2MG	N9-C8-N7	-2.02	109.60	113.39
2	2	1519	MA6	C5-N7-C8	2.01	106.37	103.51
2	2	1207	2MG	N9-C8-N7	-2.00	109.62	113.39

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	745	1MG	C4'
1	1	745	1MG	C3'
1	1	746	PSU	C4'
1	1	746	PSU	C3'
1	1	747	5MU	C2'
1	1	747	5MU	C4'
1	1	955	PSU	C4'
1	1	955	PSU	C3'
1	1	1618	6MZ	C2'
1	1	1618	6MZ	C3'
1	1	1911	PSU	C4'
1	1	1911	PSU	C3'
1	1	1915	3TD	C3'
1	1	1917	PSU	C4'
1	1	1917	PSU	C3'
1	1	1939	5MU	C2'
1	1	1939	5MU	C4'
1	1	2030	6MZ	C2'
1	1	2030	6MZ	C3'
1	1	2069	G7M	C2'
1	1	2251	OMG	C2'
1	1	2457	PSU	C4'
1	1	2457	PSU	C3'
1	1	2498	OMC	C4'
1	1	2503	2MA	C2'
1	1	2503	2MA	C3'
1	1	2504	PSU	C4'
1	1	2504	PSU	C3'
1	1	2552	OMU	C2'
1	1	2552	OMU	C3'
1	1	2580	PSU	C4'
1	1	2580	PSU	C3'
1	1	2605	PSU	C4'

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Mol	Chain	Res	Type	Atom
1	1	2605	PSU	C3'
2	2	516	PSU	C4'
2	2	516	PSU	C3'
2	2	527	7MG	C3'
2	2	1402	4OC	C1'
2	2	1402	4OC	C3'

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	q	89	0TD	CG-CB-SB-CSB
1	1	745	1MG	C3'-C4'-C5'-O5'
1	1	746	PSU	C2'-C1'-C5-C4
1	1	746	PSU	C2'-C1'-C5-C6
1	1	747	5MU	C3'-C4'-C5'-O5'
1	1	747	5MU	O4'-C4'-C5'-O5'
1	1	955	PSU	C2'-C1'-C5-C4
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	C2'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	2069	G7M	C3'-C4'-C5'-O5'
1	1	2251	OMG	O4'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2498	OMC	C3'-C4'-C5'-O5'
1	1	2498	OMC	C4'-C5'-O5'-P
1	1	2503	2MA	O4'-C1'-N9-C8
1	1	2503	2MA	O4'-C1'-N9-C4
1	1	2504	PSU	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
1	1	2552	OMU	O4'-C4'-C5'-O5'
1	1	2580	PSU	C3'-C4'-C5'-O5'
2	2	527	7MG	C3'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	1207	2MG	N1-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
2	2	1207	2MG	N3-C2-N2-CM2
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
2	2	1402	4OC	C2'-C1'-N1-C2
2	2	1518	MA6	O4'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C9
2	2	1518	MA6	C5-C6-N6-C10
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
2	2	1519	MA6	N1-C6-N6-C10
1	1	745	1MG	C4'-C5'-O5'-P
1	1	955	PSU	C3'-C4'-C5'-O5'
1	1	1911	PSU	C3'-C4'-C5'-O5'
1	1	2251	OMG	C3'-C4'-C5'-O5'
1	1	2552	OMU	C3'-C4'-C5'-O5'
1	1	2605	PSU	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	1518	MA6	C3'-C4'-C5'-O5'
2	2	1402	4OC	C2'-C1'-N1-C6
1	1	955	PSU	O4'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2580	PSU	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C2'-O2'-CM2
1	1	1911	PSU	C4'-C5'-O5'-P
1	1	1917	PSU	C4'-C5'-O5'-P
1	1	2605	PSU	C4'-C5'-O5'-P
1	1	1917	PSU	C3'-C4'-C5'-O5'
1	1	746	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	C3'-C4'-C5'-O5'
1	1	2504	PSU	C4'-C5'-O5'-P
1	1	1911	PSU	O4'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	2605	PSU	O4'-C4'-C5'-O5'
2	2	1518	MA6	N1-C6-N6-C10
1	1	746	PSU	O4'-C4'-C5'-O5'
1	1	2580	PSU	C4'-C5'-O5'-P
1	1	1917	PSU	O4'-C4'-C5'-O5'
1	1	2457	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	955	PSU	C4'-C5'-O5'-P
1	1	1618	6MZ	C4'-C5'-O5'-P
1	1	2251	OMG	C4'-C5'-O5'-P
1	1	2498	OMC	C2'-C1'-N1-C6
1	1	747	5MU	C4'-C5'-O5'-P
2	2	966	2MG	C4'-C5'-O5'-P
2	2	516	PSU	C4'-C5'-O5'-P
2	2	527	7MG	C4'-C5'-O5'-P
2	2	1519	MA6	C5-C6-N6-C9
1	1	1962	5MC	C2'-C1'-N1-C6
1	1	1939	5MU	C4'-C5'-O5'-P
1	1	2503	2MA	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	2498	OMC	C2'-C1'-N1-C2
1	1	2503	2MA	O4'-C4'-C5'-O5'
1	1	2498	OMC	C3'-C2'-O2'-CM2
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	1618	6MZ	C5-C6-N6-C9
2	2	1402	4OC	O4'-C1'-N1-C6
1	1	2552	OMU	C4'-C5'-O5'-P
2	2	516	PSU	O4'-C4'-C5'-O5'
1	1	1962	5MC	O4'-C1'-N1-C2
1	1	1962	5MC	C2'-C1'-N1-C2
2	2	966	2MG	C2'-C1'-N9-C8

