



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:56 am BST

PDB ID : 6Q98 / pdb_00006q98
EMDB ID : EMD-4477
Title : Structure of tmRNA SmpB bound in P site of E. coli 70S ribosome
Authors : Rae, C.D.
Deposited on : 2018-12-17
Resolution : 4.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

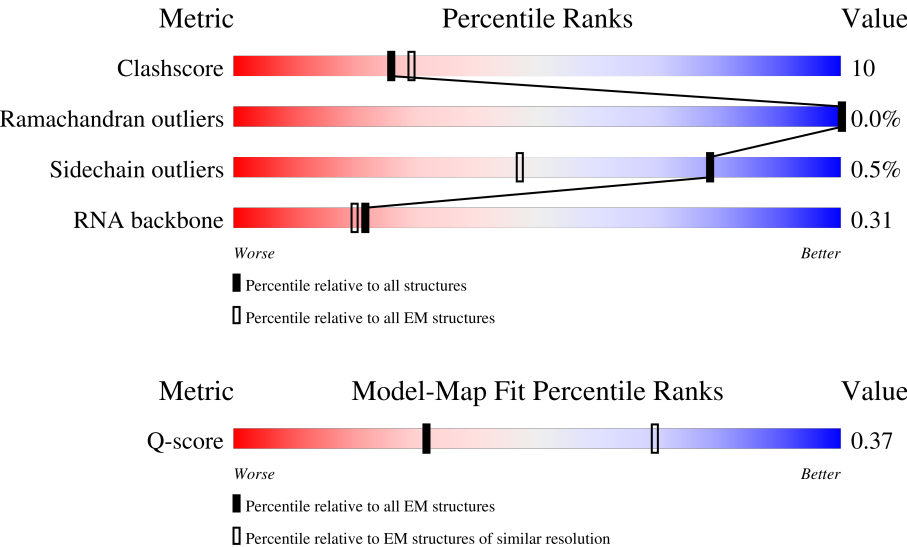
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 4.30 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	4585 (3.80 - 4.80)

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	2904	6% 43% 45% 11% .
2	2	1535	10% 41% 47% 12%
3	3	120	7% 42% 49% 9%

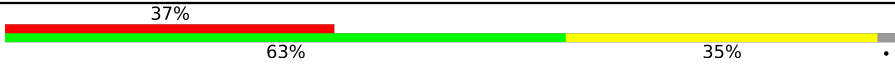
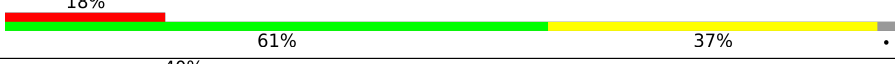
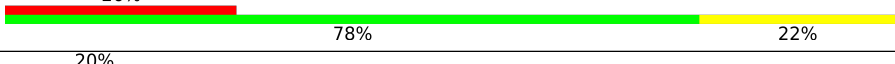
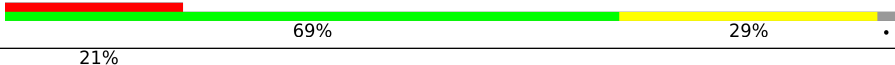
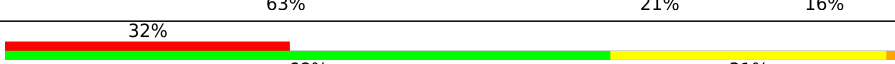
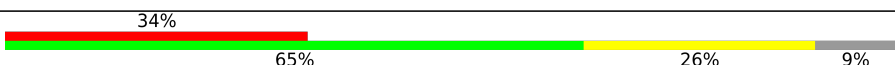
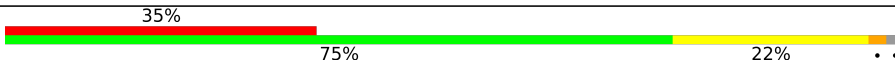
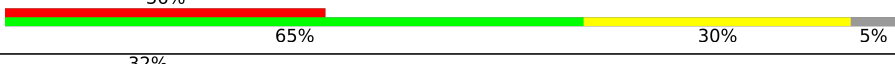
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Mol	Chain	Length	Quality of chain
4	5	160	
5	6	22	
6	B	273	
7	C	209	
8	D	201	
9	E	179	
10	F	177	
11	G	149	
12	H	165	
13	I	142	
14	J	142	
15	K	123	
16	L	144	
17	M	136	
18	N	127	
19	O	117	
20	P	115	
21	Q	118	
22	R	103	
23	S	110	
24	T	100	
25	U	104	
26	V	94	
27	W	85	
28	X	78	

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Mol	Chain	Length	Quality of chain
29	Y	63	
30	Z	59	
31	a	70	
32	b	57	
33	c	55	
34	d	46	
35	e	65	
36	f	38	
37	g	241	
38	h	233	
39	i	206	
40	j	167	
41	k	135	
42	l	179	
43	m	130	
44	n	130	
45	o	103	
46	p	129	
47	q	124	
48	r	118	
49	s	101	
50	t	89	
51	u	82	
52	v	84	
53	w	75	

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Mol	Chain	Length	Quality of chain
54	x	92	
55	y	87	
56	z	71	
57	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	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	-	-	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 153878 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 SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	150	Total	C	N	O	S	0	0
			1209	763	226	216	4		

- Molecule 5 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	6	22	Total	C	N	O	0	0
			110	66	22	22		

- 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
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- 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
			1410	899	249	256	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	149	Total	C	N	O	S	0	0
			1111	699	197	214	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	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- 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	116	Total	C	N	O	0	0
			892	552	178	162		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	114	Total	C	N	O	S	0	0
			917	574	179	163	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	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	110	Total	C	N	O	S	0	0
			857	532	166	156	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	103	Total	C	N	O	0	0
			788	498	148	142		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	76	Total	C	N	O	S	0	0
			582	360	117	104	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	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	59	Total	C	N	O	S	0	0
			472	293	89	84	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
33	c	52	Total	C	N	O	0	0
			426	275	78	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	46	Total	C	N	O	S	0	0
			377	228	90	57	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	151	Total	C	N	O	S	0	0
			1181	735	227	215	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	117	Total	C	N	O	S	0	0
			877	540	174	160	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	112	Total	C	N	O	S	0	0
			867	535	175	154	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	88	Total	C	N	O	S	0	0
			714	439	144	130	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
			648	411	121	113	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	86	Total	C	N	O	S	0	0
			669	414	138	114	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 RNA chain called transfer-messenger RNA (tmRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4	363	Total	C	N	O	P	0	0
			7758	3465	1410	2520	363		

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	1	283	Total	Mg	0
			283	283	
58	2	126	Total	Mg	0
			126	126	
58	3	8	Total	Mg	0
			8	8	
58	B	2	Total	Mg	0
			2	2	
58	C	1	Total	Mg	0
			1	1	
58	L	2	Total	Mg	0
			2	2	
58	N	1	Total	Mg	0
			1	1	
58	U	1	Total	Mg	0
			1	1	
58	f	1	Total	Mg	0
			1	1	
58	i	1	Total	Mg	0
			1	1	
58	r	2	Total	Mg	0
			2	2	
58	4	1	Total	Mg	0
			1	1	

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	a	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
59	f	1	Total	Zn	0
			1	1	

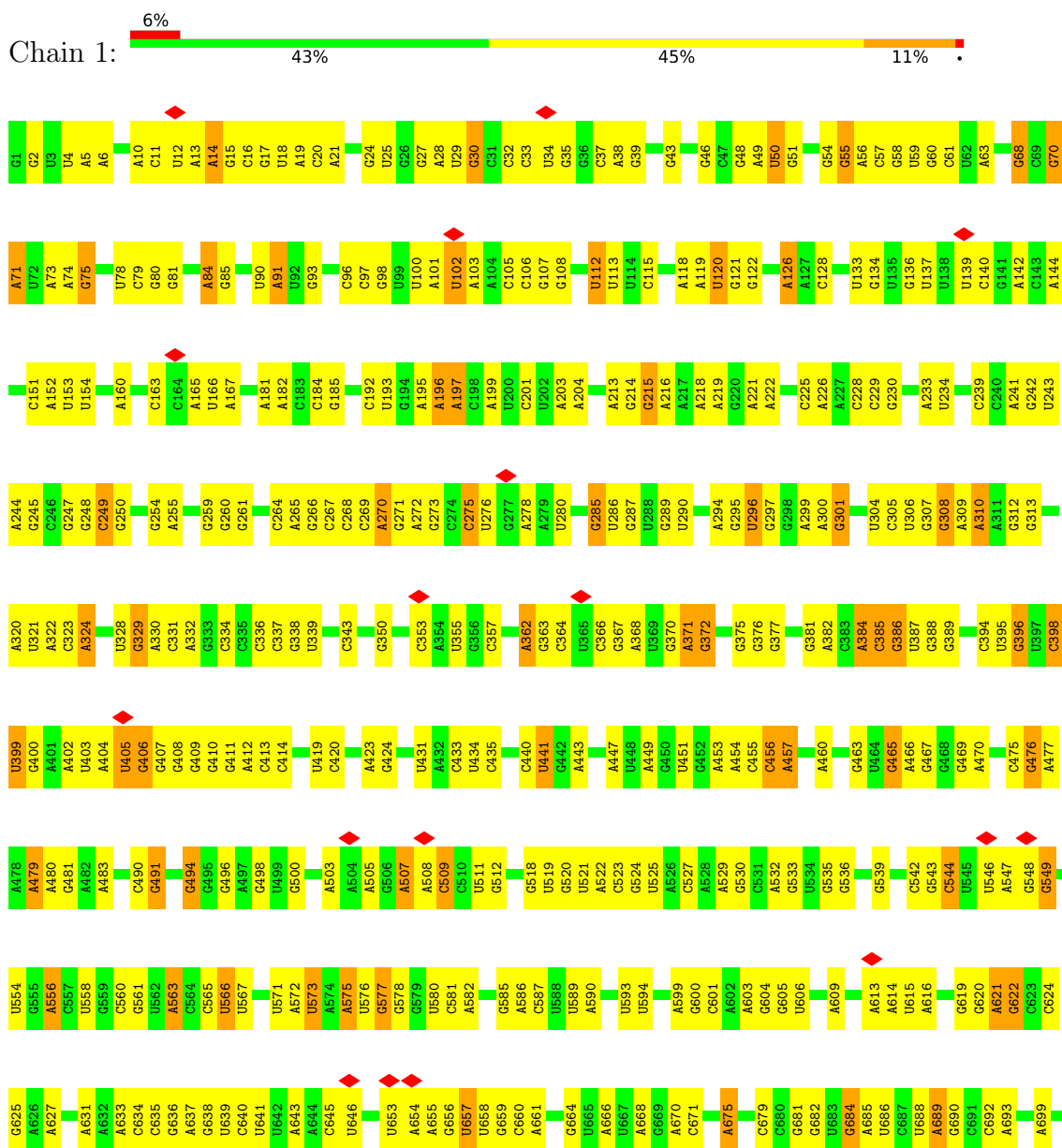
- Molecule 60 is water.

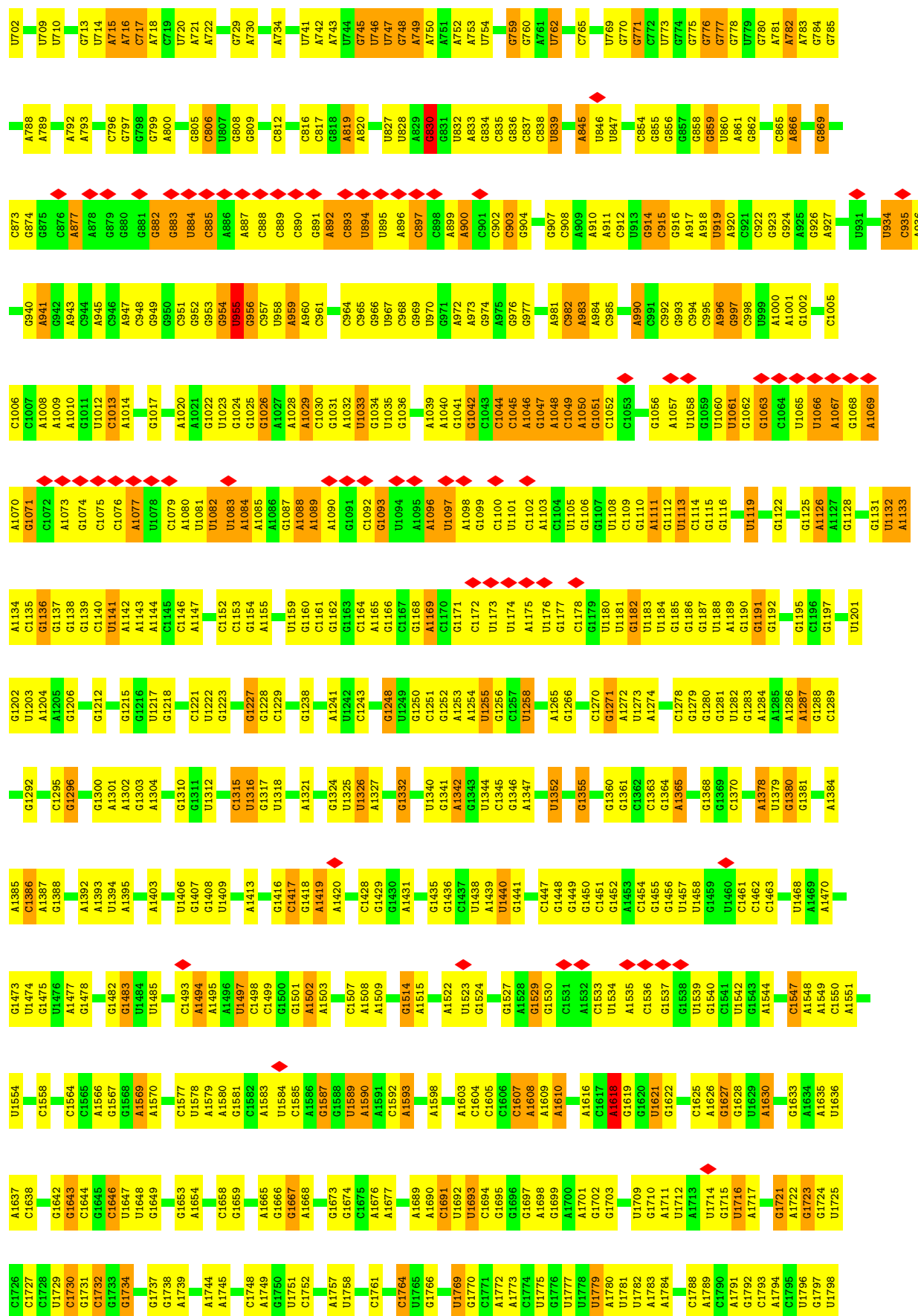
Mol	Chain	Residues	Atoms		AltConf
60	B	2	Total	O	0
			2	2	

3 Residue-property plots

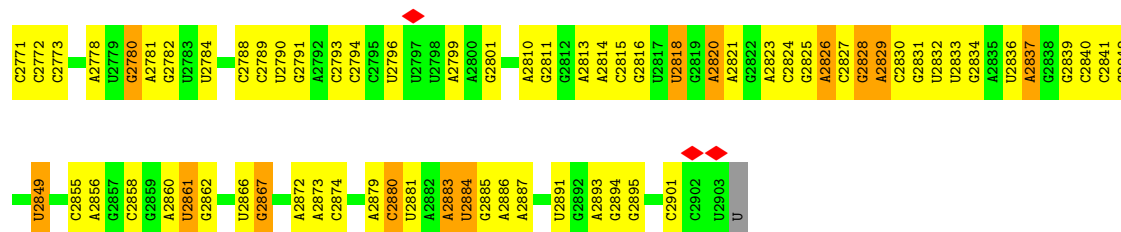
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

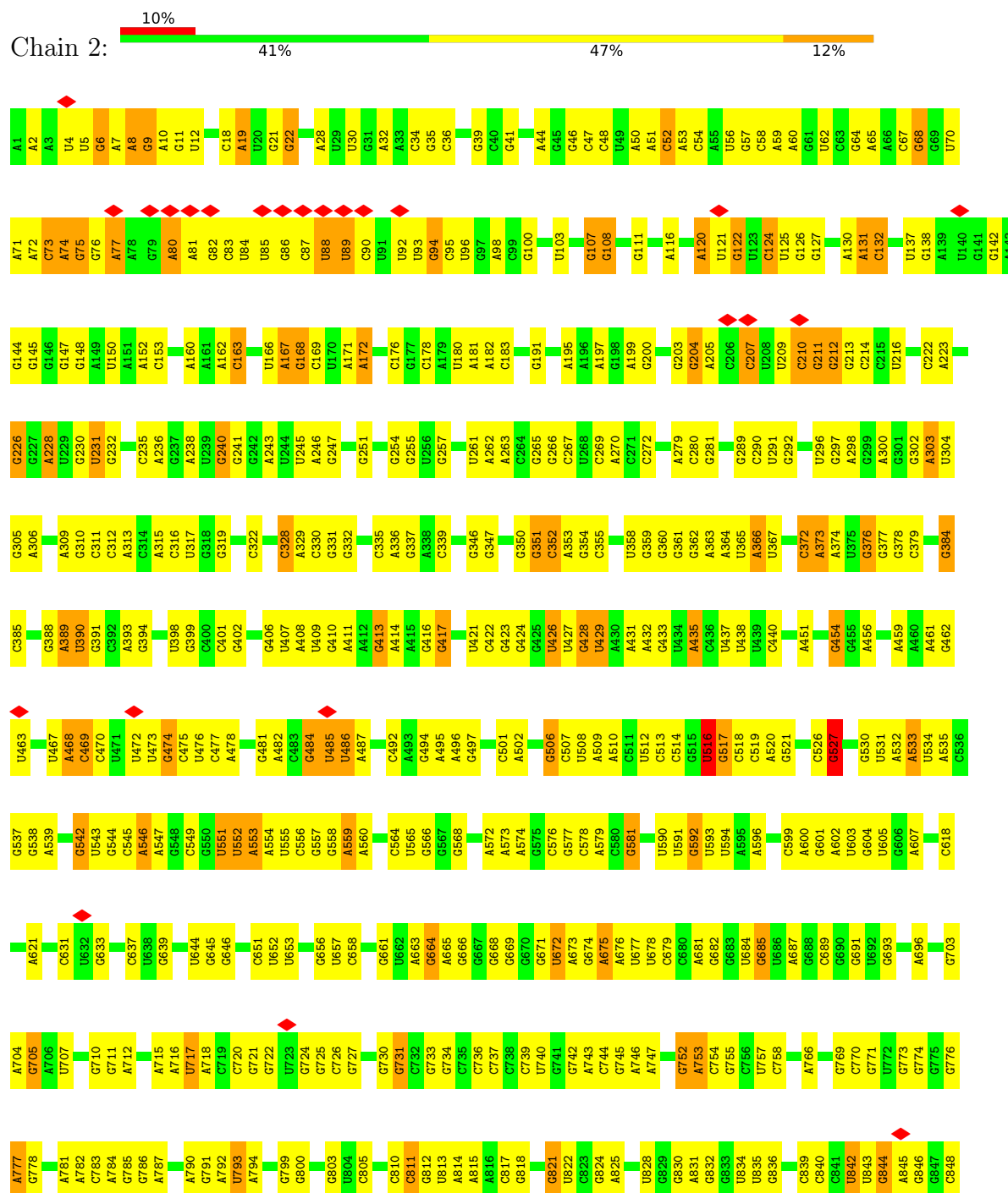


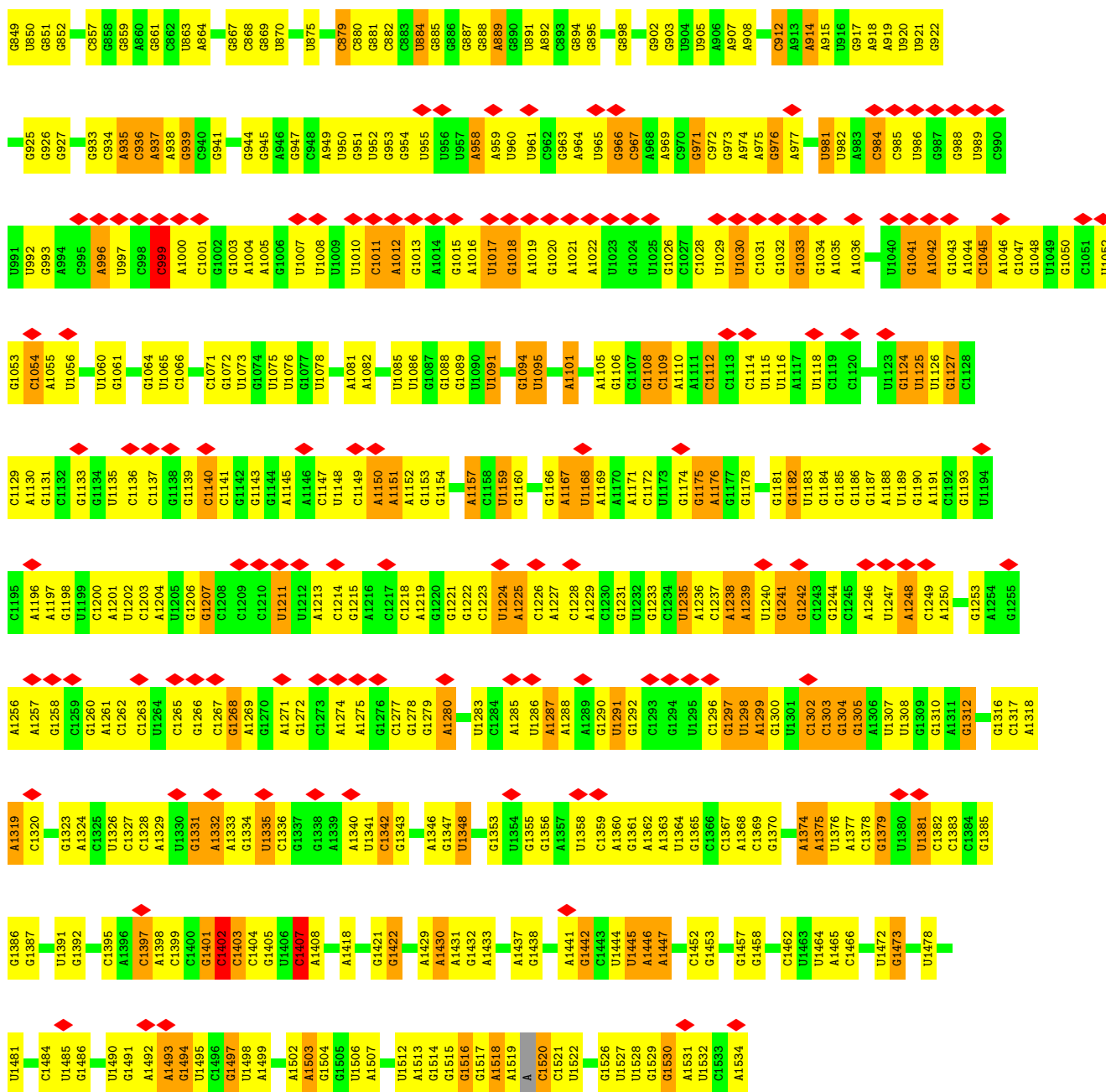


G2692	G2693	G2694	U2698	G2702	G2703	G2704	A2705	A2706	G2707	G2708	G2709	U2713	G2714	G2715	G2716	G2717	G2718	A2721	G2722	G2723	U2724	A2727	U2728	A2733	A2734	G2735	A2736	U2739	U2740	A2741	G2742	U2743	G2744	G2747	A2748	A2749	A2750	G2751	G2752	U2756	A2757	A2758	G2759	G2760	A2764	A2765	A2766	G2770											
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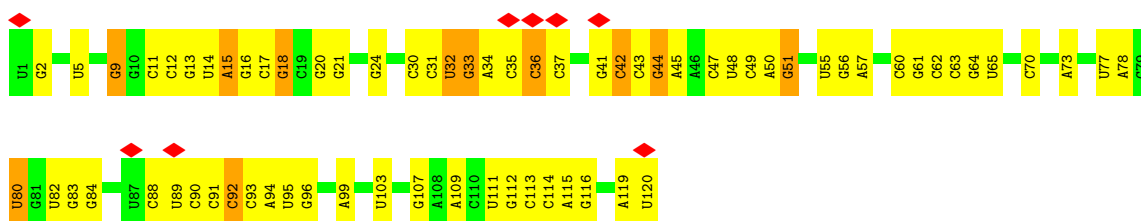
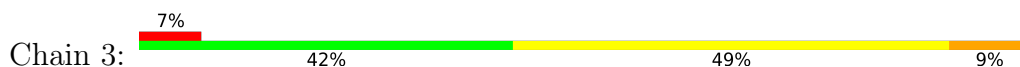


• Molecule 2: 16S ribosomal RNA

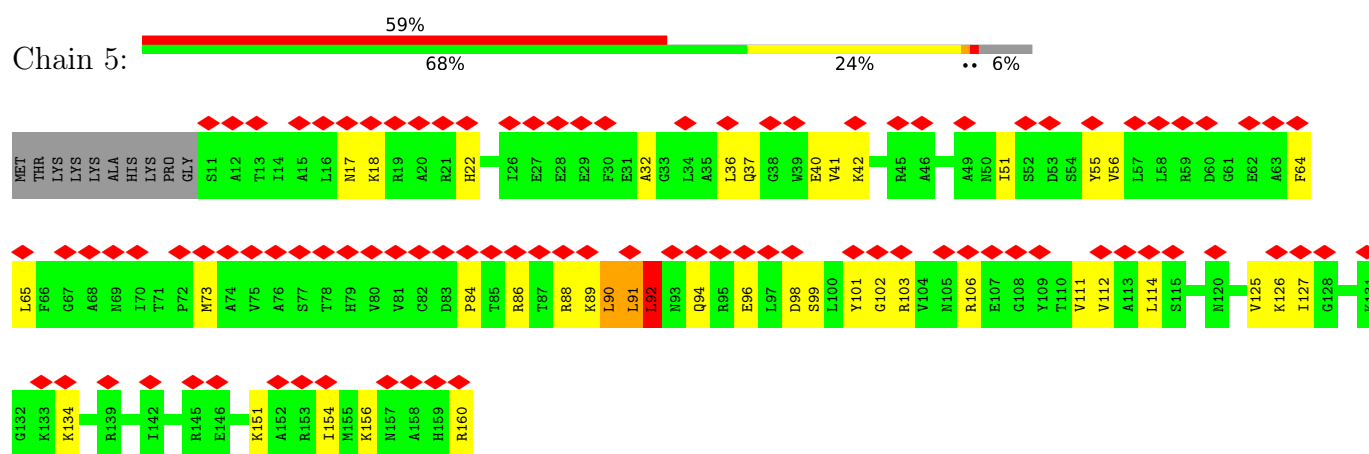




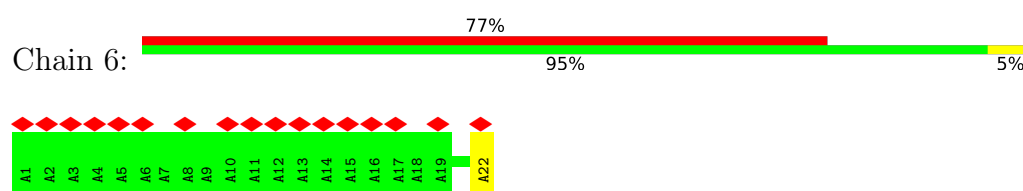
• Molecule 3: 5S ribosomal RNA



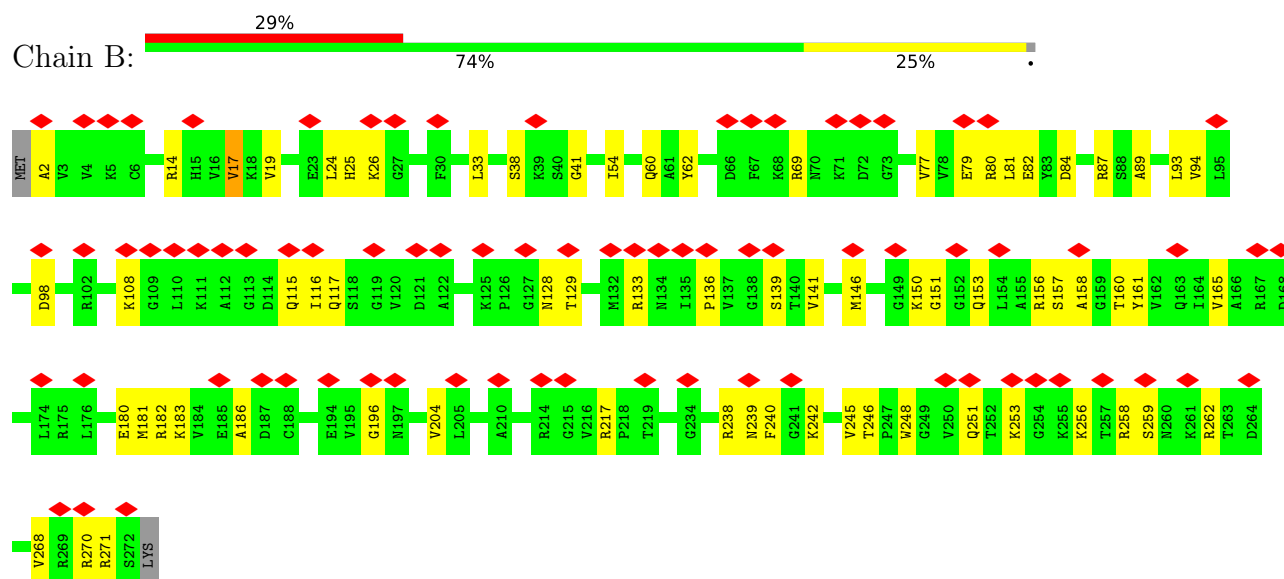
• Molecule 4: SsrA-binding protein



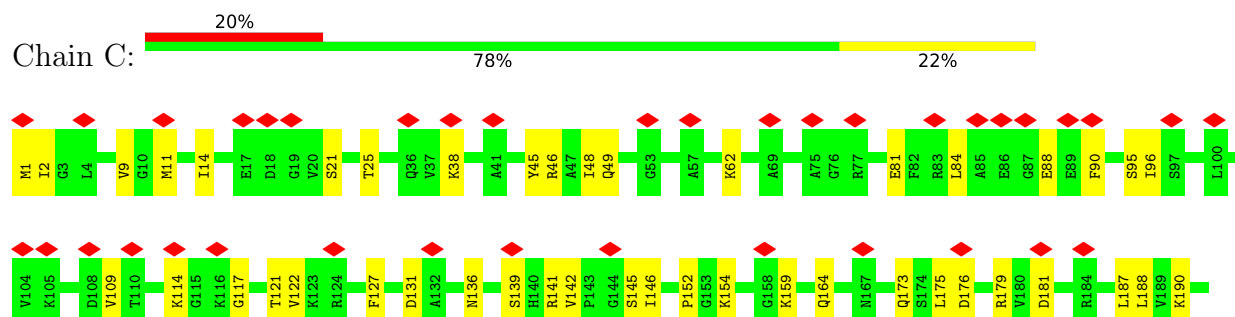
• Molecule 5: Nascent peptide



• Molecule 6: 50S ribosomal protein L2

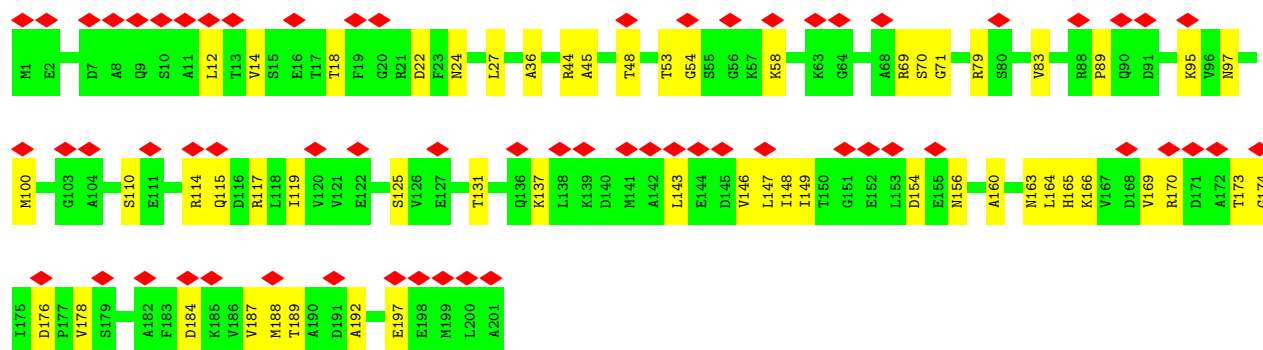
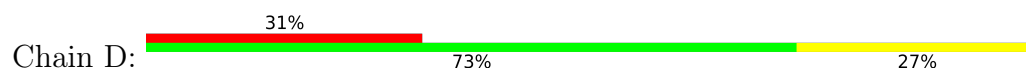


• Molecule 7: 50S ribosomal protein L3

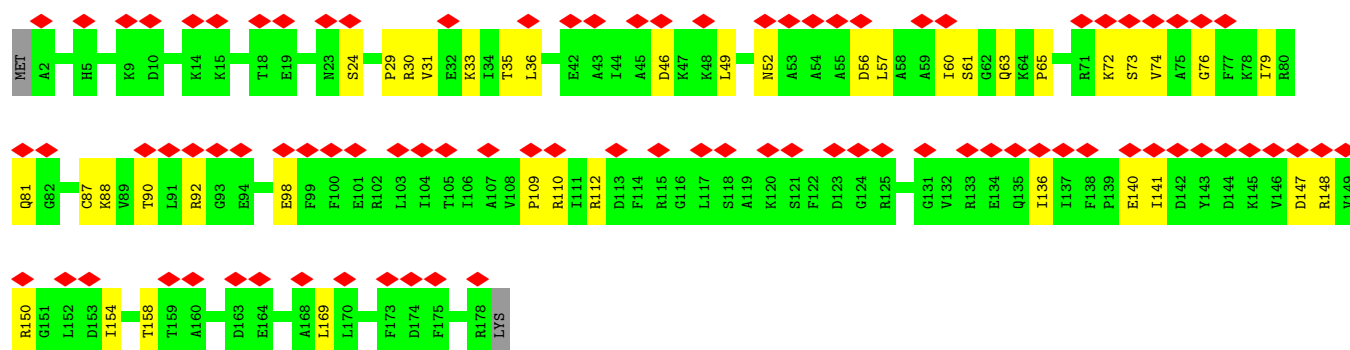
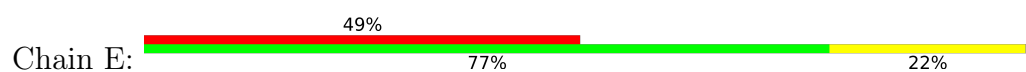




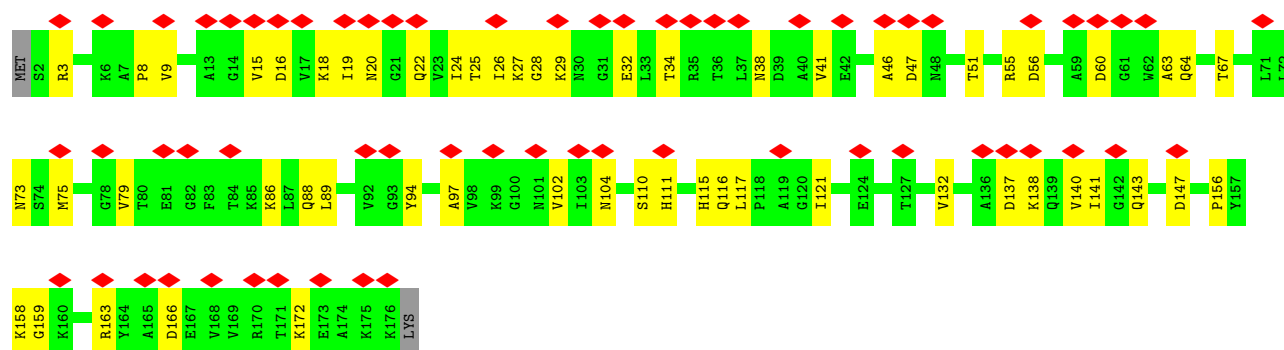
• Molecule 8: 50S ribosomal protein L4



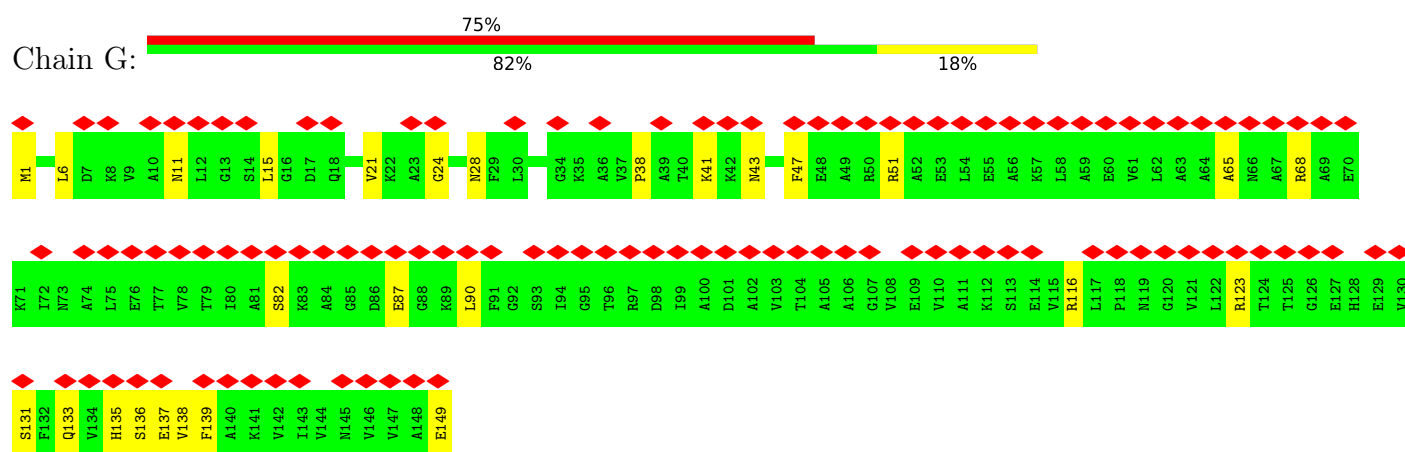
• Molecule 9: 50S ribosomal protein L5



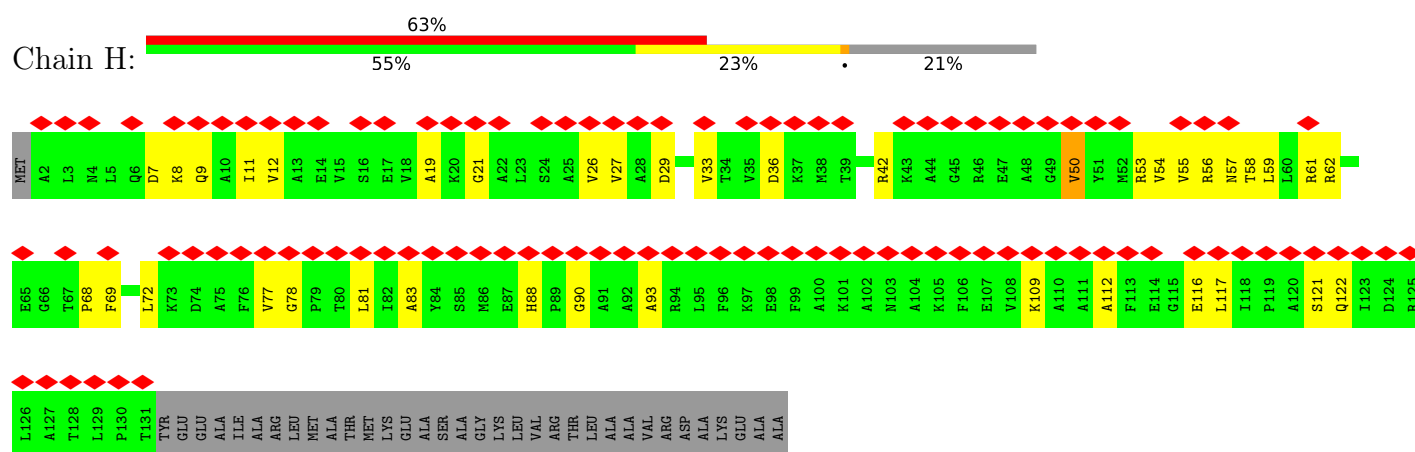
• Molecule 10: 50S ribosomal protein L6



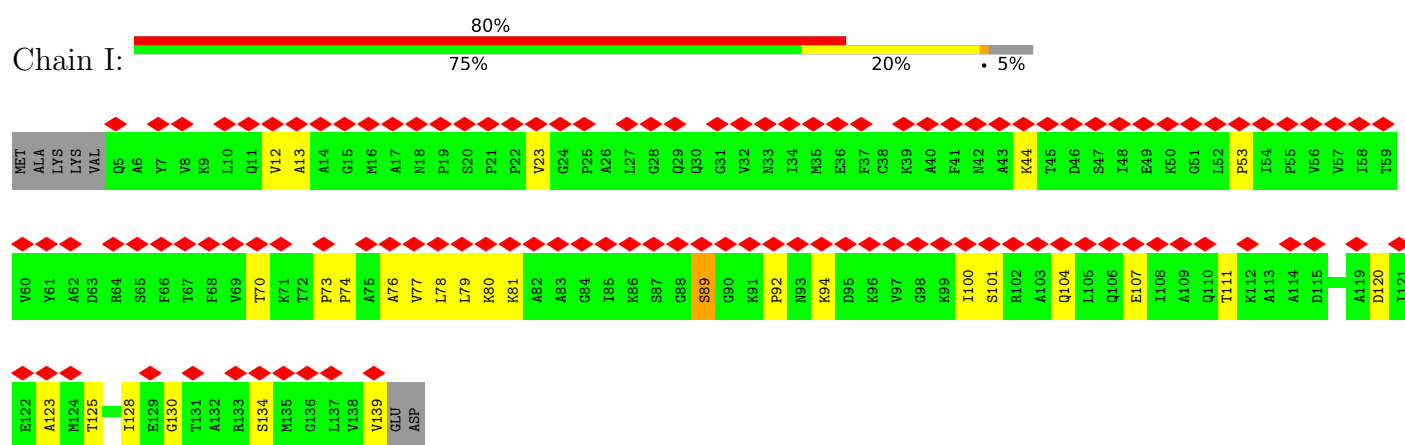
• Molecule 11: 50S ribosomal protein L9



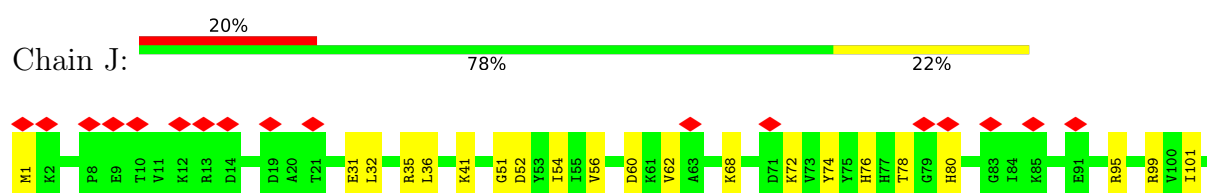
• Molecule 12: 50S ribosomal protein L10

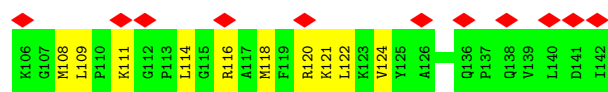


• Molecule 13: 50S ribosomal protein L11

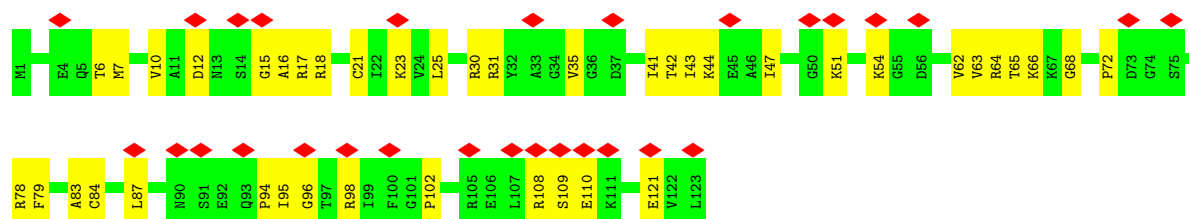


• Molecule 14: 50S ribosomal protein L13

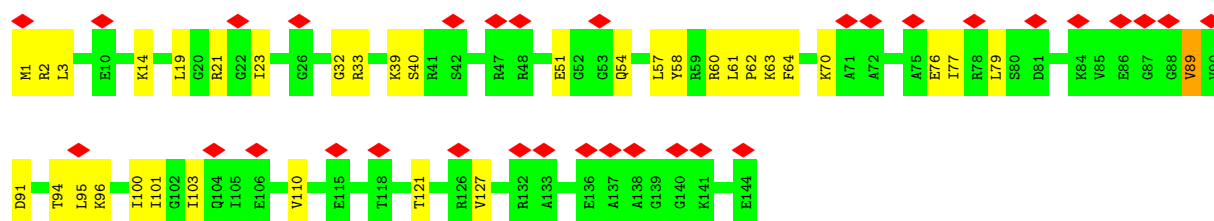
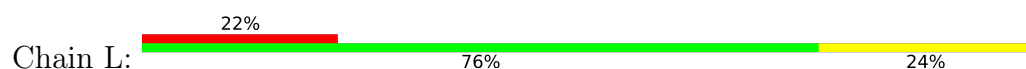