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	746	PSU	1	0
1	1	2445	2MG	1	0
1	1	1915	3TD	3	0
47	q	89	0TD	1	0
2	2	966	2MG	1	0
2	2	527	7MG	1	0
1	1	2498	OMC	1	0
1	1	1939	5MU	1	0
1	1	2504	PSU	1	0
1	1	2457	PSU	1	0
2	2	1207	2MG	1	0
1	1	747	5MU	1	0
1	1	2580	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2251	OMG	1	0
2	2	1402	4OC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 439 ligands modelled in this entry, 439 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	3
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1276:G	O3'	1277:C	P	3.78
1	1	2314:A	O3'	2315:G	P	3.57
1	2	1383:C	O3'	1384:C	P	3.26
1	2	147:G	O3'	148:G	P	3.21

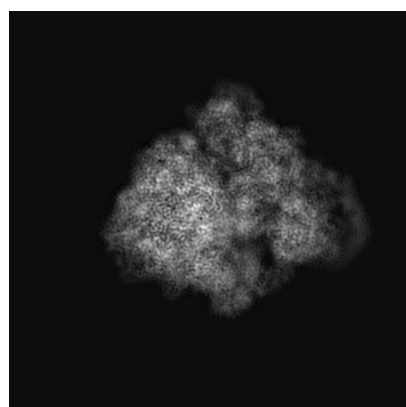
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4478. These allow visual inspection of the internal detail of the map and identification of artifacts.

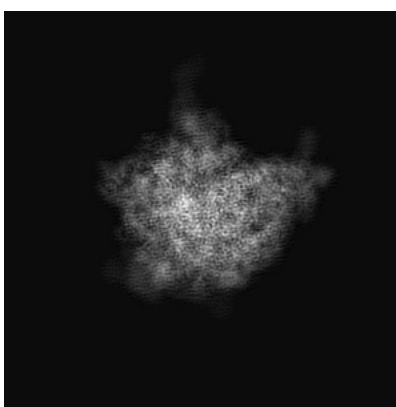
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

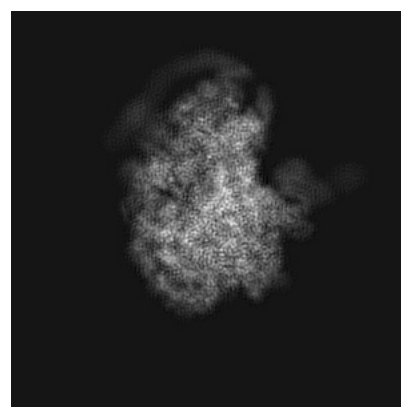
6.1.1 Primary map



X



Y

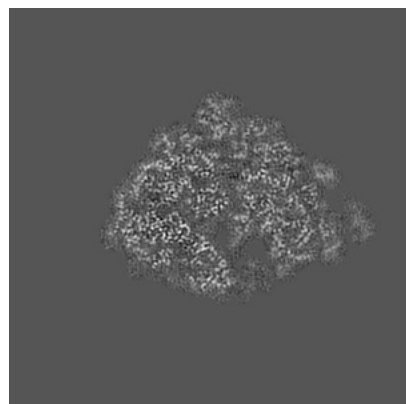


Z

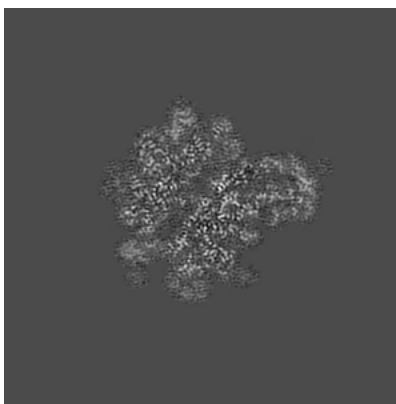
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