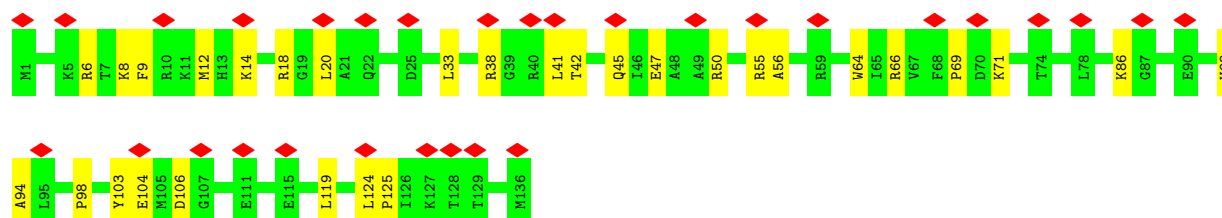
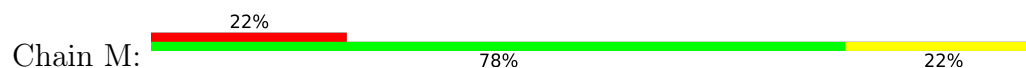
- Molecule 15: 50S ribosomal protein L14



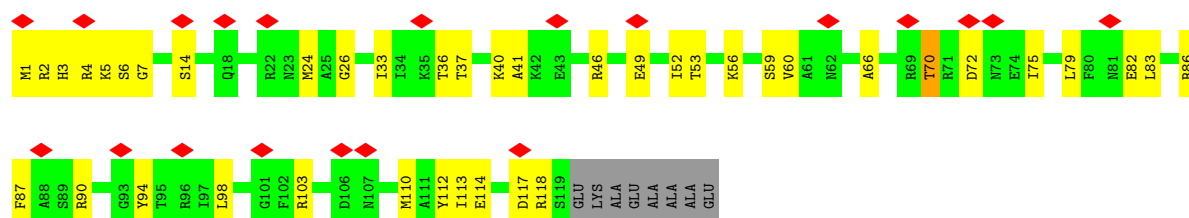
- Molecule 16: 50S ribosomal protein L15



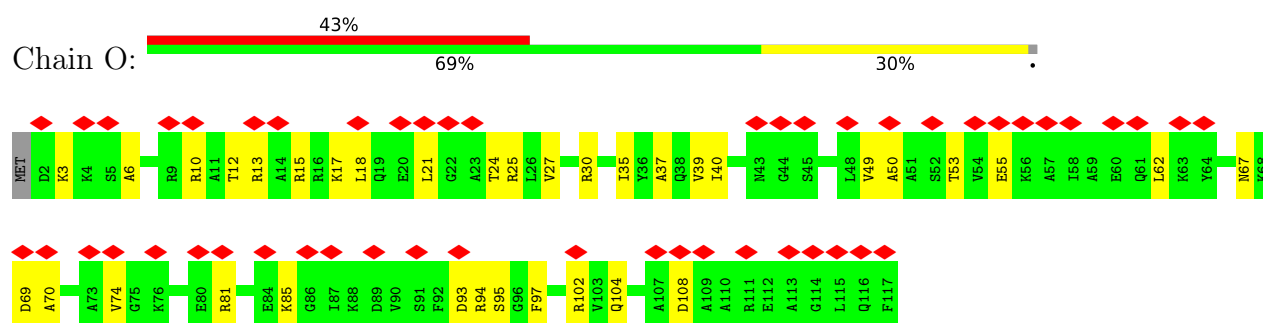
- Molecule 17: 50S ribosomal protein L16



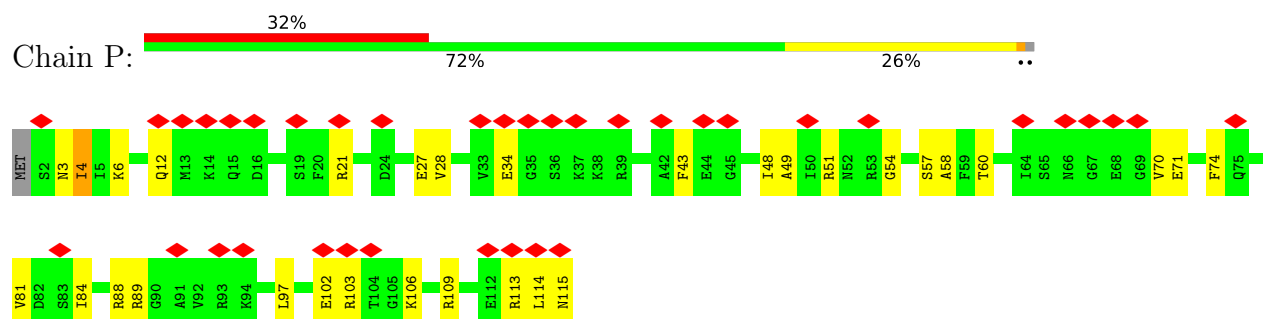
- Molecule 18: 50S ribosomal protein L17



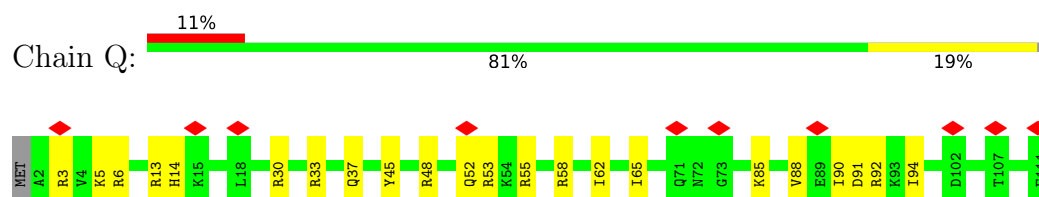
- Molecule 19: 50S ribosomal protein L18



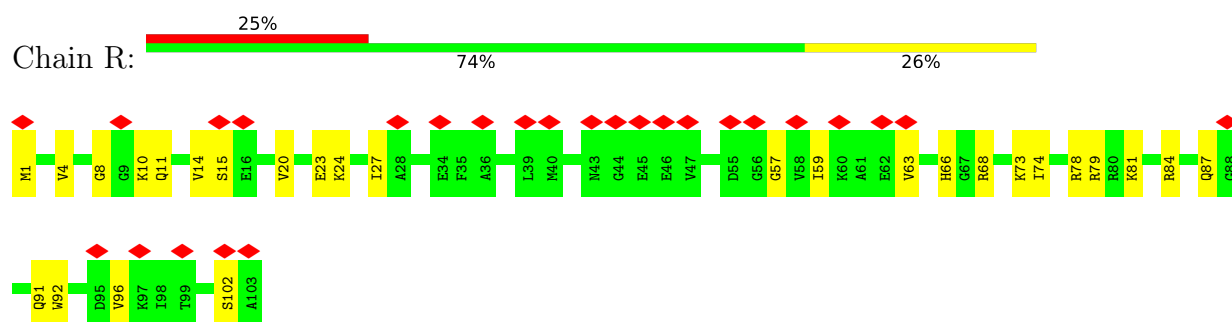
• Molecule 20: 50S ribosomal protein L19



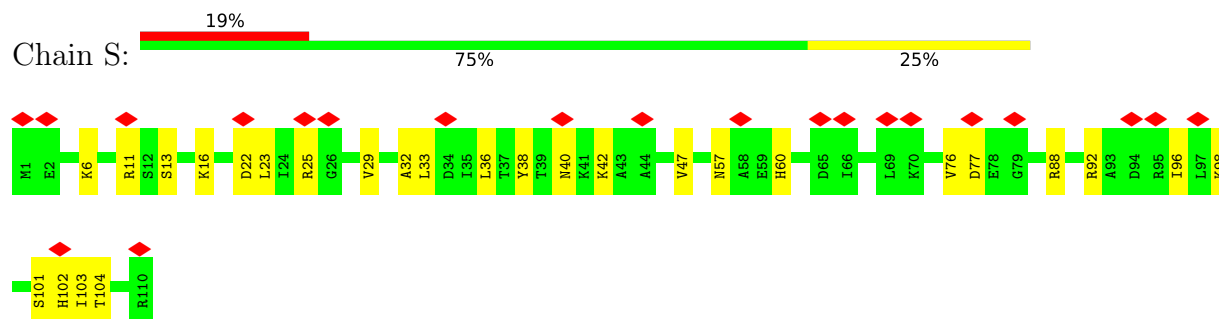
• Molecule 21: 50S ribosomal protein L20



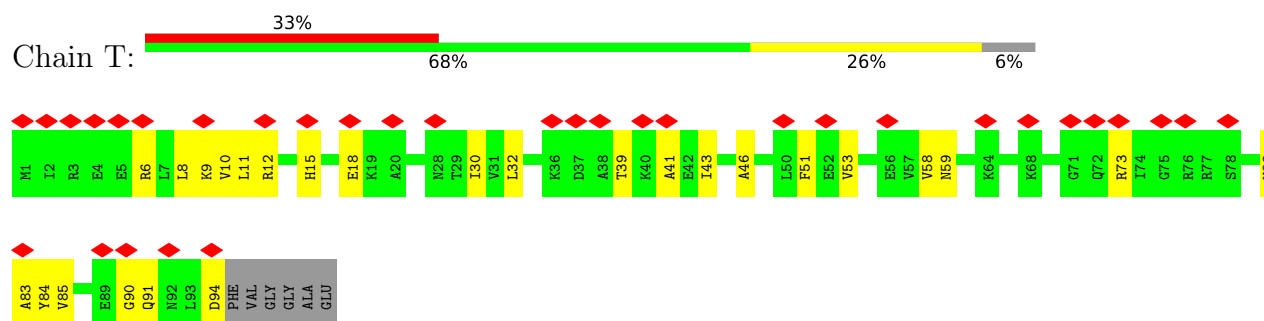
• Molecule 22: 50S ribosomal protein L21



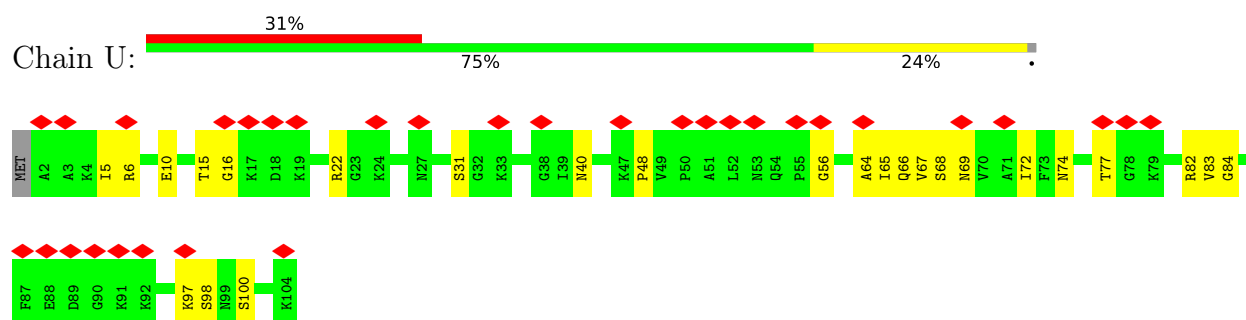
• Molecule 23: 50S ribosomal protein L22



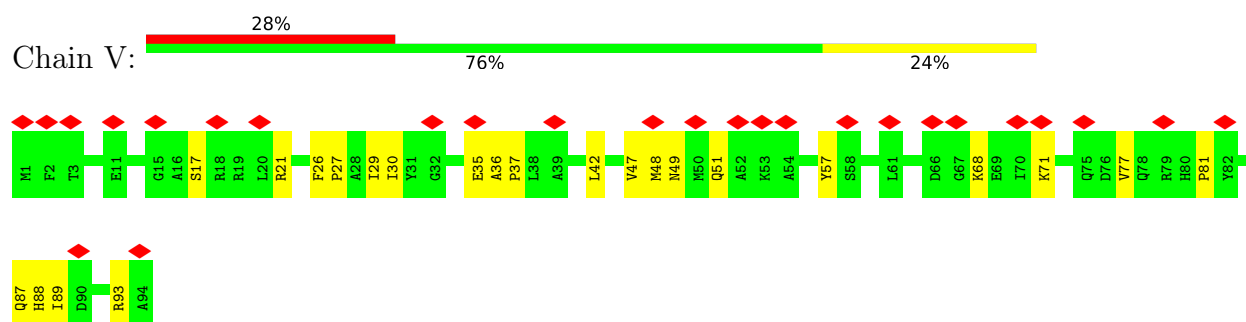
- Molecule 24: 50S ribosomal protein L23



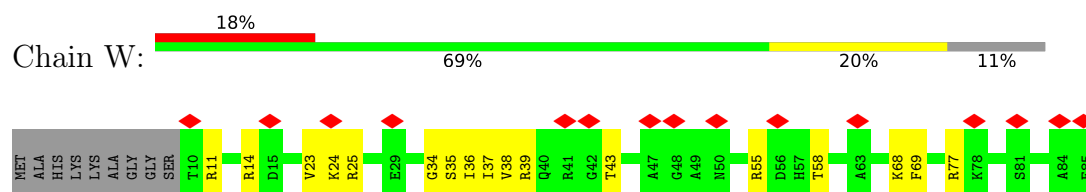
- Molecule 25: 50S ribosomal protein L24



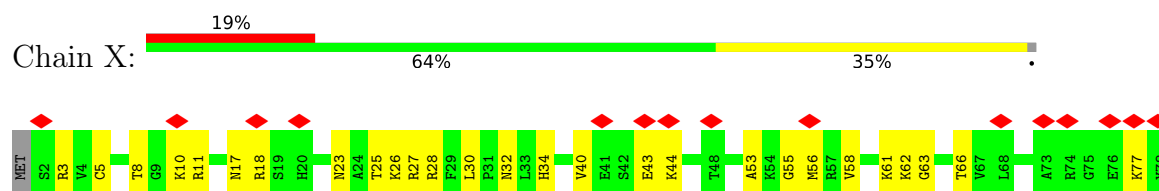
- Molecule 26: 50S ribosomal protein L25



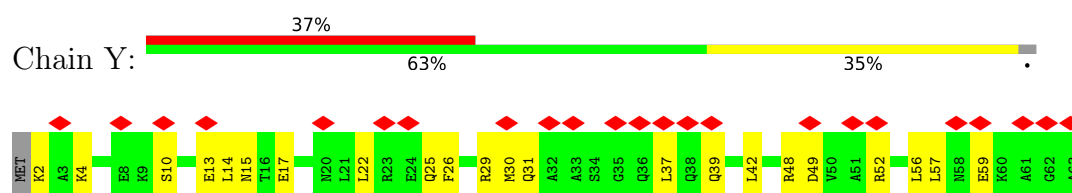
- Molecule 27: 50S ribosomal protein L27



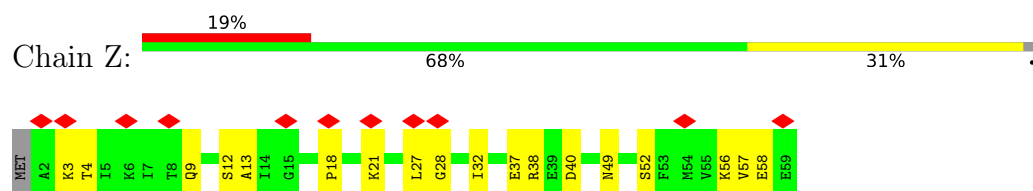
- Molecule 28: 50S ribosomal protein L28



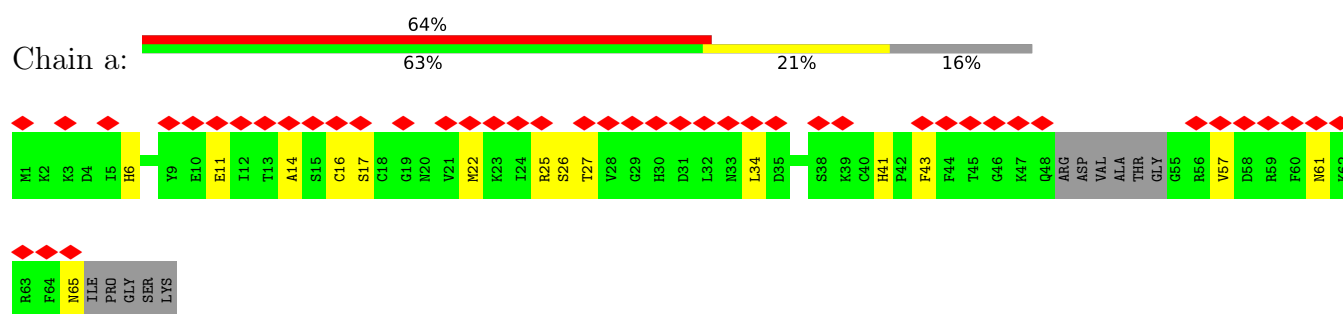
- Molecule 29: 50S ribosomal protein L29



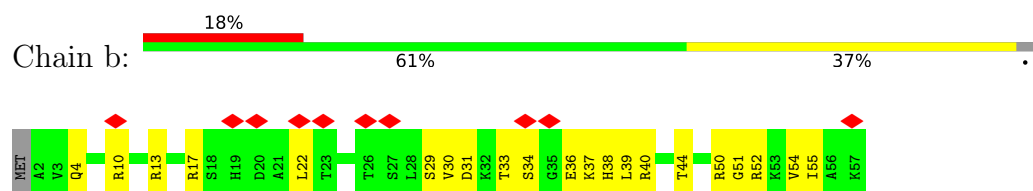
- Molecule 30: 50S ribosomal protein L30



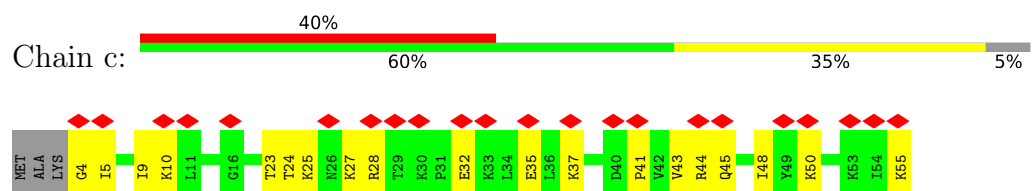
- Molecule 31: 50S ribosomal protein L31



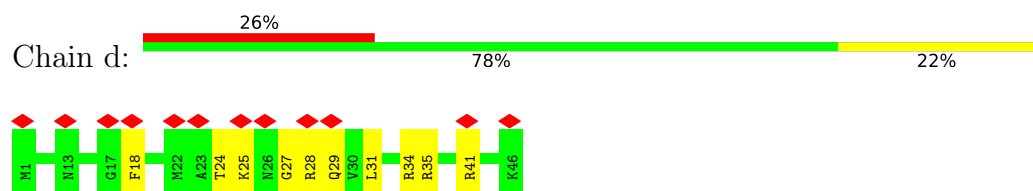
- Molecule 32: 50S ribosomal protein L32



- Molecule 33: 50S ribosomal protein L33

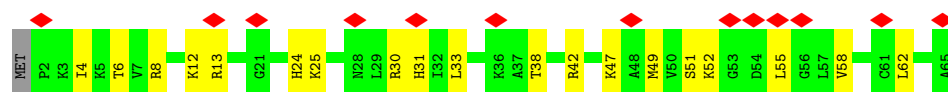


- Molecule 34: 50S ribosomal protein L34

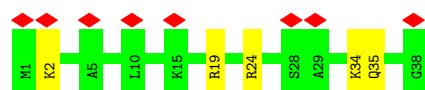
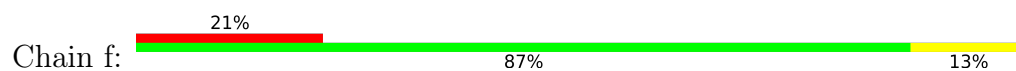


- Molecule 35: 50S ribosomal protein L35

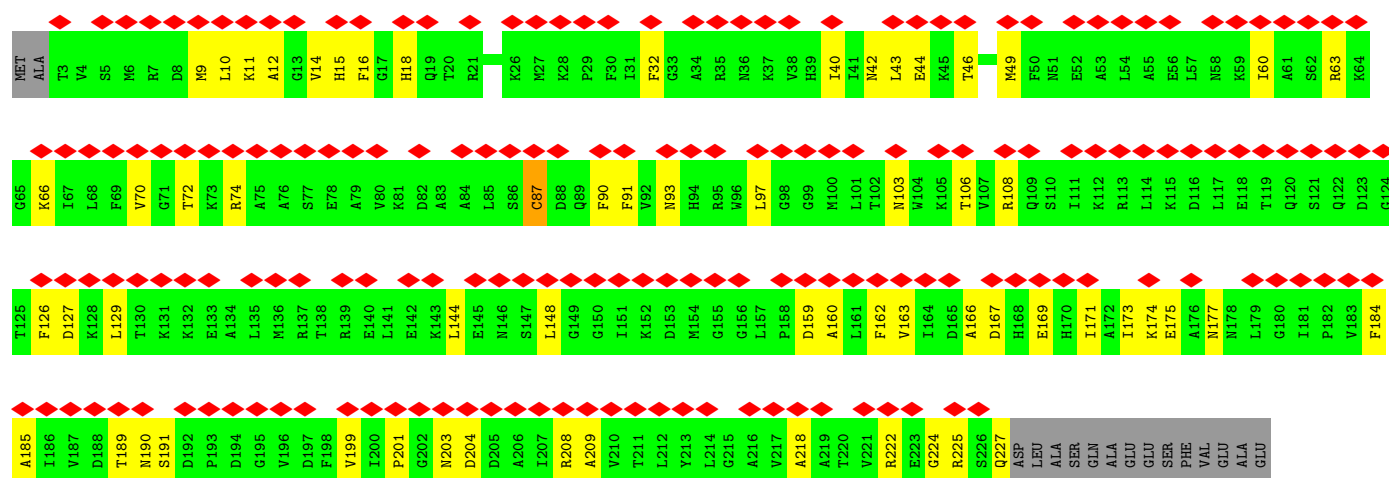
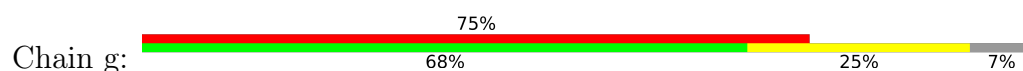




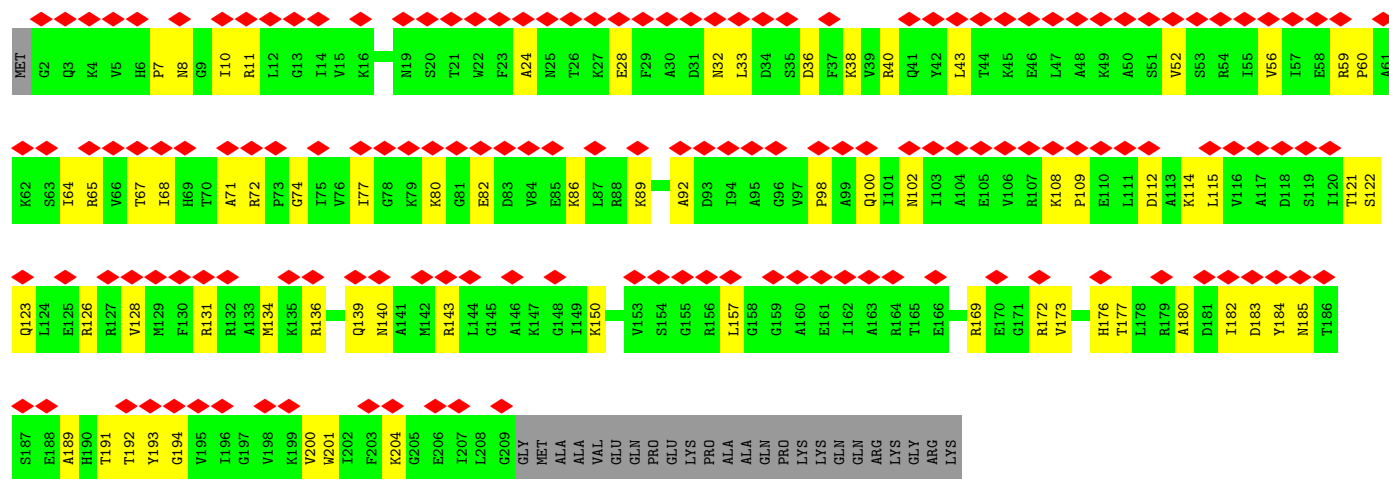
- Molecule 36: 50S ribosomal protein L36



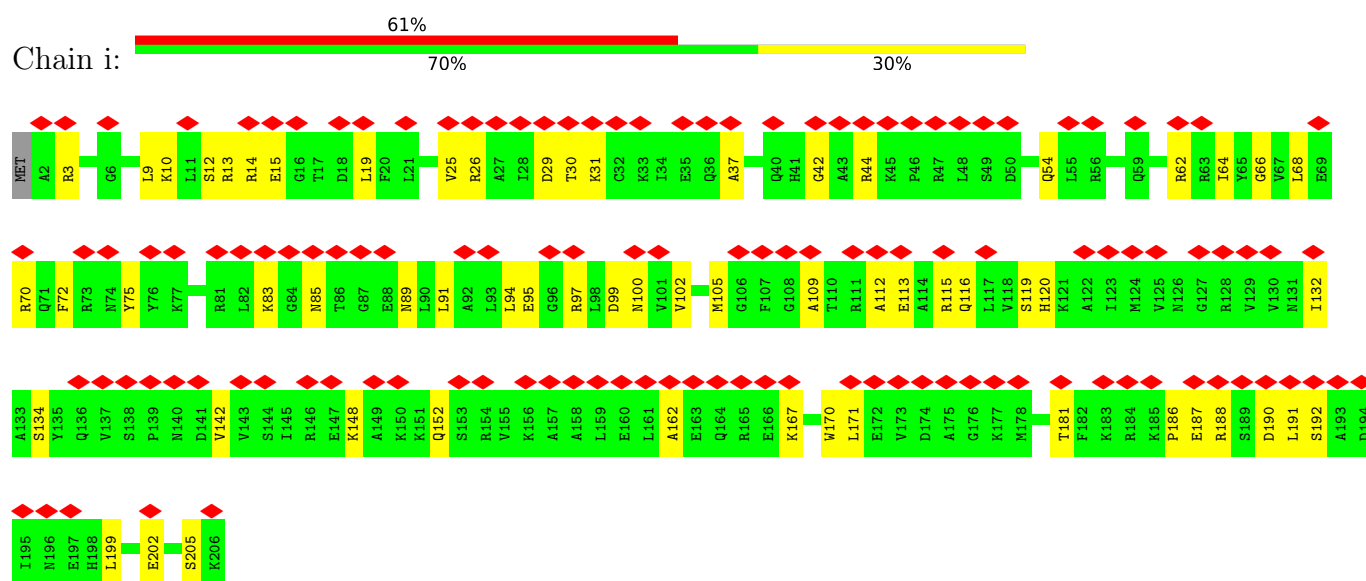
- Molecule 37: 30S ribosomal protein S2



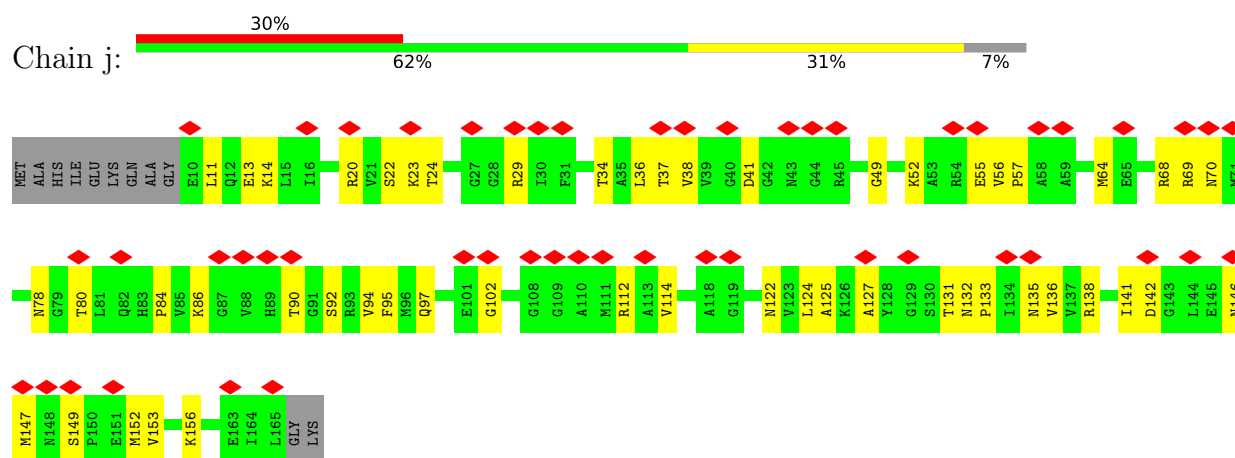
- Molecule 38: 30S ribosomal protein S3



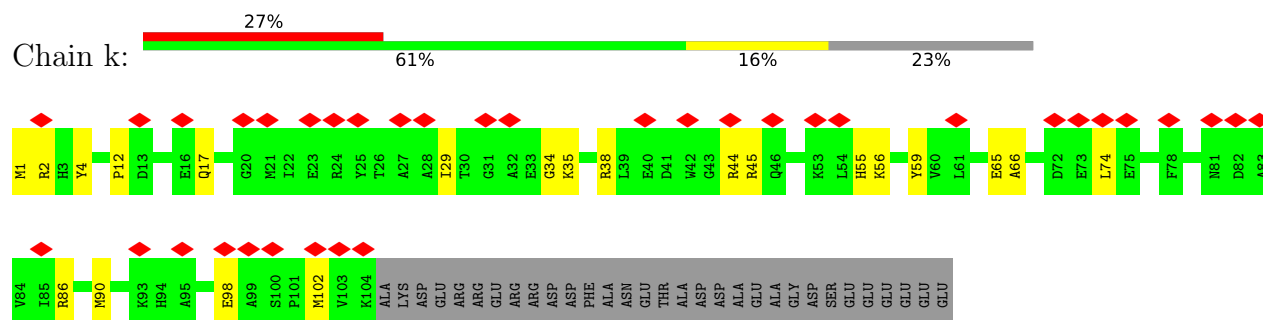
- Molecule 39: 30S ribosomal protein S4



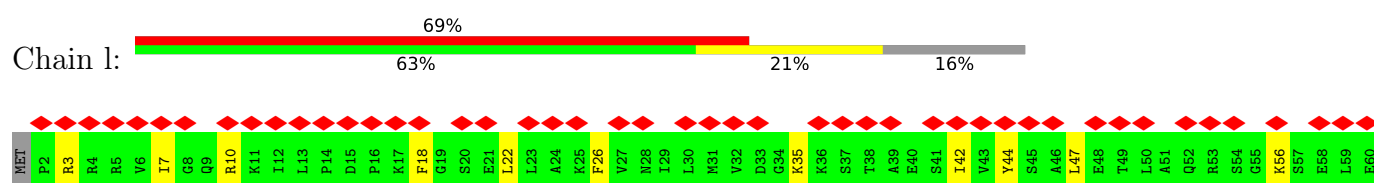
• Molecule 40: 30S ribosomal protein S5

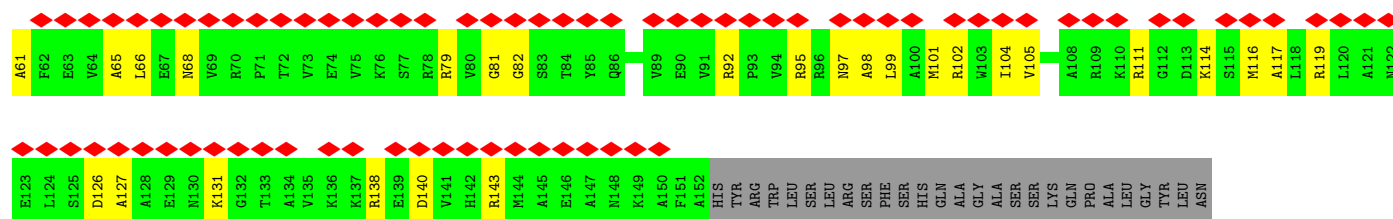


• Molecule 41: 30S ribosomal protein S6

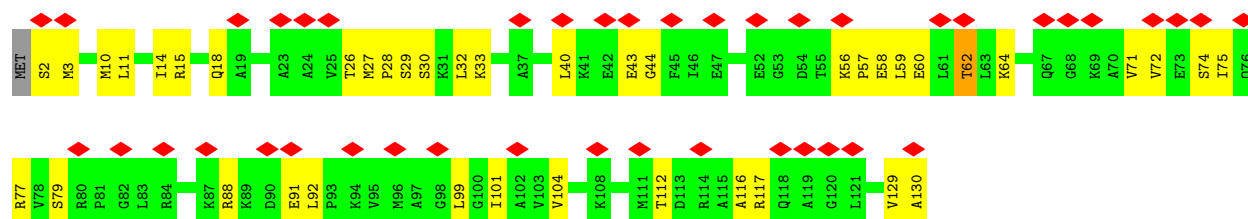


• Molecule 42: 30S ribosomal protein S7

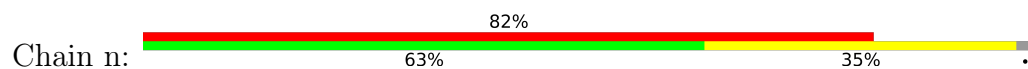




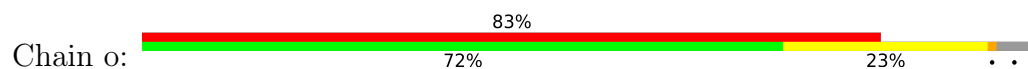
• Molecule 43: 30S ribosomal protein S8



• Molecule 44: 30S ribosomal protein S9

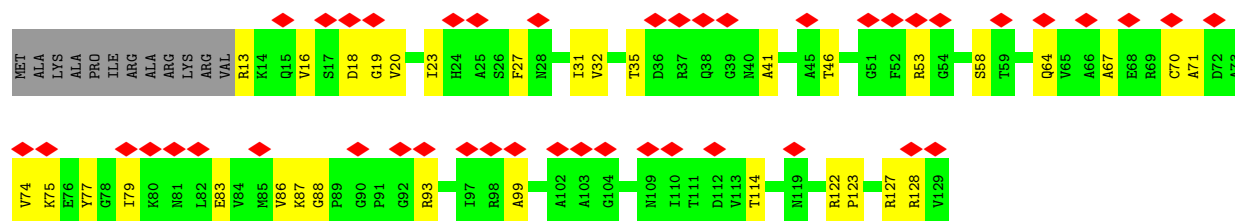


• Molecule 45: 30S ribosomal protein S10

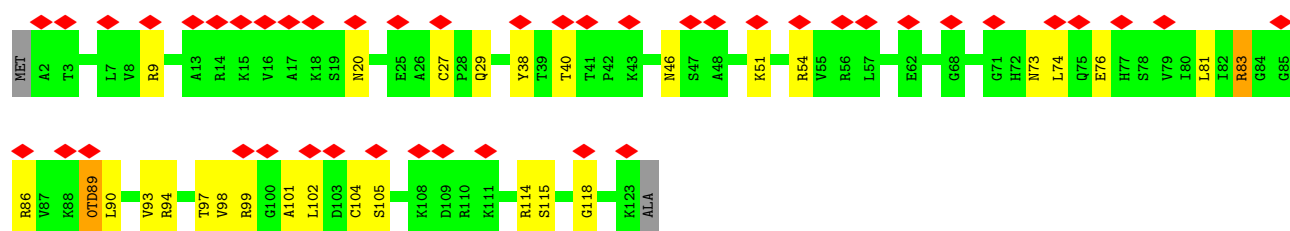
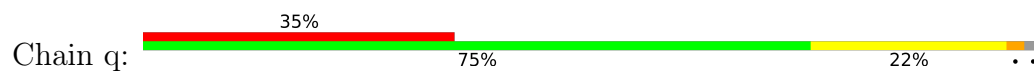


• Molecule 46: 30S ribosomal protein S11

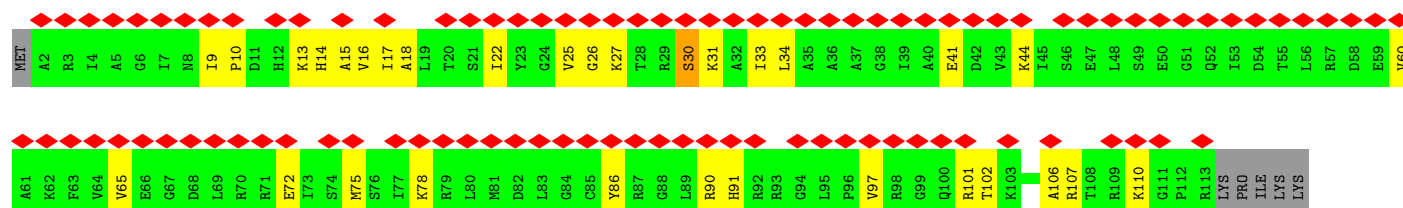
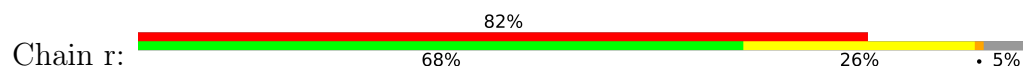




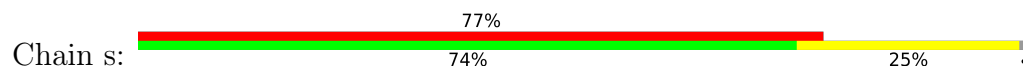
• Molecule 47: 30S ribosomal protein S12



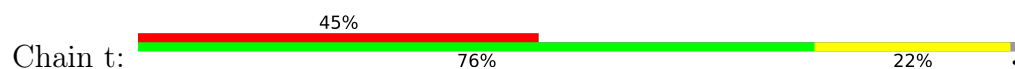
• Molecule 48: 30S ribosomal protein S13

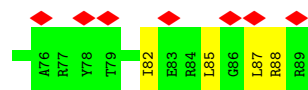


• Molecule 49: 30S ribosomal protein S14

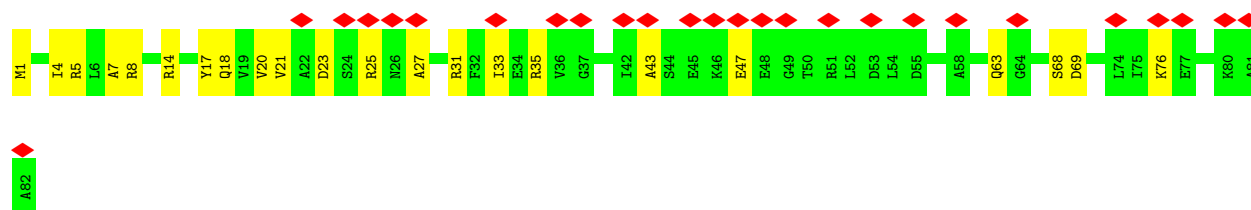
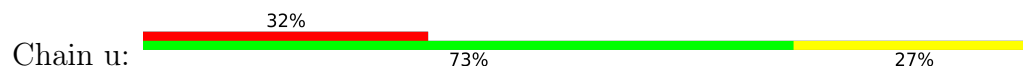


• Molecule 50: 30S ribosomal protein S15

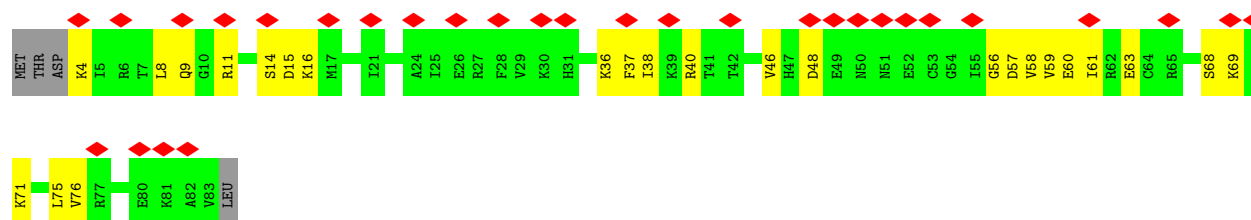




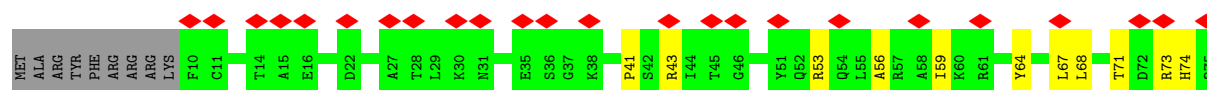
- Molecule 51: 30S ribosomal protein S16



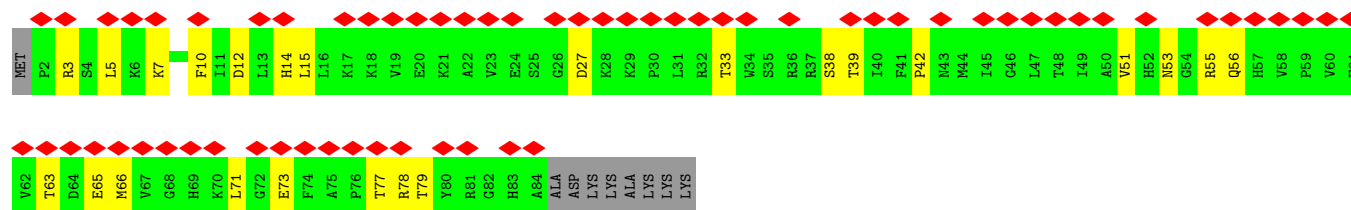
- Molecule 52: 30S ribosomal protein S17



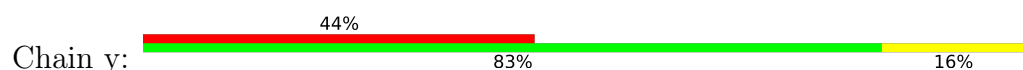
- Molecule 53: 30S ribosomal protein S18

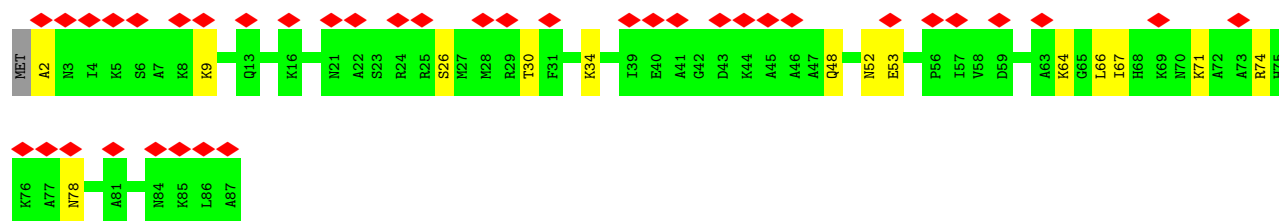


- Molecule 54: 30S ribosomal protein S19

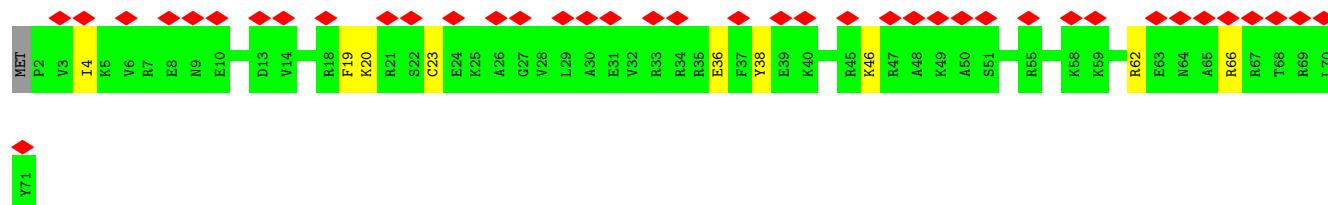
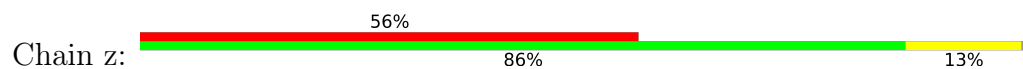


- Molecule 55: 30S ribosomal protein S20

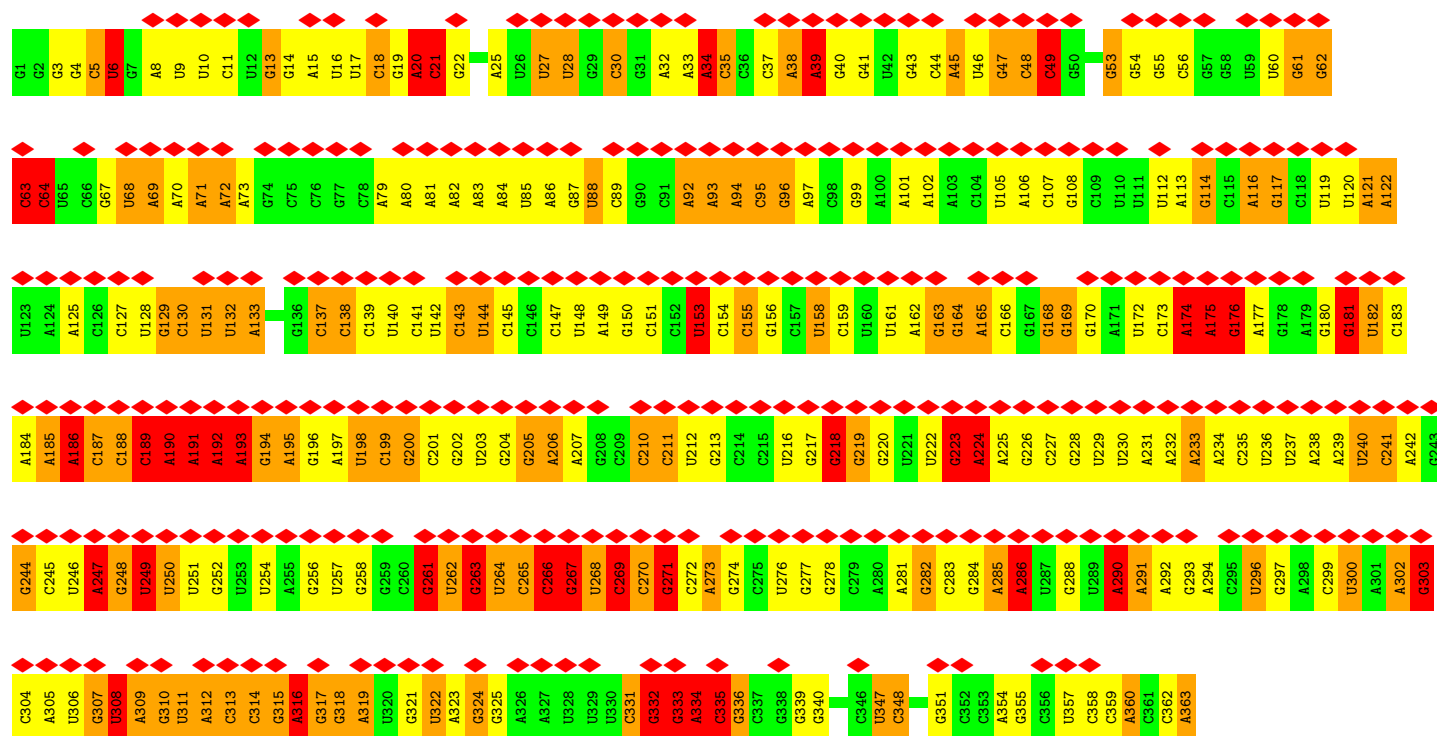
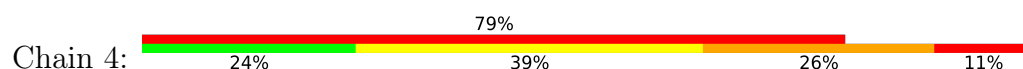




- Molecule 56: 30S ribosomal protein S21



- Molecule 57: transfer-messenger RNA (tmRNA)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18018	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	0.407	Depositor
Minimum map value	-0.269	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0934	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: 0TD, PSU, OMC, 2MA, 4OC, MG, 2MG, MA6, 6MZ, 3TD, 5MC, OMG, UR3, G7M, 7MG, 5MU, OMU, ZN, 1MG

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	0.42	1/69285 (0.0%)	0.53	2/108083 (0.0%)
2	2	0.35	0/36587	0.51	1/57062 (0.0%)
3	3	0.33	0/2872	0.45	0/4478
4	5	0.42	1/1231 (0.1%)	0.77	1/1655 (0.1%)
5	6	0.25	0/109	0.70	0/151
6	B	0.37	0/2121	0.62	0/2852
7	C	0.37	0/1586	0.63	0/2134
8	D	0.35	0/1571	0.60	0/2113
9	E	0.30	0/1434	0.67	0/1926
10	F	0.27	0/1333	0.55	0/1805
11	G	0.26	0/1122	0.59	0/1515
12	H	0.35	0/993	0.80	1/1340 (0.1%)
13	I	0.27	0/998	0.65	0/1348
14	J	0.36	0/1152	0.57	0/1551
15	K	0.37	0/955	0.61	0/1279
16	L	0.33	0/1062	0.60	0/1413
17	M	0.38	0/1093	0.59	0/1460
18	N	0.40	0/964	0.68	0/1289
19	O	0.28	0/902	0.54	0/1209
20	P	0.35	0/929	0.59	0/1242
21	Q	0.38	0/960	0.59	0/1278
22	R	0.37	0/829	0.62	0/1107
23	S	0.38	0/864	0.64	0/1156
24	T	0.31	0/752	0.55	0/1005
25	U	0.31	0/796	0.58	2/1062 (0.2%)
26	V	0.31	0/766	0.52	0/1025
27	W	0.34	0/589	0.55	0/779
28	X	0.36	0/635	0.58	0/848
29	Y	0.31	0/502	0.51	0/667
30	Z	0.32	0/452	0.57	0/605
31	a	0.21	0/480	0.50	0/638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.40	0/450	0.63	0/599
33	c	0.32	0/433	0.63	0/576
34	d	0.37	0/380	0.65	0/498
35	e	0.40	0/513	0.72	0/676
36	f	0.36	0/303	0.64	0/397
37	g	0.27	0/1791	0.62	2/2413 (0.1%)
38	h	0.27	0/1663	0.61	0/2241
39	i	0.26	0/1665	0.53	0/2227
40	j	0.34	0/1165	0.66	0/1568
41	k	0.28	0/867	0.60	0/1171
42	l	0.26	0/1195	0.61	0/1602
43	m	0.33	0/989	0.59	0/1326
44	n	0.23	0/1034	0.58	0/1375
45	o	0.25	0/800	0.57	0/1082
46	p	0.29	0/893	0.58	0/1205
47	q	0.35	0/954	0.76	2/1279 (0.2%)
48	r	0.28	0/875	0.67	0/1170
49	s	0.26	0/817	0.54	0/1088
50	t	0.32	0/722	0.60	0/964
51	u	0.29	0/659	0.63	0/884
52	v	0.30	0/657	0.59	0/881
53	w	0.29	0/553	0.52	0/743
54	x	0.24	0/680	0.57	0/915
55	y	0.27	0/675	0.54	0/895
56	z	0.28	0/597	0.55	0/792
57	4	0.52	0/8680	1.24	104/13528 (0.8%)
All	All	0.38	2/165934 (0.0%)	0.61	115/248170 (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	26	1
2	2	0	1
4	5	0	1
10	F	0	1
13	I	0	2
22	R	0	1
23	S	0	1
35	e	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	h	0	1
43	m	0	1
47	q	0	1
53	w	0	1
All	All	26	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2552	OMU	O3'-P	6.32	1.62	1.56
4	5	91	LEU	N-CA	5.25	1.53	1.46

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	4	48	C	O3'-P-O5'	10.46	119.69	104.00
57	4	266	C	O3'-P-O5'	9.61	118.41	104.00
57	4	161	U	O3'-P-O5'	9.59	118.39	104.00
57	4	163	G	O3'-P-O5'	9.26	117.89	104.00
57	4	269	C	O3'-P-O5'	9.04	117.55	104.00
57	4	137	C	O3'-P-O5'	8.99	117.48	104.00
57	4	284	G	P-O3'-C3'	8.31	132.66	120.20
57	4	34	A	O3'-P-O5'	8.17	116.26	104.00
57	4	161	U	P-O3'-C3'	8.14	132.42	120.20
57	4	137	C	P-O3'-C3'	7.65	131.68	120.20
57	4	332	G	C5'-C4'-O4'	-7.63	98.35	109.80
57	4	290	A	P-O3'-C3'	7.50	131.46	120.20
57	4	187	C	C5'-C4'-C3'	-7.37	104.94	116.00
57	4	175	A	O3'-P-O5'	7.26	114.89	104.00
57	4	360	A	O5'-C5'-C4'	6.93	121.90	111.50
57	4	193	A	O5'-C5'-C4'	6.87	121.81	111.50
57	4	161	U	C4'-C3'-O3'	-6.86	102.72	113.00
57	4	290	A	O3'-P-O5'	6.84	114.26	104.00
57	4	132	U	O3'-P-O5'	6.81	114.21	104.00
57	4	189	C	O3'-P-O5'	6.80	114.19	104.00
57	4	314	C	P-O3'-C3'	6.78	130.37	120.20
57	4	191	A	O3'-P-O5'	6.76	114.14	104.00
57	4	308	U	P-O3'-C3'	6.72	130.28	120.20
57	4	335	C	C4'-C3'-O3'	6.70	123.05	113.00
4	5	91	LEU	N-CA-C	6.59	118.15	108.86
57	4	266	C	P-O3'-C3'	6.56	130.04	120.20
57	4	233	A	P-O3'-C3'	6.50	129.95	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	4	18	C	O4'-C1'-N1	6.39	118.08	108.50
57	4	13	G	P-O3'-C3'	6.27	129.60	120.20
57	4	5	C	O3'-P-O5'	6.26	113.39	104.00
57	4	331	C	O3'-P-O5'	6.20	113.30	104.00
57	4	193	A	C5'-C4'-O4'	-6.18	100.52	109.80
57	4	303	G	O5'-C5'-C4'	6.13	120.69	111.50
57	4	211	C	C4'-C3'-O3'	-6.12	103.82	113.00
57	4	256	G	C2'-C3'-O3'	-6.12	104.53	113.70
57	4	316	A	C5'-C4'-O4'	-6.11	100.64	109.80
57	4	263	G	C5'-C4'-C3'	6.10	125.15	116.00
57	4	155	C	O3'-P-O5'	6.09	113.14	104.00
57	4	130	C	P-O3'-C3'	6.08	129.32	120.20
57	4	133	A	C5'-C4'-O4'	-6.07	100.69	109.80
57	4	174	A	O3'-P-O5'	6.07	113.10	104.00
57	4	249	U	O3'-P-O5'	6.06	113.09	104.00
57	4	336	G	P-O5'-C5'	-6.06	111.81	120.90
57	4	261	G	OP1-P-O3'	6.02	126.07	108.00
57	4	324	G	C2'-C3'-O3'	-6.00	104.70	113.70
57	4	333	G	O3'-P-O5'	-5.95	95.07	104.00
57	4	224	A	O4'-C1'-N9	5.94	117.41	108.50
57	4	49	C	P-O5'-C5'	5.92	129.79	120.90
57	4	263	G	O3'-P-O5'	5.85	112.77	104.00
57	4	270	C	C5'-C4'-O4'	-5.80	101.10	109.80
57	4	286	A	P-O3'-C3'	5.75	128.82	120.20
57	4	223	G	P-O3'-C3'	5.74	128.82	120.20
57	4	284	G	P-O5'-C5'	5.73	129.50	120.90
57	4	63	C	O3'-P-O5'	5.71	112.57	104.00
57	4	27	U	O3'-P-O5'	5.71	112.56	104.00
57	4	271	G	C5'-C4'-O4'	-5.67	101.29	109.80
57	4	131	U	P-O5'-C5'	5.67	129.40	120.90
57	4	39	A	P-O3'-C3'	5.59	128.59	120.20
57	4	261	G	P-O5'-C5'	5.55	129.23	120.90
1	1	2552	OMU	P-O3'-C3'	5.55	126.36	119.70
57	4	324	G	O4'-C1'-N9	5.54	116.80	108.50
47	q	40	THR	CA-C-N	5.53	128.08	120.67
47	q	40	THR	C-N-CA	5.53	128.08	120.67
57	4	21	C	C4'-C3'-O3'	-5.51	104.73	113.00
57	4	192	A	O3'-P-O5'	5.49	112.23	104.00
1	1	830	G	O4'-C1'-N9	-5.48	99.98	108.20
57	4	247	A	P-O3'-C3'	5.47	128.41	120.20
57	4	64	C	P-O5'-C5'	5.47	129.10	120.90
57	4	176	G	C5'-C4'-O4'	-5.46	101.62	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	4	218	G	O3'-P-O5'	5.45	112.18	104.00
57	4	61	G	P-O3'-C3'	5.44	128.37	120.20
57	4	39	A	O3'-P-O5'	5.42	112.13	104.00
57	4	20	A	O4'-C1'-C2'	-5.42	102.19	107.60
57	4	267	G	O3'-P-O5'	5.39	112.09	104.00
57	4	333	G	P-O3'-C3'	5.39	128.29	120.20
57	4	265	C	O3'-P-O5'	5.38	112.08	104.00
57	4	269	C	P-O3'-C3'	5.38	128.28	120.20
57	4	334	A	C5'-C4'-O4'	-5.38	101.73	109.80
57	4	165	A	O3'-P-O5'	5.38	112.06	104.00
57	4	193	A	O3'-P-O5'	5.37	112.05	104.00
57	4	311	U	O3'-P-O5'	5.35	112.03	104.00
57	4	163	G	P-O3'-C3'	5.33	128.19	120.20
57	4	165	A	P-O3'-C3'	5.32	128.18	120.20
57	4	307	G	P-O3'-C3'	-5.32	112.22	120.20
57	4	163	G	C5'-C4'-O4'	-5.30	101.85	109.80
25	U	98	SER	CA-C-N	5.28	135.43	125.66
25	U	98	SER	C-N-CA	5.28	135.43	125.66
57	4	181	G	P-O3'-C3'	5.28	128.12	120.20
57	4	247	A	N9-C1'-C2'	5.27	121.91	114.00
57	4	308	U	C5'-C4'-O4'	-5.24	101.23	109.10
57	4	244	G	O3'-P-O5'	5.24	111.86	104.00
57	4	313	C	O3'-P-O5'	5.24	111.86	104.00
57	4	6	U	O5'-C5'-C4'	5.22	119.33	111.50
57	4	187	C	O3'-P-O5'	5.21	111.81	104.00
57	4	116	A	O3'-P-O5'	5.20	111.80	104.00
2	2	1403	C	C4'-C3'-O3'	-5.19	105.22	113.00
12	H	81	LEU	CA-CB-CG	5.18	134.44	116.30
57	4	263	G	O5'-C5'-C4'	-5.16	103.76	111.50
57	4	286	A	O3'-P-O5'	-5.16	96.26	104.00
37	g	87	CYS	CA-C-N	5.16	130.15	122.82
37	g	87	CYS	C-N-CA	5.16	130.15	122.82
57	4	189	C	P-O3'-C3'	5.13	127.89	120.20
57	4	144	U	C5'-C4'-C3'	5.10	123.65	116.00
57	4	188	C	P-O5'-C5'	-5.10	113.25	120.90
57	4	186	A	O5'-C5'-C4'	5.08	119.12	111.50
57	4	53	G	OP2-P-O3'	-5.07	92.79	108.00
57	4	6	U	C5'-C4'-O4'	-5.06	102.21	109.80
57	4	68	U	P-O3'-C3'	5.06	127.80	120.20
57	4	190	A	P-O3'-C3'	5.06	127.79	120.20
57	4	61	G	C4'-C3'-O3'	5.05	116.98	109.40
57	4	240	U	O5'-C5'-C4'	5.04	119.06	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	4	62	G	C4'-C3'-O3'	-5.04	101.84	109.40
57	4	190	A	O3'-P-O5'	5.02	111.54	104.00
57	4	153	U	P-O5'-C5'	5.02	128.43	120.90
57	4	317	G	P-O5'-C5'	5.02	128.42	120.90

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	1618	6MZ	C2',C3'
1	1	1911	PSU	C3',C4'
1	1	1915	3TD	C3'
1	1	1917	PSU	C3',C4'
1	1	2030	6MZ	C2',C3'
1	1	2069	G7M	C2',C3',C4'
1	1	2251	OMG	C2'
1	1	2457	PSU	C3',C4'
1	1	2498	OMC	C4'
1	1	2503	2MA	C2',C3'
1	1	2504	PSU	C3',C4'
1	1	2552	OMU	C2',C3'
1	1	2580	PSU	C3',C4'
1	1	2605	PSU	C3',C4'

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	830	G	Sidechain
2	2	999	C	Sidechain
4	5	90	LEU	Mainchain
10	F	46	ALA	Peptide
13	I	89	SER	Peptide
13	I	94	LYS	Peptide
22	R	23	GLU	Peptide
23	S	60	HIS	Peptide
35	e	31	HIS	Peptide
38	h	82	GLU	Peptide
43	m	62	THR	Peptide
47	q	102	LEU	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	31363	833	0
2	2	32929	0	16585	517	0
3	3	2569	0	1301	42	0
4	5	1209	0	1228	45	0
5	6	110	0	112	1	0
6	B	2082	0	2154	49	0
7	C	1565	0	1616	34	0
8	D	1552	0	1619	38	0
9	E	1410	0	1444	27	0
10	F	1313	0	1358	39	0
11	G	1111	0	1148	17	0
12	H	980	0	1013	24	0
13	I	984	0	1035	18	0
14	J	1129	0	1162	22	0
15	K	946	0	1023	29	0
16	L	1053	0	1128	34	0
17	M	1074	0	1156	22	0
18	N	951	0	994	32	0
19	O	892	0	923	26	0
20	P	917	0	962	23	0
21	Q	947	0	1019	23	0
22	R	816	0	839	18	0
23	S	857	0	922	20	0
24	T	746	0	811	18	0
25	U	788	0	843	18	0
26	V	753	0	780	18	0
27	W	582	0	599	14	0
28	X	625	0	652	20	0
29	Y	501	0	531	16	0
30	Z	448	0	488	11	0
31	a	472	0	468	12	0
32	b	444	0	458	15	0
33	c	426	0	464	15	0
34	d	377	0	418	7	0
35	e	504	0	572	13	0
36	f	302	0	340	4	0
37	g	1760	0	1787	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	1636	0	1710	47	0
39	i	1643	0	1707	52	0
40	j	1152	0	1196	41	0
41	k	848	0	846	14	0
42	l	1181	0	1238	31	0
43	m	979	0	1031	32	0
44	n	1022	0	1070	39	0
45	o	790	0	831	22	0
46	p	877	0	887	28	0
47	q	951	0	1012	26	0
48	r	867	0	921	22	0
49	s	805	0	844	22	0
50	t	714	0	734	16	0
51	u	649	0	666	18	0
52	v	648	0	691	15	0
53	w	544	0	560	9	0
54	x	663	0	688	19	0
55	y	669	0	719	12	0
56	z	589	0	629	7	0
57	4	7758	0	3920	141	0
58	1	283	0	0	0	0
58	2	126	0	0	0	0
58	3	8	0	0	0	0
58	4	1	0	0	0	0
58	B	2	0	0	0	0
58	C	1	0	0	0	0
58	L	2	0	0	0	0
58	N	1	0	0	0	0
58	U	1	0	0	0	0
58	f	1	0	0	0	0
58	i	1	0	0	0	0
58	r	2	0	0	0	0
59	a	1	0	0	0	0
59	f	1	0	0	0	0
60	B	2	0	0	0	0
All	All	153878	0	103215	2394	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 10.