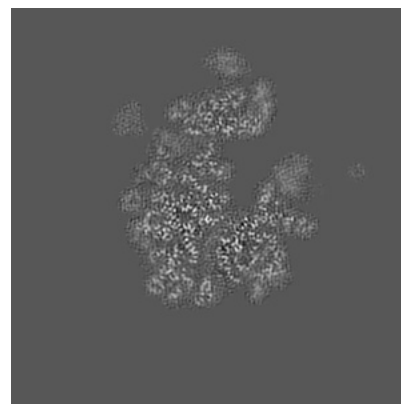
6.2.1 Primary map



X Index: 190



Y Index: 190

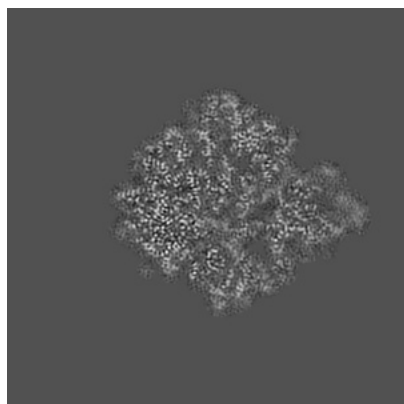


Z Index: 190

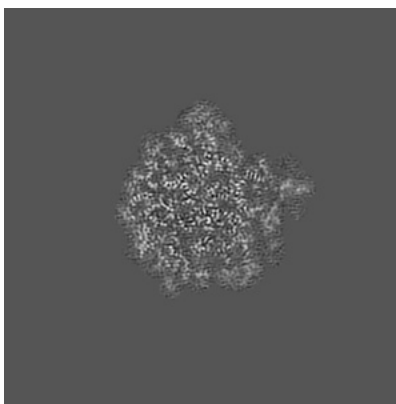
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

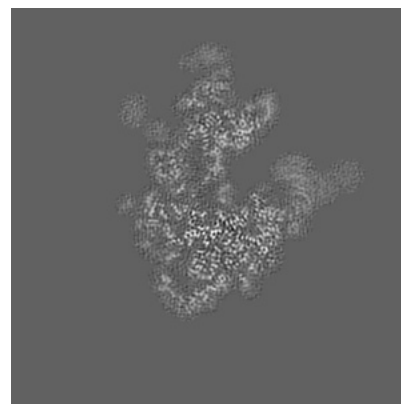
6.3.1 Primary map



X Index: 200



Y Index: 177

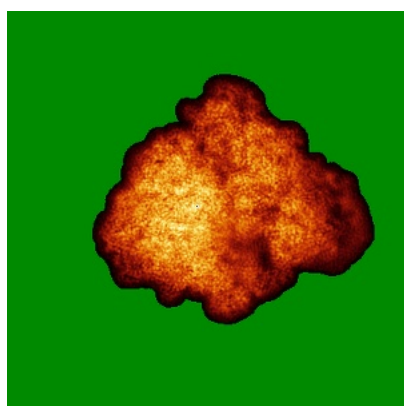


Z Index: 173

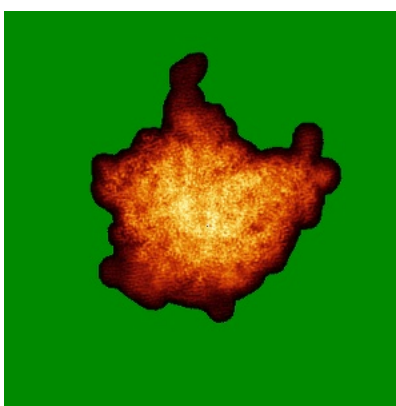
The images above show the largest variance slices of the map in three orthogonal directions.

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

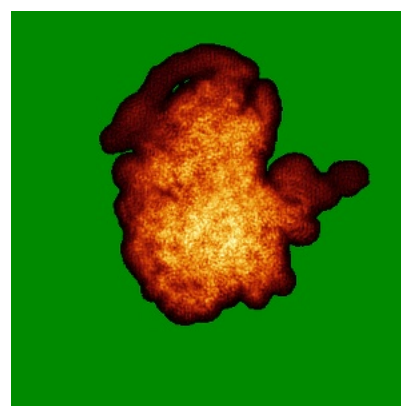
6.4.1 Primary map



X



Y



Z

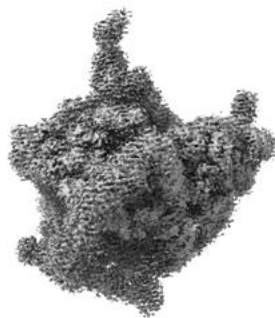
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