All (2394) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1380:G:H21	1:1:1569:A:N6	1.53	1.04
1:1:244:A:N6	1:1:254:G:H21	1.59	1.01
2:2:410:G:N2	2:2:432:A:H62	1.58	1.00
1:1:244:A:H62	1:1:254:G:N2	1.60	0.98
2:2:410:G:H21	2:2:432:A:N6	1.61	0.98
1:1:1477:A:H62	1:1:1514:G:N2	1.60	0.97
1:1:1040:A:H61	1:1:1115:G:H1	1.10	0.97
1:1:1380:G:N2	1:1:1569:A:H61	1.62	0.97
1:1:460:A:H62	1:1:469:G:N2	1.61	0.97
1:1:1477:A:N6	1:1:1514:G:H21	1.62	0.96
2:2:593:U:H3	2:2:646:G:H1	0.98	0.95
2:2:1348:U:H3	2:2:1374:A:H62	0.97	0.95
1:1:1093:G:H21	1:1:1098:A:H62	1.03	0.95
1:1:1093:G:H21	1:1:1098:A:N6	1.64	0.93
1:1:460:A:H62	1:1:469:G:H21	0.94	0.93
1:1:460:A:N6	1:1:469:G:H21	1.66	0.93
1:1:2747:G:H21	1:1:2757:A:H62	1.12	0.93
2:2:372:C:H42	2:2:389:A:H62	1.10	0.93
1:1:746:PSU:H1'	1:1:748:G:H21	1.32	0.93
10:F:16:ASP:HB3	10:F:27:LYS:O	1.70	0.91
1:1:2818:U:H3	1:1:2828:G:H1	1.11	0.91
1:1:1029:A:H62	1:1:1125:G:H21	1.12	0.91
2:2:372:C:N4	2:2:389:A:H62	1.68	0.91
1:1:2028:U:H3	1:1:2033:A:H62	0.98	0.90
1:1:883:G:OP2	1:1:883:G:N2	2.05	0.89
2:2:834:U:H3	2:2:852:G:H1	1.15	0.89
4:5:91:LEU:HA	57:4:20:A:H62	1.36	0.89
2:2:150:U:H3	2:2:171:A:H62	0.92	0.88
2:2:1304:G:H21	2:2:1333:A:H62	1.18	0.88
1:1:1042:G:H1	1:1:1113:U:H3	1.20	0.88
1:1:892:A:H4'	1:1:892:A:OP1	1.73	0.87
1:1:1380:G:H21	1:1:1569:A:H61	0.90	0.86
1:1:1093:G:N2	1:1:1098:A:H62	1.74	0.86
1:1:1477:A:H62	1:1:1514:G:H21	0.89	0.85
2:2:1401:G:H3'	2:2:1402:4OC:H6	1.58	0.85
57:4:21:C:H2'	57:4:22:G:C8	2.12	0.85
1:1:1040:A:N6	1:1:1115:G:H1	1.74	0.84
2:2:1260:G:N2	2:2:1275:A:H62	1.76	0.84
2:2:372:C:H42	2:2:389:A:N6	1.75	0.83
2:2:1348:U:H3	2:2:1374:A:N6	1.77	0.82
2:2:152:A:N6	2:2:169:C:C4	2.48	0.82
4:5:156:LYS:O	4:5:160:ARG:HB2	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1029:A:H62	1:1:1125:G:N2	1.79	0.80
2:2:950:U:H3	2:2:1231:G:H1	1.28	0.80
57:4:20:A:H3'	57:4:20:A:N3	1.97	0.79
1:1:2100:G:H22	1:1:2189:U:H1'	1.45	0.79
1:1:2706:A:H5''	1:1:2706:A:H8	1.48	0.78
1:1:2747:G:N2	1:1:2757:A:H62	1.80	0.78
57:4:21:C:H2'	57:4:22:G:H8	1.47	0.78
1:1:882:G:H5'	1:1:882:G:H8	1.49	0.78
1:1:1169:A:H61	1:1:1180:U:H3	1.33	0.77
1:1:2028:U:H3	1:1:2033:A:N6	1.81	0.77
2:2:663:A:H61	2:2:742:G:H1	1.33	0.76
2:2:150:U:H3	2:2:171:A:N6	1.77	0.76
2:2:410:G:H21	2:2:432:A:H62	0.79	0.76
1:1:1932:A:H62	1:1:1968:G:H21	1.32	0.76
2:2:152:A:H62	2:2:169:C:N4	1.84	0.75
2:2:409:U:H3	2:2:433:G:H1	1.32	0.75
1:1:244:A:H62	1:1:254:G:H21	0.81	0.75
23:S:11:ARG:HH12	23:S:98:LYS:HB3	1.50	0.75
1:1:572:A:H61	1:1:2029:G:H21	1.32	0.75
4:5:92:LEU:HG	4:5:92:LEU:O	1.87	0.75
2:2:1260:G:H21	2:2:1275:A:N6	1.85	0.74
47:q:83:ARG:HB2	47:q:83:ARG:HH21	1.51	0.74
1:1:376:G:N1	1:1:399:U:C2	2.55	0.74
2:2:1015:G:H21	2:2:1218:C:H1'	1.54	0.73
6:B:246:THR:HG23	6:B:248:TRP:H	1.52	0.72
1:1:2706:A:H5''	1:1:2706:A:C8	2.23	0.72
1:1:581:C:H2'	1:1:582:A:H8	1.54	0.72
2:2:976:G:N1	2:2:1362:A:N7	2.36	0.72
1:1:1029:A:N6	1:1:1125:G:H21	1.86	0.72
3:3:84:G:H1	3:3:92:C:H42	1.38	0.72
19:O:24:THR:HA	19:O:40:ILE:O	1.91	0.71
38:h:139:GLN:O	38:h:143:ARG:HB2	1.90	0.71
39:i:188:ARG:HH12	39:i:191:LEU:HB2	1.54	0.71
50:t:82:ILE:HD13	50:t:87:LEU:HD13	1.71	0.70
2:2:454:G:H1	2:2:478:A:H61	1.39	0.70
37:g:218:ALA:O	37:g:222:ARG:HB2	1.92	0.69
1:1:882:G:H5'	1:1:882:G:C8	2.27	0.69
3:3:13:G:H21	3:3:16:G:H1'	1.56	0.69
2:2:861:G:H1	2:2:868:C:H42	1.38	0.69
1:1:2559:C:H2'	1:1:2560:A:H8	1.58	0.69
1:1:2706:A:H8	1:1:2706:A:C5'	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2466:C:O2	1:1:2484:G:N2	2.26	0.68
11:G:47:PHE:O	11:G:51:ARG:HB2	1.93	0.68
2:2:484:G:H4'	2:2:485:U:H5'	1.75	0.68
1:1:2747:G:H21	1:1:2757:A:N6	1.90	0.68
20:P:28:VAL:HG12	20:P:84:ILE:HG12	1.74	0.68
2:2:947:G:H22	2:2:1235:U:H3	1.42	0.67
2:2:35:G:H1	2:2:549:C:H42	1.42	0.67
2:2:54:C:H2'	2:2:352:C:H41	1.60	0.67
2:2:1054:C:N4	57:4:93:A:N3	2.42	0.67
2:2:778:G:H21	46:p:122:ARG:HD3	1.60	0.67
2:2:429:U:H3	2:2:431:A:H62	1.42	0.67
2:2:456:A:H61	2:2:476:U:H3	1.41	0.67
2:2:594:U:H3	2:2:645:G:H1	1.41	0.66
1:1:668:A:H2'	1:1:670:A:H62	1.60	0.66
46:p:74:VAL:HA	46:p:77:TYR:HB2	1.75	0.66
44:n:120:LYS:HB2	44:n:123:ARG:HG2	1.78	0.66
1:1:2443:C:H2'	1:1:2444:G:H8	1.59	0.66
2:2:1304:G:N2	2:2:1333:A:H62	1.93	0.66
44:n:5:GLN:HB2	44:n:20:PHE:HB3	1.78	0.66
1:1:2473:U:OP1	1:1:2529:G:N2	2.28	0.66
1:1:892:A:H2'	1:1:892:A:N3	2.11	0.66
1:1:2010:G:H5''	23:S:42:LYS:HB2	1.76	0.66
2:2:152:A:N6	2:2:169:C:N4	2.44	0.66
12:H:59:LEU:HB2	12:H:62:ARG:HB2	1.77	0.65
2:2:34:C:H2'	2:2:35:G:H8	1.61	0.65
1:1:2069:G7M:O2'	1:1:2069:G7M:N3	2.26	0.65
2:2:527:7MG:H3'	2:2:527:7MG:H81	1.78	0.65
38:h:67:THR:HA	38:h:102:ASN:O	1.97	0.65
57:4:20:A:N3	57:4:20:A:C3'	2.60	0.65
39:i:19:LEU:HD23	39:i:64:ILE:HG13	1.77	0.65
1:1:1550:C:H2'	1:1:1551:A:H8	1.60	0.65
2:2:516:PSU:H4'	2:2:516:PSU:OP1	1.96	0.65
2:2:952:U:H2'	2:2:953:G:H8	1.61	0.65
2:2:1297:G:H1'	42:l:114:LYS:HD3	1.79	0.65
2:2:132:C:H42	2:2:230:G:H1	1.44	0.65
57:4:20:A:N3	57:4:20:A:C2'	2.60	0.65
57:4:254:U:H3	57:4:277:G:H22	1.45	0.65
2:2:1445:U:H3	2:2:1457:G:H1	1.45	0.65
19:O:25:ARG:HB2	19:O:93:ASP:HB2	1.79	0.64
57:4:48:C:H2'	57:4:49:C:H5''	1.79	0.64
2:2:1226:C:OP1	48:r:90:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4:30:C:H42	57:4:34:A:H61	1.45	0.64
2:2:1464:U:H2'	2:2:1465:A:H8	1.61	0.64
13:I:125:THR:HA	13:I:128:ILE:HB	1.79	0.64
39:i:12:SER:HA	39:i:19:LEU:HD13	1.78	0.64
2:2:769:G:N2	2:2:811:C:O2	2.31	0.64
2:2:885:G:H1	2:2:912:C:H42	1.44	0.64
47:q:83:ARG:CB	47:q:83:ARG:NH2	2.61	0.64
22:R:74:ILE:HB	22:R:87:GLN:HB3	1.80	0.64
43:m:29:SER:HB2	43:m:59:LEU:HB2	1.80	0.64
1:1:923:G:H2'	1:1:924:G:H8	1.62	0.64
46:p:71:ALA:O	46:p:75:LYS:HB2	1.98	0.64
57:4:20:A:O5'	57:4:20:A:C8	2.51	0.64
2:2:782:A:H62	2:2:800:G:H21	1.46	0.64
1:1:376:G:N1	1:1:399:U:N3	2.45	0.64
2:2:1073:U:O2	37:g:103:ASN:ND2	2.30	0.64
2:2:1223:C:H5''	2:2:1224:U:H5''	1.80	0.64
18:N:52:ILE:HD13	18:N:94:TYR:HB2	1.80	0.64
57:4:217:G:N2	57:4:218:G:O6	2.31	0.64
1:1:2070:A:H2'	1:1:2071:A:H8	1.63	0.63
1:1:2391:G:H1'	1:1:2429:G:H22	1.61	0.63
2:2:246:A:H62	2:2:281:G:H21	1.45	0.63
11:G:24:GLY:O	11:G:28:ASN:HB2	1.97	0.63
33:c:43:VAL:HG13	33:c:45:GLN:H	1.63	0.63
44:n:6:TYR:O	44:n:20:PHE:HA	1.98	0.63
9:E:29:PRO:HB2	9:E:169:LEU:HD22	1.79	0.63
17:M:42:THR:HA	17:M:93:VAL:HG12	1.81	0.63
1:1:1866:A:H62	1:1:1867:G:H21	1.47	0.63
2:2:1095:U:OP1	2:2:1108:G:N2	2.32	0.63
1:1:578:G:O2'	21:Q:33:ARG:NH1	2.31	0.63
1:1:1932:A:N6	1:1:1968:G:H21	1.97	0.63
2:2:54:C:OP1	2:2:351:G:N2	2.32	0.63
2:2:1401:G:N3	2:2:1401:G:H2'	2.14	0.63
1:1:882:G:H8	1:1:882:G:C5'	2.11	0.63
1:1:1796:U:H2'	1:1:1797:G:H8	1.63	0.63
4:5:102:GLY:O	4:5:106:ARG:NH2	2.32	0.63
10:F:20:ASN:H	10:F:24:ILE:HG12	1.64	0.63
1:1:808:G:H2'	1:1:809:G:H8	1.64	0.62
2:2:516:PSU:H3'	2:2:517:G:C8	2.34	0.62
2:2:552:U:OP1	2:2:552:U:H4'	1.98	0.62
2:2:335:C:H2'	2:2:336:A:H8	1.64	0.62
10:F:89:LEU:HD23	10:F:94:TYR:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:587:C:OP2	16:L:21:ARG:NH2	2.33	0.62
1:1:892:A:C2	1:1:893:C:H4'	2.34	0.62
1:1:443:A:N6	8:D:36:ALA:O	2.30	0.62
1:1:869:G:O3'	17:M:6:ARG:NH2	2.33	0.62
2:2:599:C:H2'	2:2:600:A:H8	1.65	0.62
1:1:1125:G:O6	1:1:1126:A:N6	2.33	0.62
44:n:52:LEU:HG	44:n:58:VAL:HG21	1.82	0.62
1:1:407:G:H2'	1:1:408:G:H8	1.65	0.62
1:1:563:A:N3	21:Q:37:GLN:NE2	2.47	0.62
4:5:114:LEU:HB2	4:5:126:LYS:HB3	1.82	0.62
26:V:48:MET:SD	26:V:51:GLN:NE2	2.71	0.62
1:1:990:A:N1	22:R:78:ARG:NH1	2.47	0.61
1:1:1033:U:O2'	1:1:2750:A:N6	2.33	0.61
15:K:64:ARG:HB2	15:K:83:ALA:HB3	1.79	0.61
21:Q:3:ARG:HH22	21:Q:5:LYS:HG3	1.64	0.61
32:b:13:ARG:O	32:b:17:ARG:NH1	2.33	0.61
2:2:1229:A:O2'	4:5:106:ARG:NH2	2.34	0.61
2:2:1310:G:O6	2:2:1327:C:N4	2.32	0.61
29:Y:10:SER:HG	29:Y:13:GLU:H	1.46	0.61
38:h:150:LYS:O	38:h:200:VAL:HA	2.00	0.61
1:1:1769:U:C2	1:1:1984:G:N1	2.68	0.61
2:2:417:G:H1	2:2:426:U:H3	1.49	0.61
39:i:188:ARG:NH1	39:i:188:ARG:O	2.33	0.61
22:R:8:GLY:O	22:R:10:LYS:NZ	2.33	0.61
52:v:68:SER:OG	52:v:69:LYS:N	2.33	0.61
1:1:334:C:OP1	1:1:336:C:N4	2.33	0.61
1:1:560:C:O2'	21:Q:48:ARG:NH2	2.34	0.61
8:D:48:THR:HA	8:D:83:VAL:H	1.66	0.61
45:o:10:LEU:HG	45:o:74:VAL:HG11	1.82	0.61
1:1:465:G:H21	1:1:684:G:H1'	1.64	0.61
50:t:69:TYR:HD1	50:t:72:ARG:HH11	1.49	0.61
21:Q:94:ILE:HD11	22:R:11:GLN:HB3	1.83	0.61
1:1:275:C:O2	1:1:362:A:N6	2.33	0.61
1:1:572:A:H61	1:1:2029:G:N2	1.97	0.61
1:1:762:U:N3	1:1:1431:A:OP1	2.33	0.61
1:1:969:G:N2	1:1:985:C:OP1	2.32	0.61
1:1:1392:A:N6	24:T:18:GLU:OE1	2.34	0.61
27:W:37:ILE:HG22	27:W:38:VAL:HG23	1.83	0.61
1:1:285:G:N1	1:1:355:U:N3	2.45	0.60
47:q:83:ARG:HB2	47:q:83:ARG:NH2	2.16	0.60
1:1:1438:U:H2'	1:1:1439:A:H8	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2099:U:H4'	1:1:2099:U:OP1	1.99	0.60
18:N:86:ARG:NH1	18:N:117:ASP:O	2.34	0.60
39:i:30:THR:HG23	39:i:31:LYS:HG3	1.83	0.60
1:1:997:G:OP2	21:Q:58:ARG:NH2	2.34	0.60
2:2:362:G:N2	2:2:365:U:OP2	2.33	0.60
3:3:34:A:N6	3:3:44:G:O2'	2.34	0.60
57:4:263:G:N2	57:4:300:U:O4	2.34	0.60
1:1:371:A:N6	1:1:402:A:OP2	2.35	0.60
1:1:631:A:OP1	35:e:47:LYS:NZ	2.33	0.60
2:2:954:G:N2	2:2:1228:C:N3	2.48	0.60
16:L:96:LYS:HD3	16:L:103:ILE:HA	1.81	0.60
48:r:106:ALA:HB3	48:r:110:LYS:HE2	1.83	0.60
2:2:107:G:H5''	2:2:108:G:H21	1.67	0.60
2:2:309:A:H2'	2:2:310:G:H8	1.66	0.60
2:2:1078:U:O2	40:j:135:ASN:ND2	2.35	0.60
1:1:456:C:N3	24:T:73:ARG:NH1	2.49	0.60
2:2:1075:U:OP2	40:j:69:ARG:NH1	2.34	0.60
2:2:1348:U:C2	2:2:1374:A:N6	2.70	0.60
39:i:132:ILE:HG22	39:i:134:SER:H	1.66	0.60
10:F:97:ALA:HB3	10:F:104:ASN:HB2	1.84	0.60
2:2:1260:G:N2	2:2:1275:A:N6	2.41	0.60
57:4:27:U:H2'	57:4:28:U:H5'	1.83	0.60
1:1:2368:C:H2'	1:1:2369:A:H8	1.65	0.60
2:2:637:C:OP1	52:v:4:LYS:N	2.35	0.60
2:2:1101:A:N6	37:g:175:GLU:OE2	2.35	0.60
8:D:125:SER:O	8:D:137:LYS:NZ	2.34	0.60
1:1:1102:C:H2'	1:1:1103:A:H8	1.67	0.59
2:2:889:A:H61	2:2:907:A:H5''	1.67	0.59
38:h:131:ARG:HA	38:h:134:MET:HE3	1.84	0.59
38:h:191:THR:HG23	38:h:193:TYR:H	1.64	0.59
1:1:2012:G:H4'	23:S:96:ILE:HD11	1.84	0.59
6:B:157:SER:OG	6:B:158:ALA:N	2.35	0.59
17:M:14:LYS:O	17:M:71:LYS:NZ	2.36	0.59
39:i:15:GLU:HB2	39:i:19:LEU:HD11	1.84	0.59
49:s:53:ARG:HG2	49:s:59:ARG:HG3	1.83	0.59
29:Y:31:GLN:HB3	29:Y:37:LEU:HD22	1.84	0.59
2:2:269:C:H2'	2:2:270:A:H8	1.66	0.59
2:2:1375:A:OP1	42:l:10:ARG:NH2	2.36	0.59
29:Y:49:ASP:OD1	29:Y:52:ARG:NH1	2.35	0.59
2:2:9:G:N7	2:2:558:G:O2'	2.36	0.59
2:2:180:U:O2	2:2:195:A:N7	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:111:U:H2'	3:3:112:G:H8	1.67	0.59
7:C:9:VAL:HG11	20:P:4:ILE:HB	1.83	0.59
1:1:1361:G:O2'	1:1:2215:C:O2'	2.20	0.59
1:1:2640:G:OP2	14:J:95:ARG:NH1	2.36	0.59
2:2:902:G:H2'	2:2:903:G:H8	1.67	0.59
1:1:1693:U:O2	6:B:14:ARG:NH1	2.36	0.59
1:1:2069:G7M:O2'	1:1:2069:G7M:C4	2.50	0.59
38:h:7:PRO:HB2	38:h:182:ILE:HD12	1.83	0.59
39:i:62:ARG:HH21	39:i:68:LEU:HA	1.67	0.59
39:i:188:ARG:NH2	39:i:192:SER:O	2.35	0.59
46:p:16:VAL:HG12	46:p:77:TYR:HB3	1.85	0.59
1:1:720:U:H2'	1:1:721:A:H8	1.68	0.59
2:2:358:U:H2'	2:2:359:G:H8	1.68	0.59
2:2:1348:U:O4	2:2:1374:A:N7	2.35	0.59
14:J:36:LEU:HD11	14:J:122:LEU:HD13	1.83	0.59
1:1:160:A:N7	1:1:166:U:O4	2.36	0.59
1:1:1791:A:N6	1:1:1828:G:O2'	2.36	0.59
1:1:2771:C:O2'	7:C:173:GLN:NE2	2.34	0.59
2:2:176:C:OP1	55:y:64:LYS:NZ	2.36	0.59
2:2:1359:C:O2'	2:2:1362:A:N6	2.34	0.59
1:1:1034:G:N2	1:1:1122:G:N3	2.50	0.58
1:1:1295:C:H2'	1:1:1296:G:H8	1.68	0.58
2:2:438:U:OP1	39:i:148:LYS:NZ	2.35	0.58
1:1:377:G:N2	1:1:398:C:O2	2.36	0.58
2:2:976:G:N1	2:2:1362:A:C5	2.72	0.58
2:2:1355:G:H2'	2:2:1356:G:H8	1.68	0.58
3:3:18:G:N1	3:3:65:U:N3	2.51	0.58
18:N:6:SER:OG	18:N:46:ARG:NH2	2.35	0.58
38:h:183:ASP:OD2	38:h:204:LYS:NZ	2.34	0.58
57:4:311:U:H2'	57:4:312:A:H8	1.68	0.58
2:2:1402:4OC:H6	2:2:1402:4OC:OP2	2.03	0.58
18:N:56:LYS:NZ	18:N:87:PHE:O	2.36	0.58
1:1:73:A:OP1	29:Y:48:ARG:NH2	2.35	0.58
1:1:144:A:OP1	24:T:6:ARG:NH2	2.36	0.58
1:1:1042:G:O6	1:1:1113:U:O4	2.22	0.58
6:B:245:VAL:HA	6:B:251:GLN:HA	1.84	0.58
44:n:6:TYR:HB2	44:n:21:ILE:HB	1.85	0.58
47:q:99:ARG:NH1	47:q:104:CYS:SG	2.77	0.58
1:1:249:C:O2	35:e:12:LYS:NZ	2.36	0.58
1:1:1666:G:HO2'	15:K:6:THR:HG1	1.43	0.58
2:2:1407:5MC:N4	2:2:1494:G:O6	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4:34:A:H1'	57:4:322:U:H1'	1.85	0.58
1:1:1932:A:H62	1:1:1968:G:N2	2.00	0.58
1:1:2553:G:H1'	1:1:2582:G:H21	1.69	0.58
2:2:339:C:O2	2:2:350:G:N2	2.35	0.58
2:2:689:C:OP2	46:p:53:ARG:NH1	2.37	0.58
4:5:40:GLU:N	57:4:335:C:N3	2.51	0.58
47:q:83:ARG:HH21	47:q:83:ARG:CB	2.17	0.58
1:1:2117:A:N6	1:1:2166:U:O4	2.37	0.58
7:C:146:ILE:HA	7:C:159:LYS:HE3	1.85	0.58
19:O:81:ARG:O	19:O:85:LYS:NZ	2.36	0.58
57:4:92:A:OP2	57:4:93:A:N6	2.37	0.58
57:4:282:G:O2'	57:4:286:A:N6	2.37	0.58
2:2:1118:U:H5'	44:n:106:ARG:HG3	1.86	0.58
2:2:1442:G:H5'	20:P:114:LEU:HD22	1.86	0.58
37:g:87:CYS:O	37:g:225:ARG:NH1	2.36	0.58
45:o:40:ILE:HD12	45:o:73:LEU:HD13	1.84	0.58
1:1:2039:U:OP1	14:J:111:LYS:NZ	2.37	0.58
1:1:2599:G:O6	6:B:239:ASN:ND2	2.37	0.58
2:2:740:U:OP1	50:t:2:SER:N	2.37	0.58
2:2:974:A:H4'	2:2:975:A:H3'	1.85	0.58
3:3:51:G:OP2	19:O:67:ASN:ND2	2.37	0.58
8:D:170:ARG:NH2	8:D:176:ASP:OD1	2.36	0.58
9:E:74:VAL:HG23	9:E:76:GLY:H	1.67	0.58
16:L:19:LEU:HD21	16:L:32:GLY:HA3	1.86	0.58
49:s:13:ARG:NH1	49:s:54:ASP:OD1	2.36	0.58
1:1:1419:A:N7	1:1:1578:U:O2	2.37	0.57
1:1:1636:U:H2'	1:1:1637:A:H8	1.68	0.57
2:2:1298:U:O4	42:l:119:ARG:NH2	2.37	0.57
10:F:15:VAL:HG12	10:F:29:LYS:H	1.69	0.57
27:W:68:LYS:NZ	27:W:69:PHE:O	2.37	0.57
57:4:20:A:N3	57:4:20:A:H2'	2.17	0.57
1:1:917:A:H5''	1:1:2268:A:H61	1.69	0.57
1:1:1066:U:H2'	1:1:1067:A:H2'	1.85	0.57
1:1:2110:G:N7	1:1:2118:U:O2'	2.37	0.57
1:1:2748:A:H1'	10:F:67:THR:HG22	1.85	0.57
2:2:1397:C:OP2	40:j:29:ARG:NH1	2.37	0.57
6:B:25:HIS:ND1	6:B:26:LYS:O	2.37	0.57
9:E:35:THR:HG22	9:E:90:THR:HG22	1.84	0.57
20:P:106:LYS:O	20:P:109:ARG:NH2	2.36	0.57
1:1:605:G:N3	1:1:657:U:O2'	2.37	0.57
2:2:228:A:H1'	51:u:63:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:159:GLY:O	10:F:163:ARG:NH1	2.36	0.57
54:x:63:THR:HB	54:x:66:MET:HG3	1.86	0.57
57:4:269:C:H42	57:4:294:A:H1'	1.67	0.57
1:1:2840:C:H5''	18:N:53:THR:HG21	1.85	0.57
2:2:363:A:N6	47:q:27:CYS:SG	2.75	0.57
2:2:996:A:N6	2:2:1044:A:N7	2.52	0.57
15:K:78:ARG:NE	20:P:71:GLU:OE2	2.37	0.57
56:z:4:ILE:HD13	56:z:19:PHE:HA	1.85	0.57
1:1:561:G:HO2'	21:Q:45:TYR:HH	1.50	0.57
2:2:1015:G:OP1	54:x:14:HIS:NE2	2.38	0.57
2:2:1045:C:N4	2:2:1211:U:O2	2.38	0.57
6:B:182:ARG:NH2	6:B:183:LYS:O	2.33	0.57
38:h:24:ALA:HB1	38:h:28:GLU:HB2	1.87	0.57
38:h:86:LYS:HA	38:h:89:LYS:HG2	1.86	0.57
43:m:29:SER:HA	43:m:33:LYS:HD2	1.87	0.57
8:D:45:ALA:HB2	8:D:89:PRO:HD3	1.85	0.57
13:I:76:ALA:HA	13:I:79:LEU:HD12	1.87	0.57
33:c:25:LYS:HE2	33:c:27:LYS:HG3	1.87	0.57
38:h:140:ASN:OD1	38:h:143:ARG:NH2	2.38	0.57
2:2:757:U:OP1	2:2:822:U:O2'	2.23	0.57
14:J:116:ARG:O	14:J:120:ARG:NH2	2.37	0.57
38:h:72:ARG:NH2	57:4:108:G:OP2	2.37	0.57
2:2:891:U:H2'	2:2:892:A:H8	1.69	0.57
2:2:963:G:H1	2:2:972:C:H42	1.51	0.57
40:j:153:VAL:HG11	43:m:99:LEU:HD13	1.85	0.57
1:1:955:PSU:H2'	1:1:955:PSU:O4	2.05	0.57
1:1:1998:A:OP2	7:C:141:ARG:NH1	2.37	0.57
2:2:673:A:H4'	41:k:86:ARG:HH21	1.70	0.57
2:2:691:G:O6	46:p:53:ARG:NH2	2.38	0.57
2:2:1316:G:N1	2:2:1319:A:OP2	2.37	0.57
21:Q:48:ARG:NH2	21:Q:52:GLN:OE1	2.38	0.57
28:X:27:ARG:NH1	28:X:28:ARG:O	2.38	0.57
38:h:100:GLN:NE2	57:4:187:C:OP1	2.34	0.57
1:1:13:A:H4'	1:1:14:A:H5'	1.87	0.57
1:1:884:U:O2	1:1:884:U:O2'	2.23	0.57
3:3:9:G:OP2	19:O:15:ARG:NH1	2.37	0.57
14:J:52:ASP:N	14:J:52:ASP:OD1	2.37	0.57
39:i:97:ARG:HH21	39:i:115:ARG:HH12	1.52	0.57
45:o:6:ILE:HA	45:o:102:LEU:HA	1.87	0.57
54:x:3:ARG:HH12	54:x:10:PHE:HB2	1.68	0.57
1:1:301:G:OP2	25:U:82:ARG:NH1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:8:A:N7	39:i:205:SER:OG	2.38	0.56
2:2:981:U:OP1	49:s:9:ARG:NH2	2.38	0.56
2:2:1168:U:O4	37:g:74:ARG:NH2	2.38	0.56
10:F:138:LYS:HA	10:F:141:ILE:HG12	1.87	0.56
1:1:599:A:H2'	1:1:600:G:H8	1.70	0.56
1:1:1084:A:N7	12:H:56:ARG:NH1	2.52	0.56
2:2:461:A:N1	2:2:470:C:N4	2.49	0.56
2:2:578:C:H2'	2:2:579:A:H8	1.70	0.56
2:2:944:G:N3	2:2:1340:A:N6	2.53	0.56
2:2:1094:G:O2'	2:2:1108:G:N2	2.38	0.56
41:k:38:ARG:NH1	41:k:98:GLU:O	2.38	0.56
45:o:7:ARG:NH1	45:o:75:ASP:OD2	2.38	0.56
1:1:377:G:N1	1:1:398:C:N3	2.53	0.56
1:1:883:G:N7	1:1:894:U:H5'	2.20	0.56
1:1:1223:G:OP2	22:R:68:ARG:NH1	2.38	0.56
1:1:1287:A:O4'	18:N:103:ARG:NH2	2.39	0.56
1:1:1792:G:O6	1:1:1828:G:N2	2.38	0.56
2:2:19:A:OP2	40:j:132:ASN:ND2	2.39	0.56
2:2:618:C:N4	2:2:621:A:OP2	2.38	0.56
17:M:47:GLU:OE2	17:M:50:ARG:NH1	2.36	0.56
26:V:77:VAL:HG12	26:V:89:ILE:HG23	1.87	0.56
30:Z:3:LYS:O	30:Z:40:ASP:N	2.39	0.56
40:j:36:LEU:HA	40:j:49:GLY:O	2.05	0.56
57:4:120:U:H3'	57:4:121:A:H2'	1.86	0.56
1:1:405:U:H3'	1:1:406:G:H8	1.69	0.56
1:1:955:PSU:OP1	1:1:955:PSU:H4'	2.06	0.56
1:1:2052:A:H2'	1:1:2053:G:H8	1.71	0.56
1:1:2116:G:N7	1:1:2171:A:N6	2.54	0.56
1:1:2818:U:O2	1:1:2828:G:N2	2.33	0.56
37:g:16:PHE:O	37:g:203:ASN:ND2	2.38	0.56
54:x:12:ASP:HB2	54:x:15:LEU:HB2	1.86	0.56
1:1:376:G:O6	1:1:399:U:C4	2.58	0.56
1:1:1665:A:H5''	15:K:66:LYS:HG2	1.88	0.56
38:h:114:LYS:HE3	38:h:185:ASN:HD22	1.70	0.56
42:l:111:ARG:O	42:l:119:ARG:NH1	2.38	0.56
1:1:1316:U:H2'	1:1:1317:G:H8	1.69	0.56
1:1:643:A:OP1	33:c:44:ARG:NH1	2.37	0.56
1:1:2396:G:H2'	1:1:2397:G:H8	1.71	0.56
1:1:2884:U:O2	32:b:50:ARG:NH1	2.39	0.56
2:2:409:U:O4	2:2:433:G:O6	2.24	0.56
2:2:744:C:H2'	2:2:745:G:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:766:A:OP2	2:2:812:G:N2	2.39	0.56
41:k:1:MET:N	41:k:66:ALA:O	2.37	0.56
1:1:20:C:H2'	1:1:21:A:H8	1.70	0.56
1:1:690:G:O3'	6:B:217:ARG:NH2	2.39	0.56
1:1:1252:G:N2	21:Q:33:ARG:O	2.39	0.56
1:1:2014:A:O2'	23:S:92:ARG:NH2	2.39	0.56
1:1:2440:C:N4	1:1:2441:U:O2	2.39	0.56
1:1:2599:G:N2	1:1:2600:A:N3	2.54	0.56
2:2:834:U:O2	2:2:852:G:N2	2.30	0.56
20:P:28:VAL:HG21	20:P:74:PHE:HE2	1.70	0.56
26:V:17:SER:OG	26:V:21:ARG:NH1	2.38	0.56
31:a:14:ALA:HB3	31:a:22:MET:O	2.05	0.56
43:m:2:SER:OG	43:m:3:MET:N	2.37	0.56
45:o:6:ILE:O	45:o:75:ASP:HA	2.05	0.56
47:q:38:TYR:OH	47:q:54:ARG:NH2	2.35	0.56
57:4:276:U:H2'	57:4:277:G:H8	1.71	0.56
1:1:544:C:H42	1:1:549:G:H22	1.53	0.56
2:2:166:U:H2'	2:2:167:A:H8	1.71	0.56
31:a:16:CYS:SG	31:a:17:SER:N	2.79	0.56
39:i:202:GLU:OE1	40:j:112:ARG:NH1	2.38	0.56
45:o:37:ARG:HH11	45:o:77:VAL:HG11	1.71	0.56
48:r:30:SER:HA	48:r:33:ILE:HB	1.87	0.56
1:1:965:C:H2'	1:1:966:G:H8	1.70	0.55
1:1:1000:A:OP2	1:1:1154:G:N1	2.37	0.55
1:1:2000:C:OP1	18:N:5:LYS:NZ	2.36	0.55
2:2:413:G:O3'	2:2:428:G:N2	2.39	0.55
2:2:1242:G:N2	2:2:1302:C:O2'	2.39	0.55
37:g:18:HIS:ND1	37:g:189:THR:OG1	2.39	0.55
1:1:376:G:C6	1:1:399:U:N3	2.74	0.55
1:1:782:A:H5'	1:1:783:A:C5	2.41	0.55
1:1:1798:U:H5''	6:B:258:ARG:HB2	1.89	0.55
2:2:1147:C:O2	44:n:18:ARG:NH2	2.38	0.55
3:3:95:U:H2'	3:3:96:G:H8	1.72	0.55
4:5:55:TYR:HA	4:5:112:VAL:HA	1.88	0.55
4:5:151:LYS:HA	4:5:154:ILE:HG12	1.89	0.55
19:O:25:ARG:NH2	19:O:93:ASP:OD2	2.33	0.55
57:4:272:C:H2'	57:4:273:A:C8	2.41	0.55
1:1:1948:G:H2'	1:1:1949:G:H8	1.70	0.55
9:E:110:ARG:O	9:E:112:ARG:NH2	2.40	0.55
1:1:102:U:O4	29:Y:2:LYS:N	2.39	0.55
1:1:877:A:N3	1:1:900:A:N6	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1047:G:OP2	12:H:62:ARG:NH2	2.40	0.55
1:1:2758:A:O2'	10:F:38:ASN:ND2	2.39	0.55
2:2:781:A:O2'	2:2:1522:U:O2	2.24	0.55
2:2:1206:G:H2'	2:2:1207:2MG:H8	1.71	0.55
18:N:112:TYR:HE2	32:b:55:ILE:HD13	1.72	0.55
28:X:32:ASN:OD1	28:X:34:HIS:NE2	2.39	0.55
41:k:12:PRO:O	41:k:44:ARG:NH2	2.37	0.55
47:q:46:ASN:ND2	47:q:89:0TD:OD2	2.40	0.55
1:1:270:A:H61	1:1:368:A:H2	1.54	0.55
1:1:572:A:OP2	22:R:79:ARG:NH2	2.40	0.55
1:1:819:A:OP2	1:1:1187:G:N2	2.40	0.55
1:1:2751:G:OP1	10:F:3:ARG:NH2	2.39	0.55
1:1:1063:G:N2	13:I:89:SER:O	2.40	0.55
1:1:2384:U:OP2	27:W:55:ARG:NH1	2.33	0.55
1:1:2706:A:C8	1:1:2706:A:C5'	2.86	0.55
2:2:331:G:O3'	55:y:2:ALA:N	2.40	0.55
2:2:1115:U:H2'	2:2:1116:U:H6	1.71	0.55
4:5:134:LYS:NZ	57:4:88:U:O2	2.39	0.55
9:E:46:ASP:HB2	9:E:49:LEU:HD13	1.88	0.55
32:b:10:ARG:HA	32:b:13:ARG:HG2	1.88	0.55
1:1:2087:G:H2'	1:1:2088:A:H8	1.72	0.55
2:2:7:A:H2'	40:j:124:LEU:HD22	1.88	0.55
2:2:1241:G:OP1	42:l:35:LYS:NZ	2.36	0.55
37:g:173:ILE:O	37:g:177:ASN:ND2	2.40	0.55
1:1:587:C:OP1	16:L:21:ARG:NH1	2.39	0.55
1:1:1057:A:N6	1:1:1088:A:OP2	2.36	0.55
1:1:1690:A:H62	1:1:1697:G:H21	1.54	0.55
1:1:1972:G:OP2	6:B:238:ARG:NH1	2.40	0.55
1:1:1997:C:H2'	1:1:1998:A:H8	1.72	0.55
1:1:2085:U:OP1	6:B:259:SER:OG	2.24	0.55
1:1:2880:C:O2'	18:N:90:ARG:NH2	2.39	0.55
2:2:1071:C:H2'	2:2:1072:G:H8	1.71	0.55
4:5:56:VAL:HB	4:5:111:VAL:HG13	1.89	0.55
26:V:21:ARG:HE	26:V:87:GLN:HA	1.72	0.55
40:j:142:ASP:O	40:j:146:ASN:ND2	2.40	0.55
57:4:49:C:H42	57:4:69:A:H61	1.54	0.55
1:1:606:U:O2	1:1:622:G:O6	2.25	0.55
1:1:2298:A:N6	1:1:2318:G:O2'	2.40	0.55
4:5:94:GLN:CG	57:4:20:A:H1'	2.37	0.55
9:E:52:ASN:O	9:E:56:ASP:N	2.40	0.55
1:1:219:A:N3	1:1:234:U:O2'	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2114:A:N6	1:1:2167:U:O2'	2.40	0.55
2:2:663:A:N6	2:2:742:G:H1	2.04	0.55
2:2:1231:G:OP1	44:n:130:ARG:NH1	2.40	0.55
3:3:18:G:H1	3:3:65:U:H3	1.55	0.55
11:G:116:ARG:HD3	11:G:133:GLN:HB3	1.88	0.55
18:N:6:SER:OG	18:N:7:GLY:N	2.40	0.55
38:h:122:SER:OG	38:h:126:ARG:NH2	2.40	0.55
1:1:244:A:OP2	35:e:8:ARG:NH2	2.40	0.54
1:1:396:G:OP2	28:X:10:LYS:NZ	2.40	0.54
1:1:745:1MG:O3'	1:1:748:G:O2'	2.24	0.54
1:1:1114:C:N4	1:1:1115:G:O6	2.39	0.54
3:3:49:C:OP2	19:O:102:ARG:NH2	2.40	0.54
43:m:77:ARG:NH2	43:m:79:SER:O	2.36	0.54
46:p:64:GLN:HB2	46:p:99:ALA:HB3	1.88	0.54
57:4:168:G:H2'	57:4:169:G:H8	1.72	0.54
1:1:854:C:H2'	1:1:855:G:H8	1.71	0.54
1:1:2780:G:OP2	14:J:120:ARG:NE	2.41	0.54
2:2:62:U:O2'	2:2:379:C:O2	2.25	0.54
2:2:1152:A:H2'	2:2:1153:G:H8	1.71	0.54
11:G:87:GLU:HG2	41:k:17:GLN:HB3	1.87	0.54
18:N:59:SER:OG	18:N:60:VAL:N	2.40	0.54
37:g:11:LYS:O	37:g:208:ARG:NH1	2.40	0.54
43:m:92:LEU:O	43:m:117:ARG:NH1	2.39	0.54
57:4:296:U:H2'	57:4:297:G:C8	2.42	0.54
57:4:331:C:H2'	57:4:332:G:H5'	1.87	0.54
1:1:1627:G:H2'	1:1:1628:G:H8	1.72	0.54
1:1:2780:G:O6	14:J:99:ARG:NH1	2.40	0.54
2:2:64:G:H4'	2:2:65:A:H3'	1.89	0.54
4:5:160:ARG:HH21	46:p:27:PHE:HZ	1.54	0.54
23:S:77:ASP:HB2	23:S:102:HIS:HB2	1.90	0.54
25:U:74:ASN:ND2	25:U:77:THR:OG1	2.38	0.54
57:4:202:G:H1'	57:4:232:A:H61	1.71	0.54
2:2:407:U:H3	2:2:435:A:H61	1.55	0.54
2:2:1347:G:O6	44:n:109:ARG:NH2	2.40	0.54
2:2:1367:C:OP1	45:o:62:ARG:NH2	2.41	0.54
18:N:2:ARG:HA	18:N:5:LYS:HD2	1.89	0.54
18:N:33:ILE:HB	18:N:114:GLU:HG3	1.89	0.54
24:T:8:LEU:HD13	29:Y:22:LEU:HB3	1.90	0.54
35:e:25:LYS:HD2	35:e:30:ARG:HH12	1.73	0.54
39:i:85:ASN:O	39:i:89:ASN:ND2	2.41	0.54
48:r:13:LYS:HB2	48:r:18:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y:48:GLN:O	55:y:52:ASN:ND2	2.41	0.54
1:1:600:G:OP1	8:D:24:ASN:ND2	2.40	0.54
1:1:2509:G:H1	1:1:2579:C:H42	1.56	0.54
2:2:80:A:H2	2:2:89:U:H3	1.54	0.54
2:2:881:G:OP1	47:q:9:ARG:NH1	2.40	0.54
7:C:48:ILE:HG12	7:C:84:LEU:HD21	1.88	0.54
7:C:131:ASP:O	7:C:136:ASN:ND2	2.36	0.54
15:K:102:PRO:HB3	15:K:121:GLU:HB2	1.89	0.54
26:V:51:GLN:OE1	26:V:57:TYR:OH	2.25	0.54
40:j:20:ARG:NH1	57:4:96:G:O4'	2.41	0.54
1:1:981:A:HO2'	1:1:2036:C:HO2'	1.56	0.54
1:1:1853:A:N7	1:1:1889:A:N6	2.56	0.54
2:2:231:U:H2'	2:2:232:G:H8	1.72	0.54
2:2:459:A:H1'	2:2:474:G:H22	1.73	0.54
2:2:552:U:OP1	2:2:552:U:C4'	2.56	0.54
10:F:60:ASP:HB2	10:F:63:ALA:HB3	1.90	0.54
38:h:74:GLY:HA2	38:h:77:ILE:HG22	1.89	0.54
39:i:148:LYS:O	39:i:152:GLN:NE2	2.41	0.54
50:t:49:ASP:OD2	50:t:52:SER:OG	2.26	0.54
57:4:251:U:H2'	57:4:252:G:H8	1.73	0.54
1:1:636:G:N1	16:L:76:GLU:OE1	2.39	0.54
1:1:729:G:H2'	1:1:1775:U:H1'	1.89	0.54
1:1:838:C:H42	1:1:940:G:H1	1.54	0.54
4:5:42:LYS:HB2	4:5:73:MET:HG2	1.89	0.54
12:H:57:ASN:ND2	12:H:62:ARG:O	2.41	0.54
16:L:58:TYR:O	35:e:13:ARG:NH2	2.40	0.54
43:m:29:SER:OG	43:m:30:SER:N	2.38	0.54
47:q:20:ASN:O	47:q:94:ARG:NH1	2.41	0.54
55:y:74:ARG:O	55:y:78:ASN:ND2	2.40	0.54
1:1:308:G:O2'	1:1:329:G:N2	2.41	0.54
1:1:2070:A:H2'	1:1:2071:A:C8	2.41	0.54
1:1:2813:A:H2'	1:1:2814:A:H8	1.72	0.54
2:2:538:G:H2'	2:2:539:A:H8	1.73	0.54
2:2:546:A:OP1	39:i:70:ARG:N	2.34	0.54
2:2:1013:G:H21	2:2:1016:A:H62	1.56	0.54
18:N:49:GLU:HA	18:N:52:ILE:HD12	1.88	0.54
19:O:53:THR:HG22	19:O:74:VAL:HG21	1.90	0.54
22:R:63:VAL:HG12	22:R:96:VAL:HG12	1.90	0.54
39:i:116:GLN:NE2	39:i:119:SER:OG	2.40	0.54
52:v:11:ARG:NH2	52:v:56:GLY:O	2.40	0.54
1:1:675:A:OP1	8:D:58:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1165:A:H2'	1:1:1166:G:H8	1.73	0.54
8:D:27:LEU:HD11	8:D:100:MET:HB2	1.89	0.54
9:E:65:PRO:HB2	9:E:87:CYS:HB3	1.89	0.54
19:O:62:LEU:HD13	19:O:70:ALA:HA	1.89	0.54
27:W:25:ARG:NH1	27:W:35:SER:OG	2.40	0.54
44:n:15:SER:OG	44:n:16:ALA:N	2.41	0.54
52:v:38:ILE:HD12	52:v:40:ARG:HD3	1.89	0.54
1:1:742:A:H2'	1:1:743:A:C8	2.43	0.54
1:1:1271:G:O2'	1:1:1618:6MZ:OP1	2.23	0.54
1:1:2525:G:H2'	1:1:2526:G:H8	1.71	0.54
2:2:770:C:H2'	2:2:771:G:H8	1.71	0.54
2:2:972:C:OP2	45:o:59:LYS:NZ	2.39	0.54
2:2:1368:A:OP2	44:n:114:LYS:NZ	2.39	0.54
2:2:1421:G:H2'	2:2:1422:G:H8	1.73	0.54
3:3:114:C:H2'	3:3:115:A:H8	1.71	0.54
45:o:5:ARG:HH11	45:o:7:ARG:HH21	1.56	0.54
46:p:93:ARG:NH1	56:z:23:CYS:SG	2.74	0.54
49:s:2:ALA:N	49:s:67:THR:O	2.41	0.54
1:1:18:U:OP1	21:Q:30:ARG:NH1	2.34	0.53
1:1:290:U:O2	1:1:350:G:O6	2.26	0.53
1:1:1069:A:O2'	1:1:1074:G:O6	2.25	0.53
1:1:1592:C:N3	1:1:1593:A:N6	2.56	0.53
1:1:1769:U:O2	1:1:1984:G:C2	2.61	0.53
1:1:2313:C:H5''	9:E:88:LYS:HD2	1.89	0.53
1:1:2485:G:N2	1:1:2486:C:O2	2.41	0.53
1:1:2572:A:O2'	1:1:2575:C:OP1	2.23	0.53
1:1:2771:C:O2'	7:C:208:LYS:NZ	2.40	0.53
2:2:1296:C:H2'	2:2:1299:A:H62	1.73	0.53
2:2:1395:C:C4'	2:2:1401:G:H21	2.21	0.53
6:B:133:ARG:HG3	6:B:186:ALA:HB1	1.90	0.53
24:T:9:LYS:O	24:T:12:ARG:NH2	2.37	0.53
36:f:2:LYS:O	36:f:35:GLN:HA	2.08	0.53
39:i:25:VAL:HG13	39:i:26:ARG:HG3	1.90	0.53
1:1:1051:G:O6	1:1:1108:U:O2	2.26	0.53
1:1:2100:G:N2	1:1:2189:U:HI'	2.21	0.53
1:1:2279:G:N7	27:W:14:ARG:NH2	2.52	0.53
2:2:501:C:OP1	47:q:114:ARG:NH2	2.41	0.53
2:2:1178:G:H3'	44:n:99:ARG:HH12	1.73	0.53
2:2:1522:U:OP1	46:p:128:ARG:NH2	2.40	0.53
23:S:88:ARG:HG3	23:S:92:ARG:HH11	1.72	0.53
44:n:84:THR:HG21	44:n:104:VAL:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:p:31:ILE:HG12	46:p:46:THR:HG22	1.90	0.53
1:1:59:U:O2	1:1:68:G:O6	2.26	0.53
2:2:263:A:OP2	55:y:74:ARG:NH2	2.41	0.53
2:2:959:A:H2	2:2:1221:G:H21	1.56	0.53
14:J:56:VAL:HB	14:J:124:VAL:HG12	1.89	0.53
19:O:50:ALA:O	19:O:81:ARG:NH2	2.40	0.53
37:g:66:LYS:O	37:g:159:ASP:N	2.41	0.53
41:k:29:ILE:HD11	41:k:74:LEU:HD22	1.91	0.53
55:y:34:LYS:NZ	55:y:53:GLU:OE1	2.41	0.53
1:1:912:C:O5'	17:M:8:LYS:NZ	2.41	0.53
1:1:1227:G:OP1	21:Q:13:ARG:NH1	2.42	0.53
2:2:1369:C:H2'	2:2:1370:G:H8	1.73	0.53
8:D:119:ILE:O	8:D:187:VAL:HA	2.09	0.53
10:F:166:ASP:OD1	10:F:166:ASP:N	2.38	0.53
1:1:75:G:O3'	29:Y:48:ARG:NH1	2.41	0.53
3:3:11:C:O2'	3:3:15:A:N6	2.41	0.53
12:H:26:VAL:HG13	12:H:116:GLU:HG2	1.90	0.53
38:h:32:ASN:HB3	38:h:59:ARG:HD2	1.90	0.53
49:s:6:MET:SD	49:s:9:ARG:NH2	2.82	0.53
52:v:15:ASP:OD1	52:v:15:ASP:N	2.42	0.53
57:4:39:A:N6	57:4:41:G:O6	2.36	0.53
1:1:903:C:N4	1:1:904:G:O6	2.41	0.53
1:1:1201:U:H2'	1:1:1202:G:H8	1.73	0.53
1:1:1951:U:O2'	1:1:1953:A:N7	2.39	0.53
2:2:261:U:OP2	55:y:74:ARG:NH1	2.41	0.53
2:2:693:G:OP1	46:p:127:ARG:NH2	2.42	0.53
2:2:1106:G:H5''	38:h:172:ARG:HB3	1.90	0.53
3:3:36:C:N4	3:3:49:C:O2'	2.42	0.53
27:W:11:ARG:O	27:W:14:ARG:NH1	2.41	0.53
56:z:62:ARG:O	56:z:66:ARG:HB2	2.09	0.53
1:1:918:A:O2'	3:3:80:U:O2	2.27	0.53
1:1:2841:C:H2'	1:1:2842:G:H8	1.72	0.53
2:2:1078:U:O2'	40:j:138:ARG:NH1	2.42	0.53
39:i:54:GLN:NE2	39:i:202:GLU:OE1	2.41	0.53
42:l:79:ARG:NH2	42:l:82:GLY:O	2.41	0.53
44:n:49:ARG:HG2	44:n:52:LEU:HD22	1.90	0.53
46:p:16:VAL:HG13	46:p:79:ILE:HG13	1.90	0.53
1:1:1077:A:N3	13:I:134:SER:OG	2.40	0.53
1:1:1365:A:O2'	28:X:11:ARG:NH1	2.42	0.53
1:1:1667:G:O2'	1:1:1991:U:O4	2.26	0.53
1:1:160:A:N6	1:1:166:U:C2	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:494:G:H21	23:S:57:ASN:HD21	1.55	0.53
1:1:572:A:N6	1:1:2029:G:H21	2.02	0.53
1:1:771:G:O2'	1:1:1355:G:O2'	2.23	0.53
1:1:2469:A:O2'	17:M:55:ARG:NH2	2.42	0.53
1:1:2828:G:H2'	1:1:2829:A:H8	1.73	0.53
2:2:126:G:OP1	2:2:605:U:O2'	2.25	0.53
13:I:100:ILE:H	13:I:139:VAL:HG13	1.74	0.53
18:N:79:LEU:HA	18:N:83:LEU:HD12	1.91	0.53
57:4:175:A:H2'	57:4:176:G:H5'	1.90	0.53
1:1:1365:A:OP1	28:X:3:ARG:NH2	2.42	0.53
1:1:2100:G:H1	1:1:2189:U:H1'	1.74	0.53
1:1:2102:G:C2	1:1:2188:U:H1'	2.44	0.53
1:1:2617:U:H2'	1:1:2618:G:H8	1.72	0.53
2:2:137:U:H2'	2:2:138:G:H8	1.74	0.53
2:2:1187:G:H2'	2:2:1188:A:C8	2.44	0.53
23:S:22:ASP:OD1	23:S:25:ARG:NH2	2.42	0.53
57:4:20:A:H3'	57:4:20:A:C4	2.44	0.53
1:1:1140:C:OP2	14:J:68:LYS:NZ	2.39	0.52
1:1:1188:U:H2'	1:1:1189:A:H8	1.73	0.52
1:1:2484:G:H4'	17:M:45:GLN:HG2	1.90	0.52
2:2:339:C:OP2	15:K:98:ARG:NH1	2.42	0.52
2:2:429:U:H2'	39:i:31:LYS:HD3	1.91	0.52
2:2:1316:G:O6	54:x:7:LYS:NZ	2.41	0.52
6:B:151:GLY:O	6:B:153:GLN:NE2	2.41	0.52
16:L:77:ILE:HD11	16:L:95:LEU:HD21	1.90	0.52
19:O:94:ARG:NH1	19:O:97:PHE:O	2.43	0.52
39:i:99:ASP:OD2	39:i:115:ARG:NH1	2.42	0.52
46:p:13:ARG:NH1	46:p:77:TYR:OH	2.38	0.52
1:1:633:A:H5''	16:L:70:LYS:HD2	1.91	0.52
1:1:960:A:HO2'	1:1:2456:C:HO2'	1.53	0.52
1:1:977:G:OP1	21:Q:55:ARG:NH1	2.40	0.52
1:1:1986:C:H2'	1:1:1987:A:H8	1.73	0.52
1:1:2292:U:OP2	19:O:13:ARG:NH2	2.40	0.52
2:2:409:U:O2	2:2:433:G:N2	2.41	0.52
2:2:935:A:N1	42:l:3:ARG:NH2	2.57	0.52
7:C:45:TYR:OH	7:C:81:GLU:OE2	2.27	0.52
12:H:121:SER:OG	12:H:122:GLN:N	2.40	0.52
16:L:33:ARG:HB3	16:L:40:SER:HA	1.91	0.52
48:r:10:PRO:HB2	48:r:13:LYS:HE3	1.91	0.52
57:4:67:G:HO2'	57:4:302:A:HO2'	1.57	0.52
1:1:558:U:OP1	14:J:114:LEU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1856:U:O2	1:1:1887:C:N4	2.42	0.52
1:1:1909:C:H2'	1:1:1910:G:C8	2.44	0.52
1:1:2066:C:H42	1:1:2444:G:H1	1.57	0.52
1:1:2393:U:H5''	16:L:62:PRO:HB3	1.90	0.52
2:2:60:A:OP1	2:2:111:G:N2	2.42	0.52
2:2:310:G:O3'	51:u:31:ARG:NH2	2.42	0.52
2:2:1342:C:H2'	2:2:1343:G:H8	1.74	0.52
40:j:69:ARG:HG3	40:j:70:ASN:HD22	1.74	0.52
1:1:395:U:O2'	1:1:396:G:N7	2.39	0.52
1:1:589:U:H2'	1:1:590:A:H8	1.75	0.52
1:1:692:C:H2'	1:1:693:A:C8	2.45	0.52
1:1:935:C:H2'	1:1:936:A:H8	1.73	0.52
1:1:1769:U:O2'	1:1:1958:C:OP1	2.25	0.52
2:2:94:G:N1	2:2:98:A:N1	2.58	0.52
3:3:80:U:OP1	17:M:18:ARG:NH2	2.43	0.52
18:N:36:THR:OG1	18:N:37:THR:N	2.42	0.52
37:g:174:LYS:HA	37:g:177:ASN:HB2	1.91	0.52
39:i:85:ASN:HA	40:j:102:GLY:HA3	1.92	0.52
39:i:109:ALA:N	39:i:113:GLU:OE1	2.41	0.52
40:j:34:THR:HG22	40:j:52:LYS:HB3	1.92	0.52
1:1:1866:A:H62	1:1:1867:G:N2	2.07	0.52
1:1:1915:3TD:O5'	1:1:1915:3TD:O3'	2.27	0.52
1:1:1919:A:N1	2:2:1495:U:O2'	2.41	0.52
1:1:2170:A:H1'	1:1:2171:A:H5''	1.92	0.52
1:1:2333:A:OP2	27:W:77:ARG:NH2	2.42	0.52
2:2:335:C:H2'	2:2:336:A:C8	2.44	0.52
2:2:416:G:H1	2:2:427:U:H3	1.57	0.52
6:B:160:THR:OG1	6:B:161:TYR:N	2.43	0.52
42:l:42:ILE:HG12	42:l:117:ALA:HB2	1.91	0.52
57:4:264:U:O4	57:4:308:U:N3	2.38	0.52
57:4:302:A:N6	57:4:306:U:O4	2.43	0.52
1:1:107:G:H2'	1:1:108:G:H8	1.73	0.52
1:1:1769:U:N3	1:1:1984:G:C6	2.78	0.52
1:1:2262:U:H2'	1:1:2263:C:H6	1.73	0.52
2:2:1512:U:H2'	2:2:1513:A:H8	1.75	0.52
32:b:33:THR:HG21	32:b:51:GLY:HA2	1.91	0.52
35:e:51:SER:OG	35:e:52:LYS:N	2.40	0.52
1:1:1723:G:O6	1:1:1737:G:O2'	2.25	0.52
1:1:2756:U:OP2	36:f:19:ARG:NE	2.33	0.52
2:2:673:A:H2'	2:2:674:G:H8	1.74	0.52
14:J:118:MET:HA	14:J:121:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:45:GLN:HE22	17:M:125:PRO:HD3	1.75	0.52
19:O:67:ASN:ND2	19:O:69:ASP:OD2	2.40	0.52
23:S:29:VAL:HA	23:S:32:ALA:HB3	1.91	0.52
24:T:10:VAL:HG23	24:T:11:LEU:HG	1.91	0.52
1:1:16:C:H2'	1:1:17:G:H8	1.75	0.52
1:1:467:G:OP2	34:d:34:ARG:NH1	2.43	0.52
1:1:491:G:N2	1:1:1321:A:OP1	2.42	0.52
2:2:150:U:O4	2:2:171:A:N7	2.43	0.52
2:2:1159:U:H4'	2:2:1160:G:H5'	1.91	0.52
11:G:116:ARG:O	11:G:131:SER:OG	2.26	0.52
41:k:4:TYR:HA	41:k:90:MET:O	2.10	0.52
43:m:11:LEU:HD22	43:m:75:ILE:HG21	1.92	0.52
46:p:123:PRO:HG2	56:z:38:TYR:HA	1.91	0.52
1:1:1047:G:O2'	1:1:1110:G:N2	2.41	0.52
1:1:1082:U:H2'	1:1:1083:U:H4'	1.91	0.52
1:1:2683:C:OP1	20:P:51:ARG:NH2	2.37	0.52
2:2:593:U:O4	2:2:646:G:O6	2.28	0.52
2:2:744:C:H2'	2:2:745:G:C8	2.45	0.52
2:2:1166:G:N2	2:2:1169:A:OP2	2.42	0.52
7:C:14:ILE:HG21	7:C:179:ARG:HH22	1.74	0.52
8:D:119:ILE:HB	8:D:187:VAL:HG12	1.91	0.52
15:K:7:MET:HB3	15:K:18:ARG:HD2	1.91	0.52
18:N:114:GLU:OE2	18:N:118:ARG:NH2	2.37	0.52
25:U:84:GLY:HA3	25:U:97:LYS:HD3	1.91	0.52
1:1:55:G:N2	1:1:115:C:O2	2.37	0.52
1:1:1045:C:H5''	1:1:1047:G:H5''	1.92	0.52
1:1:2722:G:O2'	18:N:3:HIS:O	2.25	0.52
2:2:468:A:H5''	2:2:469:C:H5	1.74	0.52
2:2:533:A:O2'	2:2:535:A:OP2	2.28	0.52
2:2:835:U:H2'	2:2:836:G:H8	1.75	0.52
6:B:79:GLU:HB3	6:B:80:ARG:HD2	1.90	0.52
7:C:1:MET:HB3	7:C:205:PRO:HG2	1.91	0.52
18:N:26:GLY:HA2	18:N:75:ILE:HD12	1.91	0.52
25:U:72:ILE:HD12	25:U:83:VAL:HG21	1.90	0.52
28:X:40:VAL:O	28:X:44:LYS:HA	2.10	0.52
45:o:26:VAL:HG13	45:o:36:VAL:HG11	1.92	0.52
1:1:573:U:O2'	1:1:575:A:OP1	2.28	0.51
1:1:1159:U:H2'	1:1:1160:G:H8	1.74	0.51
1:1:1164:C:H2'	1:1:1165:A:H8	1.74	0.51
1:1:2704:C:C2'	1:1:2705:A:H5'	2.41	0.51
1:1:2716:C:H2'	1:1:2717:C:H6	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:413:G:N1	39:i:31:LYS:O	2.36	0.51
2:2:652:U:O4	2:2:752:G:O2'	2.27	0.51
2:2:1114:C:O2	49:s:100:SER:OG	2.27	0.51
2:2:1186:G:N2	49:s:100:SER:OG	2.43	0.51
4:5:103:ARG:HA	4:5:106:ARG:HH21	1.75	0.51
8:D:53:THR:OG1	8:D:54:GLY:N	2.42	0.51
17:M:33:LEU:HB3	17:M:103:TYR:HB2	1.91	0.51
49:s:65:ARG:H	49:s:79:LEU:HD12	1.75	0.51
1:1:519:U:H2'	1:1:520:G:H8	1.75	0.51
1:1:1036:G:N2	1:1:1119:U:O2	2.40	0.51
1:1:1093:G:H22	1:1:1097:U:H5''	1.74	0.51
1:1:1146:C:H2'	1:1:1147:A:H8	1.75	0.51
1:1:1798:U:OP2	6:B:271:ARG:NH2	2.43	0.51
1:1:2287:A:O2'	1:1:2289:G:N7	2.41	0.51
2:2:222:C:H2'	2:2:223:A:H8	1.73	0.51
2:2:672:U:O2'	53:w:64:TYR:OH	2.25	0.51
1:1:1952:A:N6	1:1:1953:A:N1	2.59	0.51
1:1:2348:U:H4'	33:c:41:PRO:HB3	1.93	0.51
2:2:938:A:O2'	42:l:95:ARG:NH2	2.38	0.51
2:2:1101:A:H5''	37:g:171:ILE:HD11	1.92	0.51
2:2:1233:G:OP1	44:n:119:ARG:NH1	2.43	0.51
2:2:1458:G:OP1	55:y:30:THR:OG1	2.26	0.51
10:F:41:VAL:O	10:F:55:ARG:NH2	2.44	0.51
24:T:90:GLY:O	24:T:91:GLN:NE2	2.42	0.51
38:h:71:ALA:HB1	38:h:109:PRO:HA	1.92	0.51
43:m:15:ARG:HD3	43:m:74:SER:HA	1.93	0.51
44:n:94:LEU:HB3	44:n:98:LEU:HD13	1.92	0.51
46:p:18:ASP:N	46:p:18:ASP:OD1	2.41	0.51
1:1:372:G:OP1	28:X:62:LYS:NZ	2.42	0.51
1:1:1716:U:H2'	1:1:1717:A:H8	1.75	0.51
1:1:2101:A:C8	1:1:2101:A:O5'	2.63	0.51
1:1:2681:C:OP2	7:C:114:LYS:NZ	2.41	0.51
2:2:75:G:H2'	2:2:76:G:H8	1.74	0.51
3:3:43:C:OP1	31:a:6:HIS:NE2	2.40	0.51
11:G:65:ALA:HB1	11:G:68:ARG:HE	1.76	0.51
15:K:65:THR:OG1	15:K:66:LYS:N	2.43	0.51
57:4:20:A:C3'	57:4:20:A:C4	2.92	0.51
1:1:1665:A:H2'	1:1:1666:G:H8	1.76	0.51
2:2:297:G:N2	2:2:300:A:OP2	2.35	0.51
2:2:377:G:H2'	2:2:378:G:H8	1.75	0.51
2:2:593:U:O2	2:2:646:G:N2	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:66:ARG:NH1	17:M:104:GLU:OE2	2.43	0.51
23:S:6:LYS:HG2	23:S:104:THR:HG22	1.92	0.51
28:X:53:ALA:HA	28:X:56:MET:HE2	1.93	0.51
30:Z:56:LYS:NZ	30:Z:58:GLU:OE1	2.43	0.51
40:j:94:VAL:HG12	40:j:127:ALA:HA	1.91	0.51
1:1:688:U:H2'	1:1:689:A:H8	1.76	0.51
1:1:2171:A:O2'	1:1:2173:A:OP1	2.24	0.51
1:1:2289:G:N2	1:1:2344:U:O2	2.43	0.51
12:H:109:LYS:HB3	12:H:112:ALA:HB2	1.93	0.51
25:U:10:GLU:OE2	25:U:22:ARG:NH1	2.43	0.51
32:b:31:ASP:OD2	32:b:34:SER:N	2.42	0.51
1:1:307:G:N2	1:1:310:A:OP2	2.43	0.51
1:1:1315:C:O2'	1:1:1392:A:N3	2.41	0.51
1:1:1539:U:H2'	1:1:1540:G:H8	1.74	0.51
1:1:1901:A:OP2	6:B:253:LYS:NZ	2.36	0.51
1:1:1999:C:O2	1:1:2687:U:O2'	2.28	0.51
2:2:137:U:H3	2:2:226:G:H1	1.58	0.51
2:2:986:U:H3	2:2:1219:A:H61	1.59	0.51
11:G:38:PRO:O	11:G:43:ASN:ND2	2.39	0.51
45:o:6:ILE:HD13	45:o:102:LEU:HB2	1.92	0.51
57:4:205:G:N2	57:4:206:A:N7	2.59	0.51
1:1:30:G:H8	1:1:30:G:O5'	1.94	0.51
1:1:328:U:O3'	25:U:66:GLN:NE2	2.43	0.51
1:1:671:C:OP2	16:L:33:ARG:NH1	2.43	0.51
1:1:859:G:N2	1:1:917:A:OP2	2.39	0.51
1:1:1248:G:OP1	8:D:44:ARG:NH1	2.44	0.51
1:1:2197:U:H3	1:1:2225:A:H62	1.57	0.51
2:2:754:C:O5'	50:t:72:ARG:NH1	2.40	0.51
4:5:56:VAL:N	4:5:111:VAL:O	2.43	0.51
6:B:136:PRO:O	6:B:139:SER:OG	2.28	0.51
10:F:137:ASP:HB3	10:F:140:VAL:HG12	1.93	0.51
16:L:64:PHE:HB3	35:e:25:LYS:HE2	1.93	0.51
26:V:42:LEU:HD13	26:V:47:VAL:HG21	1.92	0.51
30:Z:28:GLY:HA3	30:Z:38:ARG:HH21	1.76	0.51
1:1:213:A:H2'	1:1:214:G:C8	2.46	0.51
1:1:328:U:O2	25:U:68:SER:OG	2.29	0.51
1:1:926:G:H2'	1:1:927:A:H8	1.76	0.51
1:1:1689:A:H2'	1:1:1690:A:C8	2.46	0.51
1:1:2751:G:OP1	1:1:2751:G:N2	2.44	0.51
2:2:1157:A:N6	2:2:1178:G:O2'	2.40	0.51
2:2:1160:G:O6	2:2:1182:G:O6	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:8:THR:HG23	50:t:31:LEU:HD21	1.92	0.51
51:u:5:ARG:NH2	51:u:27:ALA:O	2.44	0.51
1:1:1250:G:OP2	16:L:21:ARG:NE	2.43	0.51
1:1:1324:G:O2'	1:1:1326:U:OP2	2.28	0.51
1:1:1727:C:O2	1:1:1734:G:N2	2.44	0.51
2:2:36:C:H5'	47:q:118:GLY:HA2	1.93	0.51
15:K:108:ARG:NH1	20:P:34:GLU:OE1	2.44	0.51
1:1:106:C:H2'	1:1:107:G:H8	1.75	0.50
1:1:1567:G:OP1	6:B:60:GLN:NE2	2.39	0.50
1:1:2658:C:OP1	10:F:158:LYS:NZ	2.44	0.50
1:1:2810:A:H4'	7:C:62:LYS:HD2	1.93	0.50
2:2:859:G:OP2	2:2:869:G:N1	2.39	0.50
2:2:950:U:O2	2:2:1231:G:N2	2.38	0.50
6:B:84:ASP:OD2	6:B:87:ARG:N	2.44	0.50
7:C:179:ARG:HG2	7:C:181:ASP:HB2	1.93	0.50
8:D:148:ILE:HB	8:D:169:VAL:HG22	1.92	0.50
18:N:66:ALA:O	18:N:70:THR:OG1	2.29	0.50
18:N:82:GLU:OE2	18:N:86:ARG:NE	2.44	0.50
40:j:64:MET:O	40:j:68:ARG:NH2	2.44	0.50
40:j:133:PRO:HA	40:j:136:VAL:HG12	1.93	0.50
1:1:839:U:O2'	1:1:1191:G:N3	2.45	0.50
1:1:1326:U:H2'	1:1:1327:A:H8	1.77	0.50
1:1:1769:U:N3	1:1:1984:G:N1	2.59	0.50
1:1:2163:A:N6	1:1:2165:C:OP1	2.44	0.50
1:1:2329:U:H2'	1:1:2330:G:C8	2.45	0.50
2:2:1072:G:H21	37:g:106:THR:HG21	1.76	0.50
2:2:1445:U:O4	2:2:1457:G:O6	2.28	0.50
10:F:56:ASP:OD1	10:F:56:ASP:N	2.44	0.50
10:F:60:ASP:OD1	10:F:60:ASP:N	2.40	0.50
24:T:58:VAL:HG12	24:T:85:VAL:HG22	1.93	0.50
1:1:658:U:O2'	8:D:95:LYS:NZ	2.45	0.50
1:1:1088:A:N6	13:I:130:GLY:O	2.44	0.50
1:1:1592:C:H2'	1:1:1593:A:C8	2.46	0.50
1:1:2101:A:O5'	1:1:2101:A:H8	1.94	0.50
2:2:976:G:OP2	2:2:1358:U:O2'	2.27	0.50
38:h:11:ARG:NH1	38:h:180:ALA:O	2.44	0.50
52:v:36:LYS:NZ	52:v:37:PHE:O	2.44	0.50
1:1:320:A:O2'	8:D:163:ASN:ND2	2.45	0.50
1:1:624:C:H2'	1:1:625:G:H8	1.77	0.50
1:1:2233:U:H2'	1:1:2234:G:H8	1.76	0.50
1:1:2874:C:OP1	18:N:4:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:210:C:O2	2:2:211:G:N2	2.41	0.50
2:2:1152:A:H2'	2:2:1153:G:C8	2.46	0.50
2:2:1181:G:O2'	2:2:1182:G:N7	2.42	0.50
9:E:98:GLU:OE2	31:a:25:ARG:NH1	2.42	0.50
11:G:87:GLU:O	41:k:17:GLN:NE2	2.44	0.50
19:O:39:VAL:HG22	19:O:49:VAL:HG22	1.94	0.50
23:S:38:TYR:O	23:S:40:ASN:ND2	2.44	0.50
1:1:511:U:H5	1:1:512:G:C4	2.29	0.50
1:1:713:G:O2'	1:1:718:A:N6	2.44	0.50
1:1:2580:PSU:O5'	1:1:2581:G:N2	2.45	0.50
3:3:44:G:N3	3:3:47:C:N4	2.51	0.50
7:C:122:VAL:HA	7:C:127:PHE:H	1.77	0.50
14:J:78:THR:OG1	14:J:80:HIS:O	2.30	0.50
17:M:41:LEU:HD22	17:M:124:LEU:HD12	1.92	0.50
17:M:69:PRO:HA	17:M:94:ALA:HB2	1.94	0.50
18:N:72:ASP:OD2	18:N:75:ILE:N	2.35	0.50
20:P:102:GLU:HG3	20:P:103:ARG:HG3	1.92	0.50
26:V:17:SER:HG	26:V:21:ARG:HH12	1.57	0.50
37:g:166:ALA:HB3	37:g:191:SER:HB2	1.92	0.50
45:o:5:ARG:O	45:o:103:GLY:N	2.43	0.50
57:4:174:A:H2'	57:4:175:A:H8	1.77	0.50
57:4:290:A:H4'	57:4:291:A:H5'	1.93	0.50
1:1:2188:U:H2'	1:1:2189:U:O2	2.12	0.50
2:2:1238:A:OP1	2:2:1335:U:O2'	2.29	0.50
12:H:90:GLY:HA3	12:H:93:ALA:HB2	1.94	0.50
19:O:6:ALA:O	19:O:10:ARG:NH2	2.45	0.50
33:c:5:ILE:HG12	33:c:28:ARG:HE	1.76	0.50
44:n:42:GLU:OE2	44:n:45:ARG:NH1	2.44	0.50
1:1:268:C:H2'	1:1:269:C:H6	1.77	0.50
1:1:1494:A:N6	1:1:1495:A:N1	2.60	0.50
1:1:2189:U:OP2	1:1:2189:U:C2	2.65	0.50
1:1:2564:A:N6	1:1:2565:A:N1	2.60	0.50
2:2:246:A:H62	2:2:281:G:N2	2.09	0.50
2:2:261:U:OP1	55:y:71:LYS:NZ	2.42	0.50
2:2:565:U:H3'	2:2:566:G:H8	1.76	0.50
2:2:1291:U:OP1	44:n:41:ARG:NH2	2.44	0.50
3:3:18:G:O6	3:3:65:U:O4	2.30	0.50
6:B:80:ARG:HB2	6:B:93:LEU:HD23	1.93	0.50
6:B:146:MET:SD	6:B:182:ARG:NH1	2.85	0.50
12:H:21:GLY:HA2	12:H:88:HIS:HA	1.93	0.50
23:S:36:LEU:HD11	23:S:47:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:32:PHE:HB2	37:g:42:ASN:HB2	1.92	0.50
38:h:112:ASP:H	38:h:115:LEU:HD12	1.75	0.50
38:h:150:LYS:HB2	38:h:201:TRP:HB2	1.94	0.50
40:j:86:LYS:HA	40:j:94:VAL:O	2.11	0.50
57:4:3:G:H2'	57:4:4:G:H8	1.77	0.50
57:4:20:A:P	57:4:20:A:O4'	2.70	0.50
57:4:195:A:H2'	57:4:196:G:H8	1.77	0.50
57:4:277:G:H2'	57:4:278:G:H8	1.76	0.50
1:1:806:C:O2	1:1:2444:G:O2'	2.27	0.50
1:1:968:C:H2'	1:1:969:G:C8	2.46	0.50
1:1:2101:A:H2'	1:1:2102:G:O4'	2.11	0.50
2:2:521:G:OP2	47:q:51:LYS:NZ	2.43	0.50
26:V:30:ILE:O	26:V:93:ARG:NH1	2.45	0.50
34:d:31:LEU:O	34:d:35:ARG:NH1	2.45	0.50
49:s:66:GLN:HG3	49:s:79:LEU:HD11	1.94	0.50
1:1:1462:C:H2'	1:1:1463:C:H6	1.77	0.50
1:1:1691:C:H2'	1:1:1692:U:H6	1.77	0.50
1:1:1769:U:C2	1:1:1984:G:C2	3.00	0.50
1:1:2039:U:H2'	1:1:2040:G:H8	1.77	0.50
8:D:173:THR:OG1	8:D:174:GLY:N	2.44	0.50
9:E:109:PRO:HA	31:a:41:HIS:HD2	1.75	0.50
11:G:82:SER:O	11:G:149:GLU:HB3	2.11	0.50
1:1:519:U:H5''	23:S:25:ARG:HH22	1.77	0.49
1:1:2364:C:H1'	27:W:36:ILE:HD11	1.94	0.49
1:1:2380:C:H2'	1:1:2381:A:C8	2.47	0.49
2:2:1312:G:H5''	54:x:5:LEU:HD12	1.93	0.49
39:i:3:ARG:HE	39:i:115:ARG:HE	1.60	0.49
49:s:58:SER:O	49:s:58:SER:OG	2.29	0.49
50:t:36:ILE:HD12	50:t:63:ARG:HH11	1.76	0.49
57:4:21:C:H3'	57:4:21:C:OP2	2.11	0.49
1:1:78:U:OP2	29:Y:4:LYS:NZ	2.45	0.49
1:1:402:A:N6	1:1:423:A:N1	2.60	0.49
1:1:414:C:O2	1:1:1864:U:O2'	2.29	0.49
1:1:1026:G:OP2	1:1:1134:A:O2'	2.28	0.49
2:2:8:A:N6	39:i:202:GLU:O	2.45	0.49
2:2:67:C:H2'	2:2:68:G:C8	2.47	0.49
2:2:672:U:O4	2:2:734:G:O6	2.30	0.49
2:2:674:G:H2'	2:2:675:A:C8	2.48	0.49
2:2:1391:U:H2'	2:2:1392:G:H8	1.77	0.49
8:D:117:ARG:HH12	16:L:2:ARG:HH12	1.60	0.49
10:F:18:LYS:NZ	10:F:19:ILE:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:6:LEU:HA	11:G:15:LEU:HD12	1.94	0.49
16:L:96:LYS:NZ	16:L:103:ILE:O	2.44	0.49
39:i:99:ASP:HA	39:i:102:VAL:HG12	1.93	0.49
1:1:523:C:O2	1:1:554:U:O2'	2.29	0.49
1:1:882:G:C8	1:1:882:G:C5'	2.92	0.49
1:1:1665:A:H2'	1:1:1666:G:C8	2.46	0.49
1:1:2887:A:H2	32:b:40:ARG:HH22	1.60	0.49
2:2:553:A:H2'	2:2:554:A:C8	2.46	0.49
2:2:672:U:HO2'	53:w:64:TYR:HH	1.57	0.49
2:2:947:G:H5''	48:r:107:ARG:HB2	1.94	0.49
2:2:1218:C:H2'	2:2:1219:A:H8	1.76	0.49
2:2:1250:A:H2	2:2:1370:G:H1'	1.77	0.49
3:3:55:U:O3'	9:E:24:SER:OG	2.30	0.49
4:5:160:ARG:NH2	56:z:36:GLU:OE1	2.45	0.49
20:P:89:ARG:NH2	20:P:115:ASN:O	2.41	0.49
48:r:86:TYR:H	54:x:73:GLU:HB3	1.78	0.49
48:r:91:HIS:CD2	48:r:97:VAL:HG21	2.47	0.49
1:1:578:G:OP1	1:1:1255:U:O2'	2.27	0.49
1:1:1278:C:H2'	1:1:1279:G:C8	2.47	0.49
1:1:1952:A:OP1	15:K:44:LYS:NZ	2.37	0.49
1:1:2693:G:H2'	1:1:2694:G:H8	1.78	0.49
2:2:1226:C:OP2	48:r:102:THR:OG1	2.28	0.49
1:1:126:A:OP2	34:d:18:PHE:N	2.45	0.49
1:1:2544:G:N2	1:1:2646:C:O2'	2.39	0.49
2:2:21:G:H2'	2:2:22:G:C8	2.46	0.49
2:2:462:G:H22	2:2:469:C:H42	1.61	0.49
2:2:1421:G:OP1	15:K:54:LYS:NZ	2.36	0.49
4:5:36:LEU:HD22	4:5:41:VAL:HG23	1.94	0.49
46:p:88:GLY:H	46:p:114:THR:HG22	1.77	0.49
57:4:34:A:H2'	57:4:35:C:H5'	1.94	0.49
1:1:182:A:H61	1:1:215:G:H1	1.60	0.49
1:1:285:G:N2	1:1:355:U:O2	2.43	0.49
1:1:994:C:OP1	21:Q:53:ARG:NH2	2.45	0.49
1:1:2690:U:OP1	18:N:14:SER:OG	2.30	0.49
1:1:2749:A:N1	1:1:2750:A:N6	2.60	0.49
9:E:147:ASP:N	9:E:147:ASP:OD1	2.45	0.49
10:F:27:LYS:NZ	10:F:28:GLY:O	2.45	0.49
30:Z:12:SER:OG	30:Z:13:ALA:N	2.42	0.49
51:u:20:VAL:HG12	51:u:35:ARG:HB3	1.95	0.49
54:x:53:ASN:HD21	54:x:56:GLN:HE21	1.61	0.49
1:1:1451:C:H4'	1:1:1452:G:H5'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1962:5MC:O2'	1:1:1964:G:OP2	2.31	0.49
1:1:2379:G:O3'	19:O:17:LYS:NZ	2.44	0.49
2:2:674:G:H2'	2:2:675:A:H8	1.77	0.49
2:2:945:G:N2	2:2:1334:G:O2'	2.45	0.49
2:2:1148:U:H5''	44:n:11:ARG:HH11	1.78	0.49
2:2:1402:4OC:HM23	2:2:1402:4OC:O3'	2.12	0.49
8:D:178:VAL:HG23	16:L:3:LEU:HD21	1.94	0.49
14:J:32:LEU:HD22	14:J:54:ILE:HG21	1.95	0.49
51:u:68:SER:OG	51:u:69:ASP:N	2.46	0.49
57:4:192:A:H2'	57:4:193:A:H5'	1.95	0.49
1:1:90:U:H3'	1:1:91:A:H2'	1.94	0.49
1:1:715:A:OP2	50:t:88:ARG:NH2	2.46	0.49
1:1:1483:G:H22	1:1:1507:C:H1'	1.77	0.49
1:1:1779:U:H2'	1:1:1783:A:H62	1.77	0.49
1:1:2108:A:OP1	1:1:2150:C:O2'	2.30	0.49
1:1:2841:C:H2'	1:1:2842:G:C8	2.47	0.49
2:2:473:U:OP1	51:u:76:LYS:NZ	2.44	0.49
2:2:551:U:O2	2:2:551:U:H2'	2.11	0.49
2:2:783:C:H2'	2:2:784:A:H8	1.78	0.49
2:2:1303:C:H3'	2:2:1304:G:H8	1.77	0.49
6:B:117:GLN:OE1	6:B:128:ASN:ND2	2.39	0.49
12:H:53:ARG:HB3	12:H:55:VAL:HG23	1.95	0.49
40:j:20:ARG:NH1	57:4:96:G:N3	2.61	0.49
42:l:126:ASP:OD1	42:l:131:LYS:NZ	2.34	0.49
43:m:60:GLU:OE2	43:m:62:THR:OG1	2.30	0.49
44:n:42:GLU:HA	44:n:45:ARG:HB2	1.95	0.49
45:o:40:ILE:O	45:o:73:LEU:N	2.46	0.49
49:s:66:GLN:HE21	49:s:79:LEU:HD21	1.78	0.49
1:1:873:C:H2'	1:1:874:G:H8	1.78	0.49
1:1:1527:G:N2	1:1:1544:A:OP2	2.45	0.49
1:1:2064:C:O2'	1:1:2251:OMG:N2	2.38	0.49
1:1:2064:C:HO2'	1:1:2251:OMG:HN22	1.59	0.49
4:5:94:GLN:HG3	57:4:20:A:H1'	1.95	0.49
7:C:2:ILE:HD13	7:C:90:PHE:HZ	1.77	0.49
7:C:176:ASP:HB2	7:C:190:LYS:HB3	1.95	0.49
8:D:184:ASP:OD1	16:L:2:ARG:NH2	2.45	0.49
39:i:66:GLY:O	39:i:115:ARG:NH2	2.45	0.49
40:j:41:ASP:OD1	40:j:41:ASP:N	2.45	0.49
55:y:66:LEU:HD23	55:y:67:ILE:HG23	1.95	0.49
1:1:197:A:O2'	1:1:2244:U:OP1	2.31	0.49
1:1:1152:C:H2'	1:1:1153:C:H6	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2100:G:H3'	1:1:2100:G:H8	1.77	0.49
1:1:2401:U:O2	1:1:2415:G:O6	2.30	0.49
2:2:842:U:O2'	2:2:844:G:N2	2.42	0.49
2:2:1149:C:OP2	44:n:11:ARG:NH1	2.45	0.49
3:3:49:C:H2'	3:3:50:A:H8	1.78	0.49
3:3:114:C:H2'	3:3:115:A:C8	2.47	0.49
6:B:25:HIS:NE2	6:B:82:GLU:OE2	2.43	0.49
25:U:100:SER:O	25:U:100:SER:OG	2.27	0.49
43:m:101:ILE:HG12	43:m:129:VAL:HB	1.95	0.49
43:m:112:THR:O	43:m:116:ALA:HB2	2.12	0.49
51:u:4:ILE:HG12	51:u:21:VAL:HG22	1.93	0.49
54:x:38:SER:O	54:x:71:LEU:N	2.43	0.49
57:4:53:G:H22	57:4:63:C:H42	1.60	0.49
57:4:113:A:H2'	57:4:114:G:H8	1.78	0.49
1:1:742:A:H2'	1:1:743:A:H8	1.77	0.48
1:1:885:C:H1'	1:1:892:A:C8	2.47	0.48
1:1:926:G:H2'	1:1:927:A:C8	2.48	0.48
1:1:1020:A:N1	1:1:1141:U:O2'	2.44	0.48
1:1:1435:G:H2'	1:1:1436:G:C8	2.48	0.48
1:1:2353:G:N2	27:W:34:GLY:O	2.43	0.48
2:2:152:A:N6	2:2:169:C:N3	2.61	0.48
2:2:222:C:H2'	2:2:223:A:C8	2.47	0.48
2:2:935:A:H2	2:2:1383:C:H42	1.61	0.48
9:E:73:SER:HA	9:E:79:ILE:HG13	1.95	0.48
12:H:27:VAL:O	12:H:83:ALA:N	2.44	0.48
16:L:1:MET:O	16:L:2:ARG:NH1	2.46	0.48
38:h:33:LEU:HA	38:h:36:ASP:HB2	1.95	0.48
40:j:38:VAL:HG21	40:j:114:VAL:HA	1.94	0.48
57:4:174:A:H2'	57:4:175:A:C8	2.48	0.48
1:1:20:C:H2'	1:1:21:A:C8	2.47	0.48
1:1:300:A:OP2	25:U:82:ARG:NH2	2.45	0.48
1:1:1109:C:N3	1:1:1110:G:N2	2.61	0.48
1:1:1303:G:H2'	1:1:1304:A:C8	2.47	0.48
1:1:1539:U:H2'	1:1:1540:G:C8	2.47	0.48
2:2:167:A:N1	2:2:168:G:N2	2.61	0.48
2:2:1054:C:N4	57:4:93:A:O2'	2.46	0.48
11:G:1:MET:N	11:G:21:VAL:O	2.41	0.48
13:I:101:SER:OG	13:I:104:GLN:OE1	2.30	0.48
16:L:54:GLN:HE21	16:L:60:ARG:HH22	1.60	0.48
24:T:32:LEU:HB2	24:T:83:ALA:HB3	1.95	0.48
38:h:92:ALA:HB1	38:h:98:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:70:G:OP1	1:1:112:U:N3	2.46	0.48
1:1:1026:G:N2	1:1:2489:U:OP1	2.46	0.48
1:1:1793:C:H2'	1:1:1794:A:H8	1.78	0.48
1:1:1817:G:H3'	6:B:156:ARG:HH21	1.77	0.48
2:2:401:C:O2'	2:2:621:A:N3	2.41	0.48
2:2:517:G:N1	2:2:533:A:OP2	2.45	0.48
2:2:963:G:H2'	2:2:964:A:H8	1.78	0.48
3:3:32:U:H2'	3:3:33:G:C8	2.49	0.48
8:D:131:THR:HG22	8:D:160:ALA:HA	1.95	0.48
20:P:27:GLU:HA	20:P:43:PHE:O	2.13	0.48
42:l:56:LYS:HB2	42:l:61:ALA:HB2	1.95	0.48
43:m:11:LEU:HA	43:m:14:ILE:HG22	1.95	0.48
1:1:646:U:O4	1:1:2368:C:O2'	2.27	0.48
1:1:897:C:OP2	1:1:897:C:H6	1.96	0.48
1:1:922:C:N4	1:1:923:G:O6	2.46	0.48
1:1:1419:A:N7	1:1:1578:U:C2	2.82	0.48
1:1:2095:A:OP1	11:G:11:ASN:ND2	2.47	0.48
2:2:76:G:H2'	2:2:77:A:C8	2.48	0.48
2:2:958:A:N3	2:2:985:C:O2'	2.47	0.48
2:2:1029:U:H5'	2:2:1030:U:H5''	1.95	0.48
2:2:1125:U:H4'	45:o:7:ARG:HH22	1.78	0.48
2:2:1346:A:N1	42:l:10:ARG:NH2	2.62	0.48
20:P:48:ILE:O	20:P:97:LEU:N	2.44	0.48
28:X:63:GLY:O	28:X:66:THR:OG1	2.31	0.48
37:g:15:HIS:HD2	37:g:40:ILE:HG23	1.79	0.48
52:v:9:GLN:HA	52:v:59:VAL:O	2.14	0.48
57:4:64:C:H42	57:4:72:A:H2	1.62	0.48
1:1:247:G:HO2'	1:1:386:G:H1	1.62	0.48
1:1:419:U:H2'	1:1:420:C:C6	2.49	0.48
1:1:1030:C:H2'	1:1:1031:G:C8	2.48	0.48
1:1:1457:U:O2	1:1:2702:G:O6	2.31	0.48
1:1:2365:G:OP1	27:W:55:ARG:N	2.47	0.48
2:2:56:U:H2'	2:2:57:G:H8	1.79	0.48
2:2:543:U:H2'	2:2:544:G:C8	2.48	0.48
2:2:999:C:O2	2:2:1043:G:N2	2.46	0.48
3:3:48:U:OP2	19:O:30:ARG:NH2	2.46	0.48
39:i:29:ASP:OD1	39:i:29:ASP:N	2.45	0.48
50:t:69:TYR:OH	50:t:73:LYS:NZ	2.38	0.48
1:1:2291:U:O2'	1:1:2374:C:O2	2.31	0.48
2:2:917:G:H2'	2:2:918:A:C8	2.49	0.48
3:3:77:U:H2'	3:3:78:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:65:LEU:HG	4:5:90:LEU:HD11	1.94	0.48
32:b:52:ARG:HG3	32:b:54:VAL:HG13	1.96	0.48
57:4:37:C:N4	57:4:315:G:O6	2.47	0.48
1:1:308:G:H1'	1:1:329:G:H21	1.79	0.48
1:1:660:C:H2'	1:1:661:A:H8	1.79	0.48
1:1:1386:C:H2'	1:1:1387:A:C8	2.48	0.48
1:1:1872:A:H3'	1:1:1873:G:H8	1.78	0.48
1:1:2220:U:H2'	1:1:2221:G:H8	1.79	0.48
1:1:2549:G:H2'	1:1:2550:G:H8	1.78	0.48
1:1:2781:A:H5''	1:1:2782:G:H5'	1.95	0.48
2:2:6:G:H2'	40:j:124:LEU:HD11	1.95	0.48
2:2:1222:G:OP1	54:x:78:ARG:NH1	2.45	0.48
2:2:1268:G:O2'	2:2:1326:U:O2'	2.31	0.48
2:2:1530:G:O6	56:z:46:LYS:NZ	2.44	0.48
10:F:102:VAL:HG22	10:F:116:GLN:HE22	1.78	0.48
43:m:26:THR:OG1	43:m:58:GLU:OE2	2.27	0.48
1:1:1608:A:O2'	1:1:1610:A:OP2	2.31	0.48
1:1:1825:U:H2'	1:1:1826:G:H8	1.78	0.48
1:1:2576:G:O2'	1:1:2579:C:OP2	2.22	0.48
2:2:205:A:OP2	2:2:207:C:N4	2.45	0.48
9:E:31:VAL:HA	9:E:158:THR:HA	1.95	0.48
9:E:61:SER:OG	9:E:63:GLN:O	2.32	0.48
28:X:40:VAL:HG22	28:X:43:GLU:H	1.77	0.48
38:h:40:ARG:HA	38:h:43:LEU:HB3	1.96	0.48
1:1:121:G:H2'	1:1:122:G:H8	1.79	0.48
1:1:1862:G:N1	1:1:1863:G:O6	2.47	0.48
1:1:2250:G:O2'	1:1:2497:A:OP2	2.31	0.48
1:1:2825:G:H3'	1:1:2826:A:H8	1.78	0.48
2:2:1342:C:H2'	2:2:1343:G:C8	2.49	0.48
2:2:1391:U:H2'	2:2:1392:G:C8	2.48	0.48
2:2:1515:G:H2'	2:2:1516:2MG:C8	2.49	0.48
4:5:91:LEU:CA	57:4:20:A:H62	2.17	0.48
40:j:92:SER:HB3	40:j:136:VAL:HG23	1.96	0.48
1:1:296:U:H2'	1:1:297:G:H8	1.78	0.48
1:1:660:C:H2'	1:1:661:A:C8	2.49	0.48
1:1:714:U:O5'	50:t:88:ARG:NH2	2.47	0.48
1:1:1258:U:O2'	8:D:79:ARG:NH1	2.47	0.48
1:1:1417:C:O2'	1:1:1587:G:O2'	2.27	0.48
1:1:1822:C:H2'	1:1:1823:G:H8	1.78	0.48
1:1:1837:C:H2'	1:1:1899:A:H61	1.79	0.48
1:1:2705:A:H8	1:1:2705:A:O5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:60:C:H2'	3:3:61:G:H8	1.78	0.48
19:O:30:ARG:HG2	19:O:35:ILE:HD12	1.95	0.48
21:Q:94:ILE:HG21	22:R:4:VAL:HG21	1.95	0.48
28:X:55:GLY:HA2	28:X:58:VAL:HG12	1.96	0.48
34:d:24:THR:HG23	34:d:27:GLY:H	1.79	0.48
45:o:85:ASP:OD1	45:o:85:ASP:N	2.43	0.48
47:q:73:ASN:OD1	47:q:105:SER:OG	2.32	0.48
1:1:746:PSU:C1'	1:1:748:G:H21	2.17	0.47
1:1:2098:U:H2'	1:1:2099:U:O4'	2.14	0.47
1:1:2678:C:H2'	1:1:2679:A:H8	1.79	0.47
2:2:739:C:OP2	41:k:2:ARG:NH2	2.45	0.47
2:2:1032:G:N2	2:2:1033:G:O4'	2.47	0.47
4:5:36:LEU:HB3	57:4:335:C:N4	2.29	0.47
7:C:38:LYS:NZ	7:C:49:GLN:OE1	2.47	0.47
38:h:114:LYS:HB2	38:h:185:ASN:HD22	1.79	0.47
47:q:83:ARG:NH2	47:q:83:ARG:HB3	2.29	0.47
57:4:95:C:O2	57:4:96:G:N2	2.47	0.47
57:4:176:G:H2'	57:4:177:A:H8	1.79	0.47
1:1:641:U:O2'	1:1:2350:C:OP1	2.32	0.47
1:1:776:G:N2	1:1:2241:A:OP1	2.38	0.47
1:1:873:C:H2'	1:1:874:G:C8	2.49	0.47
1:1:956:G:HO2'	1:1:959:A:H62	1.57	0.47
1:1:2047:C:H2'	1:1:2048:G:C8	2.49	0.47
2:2:429:U:H3'	39:i:9:LEU:HD12	1.96	0.47
2:2:715:A:H2'	2:2:716:A:C8	2.49	0.47
2:2:742:G:H2'	2:2:743:A:H8	1.80	0.47
2:2:976:G:C6	2:2:1362:A:N7	2.82	0.47
2:2:1091:U:N3	2:2:1095:U:O4	2.47	0.47
13:I:120:ASP:H	13:I:123:ALA:HB2	1.79	0.47
1:1:18:U:H2'	1:1:19:A:C8	2.49	0.47
1:1:860:U:H2'	1:1:861:A:H8	1.78	0.47
1:1:1071:G:N3	1:1:1089:A:O2'	2.39	0.47
1:1:1380:G:N2	1:1:1569:A:N6	2.35	0.47
2:2:1153:G:H2'	2:2:1154:G:C8	2.49	0.47
4:5:17:ASN:ND2	4:5:51:ILE:O	2.48	0.47
25:U:40:ASN:HD22	25:U:65:ILE:HB	1.78	0.47
48:r:9:ILE:HD12	48:r:18:ALA:HB1	1.95	0.47
53:w:41:PRO:HG2	53:w:43:ARG:HH21	1.79	0.47
54:x:55:ARG:HH21	54:x:56:GLN:HB3	1.78	0.47
1:1:243:U:H2'	1:1:244:A:H8	1.79	0.47
2:2:527:7MG:H81	2:2:527:7MG:C3'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:156:PRO:O	10:F:172:LYS:N	2.48	0.47
28:X:18:ARG:NE	28:X:23:ASN:O	2.48	0.47
1:1:770:G:H2'	1:1:771:G:C8	2.49	0.47
1:1:1872:A:H3'	1:1:1873:G:C8	2.48	0.47
1:1:2277:G:O6	1:1:2278:A:N6	2.47	0.47
2:2:1376:U:O3'	42:l:92:ARG:NH2	2.47	0.47
2:2:1397:C:H42	57:4:94:A:H5''	1.79	0.47
4:5:36:LEU:HB3	57:4:335:C:H41	1.79	0.47
9:E:31:VAL:HG12	9:E:158:THR:HG22	1.96	0.47
13:I:78:LEU:HD23	13:I:81:LYS:HD3	1.97	0.47
15:K:35:VAL:HA	15:K:62:VAL:HG23	1.96	0.47
16:L:95:LEU:HD23	16:L:101:ILE:HD13	1.96	0.47
48:r:27:LYS:O	48:r:31:LYS:NZ	2.41	0.47
1:1:151:C:H2'	1:1:152:A:H8	1.79	0.47
1:1:296:U:H2'	1:1:297:G:C8	2.50	0.47
1:1:820:A:H2	1:1:943:A:H4'	1.80	0.47
1:1:1296:G:OP1	1:1:2709:G:O2'	2.21	0.47
2:2:1081:A:H2'	2:2:1082:A:H8	1.79	0.47
12:H:58:THR:OG1	12:H:78:GLY:O	2.32	0.47
20:P:21:ARG:HD3	20:P:113:ARG:HH12	1.79	0.47
20:P:49:ALA:H	20:P:60:THR:HG1	1.62	0.47
29:Y:56:LEU:HA	29:Y:59:GLU:HB2	1.97	0.47
54:x:33:THR:O	54:x:51:VAL:HA	2.15	0.47
57:4:95:C:H1'	57:4:96:G:H21	1.80	0.47
1:1:30:G:O5'	1:1:30:G:C8	2.68	0.47
1:1:507:A:H1'	1:1:509:C:C2	2.49	0.47
1:1:575:A:OP2	1:1:2055:C:N4	2.48	0.47
1:1:643:A:H61	1:1:2370:G:H1'	1.79	0.47
1:1:972:A:H5''	22:R:81:LYS:HE2	1.96	0.47
1:1:1184:U:H2'	1:1:1185:G:H8	1.79	0.47
1:1:1710:G:H2'	1:1:1711:A:H8	1.80	0.47
1:1:1796:U:H2'	1:1:1797:G:C8	2.46	0.47
1:1:2215:C:H2'	1:1:2216:G:C8	2.49	0.47
1:1:2250:G:OP1	1:1:2275:C:O2'	2.30	0.47
1:1:2385:C:H2'	1:1:2386:A:C8	2.50	0.47
1:1:2472:G:N2	1:1:2477:U:OP1	2.42	0.47
2:2:391:G:O3'	51:u:8:ARG:NH2	2.47	0.47
2:2:401:C:H2'	2:2:402:G:C8	2.50	0.47
2:2:973:G:H5''	45:o:52:LEU:HD13	1.97	0.47
2:2:1109:C:H2'	2:2:1110:A:C8	2.50	0.47
2:2:1369:C:H2'	2:2:1370:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1462:C:OP1	20:P:88:ARG:NH2	2.47	0.47
3:3:5:U:OP1	3:3:61:G:O2'	2.29	0.47
22:R:27:ILE:O	22:R:66:HIS:NE2	2.47	0.47
25:U:48:PRO:HG3	25:U:56:GLY:HA3	1.97	0.47
38:h:8:ASN:OD1	38:h:8:ASN:N	2.45	0.47
38:h:11:ARG:NH2	38:h:177:THR:O	2.47	0.47
38:h:157:LEU:HD13	38:h:157:LEU:HA	1.81	0.47
43:m:44:GLY:O	43:m:64:LYS:NZ	2.37	0.47
44:n:39:PHE:O	44:n:45:ARG:NH2	2.48	0.47
44:n:119:ARG:HG3	44:n:125:PRO:HG3	1.97	0.47
57:4:185:A:H3'	57:4:186:A:C8	2.50	0.47
57:4:249:U:O2'	57:4:250:U:OP2	2.30	0.47
1:1:1044:C:H5''	1:1:1048:A:H1'	1.96	0.47
1:1:1418:G:O2'	1:1:1580:A:N6	2.46	0.47
1:1:2523:G:O2'	1:1:2764:A:O2'	2.30	0.47
1:1:2567:G:H2'	1:1:2568:U:C6	2.50	0.47
2:2:111:G:H5''	51:u:27:ALA:HB2	1.96	0.47
2:2:269:C:H2'	2:2:270:A:C8	2.47	0.47
2:2:409:U:N3	2:2:433:G:N1	2.44	0.47
2:2:757:U:O2'	2:2:879:C:O2	2.27	0.47
2:2:1228:C:O2'	4:5:99:SER:O	2.30	0.47
2:2:1503:A:OP1	2:2:1531:A:O2'	2.28	0.47
3:3:116:G:H5'	19:O:55:GLU:HG2	1.97	0.47
10:F:25:THR:OG1	10:F:26:ILE:N	2.44	0.47
15:K:12:ASP:HB2	15:K:96:GLY:HA3	1.96	0.47
26:V:26:PHE:HE1	26:V:89:ILE:HD11	1.79	0.47
31:a:41:HIS:CE1	31:a:43:PHE:HB2	2.50	0.47
37:g:46:THR:HG23	37:g:201:PRO:HD2	1.97	0.47
37:g:162:PHE:HA	37:g:184:PHE:O	2.15	0.47
37:g:163:VAL:O	37:g:185:ALA:HA	2.15	0.47
38:h:60:PRO:O	38:h:65:ARG:NH1	2.48	0.47
42:l:26:PHE:HD1	42:l:101:MET:HE3	1.79	0.47
42:l:65:ALA:HB1	42:l:127:ALA:HB3	1.96	0.47
43:m:43:GLU:HG2	43:m:101:ILE:HG21	1.97	0.47
1:1:1050:A:H2	1:1:2751:G:H2'	1.79	0.47
1:1:1270:C:H42	1:1:2010:G:H1	1.62	0.47
1:1:2595:G:N2	1:1:2598:A:OP2	2.41	0.47
2:2:145:G:N2	2:2:178:C:N3	2.63	0.47
2:2:1168:U:H3	37:g:74:ARG:HH12	1.61	0.47
4:5:84:PRO:O	4:5:88:ARG:NH2	2.41	0.47
7:C:121:THR:OG1	7:C:122:VAL:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:26:LYS:HA	28:X:26:LYS:HD2	1.78	0.47
33:c:35:GLU:OE1	33:c:50:LYS:NZ	2.36	0.47
46:p:58:SER:O	46:p:58:SER:OG	2.33	0.47
57:4:199:C:H2'	57:4:200:G:C8	2.50	0.47
57:4:283:C:H4'	57:4:285:A:H62	1.79	0.47
1:1:1394:U:H4'	1:1:1603:A:H4'	1.97	0.47
1:1:1607:C:N4	1:1:1622:G:OP2	2.47	0.47
1:1:1627:G:H2'	1:1:1628:G:C8	2.49	0.47
1:1:2078:C:H2'	1:1:2079:U:C6	2.50	0.47
2:2:58:C:H2'	2:2:59:A:H8	1.80	0.47
2:2:839:C:H2'	2:2:840:C:H6	1.80	0.47
6:B:115:GLN:OE1	6:B:117:GLN:NE2	2.43	0.47
21:Q:62:ILE:HA	21:Q:65:ILE:HG22	1.97	0.47
24:T:94:ASP:N	24:T:94:ASP:OD1	2.48	0.47
34:d:24:THR:OG1	34:d:25:LYS:N	2.48	0.47
40:j:149:SER:HB2	40:j:152:MET:HG3	1.97	0.47
44:n:12:ARG:O	44:n:106:ARG:NH2	2.41	0.47
1:1:120:U:H4'	1:1:121:G:H5''	1.97	0.46
1:1:376:G:O6	1:1:399:U:O4	2.33	0.46
1:1:1303:G:OP1	1:1:1643:G:O2'	2.32	0.46
1:1:2081:U:H5''	28:X:25:THR:HG21	1.96	0.46
1:1:2395:C:OP1	16:L:63:LYS:NZ	2.36	0.46
1:1:2704:C:H2'	1:1:2705:A:H5'	1.97	0.46
2:2:309:A:H2'	2:2:310:G:C8	2.49	0.46
2:2:1167:A:O2'	2:2:1169:A:N7	2.47	0.46
2:2:1355:G:H2'	2:2:1356:G:C8	2.49	0.46
46:p:19:GLY:HA3	46:p:35:THR:O	2.14	0.46
54:x:63:THR:HG22	54:x:65:GLU:H	1.80	0.46
1:1:37:C:H2'	1:1:38:A:C8	2.51	0.46
1:1:106:C:H2'	1:1:107:G:C8	2.50	0.46
1:1:195:A:H3'	1:1:196:A:H4'	1.97	0.46
1:1:753:A:H2'	1:1:754:U:H6	1.80	0.46
1:1:835:C:H2'	1:1:836:G:H8	1.81	0.46
1:1:1278:C:H2'	1:1:1279:G:H8	1.79	0.46
1:1:2307:G:OP2	57:4:25:A:O2'	2.30	0.46
2:2:254:G:H2'	2:2:255:G:H8	1.80	0.46
2:2:672:U:H3	2:2:734:G:H1	1.62	0.46
16:L:14:LYS:HE3	16:L:14:LYS:HB2	1.70	0.46
39:i:170:TRP:CD2	39:i:186:PRO:HB3	2.50	0.46
39:i:202:GLU:O	39:i:205:SER:OG	2.33	0.46
42:l:18:PHE:HE2	42:l:47:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4:181:G:H2'	57:4:182:U:H4'	1.96	0.46
1:1:259:G:O2'	1:1:621:A:O3'	2.33	0.46
1:1:372:G:O2'	1:1:400:G:O6	2.33	0.46
1:1:1274:A:OP1	1:1:1646:C:N4	2.48	0.46
1:1:1710:G:H2'	1:1:1711:A:C8	2.51	0.46
1:1:1788:C:H2'	1:1:1789:A:C8	2.50	0.46
1:1:1827:U:OP1	1:1:1971:U:O2'	2.33	0.46
1:1:2439:A:N6	57:4:363:A:OP1	2.48	0.46
1:1:2579:C:O2'	7:C:136:ASN:OD1	2.27	0.46
2:2:502:A:OP1	47:q:115:SER:N	2.40	0.46
2:2:542:G:O3'	39:i:14:ARG:NH2	2.41	0.46
2:2:912:C:OP2	47:q:86:ARG:NH2	2.42	0.46
2:2:955:U:H3	2:2:1226:C:H42	1.62	0.46
4:5:94:GLN:HG2	57:4:20:A:H1'	1.96	0.46
19:O:104:GLN:NE2	19:O:108:ASP:OD2	2.48	0.46
38:h:150:LYS:HD3	38:h:169:ARG:HE	1.79	0.46
40:j:95:PHE:O	40:j:125:ALA:HA	2.16	0.46
43:m:112:THR:O	43:m:116:ALA:CB	2.63	0.46
51:u:7:ALA:O	51:u:17:TYR:HA	2.15	0.46
1:1:1132:U:OP2	1:1:1133:A:O2'	2.32	0.46
1:1:1303:G:H2'	1:1:1304:A:H8	1.80	0.46
2:2:204:G:H3'	2:2:205:A:H8	1.79	0.46
2:2:317:U:OP1	2:2:353:A:N6	2.48	0.46
2:2:1066:C:H42	2:2:1191:A:H62	1.64	0.46
3:3:24:G:N7	3:3:56:G:O2'	2.42	0.46
9:E:72:LYS:HA	9:E:81:GLN:HG2	1.97	0.46
28:X:3:ARG:HD2	28:X:30:LEU:HD12	1.96	0.46
1:1:580:U:H2'	1:1:581:C:C6	2.50	0.46
1:1:1161:C:H2'	1:1:1162:G:C8	2.50	0.46
1:1:1501:G:H2'	1:1:1502:A:H8	1.81	0.46
1:1:1796:U:H3	1:1:1823:G:H1	1.63	0.46
1:1:1924:C:H2'	1:1:1925:C:C6	2.50	0.46
1:1:2037:A:H2'	1:1:2038:G:H8	1.81	0.46
1:1:2039:U:H2'	1:1:2040:G:C8	2.50	0.46
1:1:2531:A:H61	1:1:2662:A:H61	1.64	0.46
1:1:2591:C:H2'	1:1:2592:G:C8	2.51	0.46
2:2:124:C:H2'	2:2:125:U:C6	2.49	0.46
2:2:601:G:H2'	2:2:602:A:H8	1.80	0.46
2:2:1296:C:O2'	2:2:1302:C:OP1	2.33	0.46
4:5:64:PHE:HD1	4:5:89:LYS:HA	1.80	0.46
8:D:22:ASP:HA	8:D:114:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:32:GLU:OE2	10:F:34:THR:OG1	2.32	0.46
17:M:86:LYS:HE2	17:M:86:LYS:HB3	1.76	0.46
21:Q:88:VAL:HG22	21:Q:90:ILE:HG13	1.97	0.46
30:Z:37:GLU:O	30:Z:38:ARG:NH1	2.42	0.46
51:u:43:ALA:HB1	51:u:47:GLU:HB2	1.97	0.46
52:v:8:LEU:O	52:v:60:GLU:HA	2.16	0.46
1:1:290:U:C2	1:1:350:G:O6	2.69	0.46
1:1:476:G:N2	1:1:479:A:O4'	2.44	0.46
1:1:635:C:O2'	1:1:639:U:OP1	2.34	0.46
1:1:833:A:H1'	16:L:51:GLU:HG3	1.96	0.46
1:1:976:G:O2'	1:1:1155:A:O2'	2.28	0.46
1:1:2855:C:H2'	1:1:2856:A:H8	1.80	0.46
2:2:235:C:H2'	2:2:236:A:H8	1.79	0.46
2:2:1514:G:H2'	2:2:1515:G:C8	2.50	0.46
9:E:46:ASP:OD1	9:E:46:ASP:N	2.44	0.46
15:K:25:LEU:O	15:K:30:ARG:NH1	2.49	0.46
32:b:29:SER:O	32:b:37:LYS:HA	2.16	0.46
51:u:7:ALA:HB3	51:u:18:GLN:HB2	1.98	0.46
1:1:523:C:H2'	1:1:524:G:H8	1.80	0.46
1:1:685:A:O2'	1:1:773:U:O4	2.24	0.46
1:1:954:G:H3'	1:1:955:PSU:H6	1.80	0.46
1:1:1658:C:H2'	1:1:1659:G:C8	2.50	0.46
1:1:1748:C:H2'	1:1:1749:A:H8	1.81	0.46
2:2:328:C:H4'	2:2:329:A:H5'	1.97	0.46
2:2:821:G:O6	2:2:880:C:N4	2.49	0.46
23:S:13:SER:OG	23:S:16:LYS:N	2.45	0.46
23:S:13:SER:O	23:S:101:SER:OG	2.26	0.46
1:1:769:U:H2'	1:1:770:G:H8	1.81	0.46
1:1:1801:A:H2'	6:B:262:ARG:HH22	1.80	0.46
2:2:933:G:O6	42:l:3:ARG:NH2	2.49	0.46
2:2:974:A:H5'	49:s:71:HIS:HB3	1.97	0.46
39:i:75:TYR:OH	39:i:97:ARG:NH1	2.49	0.46
40:j:78:ASN:OD1	40:j:78:ASN:N	2.47	0.46
43:m:74:SER:OG	43:m:130:ALA:OXT	2.32	0.46
50:t:65:LYS:HA	50:t:65:LYS:HD3	1.83	0.46
57:4:53:G:H1	57:4:63:C:H42	1.63	0.46
57:4:223:G:OP2	57:4:224:A:N6	2.49	0.46
1:1:107:G:H2'	1:1:108:G:C8	2.50	0.46
1:1:883:G:H3'	1:1:885:C:N3	2.31	0.46
1:1:2422:C:N3	1:1:2424:C:N4	2.64	0.46
1:1:2548:U:O2	15:K:23:LYS:NZ	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:209:U:OP2	2:2:210:C:N4	2.49	0.46
2:2:824:G:H2'	2:2:825:A:H8	1.79	0.46
2:2:1017:U:O2'	2:2:1018:G:O4'	2.34	0.46
2:2:1116:U:H4'	44:n:113:ARG:HH21	1.81	0.46
2:2:1248:A:H2	44:n:72:ILE:HG23	1.81	0.46
2:2:1446:A:N1	2:2:1447:A:N6	2.64	0.46
3:3:63:C:H2'	3:3:64:G:C8	2.51	0.46
11:G:135:HIS:HB3	11:G:138:VAL:HG22	1.97	0.46
15:K:23:LYS:HB2	15:K:23:LYS:HE2	1.70	0.46
16:L:57:LEU:HG	16:L:61:LEU:HD13	1.97	0.46
29:Y:30:MET:HE3	29:Y:30:MET:HB3	1.82	0.46
40:j:37:THR:OG1	40:j:38:VAL:N	2.49	0.46
57:4:38:A:N6	57:4:313:C:OP2	2.38	0.46
1:1:604:G:H2'	1:1:605:G:C8	2.50	0.46
1:1:1352:U:H3	1:1:1378:A:H62	1.64	0.46
1:1:1638:C:O2	1:1:2698:U:O2'	2.34	0.46
1:1:2273:A:H2'	1:1:2274:A:C8	2.51	0.46
1:1:2641:G:P	14:J:76:HIS:HE2	2.39	0.46
2:2:120:A:O2'	2:2:122:G:N7	2.45	0.46
2:2:556:C:H2'	2:2:557:G:H8	1.81	0.46
2:2:711:G:H2'	2:2:712:A:C8	2.51	0.46
2:2:1401:G:N3	2:2:1401:G:C2'	2.78	0.46
11:G:136:SER:OG	11:G:137:GLU:OE1	2.33	0.46
32:b:38:HIS:HB3	32:b:44:THR:HG23	1.98	0.46
34:d:28:ARG:O	34:d:29:GLN:NE2	2.49	0.46
39:i:187:GLU:N	39:i:190:ASP:OD2	2.48	0.46
57:4:163:G:H2'	57:4:164:G:H5'	1.98	0.46
57:4:174:A:O2'	57:4:175:A:H5'	2.16	0.46
57:4:189:C:H2'	57:4:190:A:H5''	1.97	0.46
1:1:24:G:H2'	1:1:25:U:C6	2.51	0.45
1:1:153:U:OP1	28:X:77:LYS:NZ	2.41	0.45
1:1:184:C:H2'	1:1:185:G:H8	1.81	0.45
1:1:519:U:H2'	1:1:520:G:C8	2.51	0.45
1:1:521:U:H2'	1:1:522:A:H8	1.81	0.45
1:1:992:C:H2'	1:1:993:G:C8	2.51	0.45
2:2:103:U:OP2	55:y:9:LYS:NZ	2.40	0.45
2:2:373:A:H2'	2:2:374:A:H8	1.81	0.45
2:2:390:U:H2'	2:2:391:G:C8	2.51	0.45
2:2:710:G:H2'	2:2:711:G:H8	1.81	0.45
2:2:925:G:O2'	2:2:927:G:OP1	2.34	0.45
2:2:1150:A:H4'	45:o:43:PRO:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:58:LYS:NZ	8:D:70:SER:O	2.49	0.45
10:F:26:ILE:HG21	10:F:79:VAL:HG11	1.97	0.45
30:Z:4:THR:HA	30:Z:40:ASP:H	1.81	0.45
31:a:11:GLU:HA	31:a:25:ARG:HA	1.98	0.45
37:g:91:PHE:HE2	37:g:93:ASN:HD22	1.63	0.45
57:4:240:U:H2'	57:4:241:C:C6	2.51	0.45
1:1:892:A:N3	1:1:892:A:C2'	2.79	0.45
1:1:2647:U:H2'	1:1:2648:G:H8	1.81	0.45
2:2:502:A:OP1	47:q:114:ARG:N	2.49	0.45
2:2:1060:U:OP1	49:s:85:ARG:NH1	2.49	0.45
2:2:1386:G:H2'	2:2:1387:G:H8	1.81	0.45
4:5:92:LEU:CD1	4:5:96:GLU:HB2	2.47	0.45
9:E:33:LYS:HB3	9:E:92:ARG:HG2	1.97	0.45
13:I:12:VAL:HG12	13:I:13:ALA:H	1.81	0.45
13:I:78:LEU:HA	13:I:81:LYS:HG2	1.99	0.45
35:e:55:LEU:HA	35:e:58:VAL:HG22	1.97	0.45
38:h:28:GLU:O	38:h:32:ASN:ND2	2.49	0.45
44:n:27:LYS:N	44:n:62:ASP:OD1	2.43	0.45
57:4:143:C:H2'	57:4:144:U:C6	2.52	0.45
1:1:300:A:H2'	1:1:334:C:H1'	1.98	0.45
1:1:619:G:H3'	1:1:620:G:H21	1.82	0.45
1:1:716:A:N6	1:1:717:C:N3	2.64	0.45
1:1:2683:C:H5''	20:P:51:ARG:HH12	1.81	0.45
1:1:2756:U:H1'	1:1:2757:A:H5''	1.99	0.45
2:2:153:C:H42	2:2:168:G:H22	1.63	0.45
2:2:527:7MG:H81	2:2:527:7MG:C5'	2.46	0.45
2:2:527:7MG:C3'	2:2:527:7MG:C8	2.99	0.45
2:2:914:A:H2'	2:2:915:A:C8	2.51	0.45
2:2:1328:C:H2'	2:2:1329:A:H8	1.81	0.45
7:C:109:VAL:HG12	7:C:203:VAL:HG22	1.99	0.45
15:K:15:GLY:O	15:K:47:ILE:N	2.48	0.45
38:h:67:THR:HB	38:h:102:ASN:HB3	1.98	0.45
42:l:140:ASP:OD1	42:l:143:ARG:NH1	2.47	0.45
46:p:23:ILE:HG12	46:p:32:VAL:HG12	1.96	0.45
57:4:20:A:C8	57:4:20:A:P	3.10	0.45
57:4:20:A:O4'	57:4:20:A:OP1	2.34	0.45
1:1:463:G:N2	1:1:466:A:OP2	2.44	0.45
1:1:500:G:N1	1:1:503:A:OP2	2.49	0.45
1:1:956:G:O2'	1:1:959:A:N6	2.43	0.45
1:1:2511:U:O2	7:C:145:SER:OG	2.28	0.45
2:2:407:U:H5''	39:i:112:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:722:G:H1	2:2:733:G:H1	1.63	0.45
2:2:937:A:H61	2:2:1379:G:H1	1.63	0.45
2:2:1112:C:N4	38:h:176:HIS:O	2.46	0.45
13:I:13:ALA:HA	13:I:53:PRO:HA	1.99	0.45
15:K:87:LEU:HA	15:K:94:PRO:HA	1.99	0.45
28:X:5:CYS:HG	28:X:8:THR:H	1.63	0.45
31:a:14:ALA:HB1	31:a:34:LEU:HD21	1.99	0.45
37:g:10:LEU:HA	37:g:15:HIS:HE1	1.82	0.45
38:h:123:GLN:HE21	38:h:128:VAL:HG21	1.81	0.45
38:h:191:THR:OG1	38:h:192:THR:N	2.49	0.45
40:j:102:GLY:N	40:j:122:ASN:OD1	2.50	0.45
57:4:137:C:H3'	57:4:138:C:H5''	1.98	0.45
1:1:866:A:N7	1:1:914:G:N1	2.64	0.45
1:1:1093:G:N2	1:1:1098:A:N6	2.45	0.45
1:1:1136:G:H2'	1:1:1137:G:H8	1.82	0.45
1:1:1283:G:N1	1:1:1286:A:OP2	2.49	0.45
1:1:2215:C:H2'	1:1:2216:G:H8	1.80	0.45
2:2:171:A:H2'	2:2:172:A:C8	2.51	0.45
8:D:14:VAL:HG23	8:D:197:GLU:HB2	1.98	0.45
22:R:14:VAL:HG12	22:R:20:VAL:HG11	1.99	0.45
24:T:43:ILE:HA	24:T:46:ALA:HB3	1.98	0.45
29:Y:15:ASN:HD21	29:Y:57:LEU:HD11	1.82	0.45
33:c:25:LYS:NZ	33:c:32:GLU:O	2.49	0.45
39:i:95:GLU:HA	39:i:100:ASN:HD22	1.81	0.45
45:o:21:ALA:HB1	45:o:92:LEU:HD12	1.98	0.45
1:1:690:G:O2'	1:1:780:G:OP1	2.32	0.45
1:1:981:A:OP2	1:1:982:C:N4	2.47	0.45
1:1:1047:G:O6	12:H:61:ARG:NH2	2.38	0.45
1:1:1406:U:H2'	1:1:1407:G:H8	1.81	0.45
2:2:753:A:OP1	50:t:73:LYS:NZ	2.46	0.45
6:B:165:VAL:HG11	6:B:181:MET:HE2	1.99	0.45
10:F:25:THR:OG1	10:F:32:GLU:OE2	2.34	0.45
10:F:115:HIS:NE2	10:F:147:ASP:OD2	2.50	0.45
30:Z:27:LEU:O	30:Z:38:ARG:NE	2.48	0.45
31:a:61:ASN:OD1	31:a:65:ASN:ND2	2.50	0.45
40:j:14:LYS:C	40:j:37:THR:HG1	2.25	0.45
43:m:27:MET:HE2	43:m:27:MET:HB2	1.75	0.45
43:m:28:PRO:O	43:m:33:LYS:NZ	2.38	0.45
43:m:74:SER:OG	43:m:74:SER:O	2.33	0.45
52:v:63:GLU:H	52:v:63:GLU:HG2	1.66	0.45
57:4:168:G:H2'	57:4:169:G:C8	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:G:N2	1:1:441:U:O2	2.50	0.45
1:1:1363:C:H2'	1:1:1364:G:H8	1.82	0.45
1:1:1730:C:O2	1:1:1731:G:N1	2.50	0.45
1:1:2220:U:H2'	1:1:2221:G:C8	2.52	0.45
1:1:2815:C:H2'	1:1:2816:G:H8	1.80	0.45
2:2:131:A:O2'	2:2:262:A:N3	2.43	0.45
2:2:581:G:H3'	2:2:758:C:H42	1.82	0.45
2:2:668:G:H2'	2:2:669:G:H8	1.82	0.45
2:2:1319:A:O2'	2:2:1323:G:N7	2.43	0.45
2:2:1512:U:H2'	2:2:1513:A:C8	2.52	0.45
6:B:33:LEU:HD23	6:B:33:LEU:HA	1.78	0.45
24:T:39:THR:HG23	24:T:41:ALA:H	1.80	0.45
39:i:83:LYS:O	39:i:89:ASN:ND2	2.37	0.45
41:k:45:ARG:HH11	41:k:102:MET:HE3	1.82	0.45
48:r:75:MET:HA	48:r:78:LYS:HD2	1.97	0.45
57:4:309:A:H4'	57:4:310:G:O4'	2.17	0.45
1:1:29:U:O5'	1:1:29:U:H6	1.99	0.45
1:1:312:G:H2'	1:1:313:G:C8	2.52	0.45
1:1:577:G:H2'	1:1:578:G:C8	2.51	0.45
1:1:746:PSU:N1	1:1:2611:C:H4'	2.31	0.45
1:1:897:C:OP2	1:1:897:C:C6	2.70	0.45
1:1:1448:G:H2'	1:1:1449:G:H8	1.82	0.45
1:1:2831:G:H1'	1:1:2883:A:H2'	1.99	0.45
2:2:1125:U:O2'	2:2:1127:G:N7	2.47	0.45
2:2:1332:A:H2'	2:2:1333:A:C8	2.52	0.45
2:2:1472:U:H2'	2:2:1473:G:C8	2.52	0.45
15:K:42:THR:OG1	15:K:43:ILE:N	2.49	0.45
20:P:49:ALA:N	20:P:60:THR:OG1	2.50	0.45
33:c:23:THR:HG22	33:c:24:THR:H	1.81	0.45
37:g:18:HIS:NE2	37:g:204:ASP:OD2	2.39	0.45
38:h:121:THR:HA	38:h:189:ALA:HB2	1.99	0.45
42:l:68:ASN:O	42:l:138:ARG:NH1	2.50	0.45
43:m:29:SER:HG	43:m:30:SER:H	1.59	0.45
48:r:60:VAL:HG12	48:r:65:VAL:HG22	1.99	0.45
57:4:20:A:H5'	57:4:21:C:C5	2.52	0.45
1:1:381:G:O6	1:1:382:A:N6	2.50	0.45
1:1:1370:C:H1'	1:1:1810:A:H2	1.81	0.45
1:1:2100:G:H3'	1:1:2100:G:C8	2.51	0.45
1:1:2743:U:OP1	36:f:34:LYS:NZ	2.35	0.45
2:2:12:U:H4'	2:2:526:C:H4'	1.98	0.45
2:2:1237:C:H4'	2:2:1300:G:H22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:110:SER:OG	10:F:111:HIS:N	2.50	0.45
18:N:4:ARG:HA	18:N:4:ARG:HD2	1.64	0.45
38:h:59:ARG:HB3	38:h:64:ILE:HD13	1.99	0.45
49:s:14:VAL:HG22	49:s:60:GLN:HE21	1.81	0.45
57:4:332:G:H1'	57:4:333:G:C6	2.52	0.45
1:1:160:A:N7	1:1:166:U:C4	2.85	0.45
1:1:604:G:H2'	1:1:605:G:H8	1.81	0.45
1:1:951:C:H2'	1:1:952:G:C8	2.52	0.45
1:1:1036:G:H1	1:1:1119:U:H3	1.65	0.45
1:1:2836:U:H2'	1:1:2837:A:H8	1.82	0.45
2:2:791:G:OP1	4:5:18:LYS:NZ	2.39	0.45
2:2:884:U:H4'	2:2:885:G:H5''	1.99	0.45
2:2:1464:U:OP1	20:P:109:ARG:NH1	2.50	0.45
35:e:38:THR:HG22	35:e:42:ARG:HE	1.81	0.45
37:g:108:ARG:NH2	57:4:122:A:OP1	2.50	0.45
39:i:26:ARG:HD3	39:i:30:THR:HG21	1.99	0.45
39:i:95:GLU:OE2	39:i:100:ASN:ND2	2.46	0.45
40:j:13:GLU:HA	40:j:38:VAL:O	2.17	0.45
40:j:152:MET:HE2	40:j:152:MET:HB3	1.79	0.45
53:w:71:THR:H	53:w:74:HIS:CE1	2.35	0.45
57:4:277:G:H2'	57:4:278:G:C8	2.51	0.45
57:4:304:C:H2'	57:4:305:A:H8	1.82	0.45
1:1:832:U:H5''	16:L:39:LYS:HG3	1.99	0.44
1:1:845:A:N6	1:1:934:U:O2	2.51	0.44
1:1:1063:G:O2'	13:I:80:LYS:NZ	2.49	0.44
1:1:1190:G:H2'	1:1:1191:G:C8	2.52	0.44
1:1:1474:U:H2'	1:1:1732:C:H41	1.81	0.44
1:1:2539:C:O2	1:1:2741:A:O2'	2.35	0.44
2:2:711:G:H2'	2:2:712:A:H8	1.82	0.44
2:2:936:C:N3	2:2:937:A:N6	2.66	0.44
2:2:959:A:H62	54:x:79:THR:HG23	1.82	0.44
3:3:20:G:H2'	3:3:21:G:C8	2.52	0.44
25:U:15:THR:OG1	25:U:16:GLY:N	2.51	0.44
26:V:27:PRO:HG2	26:V:88:HIS:HD2	1.81	0.44
39:i:72:PHE:HE1	39:i:94:LEU:HD11	1.82	0.44
53:w:67:LEU:HA	53:w:67:LEU:HD23	1.86	0.44
57:4:153:U:O2'	57:4:192:A:N7	2.42	0.44
57:4:192:A:C2'	57:4:193:A:H5'	2.47	0.44
57:4:281:A:H2'	57:4:282:G:H8	1.82	0.44
1:1:741:U:H2'	1:1:742:A:H8	1.82	0.44
1:1:832:U:H2'	1:1:833:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:884:U:O2	1:1:884:U:C2'	2.64	0.44
1:1:923:G:H2'	1:1:924:G:C8	2.49	0.44
1:1:1048:A:OP2	1:1:1109:C:N4	2.49	0.44
1:1:1049:C:H2'	1:1:1050:A:C8	2.52	0.44
2:2:240:G:H2'	2:2:241:G:H8	1.82	0.44
2:2:1041:G:H21	2:2:1042:A:H62	1.65	0.44
2:2:1429:A:H2'	2:2:1430:A:H8	1.82	0.44
8:D:58:LYS:HZ2	8:D:71:GLY:HA2	1.82	0.44
25:U:5:ILE:HD13	25:U:67:VAL:HG13	1.99	0.44
26:V:36:ALA:HA	26:V:37:PRO:HD3	1.81	0.44
57:4:158:U:H2'	57:4:159:C:C6	2.52	0.44
57:4:219:G:H2'	57:4:220:G:C8	2.53	0.44
1:1:105:C:H2'	1:1:106:C:H6	1.82	0.44
1:1:741:U:H2'	1:1:742:A:C8	2.51	0.44
1:1:833:A:H2'	1:1:834:G:H8	1.82	0.44
1:1:1062:G:H2'	1:1:1063:G:C8	2.52	0.44
1:1:1282:U:H3	1:1:1286:A:H62	1.65	0.44
1:1:1447:C:H2'	1:1:1448:G:C8	2.52	0.44
1:1:2100:G:H2'	1:1:2101:A:C4	2.52	0.44
1:1:2708:G:H2'	1:1:2709:G:H8	1.82	0.44
2:2:1048:G:OP1	49:s:4:GLN:N	2.49	0.44
2:2:1515:G:H2'	2:2:1516:2MG:H8	1.82	0.44
10:F:9:VAL:HG12	10:F:73:ASN:HD22	1.83	0.44
14:J:60:ASP:N	14:J:60:ASP:OD1	2.48	0.44
44:n:11:ARG:H	44:n:81:HIS:HD1	1.65	0.44
46:p:20:VAL:HA	46:p:83:GLU:O	2.16	0.44
50:t:33:THR:HG21	50:t:85:LEU:HD21	1.98	0.44
1:1:81:G:HO2'	1:1:295:G:HO2'	1.59	0.44
1:1:286:U:H2'	1:1:287:G:C8	2.53	0.44
1:1:1039:A:H2	1:1:1116:G:H22	1.65	0.44
1:1:1084:A:H8	12:H:54:VAL:HG13	1.82	0.44
1:1:1288:G:OP2	1:1:1288:G:N2	2.49	0.44
1:1:2329:U:H2'	1:1:2330:G:H8	1.80	0.44
1:1:2405:G:O2'	1:1:2411:A:N6	2.46	0.44
2:2:360:G:H2'	2:2:361:G:C8	2.53	0.44
6:B:69:ARG:NH1	6:B:129:THR:OG1	2.49	0.44
10:F:25:THR:HB	10:F:34:THR:HG23	1.98	0.44
26:V:88:HIS:ND1	26:V:89:ILE:O	2.50	0.44
31:a:26:SER:OG	31:a:27:THR:N	2.51	0.44
39:i:142:VAL:HG12	39:i:181:THR:HG22	1.99	0.44
46:p:16:VAL:N	46:p:77:TYR:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:255:A:O2'	1:1:384:A:OP1	2.34	0.44
1:1:1048:A:N6	1:1:1111:A:N7	2.65	0.44
2:2:454:G:H1	2:2:478:A:N6	2.12	0.44
2:2:603:U:H2'	2:2:604:G:C8	2.53	0.44
11:G:90:LEU:HD22	11:G:123:ARG:HA	1.98	0.44
25:U:40:ASN:ND2	25:U:65:ILE:HB	2.32	0.44
26:V:35:GLU:OE1	26:V:93:ARG:NH2	2.50	0.44
42:l:95:ARG:HA	42:l:98:ALA:HB3	1.98	0.44
44:n:120:LYS:HA	44:n:120:LYS:HD3	1.80	0.44
47:q:29:GLN:HB3	47:q:81:LEU:HD11	1.99	0.44
49:s:93:ILE:HD12	49:s:94:PRO:HD2	1.99	0.44
1:1:285:G:O6	1:1:355:U:O4	2.35	0.44
1:1:463:G:N1	1:1:467:G:O6	2.50	0.44
1:1:519:U:O3'	23:S:25:ARG:NH1	2.51	0.44
1:1:658:U:H1'	8:D:97:ASN:HD21	1.82	0.44
1:1:1630:A:H61	1:1:1637:A:N6	2.15	0.44
1:1:2089:C:H2'	1:1:2090:A:H8	1.81	0.44
2:2:46:G:N2	2:2:366:A:O4'	2.51	0.44
2:2:153:C:H42	2:2:168:G:H1	1.66	0.44
2:2:914:A:H2'	2:2:915:A:H8	1.83	0.44
9:E:148:ARG:HB3	9:E:150:ARG:HH12	1.82	0.44
37:g:9:MET:HB3	37:g:14:VAL:HB	1.99	0.44
40:j:156:LYS:HZ1	43:m:71:VAL:HG22	1.83	0.44
57:4:113:A:H2'	57:4:114:G:C8	2.53	0.44
1:1:5:A:H2'	1:1:6:A:H8	1.83	0.44
1:1:525:U:OP1	1:1:556:A:O2'	2.35	0.44
1:1:666:A:H1'	35:e:4:ILE:HD12	2.00	0.44
1:1:883:G:H3'	1:1:885:C:C4	2.53	0.44
2:2:726:C:H2'	2:2:727:G:C8	2.53	0.44
4:5:65:LEU:HB2	4:5:90:LEU:HD21	2.00	0.44
15:K:10:VAL:HG11	15:K:16:ALA:HB3	2.00	0.44
57:4:3:G:H2'	57:4:4:G:C8	2.53	0.44
57:4:158:U:H2'	57:4:159:C:H6	1.83	0.44
57:4:193:A:C2'	57:4:194:G:H5'	2.48	0.44
1:1:242:G:O2'	1:1:254:G:O6	2.35	0.44
1:1:746:PSU:O2'	1:1:748:G:N2	2.50	0.44
1:1:796:C:H2'	1:1:797:G:C8	2.53	0.44
1:1:883:G:O2'	1:1:892:A:N6	2.44	0.44
1:1:1001:A:H3'	1:1:1002:G:H8	1.83	0.44
1:1:1040:A:N1	1:1:1115:G:N2	2.61	0.44
1:1:1181:U:H2'	1:1:1182:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2100:G:C8	1:1:2100:G:C3'	3.01	0.44
1:1:2118:U:OP1	1:1:2148:G:O2'	2.28	0.44
1:1:2660:A:O2'	1:1:2661:G:O4'	2.35	0.44
1:1:2821:A:O2'	1:1:2827:C:O2	2.32	0.44
2:2:431:A:H2'	2:2:432:A:H8	1.83	0.44
2:2:553:A:H2'	2:2:554:A:H8	1.82	0.44
2:2:1239:A:H5''	42:l:116:MET:HG3	2.00	0.44
2:2:1305:G:N2	2:2:1331:G:O2'	2.43	0.44
2:2:1320:C:H1'	54:x:73:GLU:HG3	2.00	0.44
2:2:1437:A:H2'	2:2:1438:G:H8	1.83	0.44
4:5:37:GLN:HB2	4:5:86:ARG:CZ	2.48	0.44
6:B:98:ASP:N	6:B:98:ASP:OD1	2.47	0.44
10:F:117:LEU:HD13	10:F:121:ILE:HB	1.99	0.44
33:c:55:LYS:HB3	33:c:55:LYS:HE2	1.79	0.44
37:g:126:PHE:HB3	37:g:129:LEU:HD13	1.99	0.44
38:h:56:VAL:HB	38:h:67:THR:HG23	2.00	0.44
40:j:55:GLU:HG3	40:j:57:PRO:HD2	2.00	0.44
43:m:88:ARG:NE	43:m:91:GLU:OE2	2.51	0.44
1:1:324:A:N6	1:1:339:U:O2'	2.50	0.44
1:1:1061:U:C2	1:1:1069:A:H5''	2.53	0.44
1:1:2368:C:H2'	1:1:2369:A:C8	2.49	0.44
2:2:11:G:O2'	2:2:506:G:N2	2.49	0.44
2:2:537:G:H2'	2:2:538:G:C8	2.53	0.44
2:2:727:G:N2	2:2:730:G:OP2	2.50	0.44
8:D:143:LEU:HD13	8:D:146:VAL:HG11	2.00	0.44
9:E:74:VAL:HG22	9:E:79:ILE:HD11	2.00	0.44
11:G:41:LYS:HE3	11:G:41:LYS:HB2	1.82	0.44
12:H:33:VAL:HG23	12:H:36:ASP:HB2	2.00	0.44
41:k:35:LYS:HG3	41:k:65:GLU:HB3	2.00	0.44
51:u:23:ASP:OD1	51:u:25:ARG:NE	2.46	0.44
54:x:27:ASP:N	54:x:27:ASP:OD1	2.49	0.44
1:1:585:G:N7	21:Q:6:ARG:NH1	2.66	0.43
1:1:796:C:H2'	1:1:797:G:H8	1.82	0.43
1:1:956:G:N7	17:M:14:LYS:NZ	2.66	0.43
1:1:1751:U:H2'	1:1:1752:C:C6	2.54	0.43
1:1:2060:A:N7	8:D:69:ARG:NH2	2.66	0.43
1:1:2189:U:O2	1:1:2189:U:O4'	2.36	0.43
2:2:81:A:N3	2:2:89:U:O2'	2.41	0.43
2:2:918:A:H2'	2:2:919:A:C8	2.53	0.43
10:F:8:PRO:HG3	10:F:51:THR:HG22	1.99	0.43
21:Q:85:LYS:HA	21:Q:85:LYS:HD2	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:43:LEU:HD13	37:g:46:THR:HB	2.00	0.43
57:4:142:U:O2'	57:4:143:C:H5'	2.18	0.43
57:4:199:C:H2'	57:4:200:G:H8	1.83	0.43
1:1:133:U:H2'	1:1:134:G:C8	2.53	0.43
1:1:153:U:H2'	1:1:154:U:C6	2.53	0.43
1:1:299:A:H2'	1:1:300:A:C4	2.54	0.43
1:1:535:G:H2'	1:1:536:G:H8	1.83	0.43
1:1:1440:U:H2'	1:1:1441:G:H8	1.82	0.43
1:1:1798:U:OP1	6:B:256:LYS:NZ	2.42	0.43
1:1:2355:G:O3'	27:W:24:LYS:NZ	2.51	0.43
2:2:717:U:H2'	2:2:734:G:C8	2.52	0.43
2:2:875:U:O3'	43:m:15:ARG:NH1	2.35	0.43
4:5:91:LEU:HB3	57:4:20:A:N7	2.33	0.43
7:C:117:GLY:O	7:C:164:GLN:NE2	2.47	0.43
16:L:79:LEU:HD23	16:L:79:LEU:HA	1.87	0.43
18:N:1:MET:SD	18:N:1:MET:N	2.79	0.43
22:R:91:GLN:HE21	22:R:92:TRP:H	1.66	0.43
43:m:30:SER:OG	43:m:32:LEU:N	2.51	0.43
46:p:67:ALA:HA	46:p:70:CYS:HB3	1.99	0.43
51:u:21:VAL:HG12	51:u:33:ILE:HD12	2.00	0.43
1:1:75:G:O2'	29:Y:48:ARG:NH1	2.51	0.43
1:1:406:G:H2'	1:1:407:G:C8	2.53	0.43
1:1:759:G:H2'	1:1:760:G:H8	1.83	0.43
1:1:998:C:P	21:Q:92:ARG:HH22	2.40	0.43
1:1:1346:G:H2'	1:1:1347:A:H8	1.82	0.43
1:1:1569:A:H2'	1:1:1570:A:C8	2.54	0.43
1:1:1709:U:H2'	1:1:1710:G:H8	1.82	0.43
1:1:1793:C:H2'	1:1:1794:A:C8	2.53	0.43
2:2:475:C:H2'	2:2:476:U:H6	1.84	0.43
2:2:684:U:O2	46:p:41:ALA:N	2.51	0.43
2:2:894:G:H2'	2:2:895:G:C8	2.54	0.43
2:2:925:G:O6	2:2:1391:U:C4	2.71	0.43
6:B:77:VAL:HA	6:B:115:GLN:HA	2.01	0.43
6:B:94:VAL:HG21	6:B:116:ILE:HD11	2.01	0.43
7:C:152:PRO:HB2	7:C:154:LYS:HG2	1.99	0.43
18:N:41:ALA:HB1	18:N:113:ILE:HD11	2.00	0.43
52:v:57:ASP:OD1	52:v:58:VAL:N	2.48	0.43
57:4:71:A:H2'	57:4:72:A:C8	2.53	0.43
57:4:128:U:H2'	57:4:129:G:O4'	2.17	0.43
1:1:1222:U:H1'	1:1:1228:G:H1	1.83	0.43
1:1:1954:G:O2'	1:1:1956:U:O4	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2542:A:H4'	1:1:2543:G:H8	1.83	0.43
1:1:2703:C:H2'	1:1:2704:C:C6	2.53	0.43
2:2:304:U:H2'	2:2:305:G:C8	2.53	0.43
2:2:552:U:H2'	2:2:553:A:H5'	2.00	0.43
2:2:559:A:H4'	2:2:560:A:H3'	2.00	0.43
2:2:707:U:OP1	46:p:87:LYS:NZ	2.42	0.43
2:2:715:A:OP1	2:2:805:C:O2'	2.30	0.43
7:C:175:LEU:HD23	7:C:175:LEU:HA	1.86	0.43
39:i:105:MET:HG3	39:i:171:LEU:HD13	2.00	0.43
44:n:31:ASN:HD21	44:n:67:VAL:H	1.65	0.43
1:1:290:U:O2	1:1:350:G:C6	2.72	0.43
1:1:511:U:C5	1:1:512:G:C4	3.07	0.43
1:1:566:U:O2'	1:1:809:G:OP2	2.33	0.43
1:1:817:C:O2'	1:1:839:U:OP1	2.31	0.43
1:1:956:G:N2	1:1:960:A:OP2	2.51	0.43
1:1:1006:C:H1'	14:J:108:MET:HG2	2.01	0.43
1:1:1748:C:H2'	1:1:1749:A:C8	2.54	0.43
1:1:1889:A:H2'	1:1:1890:A:H8	1.83	0.43
1:1:2069:G7M:C4	1:1:2069:G7M:HO2'	2.27	0.43
2:2:10:A:OP2	40:j:131:THR:OG1	2.32	0.43
2:2:401:C:H2'	2:2:402:G:H8	1.83	0.43
2:2:472:U:H2'	2:2:473:U:C6	2.53	0.43
2:2:705:G:H21	46:p:31:ILE:HD13	1.83	0.43
6:B:17:VAL:HG12	6:B:204:VAL:HG22	2.01	0.43
10:F:19:ILE:HG22	10:F:24:ILE:HD13	2.01	0.43
11:G:133:GLN:HG3	11:G:139:PHE:HB3	2.00	0.43
19:O:27:VAL:O	19:O:37:ALA:HA	2.18	0.43
31:a:16:CYS:HB2	31:a:34:LEU:HB2	1.99	0.43
48:r:14:HIS:CD2	48:r:44:LYS:HG2	2.53	0.43
49:s:87:ALA:HA	49:s:90:ARG:HB2	2.00	0.43
1:1:507:A:H1'	1:1:509:C:N3	2.34	0.43
1:1:919:U:H2'	1:1:920:A:H8	1.83	0.43
1:1:1047:G:HO2'	1:1:1110:G:H22	1.63	0.43
1:1:1547:C:H2'	1:1:1548:A:C8	2.53	0.43
1:1:1709:U:H2'	1:1:1710:G:C8	2.53	0.43
2:2:147:G:H2'	2:2:148:G:C8	2.54	0.43
2:2:291:U:H2'	2:2:292:G:C8	2.54	0.43
2:2:745:G:H2'	2:2:746:A:H8	1.83	0.43
2:2:1260:G:C2	2:2:1275:A:N6	2.84	0.43
6:B:240:PHE:O	6:B:242:LYS:N	2.49	0.43
7:C:21:SER:N	15:K:72:PRO:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:189:THR:HB	8:D:192:ALA:HB3	2.00	0.43
17:M:106:ASP:OD1	17:M:106:ASP:N	2.49	0.43
22:R:57:GLY:HA2	22:R:102:SER:O	2.19	0.43
37:g:224:GLY:HA2	37:g:227:GLN:HB2	2.01	0.43
39:i:10:LYS:HA	39:i:13:ARG:HD3	2.00	0.43
45:o:25:ILE:HG21	45:o:74:VAL:HG23	2.00	0.43
48:r:16:VAL:HG21	48:r:41:GLU:HB2	2.01	0.43
51:u:1:MET:SD	51:u:1:MET:N	2.81	0.43
53:w:56:ALA:HA	53:w:59:ILE:HD12	2.01	0.43
57:4:247:A:N6	57:4:283:C:O2	2.50	0.43
1:1:213:A:H2'	1:1:214:G:H8	1.84	0.43
1:1:535:G:H2'	1:1:536:G:C8	2.54	0.43
1:1:1096:A:C5	1:1:1097:U:H1'	2.53	0.43
1:1:1589:U:H1'	1:1:1590:A:H5'	2.01	0.43
1:1:1799:G:OP2	6:B:270:ARG:NH2	2.37	0.43
1:1:2233:U:H2'	1:1:2234:G:C8	2.54	0.43
1:1:2313:C:H2'	1:1:2314:A:H8	1.82	0.43
1:1:2315:G:H2'	1:1:2316:G:H8	1.84	0.43
1:1:2463:C:H2'	1:1:2464:G:H8	1.84	0.43
1:1:2788:C:H2'	1:1:2789:C:C6	2.54	0.43
1:1:2855:C:H2'	1:1:2856:A:C8	2.53	0.43
2:2:951:G:OP2	48:r:101:ARG:NH1	2.51	0.43
2:2:1105:A:H2'	2:2:1106:G:C8	2.54	0.43
3:3:55:U:H2'	3:3:56:G:C8	2.54	0.43
8:D:165:HIS:CD2	8:D:166:LYS:HG3	2.54	0.43
10:F:26:ILE:HD13	10:F:75:MET:HB3	2.01	0.43
12:H:42:ARG:HH22	12:H:50:VAL:HG22	1.83	0.43
17:M:33:LEU:HD23	17:M:103:TYR:HD2	1.84	0.43
18:N:98:LEU:HD23	18:N:98:LEU:HA	1.85	0.43
22:R:24:LYS:HG3	22:R:92:TRP:HE3	1.83	0.43
32:b:38:HIS:ND1	32:b:39:LEU:O	2.43	0.43
38:h:136:ARG:HA	38:h:139:GLN:HB3	2.01	0.43
57:4:47:G:H2'	57:4:48:C:C6	2.54	0.43
1:1:1419:A:H5'	1:1:1579:A:H61	1.83	0.43
1:1:1462:C:H2'	1:1:1463:C:C6	2.54	0.43
1:1:2208:C:H2'	1:1:2209:G:C8	2.54	0.43
1:1:2684:U:O2	1:1:2727:A:O2'	2.32	0.43
2:2:312:C:H2'	2:2:313:A:H8	1.84	0.43
2:2:516:PSU:OP1	2:2:516:PSU:C4'	2.65	0.43
8:D:164:LEU:HD23	8:D:164:LEU:HA	1.83	0.43
12:H:77:VAL:HG21	12:H:117:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:37:THR:HA	18:N:110:MET:HA	2.01	0.43
27:W:39:ARG:HA	27:W:58:THR:HG22	2.01	0.43
31:a:57:VAL:HG13	54:x:42:PRO:HB3	2.00	0.43
42:l:42:ILE:HG23	42:l:117:ALA:HA	2.01	0.43
47:q:83:ARG:NH2	47:q:97:THR:O	2.52	0.43
57:4:210:C:H2'	57:4:240:U:H5	1.84	0.43
1:1:385:C:O2'	1:1:388:G:N2	2.52	0.43
1:1:2292:U:H2'	1:1:2293:G:C8	2.54	0.43
1:1:2723:C:OP1	7:C:114:LYS:NZ	2.42	0.43
1:1:2836:U:H2'	1:1:2837:A:C8	2.53	0.43
2:2:311:C:OP1	51:u:31:ARG:NH1	2.46	0.43
2:2:651:C:H2'	2:2:652:U:C6	2.54	0.43
2:2:736:C:H2'	2:2:737:C:C6	2.53	0.43
2:2:1493:A:O2'	2:2:1494:G:O5'	2.36	0.43
3:3:111:U:H2'	3:3:112:G:C8	2.51	0.43
6:B:2:ALA:O	6:B:19:VAL:HA	2.19	0.43
8:D:115:GLN:HE22	16:L:1:MET:HG2	1.84	0.43
18:N:24:MET:HE1	18:N:40:LYS:HD3	2.00	0.43
24:T:51:PHE:HB2	24:T:53:VAL:HG22	2.00	0.43
26:V:68:LYS:HD2	26:V:68:LYS:HA	1.89	0.43
30:Z:9:GLN:HG2	30:Z:32:ILE:HG22	2.01	0.43
37:g:66:LYS:HB3	37:g:90:PHE:HE1	1.84	0.43
41:k:29:ILE:HG22	41:k:34:GLY:HA3	2.00	0.43
43:m:10:MET:HE2	43:m:10:MET:HB3	1.75	0.43
44:n:68:LYS:HB2	44:n:68:LYS:HE3	1.69	0.43
49:s:37:SER:OG	49:s:40:ASP:N	2.44	0.43
1:1:633:A:O2'	1:1:2404:U:OP1	2.34	0.43
1:1:1992:G:N2	1:1:1996:C:O2	2.35	0.43
2:2:254:G:O3'	52:v:71:LYS:NZ	2.39	0.43
2:2:731:G:OP1	2:2:766:A:O2'	2.37	0.43
2:2:1153:G:H2'	2:2:1154:G:H8	1.83	0.43
6:B:87:ARG:HG3	6:B:89:ALA:H	1.83	0.43
7:C:95:SER:OG	7:C:96:ILE:N	2.52	0.43
12:H:8:LYS:HA	12:H:11:ILE:HG22	2.01	0.43
12:H:29:ASP:CG	12:H:56:ARG:HE	2.27	0.43
13:I:73:PRO:HA	13:I:74:PRO:HD3	1.89	0.43
16:L:23:ILE:HD13	22:R:84:ARG:HG2	2.01	0.43
33:c:9:ILE:HG12	33:c:24:THR:HA	2.01	0.43
57:4:112:U:H2'	57:4:113:A:C8	2.54	0.43
57:4:306:U:H2'	57:4:307:G:C8	2.53	0.43
1:1:1166:G:H1	1:1:1183:U:H3	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1326:U:O2'	1:1:2010:G:O2'	2.31	0.42
1:1:2183:A:O2'	1:1:2184:A:O4'	2.31	0.42
1:1:2431:U:N3	1:1:2434:A:OP2	2.47	0.42
2:2:73:C:N4	2:2:74:A:H62	2.17	0.42
2:2:254:G:H2'	2:2:255:G:C8	2.53	0.42
2:2:527:7MG:H3'	2:2:527:7MG:C8	2.50	0.42
2:2:791:G:N2	2:2:1497:G:O3'	2.52	0.42
6:B:41:GLY:HA2	6:B:54:ILE:HG22	2.01	0.42
10:F:88:GLN:HE21	10:F:163:ARG:HG3	1.84	0.42
17:M:64:TRP:HE3	17:M:104:GLU:HB2	1.83	0.42
21:Q:91:ASP:N	22:R:11:GLN:OE1	2.50	0.42
34:d:41:ARG:HD2	34:d:41:ARG:HA	1.91	0.42
43:m:72:VAL:HB	43:m:75:ILE:HD11	2.01	0.42
49:s:9:ARG:NE	49:s:10:GLU:OE2	2.50	0.42
53:w:68:LEU:HD23	53:w:68:LEU:HA	1.84	0.42
57:4:45:A:O2'	57:4:46:U:H5'	2.19	0.42
1:1:270:A:H5'	1:1:271:G:H5''	2.01	0.42
1:1:1164:C:H2'	1:1:1165:A:C8	2.54	0.42
1:1:1450:G:N2	1:1:1452:G:O6	2.49	0.42
1:1:1548:A:H2'	1:1:1549:A:C8	2.54	0.42
1:1:2593:U:H2'	1:1:2594:C:H6	1.84	0.42
2:2:211:G:N2	2:2:212:G:O4'	2.52	0.42
2:2:350:G:N1	2:2:351:G:O6	2.52	0.42
2:2:410:G:OP1	39:i:26:ARG:NH1	2.43	0.42
2:2:710:G:H2'	2:2:711:G:C8	2.54	0.42
2:2:1395:C:H4'	2:2:1401:G:H21	1.84	0.42
2:2:1513:A:H2'	2:2:1514:G:C8	2.54	0.42
12:H:19:ALA:HA	12:H:69:PHE:HE2	1.84	0.42
14:J:109:LEU:HD23	14:J:109:LEU:HA	1.86	0.42
26:V:71:LYS:HE2	26:V:71:LYS:HB2	1.84	0.42
44:n:20:PHE:O	44:n:63:LEU:HA	2.19	0.42
1:1:1136:G:H2'	1:1:1137:G:C8	2.54	0.42
1:1:2463:C:H2'	1:1:2464:G:C8	2.54	0.42
1:1:2820:A:O2'	18:N:3:HIS:ND1	2.40	0.42
2:2:35:G:N2	47:q:115:SER:OG	2.53	0.42
2:2:1513:A:H2'	2:2:1514:G:H8	1.84	0.42
4:5:42:LYS:H	4:5:73:MET:HE3	1.85	0.42
17:M:9:PHE:HB2	17:M:12:MET:HE2	2.00	0.42
19:O:3:LYS:HB2	19:O:3:LYS:HE3	1.87	0.42
22:R:1:MET:O	22:R:15:SER:OG	2.34	0.42
33:c:37:LYS:HB2	33:c:48:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:127:ASP:OD1	37:g:127:ASP:N	2.51	0.42
42:l:22:LEU:HD13	42:l:97:ASN:HD21	1.85	0.42
57:4:271:G:O2'	57:4:272:C:H5'	2.18	0.42
57:4:316:A:H2	57:4:318:G:C8	2.36	0.42
57:4:347:U:H5''	57:4:348:C:H5	1.84	0.42
1:1:49:A:H5''	1:1:50:U:H2'	2.01	0.42
1:1:693:A:OP1	6:B:38:SER:OG	2.34	0.42
1:1:862:G:O2'	3:3:78:A:N3	2.50	0.42
1:1:941:A:O2'	1:1:1190:G:O3'	2.37	0.42
1:1:1013:C:H2'	1:1:1014:A:H8	1.85	0.42
1:1:1387:A:H2'	1:1:1388:G:H8	1.84	0.42
1:1:2026:U:H2'	1:1:2027:G:C8	2.54	0.42
1:1:2204:G:OP2	6:B:150:LYS:NZ	2.35	0.42
1:1:2302:U:H2'	1:1:2303:G:H8	1.84	0.42
2:2:28:A:O2'	2:2:296:U:OP1	2.34	0.42
2:2:302:G:H2'	2:2:303:A:C8	2.55	0.42
2:2:1055:A:H2	38:h:194:GLY:HA3	1.84	0.42
2:2:1445:U:C4	2:2:1457:G:O6	2.72	0.42
6:B:24:LEU:HD23	6:B:81:LEU:HB3	2.01	0.42
10:F:117:LEU:HD23	10:F:117:LEU:HA	1.93	0.42
19:O:12:THR:HA	19:O:15:ARG:HB3	2.01	0.42
24:T:11:LEU:HB2	29:Y:26:PHE:HE1	1.85	0.42
25:U:31:SER:O	25:U:31:SER:OG	2.35	0.42
38:h:184:TYR:HB2	38:h:201:TRP:CD1	2.54	0.42
39:i:199:LEU:HD23	39:i:199:LEU:HA	1.91	0.42
48:r:14:HIS:HD2	48:r:44:LYS:HG2	1.84	0.42
55:y:26:SER:O	55:y:30:THR:OG1	2.37	0.42
1:1:84:A:OP1	25:U:6:ARG:NH1	2.52	0.42
1:1:720:U:H2'	1:1:721:A:C8	2.50	0.42
1:1:1380:G:N2	1:1:1570:A:N1	2.65	0.42
2:2:486:U:H2'	2:2:487:A:H8	1.85	0.42
2:2:551:U:H3'	2:2:552:U:H6	1.84	0.42
2:2:1061:G:H5'	45:o:61:ALA:HB2	2.01	0.42
2:2:1287:A:H2'	2:2:1288:A:C8	2.54	0.42
3:3:20:G:H2'	3:3:21:G:H8	1.84	0.42
4:5:73:MET:SD	4:5:73:MET:N	2.93	0.42
6:B:180:GLU:HG3	6:B:270:ARG:HA	2.02	0.42
9:E:36:LEU:HD21	9:E:57:LEU:HD11	2.01	0.42
15:K:51:LYS:HD3	15:K:95:ILE:HG22	2.01	0.42
16:L:100:ILE:HG22	16:L:101:ILE:HG23	2.01	0.42
24:T:30:ILE:HG13	24:T:85:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:17:ASN:ND2	28:X:27:ARG:HE	2.17	0.42
33:c:10:LYS:HB2	33:c:10:LYS:HE3	1.80	0.42
35:e:24:HIS:NE2	35:e:49:MET:O	2.52	0.42
47:q:83:ARG:HB3	47:q:83:ARG:CZ	2.49	0.42
47:q:90:LEU:HD13	47:q:93:VAL:HG21	2.01	0.42
48:r:16:VAL:HG23	48:r:17:ILE:HG12	2.01	0.42
57:4:140:U:H2'	57:4:141:C:H6	1.84	0.42
57:4:201:C:H2'	57:4:202:G:C8	2.55	0.42
1:1:561:G:O2'	21:Q:45:TYR:OH	2.23	0.42
1:1:860:U:H2'	1:1:861:A:C8	2.54	0.42
1:1:883:G:H8	1:1:884:U:C4	2.38	0.42
1:1:1764:C:H42	1:1:1989:G:H1	1.67	0.42
1:1:1889:A:H2'	1:1:1890:A:C8	2.55	0.42
1:1:2037:A:H2'	1:1:2038:G:C8	2.54	0.42
1:1:2380:C:P	19:O:17:LYS:HZ1	2.43	0.42
4:5:127:ILE:HD13	4:5:127:ILE:HA	1.87	0.42
14:J:62:VAL:HG21	14:J:101:ILE:HD11	2.00	0.42
27:W:23:VAL:HG13	27:W:38:VAL:HG22	2.01	0.42
32:b:30:VAL:HA	32:b:36:GLU:O	2.19	0.42
45:o:5:ARG:HB2	45:o:77:VAL:HA	2.00	0.42
1:1:892:A:N6	1:1:893:C:O2'	2.53	0.42
1:1:1449:G:H2'	1:1:1450:G:H8	1.85	0.42
1:1:1692:U:N3	1:1:1694:C:N3	2.68	0.42
1:1:2420:C:OP2	35:e:33:LEU:N	2.50	0.42
1:1:2840:C:H2'	1:1:2841:C:C6	2.55	0.42
2:2:1527:U:H2'	2:2:1528:U:H6	1.85	0.42
4:5:32:ALA:HB3	4:5:125:VAL:HG13	2.01	0.42
4:5:91:LEU:HG	57:4:20:A:N6	2.35	0.42
7:C:46:ARG:NH2	7:C:88:GLU:O	2.50	0.42
8:D:18:THR:O	8:D:110:SER:OG	2.38	0.42
14:J:41:LYS:NZ	14:J:51:GLY:O	2.36	0.42
15:K:17:ARG:HG3	15:K:47:ILE:HG12	2.02	0.42
57:4:261:G:H4'	57:4:262:U:OP1	2.20	0.42
57:4:264:U:H2'	57:4:265:C:C6	2.54	0.42
1:1:1161:C:H2'	1:1:1162:G:H8	1.84	0.42
1:1:1608:A:N6	1:1:1621:U:O4	2.45	0.42
1:1:1665:A:N1	1:1:1996:C:N4	2.67	0.42
1:1:1948:G:H2'	1:1:1949:G:C8	2.51	0.42
1:1:1990:C:H2'	1:1:1991:U:C2	2.55	0.42
1:1:2771:C:HO2'	7:C:173:GLN:HE22	1.62	0.42
2:2:376:G:OP2	51:u:68:SER:OG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:437:U:HO2'	39:i:120:HIS:CE1	2.37	0.42
2:2:677:U:H2'	2:2:678:U:C6	2.54	0.42
2:2:1328:C:H2'	2:2:1329:A:C8	2.55	0.42
3:3:93:C:H2'	3:3:94:A:H8	1.84	0.42
4:5:55:TYR:HB3	4:5:112:VAL:HG12	2.01	0.42
4:5:98:ASP:HA	4:5:101:TYR:HE1	1.84	0.42
15:K:68:GLY:HA3	15:K:78:ARG:HG2	2.01	0.42
23:S:33:LEU:HD23	23:S:33:LEU:HA	1.84	0.42
42:l:111:ARG:NE	42:l:119:ARG:O	2.47	0.42
57:4:219:G:H2'	57:4:220:G:H8	1.84	0.42
57:4:267:G:H2'	57:4:268:U:C6	2.55	0.42
1:1:182:A:N3	1:1:433:C:O2'	2.41	0.42
1:1:582:A:OP1	21:Q:14:HIS:ND1	2.42	0.42
1:1:1039:A:O2'	26:V:49:ASN:ND2	2.50	0.42
1:1:1721:G:O2'	1:1:1739:A:N6	2.52	0.42
1:1:2408:U:H2'	1:1:2409:G:C8	2.54	0.42
1:1:2569:G:H2'	1:1:2570:G:C8	2.55	0.42
1:1:2815:C:H2'	1:1:2816:G:C8	2.54	0.42
2:2:565:U:OP2	2:2:566:G:O2'	2.38	0.42
2:2:839:C:H2'	2:2:840:C:C6	2.55	0.42
2:2:925:G:O6	2:2:1391:U:O4	2.37	0.42
2:2:1239:A:N7	2:2:1298:U:N3	2.68	0.42
3:3:60:C:H2'	3:3:61:G:C8	2.54	0.42
3:3:77:U:H2'	3:3:78:A:C8	2.55	0.42
6:B:108:LYS:HA	6:B:196:GLY:HA2	2.02	0.42
17:M:20:LEU:HD13	26:V:81:PRO:HG2	2.02	0.42
22:R:73:LYS:HA	22:R:73:LYS:HD2	1.89	0.42
37:g:60:ILE:HA	37:g:63:ARG:HG2	2.02	0.42
41:k:59:TYR:HE2	53:w:67:LEU:HD21	1.85	0.42
44:n:38:TYR:OH	44:n:75:GLN:NE2	2.53	0.42
45:o:12:ALA:HB3	45:o:18:ILE:HD12	2.00	0.42
1:1:1342:A:O2'	1:1:1344:U:OP2	2.26	0.42
1:1:2033:A:O2'	1:1:2035:G:OP2	2.34	0.42
1:1:2258:C:O2'	1:1:2427:C:OP2	2.38	0.42
2:2:824:G:H2'	2:2:825:A:C8	2.55	0.42
2:2:949:A:O2'	2:2:971:G:O6	2.37	0.42
2:2:1124:G:O2'	2:2:1145:A:N6	2.53	0.42
2:2:1139:G:H4'	2:2:1140:C:H5'	2.01	0.42
2:2:1236:A:H4'	2:2:1304:G:H4'	2.02	0.42
2:2:1527:U:H2'	2:2:1528:U:C6	2.55	0.42
9:E:136:ILE:HA	9:E:141:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:154:ILE:HD13	9:E:154:ILE:HA	1.87	0.42
10:F:22:GLN:HE22	10:F:55:ARG:HH22	1.67	0.42
12:H:68:PRO:HA	12:H:72:LEU:HG	2.01	0.42
15:K:62:VAL:HA	15:K:84:CYS:HA	2.02	0.42
23:S:98:LYS:HD2	23:S:98:LYS:HA	1.87	0.42
24:T:59:ASN:O	24:T:84:TYR:N	2.50	0.42
28:X:25:THR:OG1	28:X:26:LYS:N	2.52	0.42
30:Z:38:ARG:HD3	30:Z:38:ARG:HA	1.80	0.42
37:g:60:ILE:HD13	37:g:160:ALA:HB2	2.02	0.42
1:1:777:G:H2'	1:1:778:G:H8	1.85	0.41
1:1:1197:G:H1'	1:1:1250:G:H22	1.85	0.41
1:1:2089:C:H2'	1:1:2090:A:C8	2.54	0.41
2:2:830:G:H2'	2:2:831:A:H8	1.85	0.41
4:5:111:VAL:HG21	4:5:127:ILE:HG23	2.02	0.41
17:M:56:ALA:HB2	17:M:119:LEU:HD12	2.02	0.41
40:j:22:SER:OG	40:j:23:LYS:N	2.53	0.41
44:n:12:ARG:HD3	44:n:77:GLY:HA3	2.02	0.41
57:4:140:U:H2'	57:4:141:C:C6	2.55	0.41
57:4:247:A:H4'	57:4:248:G:O5'	2.19	0.41
1:1:78:U:H3	1:1:108:G:H1	1.66	0.41
1:1:197:A:H62	1:1:2430:A:H2'	1.85	0.41
1:1:409:G:H2'	1:1:410:G:C8	2.55	0.41
1:1:679:C:O2	1:1:799:G:N2	2.54	0.41
1:1:816:C:N3	1:1:1192:G:N1	2.69	0.41
1:1:1081:U:H4'	13:I:123:ALA:HA	2.02	0.41
1:1:1332:G:N7	1:1:1609:A:O2'	2.45	0.41
1:1:1346:G:H2'	1:1:1347:A:C8	2.54	0.41
1:1:1822:C:H2'	1:1:1823:G:C8	2.55	0.41
1:1:2849:U:N3	1:1:2867:G:N3	2.68	0.41
2:2:429:U:H5'	39:i:9:LEU:HB2	2.02	0.41
2:2:591:U:H2'	2:2:592:G:C8	2.56	0.41
2:2:1150:A:H3'	2:2:1151:A:C8	2.55	0.41
2:2:1381:U:H2'	2:2:1382:C:O4'	2.20	0.41
2:2:1395:C:O4'	2:2:1401:G:N2	2.53	0.41
9:E:30:ARG:H	9:E:30:ARG:HG2	1.63	0.41
16:L:110:VAL:HB	16:L:127:VAL:HG12	2.01	0.41
38:h:150:LYS:HD3	38:h:173:VAL:HG21	2.02	0.41
39:i:162:ALA:HB1	39:i:167:LYS:HD3	2.02	0.41
43:m:56:LYS:HA	43:m:57:PRO:HD3	1.86	0.41
57:4:116:A:H2'	57:4:117:G:H5''	2.02	0.41
57:4:316:A:N6	57:4:319:A:N7	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4:354:A:H2'	57:4:355:G:H8	1.85	0.41
1:1:1105:U:H2'	1:1:1106:G:H8	1.85	0.41
1:1:1184:U:H2'	1:1:1185:G:C8	2.53	0.41
1:1:1344:U:O2	1:1:1384:A:O2'	2.35	0.41
1:1:2097:A:H2'	1:1:2098:U:C6	2.55	0.41
1:1:2450:A:OP1	1:1:2497:A:O2'	2.33	0.41
1:1:2676:C:P	15:K:31:ARG:HH12	2.43	0.41
2:2:358:U:H2'	2:2:359:G:C8	2.53	0.41
2:2:363:A:H2'	2:2:364:A:C8	2.56	0.41
2:2:377:G:H2'	2:2:378:G:C8	2.54	0.41
2:2:560:A:O5'	2:2:566:G:N2	2.53	0.41
2:2:790:A:H5'	4:5:22:HIS:ND1	2.35	0.41
2:2:1238:A:N7	2:2:1303:C:H1'	2.36	0.41
2:2:1326:U:H2'	2:2:1327:C:H6	1.85	0.41
19:O:18:LEU:HD23	19:O:21:LEU:HD12	2.02	0.41
23:S:23:LEU:HD11	32:b:22:LEU:HD23	2.02	0.41
27:W:43:THR:O	27:W:43:THR:OG1	2.39	0.41
37:g:72:THR:OG1	37:g:169:GLU:OE2	2.33	0.41
37:g:97:LEU:HD11	37:g:148:LEU:HD21	2.02	0.41
44:n:18:ARG:O	44:n:65:ILE:HA	2.19	0.41
49:s:13:ARG:HG3	49:s:54:ASP:CG	2.45	0.41
57:4:334:A:H4'	57:4:335:C:C6	2.56	0.41
1:1:30:G:C8	1:1:30:G:OP2	2.73	0.41
1:1:97:C:H2'	1:1:98:G:C8	2.56	0.41
1:1:2023:C:H2'	1:1:2024:G:H8	1.84	0.41
1:1:2100:G:H1	1:1:2189:U:C1'	2.33	0.41
1:1:2333:A:H5'	1:1:2335:A:H1'	2.02	0.41
1:1:2408:U:H2'	1:1:2409:G:H8	1.85	0.41
1:1:2632:A:O2'	1:1:2811:G:O2'	2.24	0.41
2:2:668:G:H2'	2:2:669:G:C8	2.55	0.41
2:2:959:A:N6	54:x:77:THR:O	2.53	0.41
2:2:1105:A:H2'	2:2:1106:G:H8	1.85	0.41
2:2:1402:4OC:HM22	2:2:1402:4OC:H1'	1.61	0.41
15:K:109:SER:OG	15:K:110:GLU:OE2	2.38	0.41
42:l:99:LEU:HD12	42:l:102:ARG:HB3	2.03	0.41
47:q:76:GLU:OE1	47:q:76:GLU:N	2.49	0.41
1:1:581:C:H2'	1:1:582:A:C8	2.43	0.41
1:1:983:A:H62	1:1:984:A:H62	1.68	0.41
1:1:1326:U:HO2'	1:1:2010:G:HO2'	1.65	0.41
1:1:1805:A:N6	1:1:1813:G:O6	2.53	0.41
1:1:2327:A:N7	1:1:2388:A:N6	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:C:P	40:j:132:ASN:HD21	2.42	0.41
2:2:664:G:OP1	53:w:53:ARG:NE	2.41	0.41
2:2:685:G:OP1	46:p:13:ARG:NH2	2.53	0.41
2:2:939:G:H1'	2:2:1376:U:H3	1.84	0.41
2:2:1076:U:OP1	37:g:174:LYS:NZ	2.49	0.41
25:U:40:ASN:ND2	25:U:64:ALA:O	2.53	0.41
37:g:15:HIS:HB3	37:g:43:LEU:HD23	2.03	0.41
44:n:49:ARG:HA	44:n:52:LEU:HB2	2.02	0.41
54:x:38:SER:OG	54:x:39:THR:N	2.52	0.41
1:1:90:U:OP2	1:1:91:A:O2'	2.31	0.41
1:1:2772:C:H2'	1:1:2773:C:H6	1.85	0.41
2:2:56:U:H2'	2:2:57:G:C8	2.55	0.41
2:2:785:G:H2'	2:2:786:G:H8	1.84	0.41
2:2:984:C:H2'	2:2:985:C:H6	1.85	0.41
2:2:1175:G:O2'	2:2:1176:A:O5'	2.37	0.41
2:2:1377:A:C6	42:l:7:ILE:HD11	2.55	0.41
2:2:1429:A:H2'	2:2:1430:A:C8	2.55	0.41
37:g:49:MET:HE3	37:g:199:VAL:HG23	2.02	0.41
40:j:84:PRO:HG3	40:j:97:GLN:HG3	2.02	0.41
42:l:98:ALA:O	42:l:102:ARG:NH1	2.54	0.41
46:p:23:ILE:HB	46:p:86:VAL:HG23	2.01	0.41
50:t:21:ASP:OD1	50:t:21:ASP:N	2.53	0.41
50:t:25:THR:HG23	50:t:66:LEU:HD12	2.03	0.41
57:4:147:C:H2'	57:4:148:U:H6	1.85	0.41
1:1:305:C:H2'	1:1:306:U:C6	2.56	0.41
1:1:593:U:H2'	1:1:594:U:C6	2.56	0.41
1:1:1447:C:H2'	1:1:1448:G:H8	1.85	0.41
1:1:2047:C:H2'	1:1:2048:G:H8	1.86	0.41
1:1:2549:G:H2'	1:1:2550:G:C8	2.56	0.41
2:2:517:G:N2	2:2:530:G:OP1	2.44	0.41
2:2:1225:A:OP2	48:r:102:THR:N	2.46	0.41
3:3:95:U:H2'	3:3:96:G:C8	2.55	0.41
8:D:149:ILE:HD11	8:D:188:MET:HG2	2.02	0.41
15:K:21:CYS:HA	15:K:41:ILE:HG22	2.03	0.41
37:g:144:LEU:HG	37:g:148:LEU:HD23	2.03	0.41
39:i:91:LEU:HD23	39:i:91:LEU:HA	1.88	0.41
52:v:14:SER:OG	52:v:16:LYS:NZ	2.54	0.41
52:v:46:VAL:HG21	52:v:61:ILE:HG21	2.01	0.41
57:4:306:U:H2'	57:4:307:G:H8	1.86	0.41
1:1:833:A:O2'	16:L:51:GLU:OE2	2.38	0.41
1:1:1723:G:H3'	1:1:1724:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2026:U:H2'	1:1:2027:G:H8	1.86	0.41
1:1:2585:U:N3	5:6:22:ALA:O	2.52	0.41
2:2:783:C:H2'	2:2:784:A:C8	2.56	0.41
2:2:1159:U:N3	2:2:1182:G:O2'	2.45	0.41
2:2:1203:C:H2'	2:2:1204:A:H8	1.86	0.41
2:2:1520:C:H2'	2:2:1521:C:C6	2.56	0.41
3:3:61:G:H2'	3:3:62:C:H6	1.85	0.41
4:5:41:VAL:HG11	57:4:335:C:H5''	2.02	0.41
4:5:151:LYS:NZ	42:l:81:GLY:O	2.48	0.41
4:5:156:LYS:HE3	4:5:156:LYS:HB3	1.84	0.41
9:E:60:ILE:HA	9:E:140:GLU:HG3	2.03	0.41
14:J:72:LYS:HZ3	14:J:74:TYR:HE1	1.68	0.41
16:L:91:ASP:H	16:L:94:THR:HB	1.86	0.41
19:O:93:ASP:OD1	19:O:95:SER:OG	2.38	0.41
29:Y:39:GLN:HB3	29:Y:42:LEU:HD23	2.03	0.41
32:b:4:GLN:H	32:b:4:GLN:HG2	1.73	0.41
37:g:12:ALA:HB1	37:g:209:ALA:HA	2.01	0.41
38:h:108:LYS:HE3	38:h:108:LYS:HB3	1.88	0.41
39:i:37:ALA:HB3	39:i:42:GLY:HA2	2.03	0.41
40:j:141:ILE:HD12	40:j:141:ILE:HA	1.96	0.41
42:l:66:LEU:HD13	42:l:104:ILE:HD11	2.03	0.41
42:l:102:ARG:HA	42:l:105:VAL:HG12	2.01	0.41
44:n:14:SER:O	44:n:70:GLY:N	2.54	0.41
47:q:74:LEU:HD13	47:q:74:LEU:HA	1.86	0.41
57:4:268:U:H2'	57:4:269:C:C6	2.56	0.41
1:1:449:A:H4'	21:Q:3:ARG:HH11	1.86	0.41
1:1:639:U:H2'	1:1:640:C:C6	2.56	0.41
1:1:749:A:H2'	1:1:750:A:H8	1.85	0.41
1:1:759:G:H2'	1:1:760:G:C8	2.55	0.41
1:1:837:C:N3	1:1:941:A:N6	2.69	0.41
1:1:1046:A:O2'	12:H:7:ASP:OD2	2.39	0.41
1:1:1817:G:OP1	6:B:62:TYR:OH	2.30	0.41
1:1:2328:A:H2'	1:1:2329:U:C6	2.56	0.41
1:1:2392:A:OP2	1:1:2422:C:N4	2.54	0.41
1:1:2734:A:N6	1:1:2770:G:O2'	2.53	0.41
2:2:162:A:C5	2:2:163:C:H1'	2.56	0.41
2:2:312:C:H2'	2:2:313:A:C8	2.55	0.41
2:2:384:G:H2'	2:2:385:C:C6	2.56	0.41
2:2:793:U:O2	2:2:1516:2MG:O2'	2.28	0.41
2:2:864:A:H5'	40:j:90:THR:O	2.20	0.41
2:2:1011:C:H2'	2:2:1012:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1091:U:O2	2:2:1095:U:N3	2.52	0.41
2:2:1329:A:H5'	48:r:26:GLY:N	2.36	0.41
2:2:1360:A:OP1	49:s:58:SER:OG	2.36	0.41
7:C:139:SER:HA	7:C:142:VAL:HG13	2.03	0.41
8:D:12:LEU:HD12	8:D:12:LEU:HA	1.85	0.41
13:I:107:GLU:O	13:I:111:THR:HB	2.21	0.41
20:P:3:ASN:HA	20:P:6:LYS:HB3	2.02	0.41
20:P:54:GLY:O	20:P:57:SER:OG	2.35	0.41
23:S:76:VAL:HG12	23:S:103:ILE:HA	2.02	0.41
30:Z:18:PRO:HA	30:Z:21:LYS:HB2	2.02	0.41
37:g:42:ASN:HD21	37:g:44:GLU:HB2	1.86	0.41
43:m:18:GLN:OE1	43:m:72:VAL:N	2.54	0.41
57:4:303:G:H2'	57:4:304:C:C6	2.55	0.41
1:1:406:G:H2'	1:1:407:G:H8	1.86	0.41
1:1:539:G:H1	1:1:554:U:H3	1.69	0.41
1:1:542:C:H2'	1:1:543:G:H8	1.86	0.41
1:1:599:A:H2'	1:1:600:G:C8	2.52	0.41
1:1:643:A:O4'	33:c:44:ARG:NH1	2.54	0.41
1:1:781:A:O2'	1:1:1788:C:O2'	2.28	0.41
1:1:2074:U:H2'	1:1:2075:U:C6	2.56	0.41
1:1:2313:C:H2'	1:1:2314:A:C8	2.55	0.41
2:2:657:U:H2'	2:2:658:C:H6	1.85	0.41
2:2:1189:U:H4'	38:h:10:ILE:HD11	2.03	0.41
3:3:32:U:H2'	3:3:33:G:H8	1.86	0.41
3:3:42:C:O2	9:E:90:THR:OG1	2.35	0.41
8:D:154:ASP:OD1	8:D:156:ASN:N	2.54	0.41
13:I:53:PRO:HG2	13:I:77:VAL:HG21	2.03	0.41
14:J:1:MET:HE2	14:J:1:MET:HB2	1.93	0.41
14:J:31:GLU:OE2	14:J:35:ARG:NE	2.43	0.41
38:h:52:VAL:HG12	38:h:68:ILE:HG21	2.02	0.41
40:j:147:MET:HE3	40:j:147:MET:HB2	1.95	0.41
42:l:44:TYR:HA	42:l:47:LEU:HB2	2.03	0.41
44:n:106:ARG:NH1	44:n:107:ASP:O	2.54	0.41
52:v:48:ASP:OD1	52:v:48:ASP:N	2.54	0.41
57:4:139:C:H2'	57:4:140:U:C6	2.56	0.41
1:1:329:G:OP2	25:U:69:ASN:ND2	2.54	0.40
1:1:967:U:H2'	1:1:968:C:C6	2.56	0.40
1:1:1280:G:H2'	1:1:1281:G:H8	1.84	0.40
1:1:2810:A:H8	1:1:2811:G:C8	2.38	0.40
2:2:555:U:H2'	2:2:556:C:C6	2.56	0.40
2:2:557:G:H2'	2:2:558:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:601:G:H2'	2:2:602:A:C8	2.57	0.40
2:2:673:A:H2'	2:2:674:G:C8	2.53	0.40
2:2:1248:A:O2'	44:n:38:TYR:O	2.39	0.40
6:B:69:ARG:HG3	6:B:129:THR:HG21	2.03	0.40
29:Y:14:LEU:HA	29:Y:17:GLU:HB3	2.02	0.40
35:e:6:THR:HG23	35:e:62:LEU:HA	2.03	0.40
36:f:19:ARG:HB2	36:f:24:ARG:HE	1.86	0.40
37:g:66:LYS:H	37:g:159:ASP:HB2	1.86	0.40
37:g:167:ASP:OD2	37:g:190:ASN:ND2	2.44	0.40
41:k:55:HIS:HB2	41:k:56:LYS:HD3	2.02	0.40
57:4:198:U:H2'	57:4:199:C:C5	2.55	0.40
57:4:251:U:H2'	57:4:252:G:C8	2.53	0.40
1:1:994:C:O2'	1:1:996:A:OP1	2.37	0.40
1:1:1497:U:O2'	1:1:1577:C:O3'	2.36	0.40
1:1:1604:C:H2'	1:1:1605:C:C6	2.56	0.40
1:1:2284:A:OP1	33:c:4:GLY:N	2.53	0.40
1:1:2303:G:H2'	1:1:2304:G:H8	1.85	0.40
1:1:2688:G:H21	1:1:2721:A:H62	1.70	0.40
1:1:2861:U:H2'	1:1:2862:G:C8	2.56	0.40
2:2:52:C:H2'	2:2:53:A:C8	2.56	0.40
2:2:677:U:O2	2:2:777:A:O2'	2.29	0.40
7:C:14:ILE:HA	20:P:12:GLN:HE22	1.85	0.40
7:C:179:ARG:HB3	7:C:188:LEU:HD23	2.04	0.40
8:D:117:ARG:HH22	16:L:2:ARG:HH12	1.68	0.40
16:L:89:VAL:HA	16:L:121:THR:HB	2.03	0.40
24:T:15:HIS:CD2	24:T:82:LYS:HE3	2.56	0.40
38:h:38:LYS:HA	38:h:38:LYS:HD2	1.78	0.40
38:h:80:LYS:HE2	38:h:80:LYS:HB2	1.97	0.40
47:q:98:VAL:HG11	47:q:101:ALA:HB3	2.03	0.40
50:t:48:LYS:HD3	50:t:48:LYS:HA	1.88	0.40
1:1:372:G:C5	28:X:61:LYS:HD3	2.56	0.40
1:1:457:A:H61	1:1:470:A:H5''	1.87	0.40
1:1:915:C:H3'	1:1:916:G:H8	1.86	0.40
1:1:1138:G:C5	1:1:1139:G:H1'	2.57	0.40
1:1:2052:A:H2'	1:1:2053:G:C8	2.53	0.40
1:1:2067:G:H4'	1:1:2068:U:OP2	2.22	0.40
1:1:2130:U:H1'	1:1:2159:G:H1	1.87	0.40
2:2:81:A:N1	2:2:88:U:N3	2.70	0.40
2:2:199:A:H2'	2:2:200:G:H8	1.86	0.40
2:2:235:C:H2'	2:2:236:A:C8	2.56	0.40
2:2:681:A:H2'	2:2:682:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:867:G:H2'	2:2:868:C:C6	2.56	0.40
2:2:921:U:O2'	40:j:24:THR:O	2.33	0.40
2:2:1403:C:O2'	2:2:1404:C:H5'	2.22	0.40
2:2:1526:G:H2'	2:2:1527:U:C6	2.56	0.40
7:C:11:MET:SD	7:C:25:THR:OG1	2.73	0.40
7:C:187:LEU:HD12	7:C:187:LEU:HA	1.91	0.40
10:F:64:GLN:O	10:F:67:THR:OG1	2.35	0.40
10:F:86:LYS:HG2	10:F:132:VAL:HG22	2.02	0.40
26:V:29:ILE:HG22	26:V:88:HIS:HE1	1.87	0.40
32:b:29:SER:OG	32:b:40:ARG:NH2	2.54	0.40
43:m:40:LEU:HD23	43:m:40:LEU:HA	1.97	0.40
48:r:15:ALA:HB3	48:r:34:LEU:HD22	2.04	0.40
48:r:72:GLU:HA	48:r:75:MET:HE3	2.04	0.40
51:u:14:ARG:HE	51:u:14:ARG:HB3	1.74	0.40
57:4:163:G:H21	57:4:191:A:H61	1.68	0.40
1:1:71:A:O3'	24:T:9:LYS:NZ	2.54	0.40
1:1:1097:U:H3'	1:1:1098:A:C8	2.55	0.40
1:1:1429:G:H1	1:1:1564:C:H42	1.70	0.40
1:1:1498:C:H2'	1:1:1499:C:H6	1.86	0.40
1:1:1818:U:O2'	6:B:153:GLN:O	2.32	0.40
1:1:1947:C:H2'	1:1:1948:G:C8	2.56	0.40
1:1:2036:C:H2'	1:1:2037:A:H8	1.86	0.40
2:2:416:G:H2'	2:2:417:G:H8	1.86	0.40
2:2:1149:C:O2'	2:2:1280:A:N1	2.54	0.40
6:B:181:MET:HB2	6:B:268:VAL:HB	2.04	0.40
12:H:9:GLN:HA	12:H:12:VAL:HG12	2.03	0.40
12:H:11:ILE:HD12	12:H:11:ILE:HA	1.97	0.40
13:I:44:LYS:NZ	13:I:70:THR:OG1	2.40	0.40
15:K:79:PHE:HD1	20:P:70:VAL:HG22	1.87	0.40
18:N:79:LEU:HD23	18:N:83:LEU:HD12	2.03	0.40
20:P:51:ARG:HD3	20:P:58:ALA:HB3	2.03	0.40
29:Y:25:GLN:HE22	29:Y:29:ARG:HH21	1.69	0.40
39:i:44:ARG:HA	39:i:44:ARG:HD3	1.92	0.40
49:s:66:GLN:NE2	49:s:79:LEU:HD21	2.35	0.40
52:v:4:LYS:HB2	52:v:4:LYS:HE2	1.93	0.40
56:z:20:LYS:HE2	56:z:20:LYS:HB3	1.93	0.40
1:1:638:G:H2'	1:1:639:U:O4'	2.22	0.40
1:1:1529:G:O6	1:1:1542:U:O4	2.39	0.40
1:1:1997:C:H2'	1:1:1998:A:C8	2.55	0.40
1:1:2064:C:HO2'	1:1:2251:OMG:N2	2.18	0.40
1:1:2073:C:H2'	1:1:2074:U:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2087:G:H2'	1:1:2088:A:C8	2.53	0.40
1:1:2127:G:O2'	1:1:2128:G:N7	2.45	0.40
1:1:2625:G:H2'	1:1:2626:C:C6	2.56	0.40
2:2:408:A:H2'	2:2:409:U:C6	2.57	0.40
2:2:574:A:HO2'	2:2:882:C:HO2'	1.67	0.40
3:3:82:U:H2'	3:3:83:G:H8	1.85	0.40
8:D:147:LEU:HD11	8:D:170:ARG:HG2	2.03	0.40
10:F:143:GLN:NE2	10:F:147:ASP:OD1	2.53	0.40
17:M:38:ARG:HG3	17:M:98:PRO:HD3	2.02	0.40
30:Z:49:ASN:HA	30:Z:52:SER:HB3	2.03	0.40
33:c:5:ILE:HD12	33:c:5:ILE:HA	1.96	0.40
43:m:92:LEU:HD23	43:m:92:LEU:HA	1.86	0.40
57:4:5:C:C2'	57:4:6:U:H5'	2.51	0.40
57:4:176:G:H2'	57:4:177:A:C8	2.56	0.40
57:4:266:C:H2'	57:4:267:G:H5''	2.03	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	5	148/160 (92%)	127 (86%)	20 (14%)	1 (1%)	18	55
5	6	20/22 (91%)	12 (60%)	8 (40%)	0	100	100
6	B	269/273 (98%)	236 (88%)	33 (12%)	0	100	100
7	C	207/209 (99%)	183 (88%)	24 (12%)	0	100	100
8	D	199/201 (99%)	177 (89%)	22 (11%)	0	100	100
9	E	175/179 (98%)	152 (87%)	23 (13%)	0	100	100
10	F	173/177 (98%)	154 (89%)	18 (10%)	1 (1%)	21	58
11	G	147/149 (99%)	128 (87%)	19 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	128/165 (78%)	94 (73%)	34 (27%)	0	100	100
13	I	133/142 (94%)	104 (78%)	28 (21%)	1 (1%)	16	52
14	J	140/142 (99%)	125 (89%)	15 (11%)	0	100	100
15	K	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
16	L	142/144 (99%)	122 (86%)	20 (14%)	0	100	100
17	M	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
18	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
19	O	114/117 (97%)	98 (86%)	16 (14%)	0	100	100
20	P	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
21	Q	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
22	R	101/103 (98%)	86 (85%)	15 (15%)	0	100	100
23	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
24	T	92/100 (92%)	84 (91%)	8 (9%)	0	100	100
25	U	101/104 (97%)	90 (89%)	11 (11%)	0	100	100
26	V	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
27	W	74/85 (87%)	63 (85%)	11 (15%)	0	100	100
28	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
29	Y	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
30	Z	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
31	a	55/70 (79%)	47 (86%)	8 (14%)	0	100	100
32	b	54/57 (95%)	45 (83%)	9 (17%)	0	100	100
33	c	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
34	d	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
35	e	62/65 (95%)	52 (84%)	10 (16%)	0	100	100
36	f	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
37	g	223/241 (92%)	195 (87%)	28 (13%)	0	100	100
38	h	206/233 (88%)	179 (87%)	27 (13%)	0	100	100
39	i	203/206 (98%)	185 (91%)	18 (9%)	0	100	100
40	j	154/167 (92%)	135 (88%)	19 (12%)	0	100	100
41	k	102/135 (76%)	97 (95%)	5 (5%)	0	100	100
42	l	149/179 (83%)	135 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	m	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
44	n	125/130 (96%)	110 (88%)	15 (12%)	0	100	100
45	o	97/103 (94%)	88 (91%)	9 (9%)	0	100	100
46	p	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
47	q	119/124 (96%)	99 (83%)	20 (17%)	0	100	100
48	r	110/118 (93%)	89 (81%)	21 (19%)	0	100	100
49	s	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
50	t	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
51	u	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
52	v	78/84 (93%)	67 (86%)	11 (14%)	0	100	100
53	w	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
54	x	81/92 (88%)	66 (82%)	15 (18%)	0	100	100
55	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
56	z	68/71 (96%)	60 (88%)	8 (12%)	0	100	100
All	All	6023/6402 (94%)	5297 (88%)	723 (12%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	47	ASP
4	5	92	LEU
13	I	92	PRO