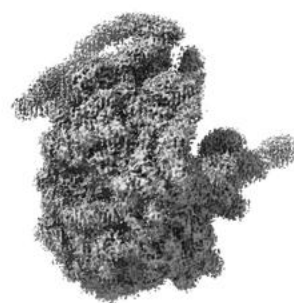
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

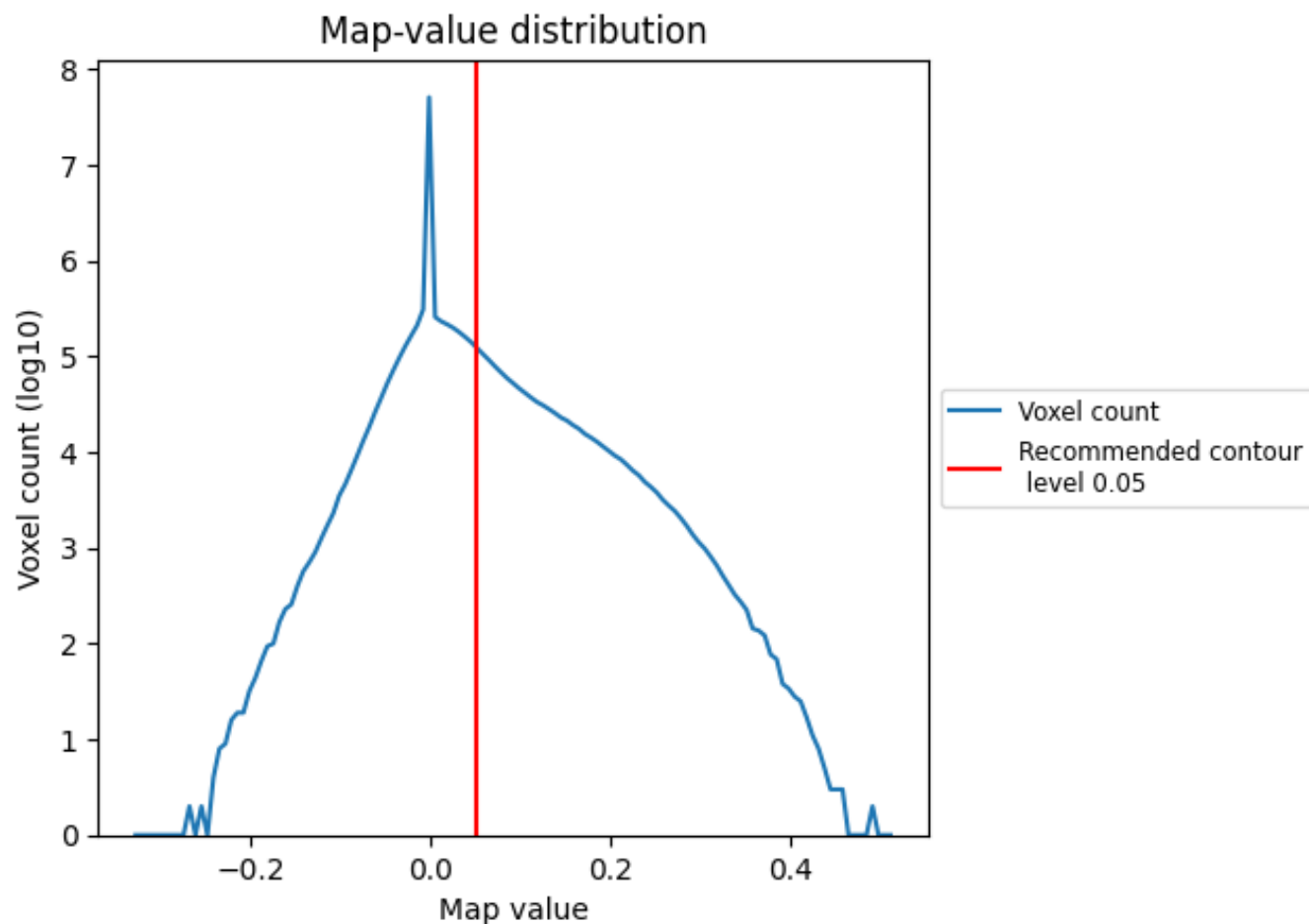
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