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	
4	5	125/133 (94%)	124 (99%)	1 (1%)	73	77
6	B	216/218 (99%)	214 (99%)	2 (1%)	70	76
7	C	164/164 (100%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	165/165 (100%)	165 (100%)	0	100	100
9	E	148/150 (99%)	148 (100%)	0	100	100
10	F	136/138 (99%)	136 (100%)	0	100	100
11	G	114/114 (100%)	114 (100%)	0	100	100
12	H	99/123 (80%)	98 (99%)	1 (1%)	68	76
13	I	104/110 (94%)	103 (99%)	1 (1%)	68	76
14	J	116/116 (100%)	116 (100%)	0	100	100
15	K	104/104 (100%)	103 (99%)	1 (1%)	68	76
16	L	103/103 (100%)	102 (99%)	1 (1%)	68	76
17	M	109/109 (100%)	109 (100%)	0	100	100
18	N	99/103 (96%)	98 (99%)	1 (1%)	68	76
19	O	86/87 (99%)	86 (100%)	0	100	100
20	P	99/100 (99%)	97 (98%)	2 (2%)	48	66
21	Q	89/90 (99%)	89 (100%)	0	100	100
22	R	84/84 (100%)	83 (99%)	1 (1%)	63	73
23	S	93/93 (100%)	93 (100%)	0	100	100
24	T	81/84 (96%)	81 (100%)	0	100	100
25	U	84/85 (99%)	84 (100%)	0	100	100
26	V	78/78 (100%)	78 (100%)	0	100	100
27	W	58/63 (92%)	58 (100%)	0	100	100
28	X	67/68 (98%)	67 (100%)	0	100	100
29	Y	54/55 (98%)	54 (100%)	0	100	100
30	Z	48/49 (98%)	47 (98%)	1 (2%)	47	65
31	a	54/62 (87%)	54 (100%)	0	100	100
32	b	47/48 (98%)	47 (100%)	0	100	100
33	c	47/49 (96%)	47 (100%)	0	100	100
34	d	38/38 (100%)	38 (100%)	0	100	100
35	e	51/52 (98%)	51 (100%)	0	100	100
36	f	34/34 (100%)	34 (100%)	0	100	100
37	g	187/199 (94%)	186 (100%)	1 (0%)	81	81
38	h	171/190 (90%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	i	172/173 (99%)	172 (100%)	0	100	100
40	j	119/126 (94%)	116 (98%)	3 (2%)	42	62
41	k	91/116 (78%)	91 (100%)	0	100	100
42	l	124/147 (84%)	124 (100%)	0	100	100
43	m	104/105 (99%)	103 (99%)	1 (1%)	68	76
44	n	105/107 (98%)	105 (100%)	0	100	100
45	o	86/90 (96%)	85 (99%)	1 (1%)	63	73
46	p	90/99 (91%)	90 (100%)	0	100	100
47	q	102/103 (99%)	101 (99%)	1 (1%)	68	76
48	r	90/96 (94%)	87 (97%)	3 (3%)	33	55
49	s	83/84 (99%)	83 (100%)	0	100	100
50	t	76/77 (99%)	76 (100%)	0	100	100
51	u	65/65 (100%)	65 (100%)	0	100	100
52	v	74/78 (95%)	72 (97%)	2 (3%)	39	60
53	w	57/65 (88%)	57 (100%)	0	100	100
54	x	72/79 (91%)	72 (100%)	0	100	100
55	y	65/66 (98%)	65 (100%)	0	100	100
56	z	60/61 (98%)	60 (100%)	0	100	100
All	All	4987/5195 (96%)	4963 (100%)	24 (0%)	78	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	92	LEU
6	B	17	VAL
6	B	141	VAL
12	H	50	VAL
13	I	23	VAL
15	K	63	VAL
16	L	89	VAL
18	N	70	THR
20	P	4	ILE
20	P	81	VAL
22	R	59	ILE
30	Z	57	VAL
37	g	70	VAL