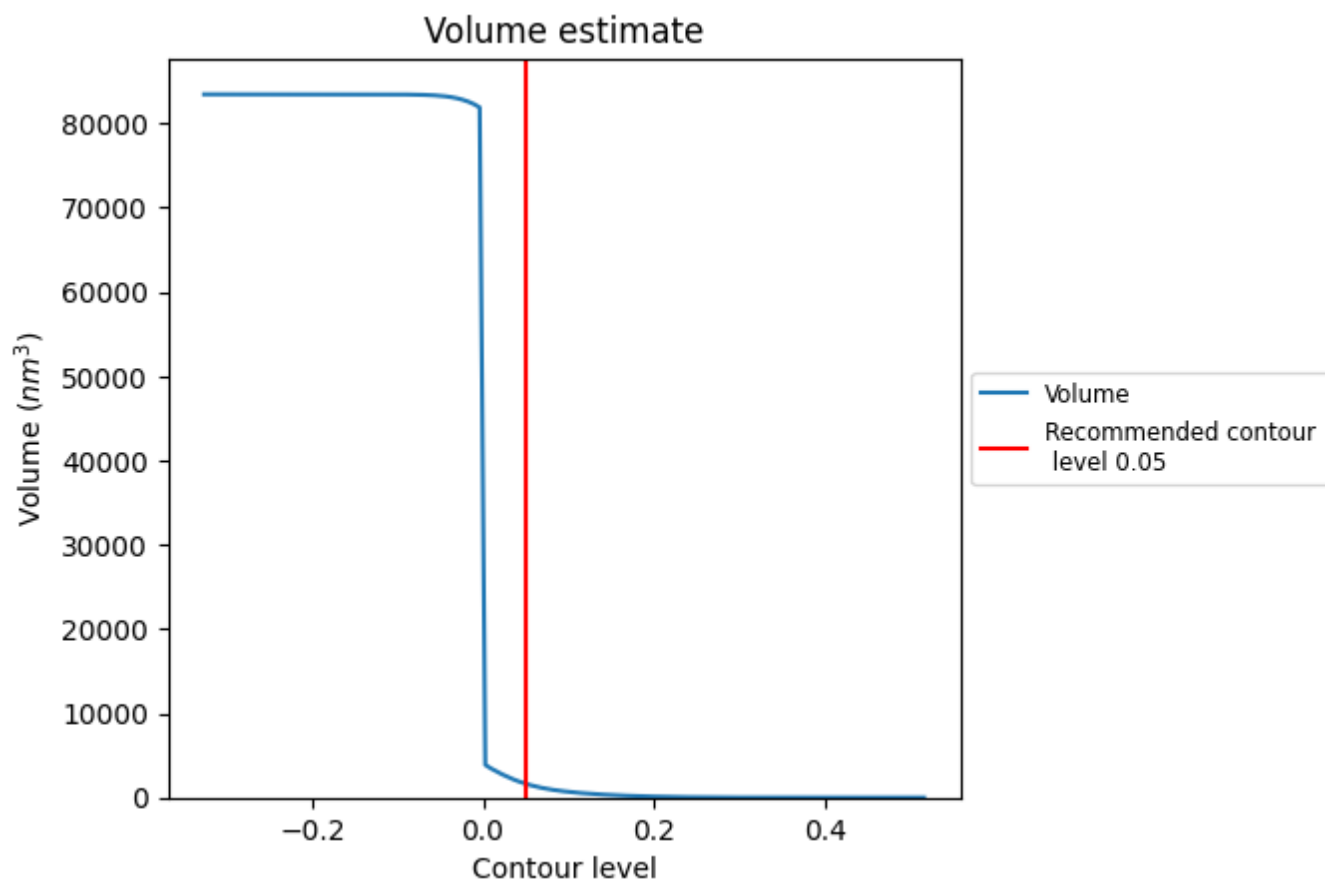
This section contains the results of statistical analysis of the map.

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.