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Mol	Chain	Res	Type
40	j	11	LEU
40	j	56	VAL
40	j	80	THR
43	m	104	VAL
45	o	74	VAL
47	q	83	ARG
48	r	22	ILE
48	r	25	VAL
48	r	30	SER
52	v	75	LEU
52	v	76	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
4	5	37	GLN
4	5	148	GLN
6	B	70	ASN
6	B	134	ASN
7	C	42	ASN
7	C	173	GLN
8	D	115	GLN
8	D	163	ASN
9	E	5	HIS
10	F	22	GLN
10	F	73	ASN
11	G	11	ASN
11	G	28	ASN
13	I	11	GLN
15	K	90	ASN
15	K	93	GLN
16	L	38	GLN
17	M	45	GLN
17	M	60	GLN
19	O	61	GLN
20	P	12	GLN
20	P	15	GLN
20	P	115	ASN
21	Q	66	ASN
22	R	6	GLN
22	R	86	GLN
22	R	91	GLN

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Mol	Chain	Res	Type
23	S	40	ASN
23	S	57	ASN
23	S	60	HIS
23	S	61	ASN
23	S	102	HIS
24	T	15	HIS
24	T	48	GLN
24	T	59	ASN
25	U	46	GLN
27	W	76	ASN
28	X	16	ASN
29	Y	15	ASN
29	Y	25	GLN
29	Y	27	ASN
30	Z	49	ASN
31	a	30	HIS
31	a	33	ASN
31	a	41	HIS
31	a	61	ASN
31	a	65	ASN
32	b	4	GLN
34	d	29	GLN
35	e	26	HIS
35	e	43	HIS
37	g	42	ASN
37	g	109	GLN
38	h	3	GLN
38	h	32	ASN
38	h	123	GLN
38	h	185	ASN
39	i	116	GLN
39	i	136	GLN
39	i	152	GLN
40	j	70	ASN
41	k	46	GLN
41	k	94	HIS
42	l	86	GLN
42	l	97	ASN
43	m	16	ASN
44	n	31	ASN
45	o	15	HIS
49	s	4	GLN

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Mol	Chain	Res	Type
49	s	66	GLN
51	u	26	ASN
51	u	79	ASN
54	x	53	ASN
55	y	3	ASN
55	y	52	ASN
55	y	55	GLN
55	y	68	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2904 (99%)	994 (34%)	22 (0%)
2	2	1532/1535 (99%)	498 (32%)	7 (0%)
3	3	119/120 (99%)	35 (29%)	0
57	4	361/363 (99%)	211 (58%)	31 (8%)
All	All	4914/4922 (99%)	1738 (35%)	60 (1%)

All (1738) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	G
1	1	4	U
1	1	10	A
1	1	11	C
1	1	12	U
1	1	14	A
1	1	15	G
1	1	27	G
1	1	28	A
1	1	30	G
1	1	32	C
1	1	33	C
1	1	34	U
1	1	35	G
1	1	43	G
1	1	46	G
1	1	48	G
1	1	50	U
1	1	51	G
1	1	54	G

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Mol	Chain	Res	Type
1	1	55	G
1	1	57	C
1	1	58	G
1	1	60	G
1	1	61	C
1	1	63	A
1	1	68	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	79	C
1	1	80	G
1	1	84	A
1	1	85	G
1	1	91	A
1	1	93	G
1	1	96	C
1	1	100	U
1	1	101	A
1	1	102	U
1	1	103	A
1	1	112	U
1	1	113	U
1	1	118	A
1	1	119	A
1	1	120	U
1	1	126	A
1	1	128	C
1	1	136	G
1	1	137	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	165	A
1	1	167	A
1	1	181	A
1	1	192	C
1	1	193	U
1	1	196	A
1	1	197	A
1	1	199	A

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Mol	Chain	Res	Type
1	1	201	C
1	1	203	A
1	1	204	A
1	1	215	G
1	1	216	A
1	1	218	A
1	1	221	A
1	1	222	A
1	1	225	C
1	1	226	A
1	1	228	C
1	1	229	C
1	1	230	G
1	1	233	A
1	1	239	C
1	1	241	A
1	1	245	G
1	1	248	G
1	1	249	C
1	1	250	G
1	1	260	G
1	1	261	G
1	1	264	C
1	1	265	A
1	1	266	G
1	1	267	C
1	1	270	A
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	278	A
1	1	280	U
1	1	285	G
1	1	289	G
1	1	294	A
1	1	296	U
1	1	301	G
1	1	304	U
1	1	308	G
1	1	309	A
1	1	310	A

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Mol	Chain	Res	Type
1	1	321	U
1	1	322	A
1	1	323	C
1	1	324	A
1	1	329	G
1	1	330	A
1	1	331	C
1	1	332	A
1	1	337	C
1	1	338	G
1	1	343	C
1	1	353	C
1	1	357	C
1	1	362	A
1	1	363	G
1	1	364	C
1	1	366	C
1	1	367	G
1	1	370	G
1	1	371	A
1	1	372	G
1	1	375	G
1	1	384	A
1	1	385	C
1	1	386	G
1	1	387	U
1	1	389	G
1	1	394	C
1	1	396	G
1	1	398	C
1	1	399	U
1	1	403	U
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	413	C
1	1	424	G
1	1	431	U
1	1	434	U
1	1	435	C

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Mol	Chain	Res	Type
1	1	440	C
1	1	441	U
1	1	447	A
1	1	451	U
1	1	453	A
1	1	454	A
1	1	455	C
1	1	456	C
1	1	457	A
1	1	465	G
1	1	475	C
1	1	476	G
1	1	477	A
1	1	479	A
1	1	480	A
1	1	481	G
1	1	483	A
1	1	490	C
1	1	491	G
1	1	494	G
1	1	496	G
1	1	498	G
1	1	505	A
1	1	507	A
1	1	508	A
1	1	509	C
1	1	518	G
1	1	527	C
1	1	529	A
1	1	530	G
1	1	532	A
1	1	533	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	556	A
1	1	563	A
1	1	565	C
1	1	566	U
1	1	567	U

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Mol	Chain	Res	Type
1	1	571	U
1	1	573	U
1	1	575	A
1	1	576	U
1	1	577	G
1	1	586	A
1	1	601	C
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	622	G
1	1	627	A
1	1	634	C
1	1	637	A
1	1	645	C
1	1	653	U
1	1	654	A
1	1	655	A
1	1	656	G
1	1	657	U
1	1	659	G
1	1	664	G
1	1	675	A
1	1	681	G
1	1	682	G
1	1	684	G
1	1	686	U
1	1	689	A
1	1	699	A
1	1	702	U
1	1	709	U
1	1	710	U
1	1	715	A
1	1	716	A
1	1	717	C
1	1	722	A
1	1	730	A
1	1	734	A

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Mol	Chain	Res	Type
1	1	747	5MU
1	1	748	G
1	1	749	A
1	1	752	A
1	1	759	G
1	1	762	U
1	1	765	C
1	1	771	G
1	1	775	G
1	1	776	G
1	1	777	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	788	A
1	1	789	A
1	1	792	A
1	1	793	A
1	1	800	A
1	1	805	G
1	1	806	C
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	830	G
1	1	839	U
1	1	845	A
1	1	846	U
1	1	847	U
1	1	856	G
1	1	858	G
1	1	859	G
1	1	865	C
1	1	866	A
1	1	869	G
1	1	877	A
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C

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Mol	Chain	Res	Type
1	1	889	C
1	1	890	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	899	A
1	1	900	A
1	1	902	C
1	1	903	C
1	1	907	G
1	1	908	C
1	1	910	A
1	1	911	A
1	1	914	G
1	1	915	C
1	1	919	U
1	1	934	U
1	1	935	C
1	1	941	A
1	1	945	A
1	1	947	A
1	1	948	C
1	1	949	G
1	1	953	G
1	1	954	G
1	1	955	PSU
1	1	956	G
1	1	957	C
1	1	958	U
1	1	959	A
1	1	961	C
1	1	964	C
1	1	970	U
1	1	973	A
1	1	974	G
1	1	982	C
1	1	983	A
1	1	990	A
1	1	995	C