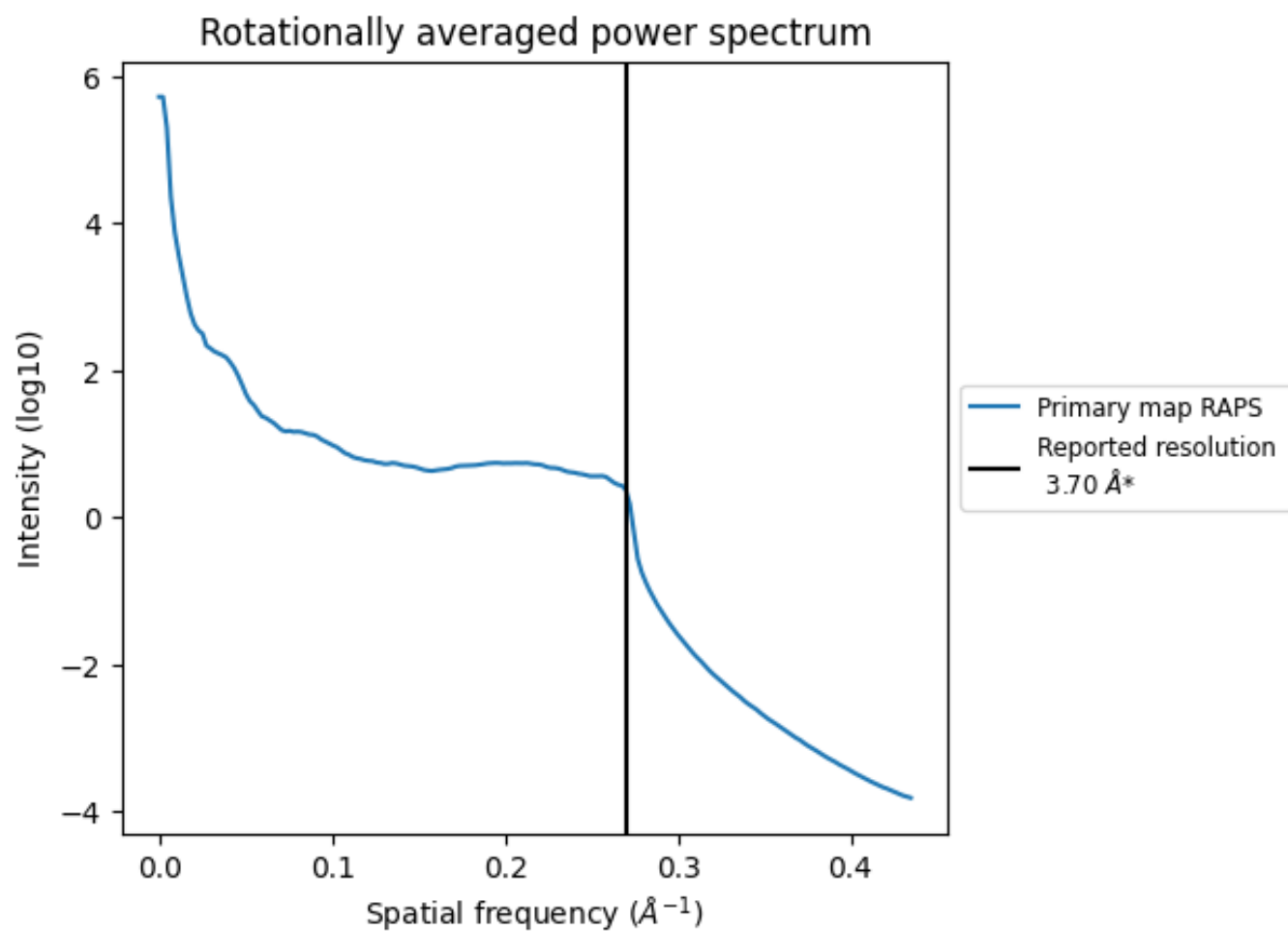
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1641 nm³; this corresponds to an approximate mass of 1482 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 0.270 $\text{\AA}^{-1}$

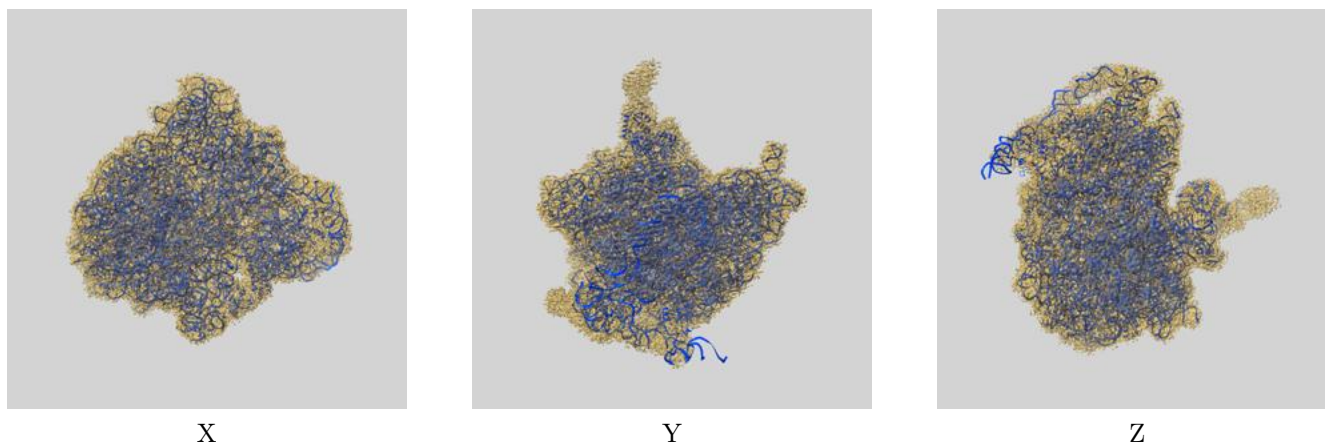
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

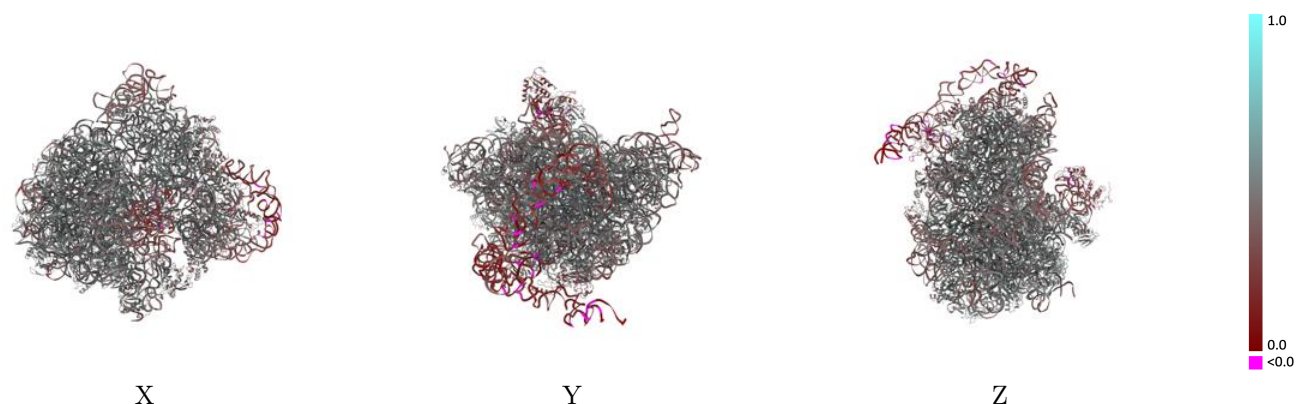
This section contains information regarding the fit between EMDB map EMD-4478 and PDB model 6Q9A. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



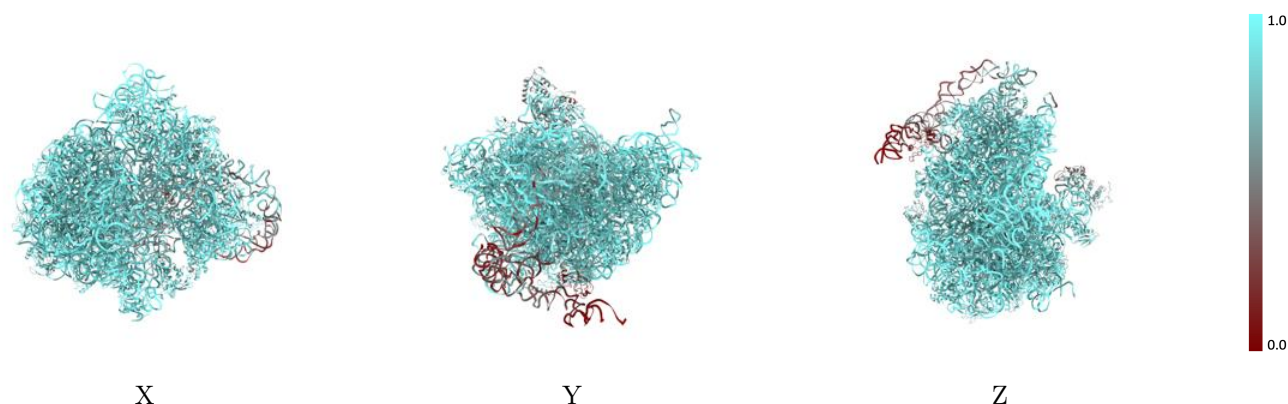
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



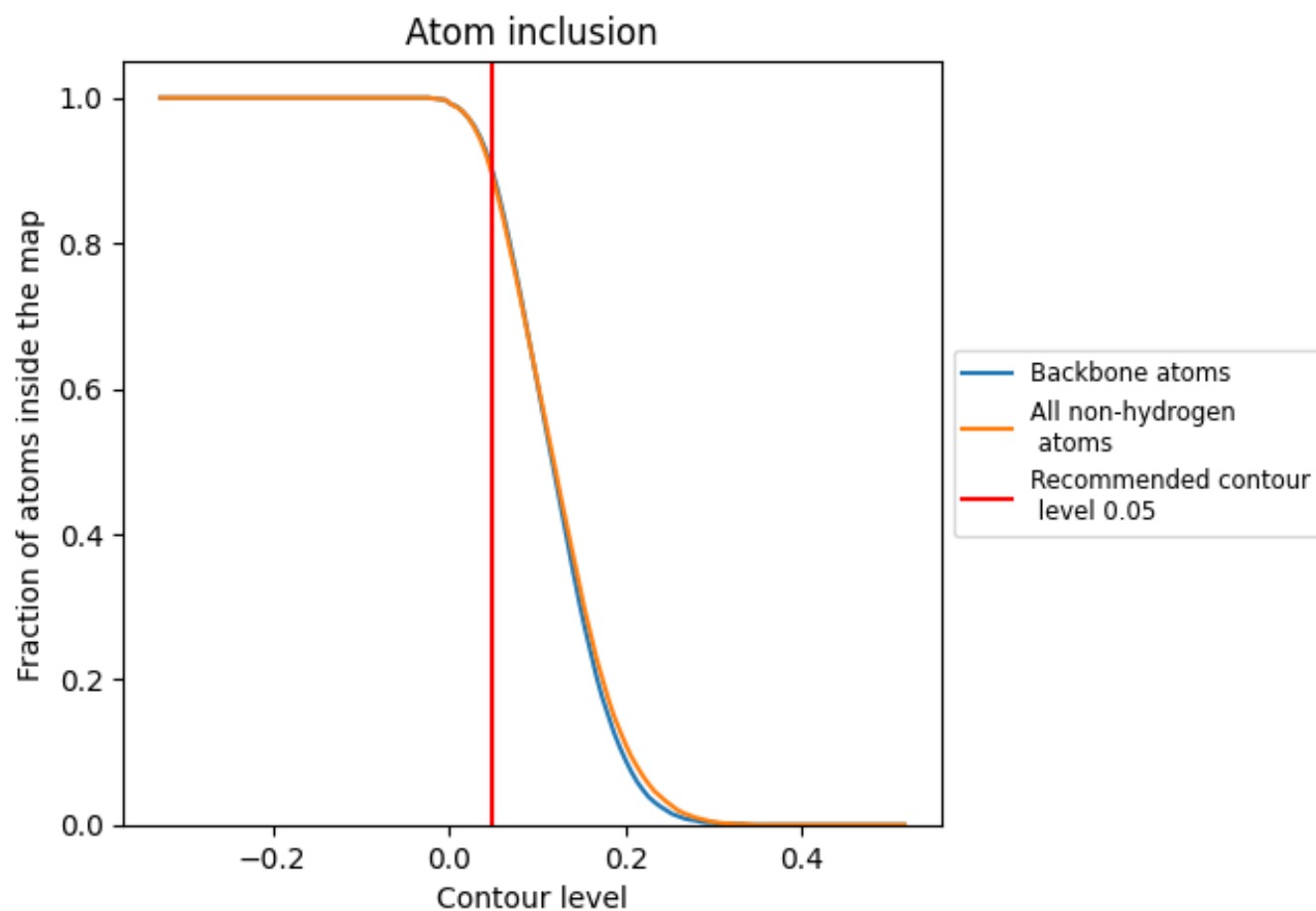
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.4400
1	 0.9460	 0.4520
2	 0.9620	 0.4470
3	 0.9600	 0.4340
4	 0.4070	 0.1720
5	 0.1950	 0.2830
6	 0.6170	 0.4430
7	 0.8820	 0.4010
B	 0.9020	 0.5200
C	 0.9000	 0.5110
D	 0.8700	 0.4760
E	 0.8710	 0.4570
F	 0.8910	 0.4530
G	 0.7570	 0.3830
H	 0.6220	 0.2760
I	 0.5530	 0.2680
J	 0.8990	 0.5000
K	 0.8660	 0.5100
L	 0.9010	 0.5030
M	 0.9000	 0.5180
N	 0.9130	 0.5110
O	 0.9090	 0.4680
P	 0.8830	 0.5110
Q	 0.8930	 0.4990
R	 0.8910	 0.4990
S	 0.8810	 0.5060
T	 0.8790	 0.4840
U	 0.8940	 0.4730
V	 0.8950	 0.4810
W	 0.9150	 0.5310
X	 0.8920	 0.4980
Y	 0.8830	 0.4600
Z	 0.8960	 0.4850
a	 0.8560	 0.4120
b	 0.9190	 0.5060



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Chain	Atom inclusion	Q-score
c	 0.8560	 0.4800
d	 0.9190	 0.5290
e	 0.9140	 0.5240
f	 0.9050	 0.5190
g	 0.8360	 0.4240
h	 0.8430	 0.4720
i	 0.8660	 0.4610
j	 0.8740	 0.4820
k	 0.8890	 0.4690
l	 0.8500	 0.4450
m	 0.8740	 0.4870
n	 0.8990	 0.4590
o	 0.8310	 0.4440
p	 0.8570	 0.4700
q	 0.8850	 0.5110
r	 0.8850	 0.4620
s	 0.9020	 0.4770
t	 0.8950	 0.4720
u	 0.8850	 0.4750
v	 0.8630	 0.4900
w	 0.8850	 0.4710
x	 0.9160	 0.4720
y	 0.9140	 0.4600
z	 0.7660	 0.4220