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Mol	Chain	Res	Type
1	1	996	A
1	1	997	G
1	1	1005	C
1	1	1008	A
1	1	1009	A
1	1	1010	A
1	1	1012	U
1	1	1013	C
1	1	1017	G
1	1	1022	G
1	1	1023	U
1	1	1024	G
1	1	1025	G
1	1	1026	G
1	1	1028	A
1	1	1029	A
1	1	1032	A
1	1	1033	U
1	1	1035	U
1	1	1041	G
1	1	1042	G
1	1	1044	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1048	A
1	1	1049	C
1	1	1050	A
1	1	1051	G
1	1	1052	C
1	1	1056	G
1	1	1058	U
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1071	G

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Mol	Chain	Res	Type
1	1	1073	A
1	1	1075	C
1	1	1076	C
1	1	1077	A
1	1	1079	C
1	1	1080	A
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1085	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1090	A
1	1	1092	C
1	1	1093	G
1	1	1096	A
1	1	1097	U
1	1	1099	G
1	1	1100	C
1	1	1101	U
1	1	1111	A
1	1	1112	G
1	1	1113	U
1	1	1119	U
1	1	1126	A
1	1	1128	G
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1135	C
1	1	1136	G
1	1	1141	U
1	1	1142	A
1	1	1143	A
1	1	1144	A
1	1	1168	G
1	1	1169	A
1	1	1171	G
1	1	1172	C
1	1	1173	U
1	1	1174	U

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Mol	Chain	Res	Type
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1182	G
1	1	1186	G
1	1	1191	G
1	1	1195	G
1	1	1203	U
1	1	1204	A
1	1	1206	G
1	1	1212	G
1	1	1215	G
1	1	1217	U
1	1	1218	G
1	1	1221	C
1	1	1227	G
1	1	1229	C
1	1	1238	G
1	1	1241	A
1	1	1243	C
1	1	1248	G
1	1	1251	C
1	1	1253	A
1	1	1254	A
1	1	1255	U
1	1	1256	G
1	1	1258	U
1	1	1265	A
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1284	A
1	1	1287	A
1	1	1289	C
1	1	1292	G
1	1	1296	G
1	1	1300	G
1	1	1301	A
1	1	1302	A
1	1	1310	G

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Mol	Chain	Res	Type
1	1	1312	U
1	1	1315	C
1	1	1316	U
1	1	1318	U
1	1	1325	U
1	1	1326	U
1	1	1332	G
1	1	1340	U
1	1	1341	G
1	1	1342	A
1	1	1345	C
1	1	1352	U
1	1	1355	G
1	1	1360	G
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1381	G
1	1	1385	A
1	1	1386	C
1	1	1393	A
1	1	1395	A
1	1	1403	A
1	1	1408	G
1	1	1409	U
1	1	1413	A
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1440	U
1	1	1454	C
1	1	1455	G
1	1	1456	G
1	1	1458	U
1	1	1461	C
1	1	1468	U
1	1	1470	A
1	1	1473	G

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Mol	Chain	Res	Type
1	1	1475	G
1	1	1478	G
1	1	1482	G
1	1	1483	G
1	1	1485	U
1	1	1493	C
1	1	1494	A
1	1	1497	U
1	1	1502	A
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1514	G
1	1	1515	A
1	1	1522	A
1	1	1523	U
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1533	C
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1547	C
1	1	1554	U
1	1	1558	C
1	1	1566	A
1	1	1569	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	1593	A
1	1	1598	A
1	1	1607	C
1	1	1608	A
1	1	1610	A
1	1	1616	A

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Mol	Chain	Res	Type
1	1	1618	6MZ
1	1	1619	G
1	1	1621	U
1	1	1625	C
1	1	1626	A
1	1	1627	G
1	1	1630	A
1	1	1633	G
1	1	1635	A
1	1	1642	G
1	1	1643	G
1	1	1644	C
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1653	G
1	1	1654	A
1	1	1667	G
1	1	1668	A
1	1	1673	G
1	1	1674	G
1	1	1676	A
1	1	1677	A
1	1	1691	C
1	1	1693	U
1	1	1695	G
1	1	1698	A
1	1	1699	G
1	1	1701	A
1	1	1702	G
1	1	1703	G
1	1	1712	U
1	1	1714	U
1	1	1715	G
1	1	1716	U
1	1	1721	G
1	1	1722	A
1	1	1723	G
1	1	1725	U
1	1	1729	U
1	1	1730	C

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Mol	Chain	Res	Type
1	1	1732	C
1	1	1734	G
1	1	1738	G
1	1	1744	A
1	1	1745	A
1	1	1757	A
1	1	1758	U
1	1	1761	C
1	1	1764	C
1	1	1766	G
1	1	1769	U
1	1	1770	G
1	1	1772	A
1	1	1773	A
1	1	1777	U
1	1	1779	U
1	1	1780	A
1	1	1781	U
1	1	1782	U
1	1	1784	A
1	1	1800	C
1	1	1802	A
1	1	1803	A
1	1	1804	C
1	1	1808	A
1	1	1809	A
1	1	1811	G
1	1	1813	G
1	1	1816	C
1	1	1819	A
1	1	1820	U
1	1	1821	A
1	1	1828	G
1	1	1830	C
1	1	1833	C
1	1	1834	U
1	1	1835	2MG
1	1	1842	G
1	1	1845	G
1	1	1848	A
1	1	1853	A
1	1	1855	U

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Mol	Chain	Res	Type
1	1	1857	G
1	1	1860	G
1	1	1863	G
1	1	1865	U
1	1	1866	A
1	1	1867	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1875	G
1	1	1877	A
1	1	1879	C
1	1	1880	U
1	1	1894	C
1	1	1896	G
1	1	1897	G
1	1	1906	G
1	1	1907	G
1	1	1911	PSU
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	1919	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1939	5MU
1	1	1940	U
1	1	1942	C
1	1	1943	U
1	1	1953	A
1	1	1955	U
1	1	1960	A
1	1	1962	5MC
1	1	1965	C
1	1	1966	A
1	1	1967	C

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Mol	Chain	Res	Type
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1981	A
1	1	1983	G
1	1	1989	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	1999	C
1	1	2014	A
1	1	2015	A
1	1	2022	U
1	1	2023	C
1	1	2030	6MZ
1	1	2031	A
1	1	2032	G
1	1	2033	A
1	1	2035	G
1	1	2043	C
1	1	2044	C
1	1	2046	G
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2066	C
1	1	2068	U
1	1	2069	G7M
1	1	2070	A
1	1	2072	C
1	1	2076	U
1	1	2077	A
1	1	2081	U
1	1	2092	U
1	1	2093	G
1	1	2094	A
1	1	2095	A

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Mol	Chain	Res	Type
1	1	2096	C
1	1	2097	A
1	1	2099	U
1	1	2100	G
1	1	2102	G
1	1	2104	C
1	1	2105	U
1	1	2106	U
1	1	2108	A
1	1	2110	G
1	1	2111	U
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	2122	U
1	1	2123	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	2136	G
1	1	2137	U
1	1	2138	G
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2143	C
1	1	2144	G
1	1	2146	C

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Mol	Chain	Res	Type
1	1	2147	A
1	1	2148	G
1	1	2149	U
1	1	2150	C
1	1	2151	U
1	1	2153	C
1	1	2154	A
1	1	2155	U
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2160	C
1	1	2162	G
1	1	2164	C
1	1	2165	C
1	1	2167	U
1	1	2168	G
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2176	A
1	1	2178	C
1	1	2179	C
1	1	2180	U
1	1	2181	U
1	1	2183	A
1	1	2185	U
1	1	2186	G
1	1	2189	U
1	1	2190	G
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2199	A
1	1	2203	U
1	1	2204	G
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2214	C

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Mol	Chain	Res	Type
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	2244	U
1	1	2247	A
1	1	2249	U
1	1	2250	G
1	1	2258	C
1	1	2259	U
1	1	2266	A
1	1	2267	A
1	1	2269	G
1	1	2279	G
1	1	2283	C
1	1	2286	G
1	1	2298	A
1	1	2305	U
1	1	2307	G
1	1	2309	A
1	1	2312	U
1	1	2318	G
1	1	2319	G
1	1	2320	U
1	1	2321	U
1	1	2325	G
1	1	2327	A
1	1	2334	U
1	1	2335	A
1	1	2336	A
1	1	2337	G
1	1	2343	U
1	1	2345	G
1	1	2346	A
1	1	2347	C
1	1	2350	C
1	1	2352	A
1	1	2355	G
1	1	2357	G
1	1	2359	C

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Mol	Chain	Res	Type
1	1	2361	G
1	1	2365	G
1	1	2374	C
1	1	2383	G
1	1	2385	C
1	1	2388	A
1	1	2389	G
1	1	2394	C
1	1	2402	U
1	1	2403	C
1	1	2407	A
1	1	2410	G
1	1	2412	A
1	1	2413	G
1	1	2421	G
1	1	2422	C
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2428	G
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2433	A
1	1	2435	A
1	1	2440	C
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2452	C
1	1	2457	PSU
1	1	2458	G
1	1	2468	A
1	1	2469	A
1	1	2470	G
1	1	2476	A
1	1	2477	U
1	1	2478	A
1	1	2484	G
1	1	2486	C

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Mol	Chain	Res	Type
1	1	2487	G
1	1	2489	U
1	1	2491	U
1	1	2497	A
1	1	2498	OMC
1	1	2499	C
1	1	2501	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	2534	A
1	1	2535	G
1	1	2538	C
1	1	2543	G
1	1	2545	G
1	1	2547	A
1	1	2552	OMU
1	1	2553	G
1	1	2554	U
1	1	2562	U
1	1	2564	A
1	1	2565	A
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2575	C
1	1	2577	A
1	1	2578	G
1	1	2580	PSU
1	1	2581	G
1	1	2584	U
1	1	2585	U
1	1	2587	A
1	1	2599	G
1	1	2601	C

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Mol	Chain	Res	Type
1	1	2602	A
1	1	2603	G
1	1	2605	PSU
1	1	2606	C
1	1	2608	G
1	1	2609	U
1	1	2612	C
1	1	2613	U
1	1	2621	G
1	1	2629	U
1	1	2630	G
1	1	2634	A
1	1	2640	G
1	1	2641	G
1	1	2645	G
1	1	2646	C
1	1	2650	U
1	1	2661	G
1	1	2662	A
1	1	2663	G
1	1	2668	G
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2692	G
1	1	2698	U
1	1	2706	A
1	1	2707	U
1	1	2713	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2722	G
1	1	2724	U
1	1	2727	A
1	1	2728	U
1	1	2733	A
1	1	2736	A
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2751	G

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Mol	Chain	Res	Type
1	1	2752	C
1	1	2757	A
1	1	2759	G
1	1	2760	C
1	1	2764	A
1	1	2765	A
1	1	2766	A
1	1	2778	A
1	1	2780	G
1	1	2784	U
1	1	2790	U
1	1	2791	G
1	1	2793	C
1	1	2794	C
1	1	2796	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2824	C
1	1	2826	A
1	1	2828	G
1	1	2829	A
1	1	2830	C
1	1	2832	U
1	1	2833	U
1	1	2834	G
1	1	2837	A
1	1	2839	G
1	1	2849	U
1	1	2858	C
1	1	2860	A
1	1	2861	U
1	1	2866	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2881	U
1	1	2883	A

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Mol	Chain	Res	Type
1	1	2884	U
1	1	2885	G
1	1	2886	A
1	1	2891	U
1	1	2893	A
1	1	2894	G
1	1	2895	G
1	1	2901	C
2	2	2	A
2	2	4	U
2	2	5	U
2	2	6	G
2	2	9	G
2	2	19	A
2	2	22	G
2	2	30	U
2	2	32	A
2	2	39	G
2	2	41	G
2	2	44	A
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	68	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	73	C
2	2	74	A
2	2	75	G
2	2	77	A
2	2	80	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	88	U
2	2	89	U

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Mol	Chain	Res	Type
2	2	90	C
2	2	92	U
2	2	93	U
2	2	94	G
2	2	95	C
2	2	96	U
2	2	100	G
2	2	107	G
2	2	108	G
2	2	116	A
2	2	120	A
2	2	121	U
2	2	122	G
2	2	124	C
2	2	127	G
2	2	130	A
2	2	131	A
2	2	132	C
2	2	142	G
2	2	144	G
2	2	160	A
2	2	163	C
2	2	167	A
2	2	168	G
2	2	172	A
2	2	181	A
2	2	182	A
2	2	183	C
2	2	191	G
2	2	197	A
2	2	203	G
2	2	204	G
2	2	207	C
2	2	210	C
2	2	211	G
2	2	212	G
2	2	213	G
2	2	214	C
2	2	216	U
2	2	226	G
2	2	228	A
2	2	231	U

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Mol	Chain	Res	Type
2	2	238	A
2	2	240	G
2	2	243	A
2	2	245	U
2	2	247	G
2	2	251	G
2	2	257	G
2	2	265	G
2	2	266	G
2	2	267	C
2	2	272	C
2	2	279	A
2	2	280	C
2	2	289	G
2	2	290	C
2	2	298	A
2	2	303	A
2	2	306	A
2	2	315	A
2	2	316	C
2	2	319	G
2	2	322	C
2	2	328	C
2	2	330	C
2	2	332	G
2	2	337	G
2	2	346	G
2	2	347	G
2	2	351	G
2	2	352	C
2	2	354	G
2	2	355	C
2	2	366	A
2	2	367	U
2	2	372	C
2	2	373	A
2	2	376	G
2	2	384	G
2	2	388	G
2	2	389	A
2	2	390	U
2	2	393	A

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Mol	Chain	Res	Type
2	2	394	G
2	2	398	U
2	2	399	G
2	2	406	G
2	2	411	A
2	2	413	G
2	2	414	A
2	2	417	G
2	2	421	U
2	2	422	C
2	2	423	G
2	2	424	G
2	2	426	U
2	2	428	G
2	2	429	U
2	2	435	A
2	2	440	C
2	2	451	A
2	2	454	G
2	2	463	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	474	G
2	2	477	C
2	2	481	G
2	2	482	A
2	2	484	G
2	2	485	U
2	2	486	U
2	2	492	C
2	2	494	G
2	2	495	A
2	2	496	A
2	2	497	G
2	2	506	G
2	2	507	C
2	2	508	U
2	2	509	A
2	2	510	A
2	2	513	C
2	2	514	C

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Mol	Chain	Res	Type
2	2	516	PSU
2	2	517	G
2	2	518	C
2	2	519	C
2	2	520	A
2	2	527	7MG
2	2	531	U
2	2	532	A
2	2	533	A
2	2	534	U
2	2	542	G
2	2	545	C
2	2	546	A
2	2	547	A
2	2	551	U
2	2	552	U
2	2	553	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	581	G
2	2	590	U
2	2	592	G
2	2	596	A
2	2	607	A
2	2	631	C
2	2	633	G
2	2	639	G
2	2	644	U
2	2	653	U
2	2	656	G
2	2	661	G
2	2	664	G
2	2	665	A
2	2	666	G
2	2	671	G
2	2	672	U
2	2	675	A

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Mol	Chain	Res	Type
2	2	676	A
2	2	679	C
2	2	685	G
2	2	687	A
2	2	696	A
2	2	703	G
2	2	704	A
2	2	705	G
2	2	717	U
2	2	718	A
2	2	720	C
2	2	721	G
2	2	724	G
2	2	725	G
2	2	731	G
2	2	747	A
2	2	752	G
2	2	753	A
2	2	755	G
2	2	773	G
2	2	774	G
2	2	776	G
2	2	777	A
2	2	787	A
2	2	792	A
2	2	793	U
2	2	794	A
2	2	799	G
2	2	803	G
2	2	810	C
2	2	811	C
2	2	813	U
2	2	814	A
2	2	815	A
2	2	817	C
2	2	818	G
2	2	821	G
2	2	828	U
2	2	832	G
2	2	842	U
2	2	843	U
2	2	844	G

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Mol	Chain	Res	Type
2	2	845	A
2	2	846	G
2	2	848	C
2	2	849	G
2	2	850	U
2	2	851	G
2	2	857	C
2	2	863	U
2	2	870	U
2	2	879	C
2	2	887	G
2	2	888	G
2	2	889	A
2	2	898	G
2	2	905	U
2	2	908	A
2	2	912	C
2	2	914	A
2	2	920	U
2	2	922	G
2	2	926	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	937	A
2	2	939	G
2	2	941	G
2	2	958	A
2	2	960	U
2	2	961	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	976	G
2	2	977	A
2	2	981	U
2	2	982	U
2	2	984	C
2	2	988	G
2	2	989	U

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Mol	Chain	Res	Type
2	2	992	U
2	2	993	G
2	2	996	A
2	2	997	U
2	2	999	C
2	2	1000	A
2	2	1001	C
2	2	1003	G
2	2	1004	A
2	2	1005	A
2	2	1007	U
2	2	1008	U
2	2	1010	U
2	2	1011	C
2	2	1012	A
2	2	1017	U
2	2	1018	G
2	2	1019	A
2	2	1020	G
2	2	1021	A
2	2	1022	A
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1034	G
2	2	1035	A
2	2	1036	A
2	2	1041	G
2	2	1042	A
2	2	1045	C
2	2	1046	A
2	2	1047	G
2	2	1050	G
2	2	1052	U
2	2	1053	G
2	2	1054	C
2	2	1056	U
2	2	1064	G
2	2	1065	U
2	2	1085	U

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Mol	Chain	Res	Type
2	2	1086	U
2	2	1088	G
2	2	1089	G
2	2	1091	U
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1108	G
2	2	1112	C
2	2	1124	G
2	2	1125	U
2	2	1126	U
2	2	1127	G
2	2	1129	C
2	2	1130	A
2	2	1131	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1150	A
2	2	1151	A
2	2	1157	A
2	2	1159	U
2	2	1167	A
2	2	1168	U
2	2	1171	A
2	2	1172	C
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1182	G
2	2	1183	U
2	2	1184	G
2	2	1185	G
2	2	1190	G
2	2	1193	G
2	2	1196	A
2	2	1197	A

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Mol	Chain	Res	Type
2	2	1198	G
2	2	1200	C
2	2	1201	A
2	2	1202	U
2	2	1211	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1224	U
2	2	1225	A
2	2	1227	A
2	2	1235	U
2	2	1238	A
2	2	1239	A
2	2	1240	U
2	2	1241	G
2	2	1242	G
2	2	1244	G
2	2	1246	A
2	2	1247	U
2	2	1248	A
2	2	1249	C
2	2	1253	G
2	2	1256	A
2	2	1257	A
2	2	1258	G
2	2	1261	A
2	2	1262	C
2	2	1263	C
2	2	1265	C
2	2	1266	G
2	2	1267	C
2	2	1268	G
2	2	1269	A
2	2	1271	A
2	2	1272	G
2	2	1274	A
2	2	1277	C
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1283	U

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Mol	Chain	Res	Type
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1290	G
2	2	1291	U
2	2	1292	G
2	2	1297	G
2	2	1298	U
2	2	1299	A
2	2	1302	C
2	2	1303	C
2	2	1304	G
2	2	1305	G
2	2	1307	U
2	2	1308	U
2	2	1312	G
2	2	1317	C
2	2	1318	A
2	2	1319	A
2	2	1324	A
2	2	1331	G
2	2	1332	A
2	2	1335	U
2	2	1336	C
2	2	1341	U
2	2	1342	C
2	2	1348	U
2	2	1353	G
2	2	1361	G
2	2	1363	A
2	2	1364	U
2	2	1365	G
2	2	1374	A
2	2	1375	A
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1385	G
2	2	1397	C
2	2	1398	A
2	2	1399	C
2	2	1401	G

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Mol	Chain	Res	Type
2	2	1402	4OC
2	2	1405	G
2	2	1407	5MC
2	2	1408	A
2	2	1418	A
2	2	1422	G
2	2	1430	A
2	2	1431	A
2	2	1432	G
2	2	1433	A
2	2	1441	A
2	2	1442	G
2	2	1444	U
2	2	1445	U
2	2	1446	A
2	2	1447	A
2	2	1452	C
2	2	1453	G
2	2	1466	C
2	2	1473	G
2	2	1478	U
2	2	1481	U
2	2	1484	C
2	2	1485	U
2	2	1486	G
2	2	1490	U
2	2	1491	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1502	A
2	2	1503	A
2	2	1504	G
2	2	1506	U
2	2	1507	A
2	2	1517	G
2	2	1518	MA6
2	2	1520	C
2	2	1529	G
2	2	1530	G

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Mol	Chain	Res	Type
2	2	1532	U
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	12	C
3	3	14	U
3	3	15	A
3	3	17	C
3	3	18	G
3	3	30	C
3	3	31	C
3	3	32	U
3	3	33	G
3	3	35	C
3	3	36	C
3	3	37	C
3	3	41	G
3	3	42	C
3	3	44	G
3	3	45	A
3	3	51	G
3	3	57	A
3	3	70	C
3	3	73	A
3	3	80	U
3	3	88	C
3	3	89	U
3	3	90	C
3	3	91	C
3	3	92	C
3	3	99	A
3	3	103	U
3	3	107	G
3	3	109	A
3	3	113	C
3	3	119	A
3	3	120	U
57	4	6	U
57	4	8	A
57	4	9	U
57	4	10	U
57	4	11	C

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Mol	Chain	Res	Type
57	4	13	G
57	4	14	G
57	4	15	A
57	4	16	U
57	4	17	U
57	4	18	C
57	4	19	G
57	4	20	A
57	4	21	C
57	4	28	U
57	4	30	C
57	4	32	A
57	4	33	A
57	4	34	A
57	4	35	C
57	4	38	A
57	4	39	A
57	4	40	G
57	4	43	G
57	4	44	C
57	4	45	A
57	4	47	G
57	4	49	C
57	4	54	G
57	4	55	G
57	4	56	C
57	4	60	U
57	4	61	G
57	4	62	G
57	4	63	C
57	4	64	C
57	4	68	U
57	4	69	A
57	4	70	A
57	4	71	A
57	4	72	A
57	4	73	A
57	4	79	A
57	4	80	A
57	4	81	A
57	4	82	A
57	4	83	A

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Mol	Chain	Res	Type
57	4	84	A
57	4	85	U
57	4	86	A
57	4	87	G
57	4	88	U
57	4	89	C
57	4	92	A
57	4	93	A
57	4	94	A
57	4	95	C
57	4	96	G
57	4	97	A
57	4	99	G
57	4	101	A
57	4	102	A
57	4	105	U
57	4	106	A
57	4	107	C
57	4	114	G
57	4	117	G
57	4	119	U
57	4	121	A
57	4	122	A
57	4	125	A
57	4	127	C
57	4	129	G
57	4	130	C
57	4	131	U
57	4	132	U
57	4	133	A
57	4	138	C
57	4	143	C
57	4	145	C
57	4	149	A
57	4	150	G
57	4	151	C
57	4	154	C
57	4	155	C
57	4	156	G
57	4	158	U
57	4	162	A
57	4	164	G

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Mol	Chain	Res	Type
57	4	165	A
57	4	166	C
57	4	168	G
57	4	169	G
57	4	170	G
57	4	172	U
57	4	173	C
57	4	174	A
57	4	175	A
57	4	176	G
57	4	180	G
57	4	181	G
57	4	182	U
57	4	183	C
57	4	184	A
57	4	185	A
57	4	186	A
57	4	188	C
57	4	189	C
57	4	190	A
57	4	191	A
57	4	192	A
57	4	193	A
57	4	194	G
57	4	195	A
57	4	197	A
57	4	198	U
57	4	199	C
57	4	200	G
57	4	203	U
57	4	204	G
57	4	205	G
57	4	206	A
57	4	207	A
57	4	210	C
57	4	211	C
57	4	213	G
57	4	216	U
57	4	218	G
57	4	219	G
57	4	222	U
57	4	223	G

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Mol	Chain	Res	Type
57	4	224	A
57	4	225	A
57	4	226	G
57	4	227	C
57	4	228	G
57	4	229	U
57	4	230	U
57	4	231	A
57	4	233	A
57	4	234	A
57	4	235	C
57	4	236	U
57	4	237	U
57	4	238	A
57	4	239	A
57	4	241	C
57	4	242	A
57	4	244	G
57	4	245	C
57	4	246	U
57	4	247	A
57	4	248	G
57	4	249	U
57	4	250	U
57	4	257	U
57	4	258	G
57	4	261	G
57	4	262	U
57	4	263	G
57	4	264	U
57	4	266	C
57	4	267	G
57	4	268	U
57	4	269	C
57	4	270	C
57	4	271	G
57	4	273	A
57	4	274	G
57	4	282	G
57	4	285	A
57	4	286	A
57	4	288	G

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Mol	Chain	Res	Type
57	4	291	A
57	4	292	A
57	4	293	G
57	4	296	U
57	4	299	C
57	4	300	U
57	4	302	A
57	4	303	G
57	4	308	U
57	4	309	A
57	4	310	G
57	4	312	A
57	4	315	G
57	4	316	A
57	4	317	G
57	4	318	G
57	4	319	A
57	4	321	G
57	4	322	U
57	4	323	A
57	4	324	G
57	4	325	G
57	4	332	G
57	4	333	G
57	4	334	A
57	4	335	C
57	4	336	G
57	4	339	G
57	4	340	G
57	4	347	U
57	4	348	C
57	4	351	G
57	4	357	U
57	4	358	C
57	4	359	C
57	4	360	A
57	4	362	C
57	4	363	A

All (60) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	1	56	A
1	1	70	G
1	1	404	A
1	1	613	A
1	1	784	G
1	1	882	G
1	1	883	G
1	1	894	U
1	1	955	PSU
1	1	1379	U
1	1	1911	PSU
1	1	1917	PSU
1	1	2132	U
1	1	2146	C
1	1	2425	A
1	1	2457	PSU
1	1	2498	OMC
1	1	2504	PSU
1	1	2580	PSU
1	1	2605	PSU
1	1	2706	A
1	1	2756	U
2	2	8	A
2	2	83	C
2	2	512	U
2	2	516	PSU
2	2	884	U
2	2	1109	C
2	2	1214	C
57	4	9	U
57	4	10	U
57	4	13	G
57	4	14	G
57	4	15	A
57	4	17	U
57	4	19	G
57	4	20	A
57	4	32	A
57	4	33	A
57	4	38	A
57	4	61	G

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Mol	Chain	Res	Type
57	4	68	U
57	4	130	C
57	4	153	U
57	4	183	C
57	4	212	U
57	4	223	G
57	4	229	U
57	4	233	A
57	4	237	U
57	4	245	C
57	4	247	A
57	4	249	U
57	4	257	U
57	4	261	G
57	4	290	A
57	4	308	U
57	4	314	C
57	4	332	G
57	4	333	G

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
47	0TD	q	89	47	7,9,10	1.40	1 (14%)	6,11,13	2.63	3 (50%)
1	OMU	1	2552	1	19,22,23	2.60	7 (36%)	26,31,34	2.09	7 (26%)
1	PSU	1	2457	1	18,21,22	1.96	5 (27%)	22,30,33	2.30	5 (22%)
1	5MU	1	747	1	19,22,23	1.41	5 (26%)	28,32,35	2.17	7 (25%)
2	7MG	2	527	2	22,26,27	1.37	4 (18%)	29,39,42	2.59	8 (27%)
1	5MC	1	1962	1	18,22,23	2.08	3 (16%)	26,32,35	1.59	2 (7%)
2	MA6	2	1518	2	23,26,27	1.29	3 (13%)	34,38,41	2.18	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MA6	2	1519	2	23,26,27	1.28	4 (17%)	34,38,41	2.12	9 (26%)
1	2MA	1	2503	1,58	22,25,26	1.59	4 (18%)	33,37,40	2.27	8 (24%)
1	PSU	1	2605	1	18,21,22	1.93	5 (27%)	22,30,33	2.09	3 (13%)
1	5MU	1	1939	1,58	19,22,23	1.41	4 (21%)	28,32,35	2.35	7 (25%)
2	2MG	2	1516	2	23,26,27	2.66	6 (26%)	32,38,41	2.18	7 (21%)
1	1MG	1	745	1	22,26,27	1.18	2 (9%)	33,39,42	1.90	6 (18%)
1	PSU	1	1911	1	18,21,22	1.96	5 (27%)	22,30,33	2.14	4 (18%)
1	OMC	1	2498	1,58	19,22,23	1.86	6 (31%)	26,31,34	2.16	6 (23%)
2	PSU	2	516	2,58	18,21,22	1.44	3 (16%)	22,30,33	2.14	5 (22%)
1	OMG	1	2251	1,57	23,26,27	2.68	7 (30%)	33,38,41	1.94	7 (21%)
1	G7M	1	2069	1	23,26,27	1.65	3 (13%)	35,39,42	1.81	6 (17%)
1	2MG	1	1835	1	23,26,27	2.60	6 (26%)	32,38,41	2.51	11 (34%)
2	5MC	2	967	2	18,22,23	2.07	3 (16%)	26,32,35	1.43	4 (15%)
1	6MZ	1	1618	1	22,25,26	2.74	3 (13%)	30,36,39	2.61	11 (36%)
1	PSU	1	1917	1,58	18,21,22	2.00	5 (27%)	22,30,33	1.95	5 (22%)
2	2MG	2	1207	2	23,26,27	2.68	6 (26%)	32,38,41	2.24	7 (21%)
2	4OC	2	1402	2	20,23,24	0.83	1 (5%)	26,32,35	1.33	4 (15%)
2	2MG	2	966	2	23,26,27	2.63	6 (26%)	32,38,41	2.34	10 (31%)
1	PSU	1	746	1	18,21,22	1.40	2 (11%)	22,30,33	2.23	6 (27%)
2	5MC	2	1407	2	18,22,23	2.13	3 (16%)	26,32,35	1.40	3 (11%)
1	6MZ	1	2030	1	22,25,26	2.68	5 (22%)	30,36,39	2.96	12 (40%)
1	PSU	1	2504	1	18,21,22	2.05	6 (33%)	22,30,33	2.15	5 (22%)
1	2MG	1	2445	1	23,26,27	2.68	6 (26%)	32,38,41	2.40	7 (21%)
1	3TD	1	1915	1	18,22,23	2.71	7 (38%)	22,32,35	1.45	1 (4%)
1	PSU	1	955	1	18,21,22	1.43	3 (16%)	22,30,33	2.08	5 (22%)
1	PSU	1	2580	1	18,21,22	2.07	5 (27%)	22,30,33	2.35	6 (27%)
2	UR3	2	1498	2,58	19,22,23	2.76	6 (31%)	26,32,35	1.23	2 (7%)

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
47	0TD	q	89	47	-	2/7/12/14	-
1	OMU	1	2552	1	2/2/5/5	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	2457	1	2/2/5/5	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
2	7MG	2	527	2	-	2/7/37/38	0/3/3/3
1	5MC	1	1962	1	-	2/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	3/11/29/30	0/3/3/3
2	MA6	2	1519	2	-	3/11/29/30	0/3/3/3
1	2MA	1	2503	1,58	2/2/5/5	5/7/25/26	0/3/3/3
1	PSU	1	2605	1	2/2/5/5	3/7/25/26	0/2/2/2
1	5MU	1	1939	1,58	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	1/9/27/28	0/3/3/3
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
1	PSU	1	1911	1	2/2/5/5	3/7/25/26	0/2/2/2
1	OMC	1	2498	1,58	1/1/5/5	5/9/27/28	0/2/2/2
2	PSU	2	516	2,58	-	3/7/25/26	0/2/2/2
1	OMG	1	2251	1,57	1/1/5/5	2/9/27/28	0/3/3/3
1	G7M	1	2069	1	3/3/5/5	2/7/25/26	0/3/3/3
1	2MG	1	1835	1	-	3/9/27/28	0/3/3/3
2	5MC	2	967	2	-	3/7/25/26	0/2/2/2
1	6MZ	1	1618	1	2/2/5/6	5/9/27/28	0/3/3/3
1	PSU	1	1917	1,58	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
2	4OC	2	1402	2	-	3/9/29/30	0/2/2/2
2	2MG	2	966	2	-	0/9/27/28	0/3/3/3
1	PSU	1	746	1	-	2/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	2/7/25/26	0/2/2/2
1	6MZ	1	2030	1	2/2/5/6	4/9/27/28	0/3/3/3
1	PSU	1	2504	1	2/2/5/5	4/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	4/9/27/28	0/3/3/3
1	3TD	1	1915	1	1/1/5/5	4/7/25/26	0/2/2/2
1	PSU	1	955	1	-	3/7/25/26	0/2/2/2
1	PSU	1	2580	1	2/2/5/5	2/7/25/26	0/2/2/2
2	UR3	2	1498	2,58	-	6/7/25/26	0/2/2/2

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1618	6MZ	C6-N6	11.64	1.46	1.34
1	1	2030	6MZ	C6-N6	10.71	1.45	1.34
2	2	966	2MG	O6-C6	9.44	1.41	1.23
2	2	1207	2MG	O6-C6	9.29	1.41	1.23
1	1	2251	OMG	O6-C6	9.24	1.41	1.23
2	2	1516	2MG	O6-C6	9.15	1.41	1.23
1	1	2445	2MG	O6-C6	8.98	1.40	1.23
1	1	1835	2MG	O6-C6	8.72	1.40	1.23
2	2	1498	UR3	O4-C4	8.46	1.41	1.23
1	1	1915	3TD	O4-C4	8.18	1.40	1.23
1	1	2552	OMU	O4-C4	7.95	1.39	1.24
2	2	967	5MC	C4-N4	6.43	1.50	1.34
1	1	1962	5MC	C4-N4	6.21	1.50	1.34
2	2	1407	5MC	C4-N4	6.15	1.50	1.34
2	2	966	2MG	C2-N2	6.08	1.46	1.33
1	1	2069	G7M	C5-N7	-5.81	1.32	1.39
2	2	1516	2MG	C2-N2	5.81	1.46	1.33
2	2	1207	2MG	C2-N2	5.75	1.46	1.33
1	1	1835	2MG	C2-N2	5.41	1.45	1.33
2	2	1407	5MC	C2-N1	-5.12	1.28	1.40
1	1	2445	2MG	C2-N2	4.99	1.44	1.33
1	1	1962	5MC	C2-N1	-4.89	1.29	1.40
1	1	2251	OMG	C2-N2	4.88	1.45	1.34
1	1	2504	PSU	C4-N3	-4.87	1.29	1.38
2	2	967	5MC	C2-N1	-4.71	1.29	1.40
1	1	2498	OMC	C4-N4	4.71	1.45	1.33
1	1	2457	PSU	C4-N3	-4.61	1.30	1.38
1	1	2605	PSU	C4-N3	-4.58	1.30	1.38
1	1	2580	PSU	C2-N1	-4.45	1.30	1.36
1	1	1917	PSU	C6-C5	4.42	1.40	1.35
1	1	1911	PSU	C4-N3	-4.41	1.30	1.38
1	1	2445	2MG	C6-N1	-4.37	1.30	1.38
1	1	2580	PSU	C4-N3	-4.34	1.30	1.38
1	1	1917	PSU	C4-N3	-4.33	1.30	1.38
1	1	1915	3TD	C2-N1	-4.21	1.31	1.37
1	1	2503	2MA	C6-N6	4.20	1.44	1.34
2	2	1498	UR3	C4-N3	-4.12	1.31	1.40
2	2	1498	UR3	C2-N1	-4.11	1.32	1.38
1	1	2251	OMG	C6-N1	-4.09	1.31	1.38
1	1	2552	OMU	C4-N3	-3.91	1.31	1.38
1	1	2580	PSU	C6-N1	-3.81	1.29	1.36
1	1	1835	2MG	C6-N1	-3.80	1.31	1.38
1	1	2030	6MZ	C8-N9	-3.79	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2445	2MG	C2-N1	-3.79	1.30	1.36
1	1	2605	PSU	C6-C5	3.78	1.39	1.35
1	1	2580	PSU	C6-C5	3.75	1.39	1.35
1	1	2457	PSU	C6-C5	3.73	1.39	1.35
2	2	1207	2MG	C6-N1	-3.63	1.32	1.38
1	1	2504	PSU	C2-N1	-3.61	1.31	1.36
1	1	1911	PSU	C6-C5	3.61	1.39	1.35
1	1	1911	PSU	C2-N1	-3.60	1.31	1.36
2	2	1516	2MG	C6-N1	-3.55	1.32	1.38
1	1	2504	PSU	C6-C5	3.53	1.39	1.35
2	2	527	7MG	C4-N9	-3.49	1.33	1.37
1	1	2552	OMU	C2-N3	-3.46	1.31	1.38
2	2	1519	MA6	C8-N9	-3.45	1.31	1.37
1	1	1917	PSU	C2-N1	-3.45	1.32	1.36
1	1	2457	PSU	C6-N1	-3.43	1.30	1.36
1	1	1618	6MZ	C8-N9	-3.40	1.31	1.37
2	2	1518	MA6	C8-N9	-3.37	1.31	1.37
1	1	2552	OMU	C2-N1	-3.33	1.33	1.38
1	1	2457	PSU	C2-N1	-3.31	1.32	1.36
1	1	745	1MG	C5-C4	3.30	1.48	1.38
1	1	1911	PSU	C6-N1	-3.30	1.30	1.36
1	1	1915	3TD	C4-N3	-3.29	1.33	1.40
1	1	2503	2MA	C8-N9	-3.28	1.31	1.37
1	1	1835	2MG	C2-N1	-3.27	1.31	1.36
1	1	2504	PSU	C6-N1	-3.22	1.30	1.36
1	1	2605	PSU	C6-N1	-3.21	1.30	1.36
2	2	1498	UR3	C2-N3	-3.21	1.32	1.39
2	2	1518	MA6	C6-N6	3.20	1.46	1.36
1	1	746	PSU	C6-C5	3.19	1.39	1.35
2	2	1516	2MG	C5-N7	-3.19	1.32	1.39
1	1	1917	PSU	C6-N1	-3.19	1.30	1.36
1	1	1618	6MZ	C5-N7	-3.13	1.33	1.39
1	1	1915	3TD	C6-C5	3.12	1.39	1.35
1	1	2445	2MG	C5-N7	-3.10	1.33	1.39
1	1	2498	OMC	O2-C2	-3.09	1.18	1.23
2	2	1498	UR3	O2-C2	-3.08	1.16	1.22
1	1	2605	PSU	C2-N1	-3.06	1.32	1.36
1	1	2251	OMG	C8-N9	-3.04	1.30	1.37
2	2	516	PSU	C6-C5	3.03	1.38	1.35
1	1	955	PSU	C4-N3	-3.02	1.33	1.38
2	2	516	PSU	C4-N3	-2.99	1.33	1.38
1	1	2445	2MG	C8-N9	-2.96	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1207	2MG	C5-N7	-2.94	1.33	1.39
1	1	1939	5MU	C4-N3	-2.94	1.33	1.38
1	1	1835	2MG	C8-N9	-2.92	1.31	1.37
2	2	1516	2MG	C8-N9	-2.91	1.31	1.37
1	1	1915	3TD	C2-N3	-2.89	1.32	1.38
2	2	966	2MG	C6-N1	-2.89	1.33	1.38
2	2	1207	2MG	C8-N9	-2.87	1.31	1.37
1	1	2069	G7M	C6-N1	-2.84	1.33	1.38
1	1	747	5MU	C6-C5	2.82	1.39	1.34
2	2	1207	2MG	C2-N1	-2.82	1.32	1.36
1	1	2251	OMG	C5-N7	-2.82	1.33	1.39
1	1	746	PSU	C4-N3	-2.79	1.33	1.38
1	1	2030	6MZ	C5-N7	-2.78	1.33	1.39
1	1	955	PSU	C6-C5	2.78	1.38	1.35
2	2	1518	MA6	C5-N7	-2.78	1.33	1.39
1	1	1835	2MG	C5-N7	-2.78	1.33	1.39
1	1	2503	2MA	C5-N7	-2.77	1.33	1.39
1	1	747	5MU	C4-N3	-2.77	1.33	1.38
2	2	527	7MG	C5-C4	2.76	1.47	1.38
2	2	1498	UR3	C6-N1	-2.68	1.31	1.38
1	1	2069	G7M	C5-C4	2.66	1.45	1.38
2	2	1407	5MC	C2-N3	-2.66	1.30	1.36
1	1	2251	OMG	C2-N1	-2.62	1.31	1.37
1	1	2251	OMG	O2'-CM2	-2.62	1.33	1.42
1	1	1939	5MU	C6-N1	-2.61	1.33	1.38
2	2	966	2MG	C8-N9	-2.57	1.31	1.37
1	1	2498	OMC	C2-N1	-2.55	1.34	1.40
1	1	2498	OMC	C5-C4	-2.52	1.37	1.42
1	1	2498	OMC	C2-N3	-2.48	1.31	1.36
2	2	1519	MA6	C6-N6	2.48	1.44	1.36
2	2	1519	MA6	C5-N7	-2.48	1.34	1.39
1	1	1915	3TD	C6-N1	-2.46	1.32	1.36
1	1	2552	OMU	C6-N1	-2.46	1.32	1.38
1	1	1962	5MC	C2-N3	-2.44	1.31	1.36
2	2	527	7MG	C6-N1	-2.43	1.34	1.38
1	1	1939	5MU	C2-N3	-2.41	1.33	1.38
1	1	1939	5MU	C6-C5	2.41	1.38	1.34
1	1	2503	2MA	C6-N1	-2.40	1.31	1.35
2	2	1516	2MG	C2-N1	-2.38	1.32	1.36
2	2	966	2MG	C5-N7	-2.36	1.34	1.39
1	1	2504	PSU	C2-N3	-2.36	1.33	1.37
1	1	2552	OMU	O2-C2	-2.36	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2580	PSU	C2-N3	-2.32	1.33	1.37
1	1	747	5MU	C4-C5	2.31	1.48	1.44
1	1	1911	PSU	C2-N3	-2.30	1.33	1.37
1	1	2498	OMC	C4-N3	-2.29	1.30	1.34
1	1	2605	PSU	C2-N3	-2.29	1.33	1.37
2	2	516	PSU	C2-N3	-2.24	1.33	1.37
1	1	747	5MU	C6-N1	-2.22	1.34	1.38
2	2	527	7MG	C5-N7	-2.20	1.33	1.35
2	2	967	5MC	C2-N3	-2.20	1.31	1.36
1	1	2552	OMU	C5-C4	-2.19	1.38	1.43
1	1	955	PSU	C2-N3	-2.19	1.33	1.37
1	1	1915	3TD	O2-C2	-2.18	1.19	1.23
1	1	2504	PSU	O4'-C1'	-2.16	1.40	1.43
1	1	2030	6MZ	C4-N9	-2.16	1.32	1.37
2	2	966	2MG	C2-N1	-2.14	1.33	1.36
1	1	1917	PSU	O4'-C1'	-2.11	1.40	1.43
1	1	2030	6MZ	C6-N1	-2.08	1.31	1.35
1	1	747	5MU	C2-N3	-2.07	1.34	1.38
1	1	745	1MG	C5-N7	-2.06	1.35	1.39
2	2	1519	MA6	C4-N9	-2.04	1.33	1.37
1	1	2457	PSU	C2-N3	-2.03	1.34	1.37
2	2	1402	4OC	C6-N1	-2.03	1.33	1.38
47	q	89	0TD	CSB-SB	-2.00	1.75	1.79

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2030	6MZ	C9-N6-C6	-9.62	114.59	122.87
2	2	527	7MG	N9-C4-N3	8.69	138.46	125.47
1	1	2503	2MA	C5-C4-N3	-7.78	118.44	127.19
2	2	966	2MG	C2-N3-C4	7.67	121.54	112.04
1	1	1835	2MG	C2-N3-C4	7.63	121.50	112.04
2	2	1207	2MG	C2-N3-C4	7.03	120.75	112.04
1	1	2445	2MG	C5-C4-N3	-6.95	117.19	128.46
1	1	2445	2MG	C2-N3-C4	6.91	120.61	112.04
1	1	2498	OMC	O2-C2-N3	-6.85	111.18	122.33
1	1	2457	PSU	N1-C2-N3	6.77	122.80	115.13
2	2	516	PSU	N1-C2-N3	6.77	122.80	115.13
2	2	1516	2MG	C2-N3-C4	6.68	120.32	112.04
1	1	1835	2MG	C5-C4-N3	-6.66	117.65	128.46
2	2	1207	2MG	C5-C4-N3	-6.48	117.95	128.46
1	1	1962	5MC	C5-C6-N1	-6.46	116.69	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2580	PSU	N1-C2-N3	6.41	122.39	115.13
1	1	746	PSU	N1-C2-N3	6.39	122.37	115.13
1	1	2605	PSU	N1-C2-N3	6.36	122.33	115.13
1	1	955	PSU	N1-C2-N3	6.35	122.32	115.13
2	2	1516	2MG	C5-C4-N3	-6.30	118.24	128.46
1	1	1911	PSU	N1-C2-N3	6.25	122.21	115.13
2	2	966	2MG	C5-C4-N3	-6.17	118.45	128.46
1	1	1618	6MZ	C9-N6-C6	-6.15	117.58	122.87
1	1	2504	PSU	N1-C2-N3	6.14	122.09	115.13
1	1	2503	2MA	N3-C4-N9	5.97	135.28	126.99
1	1	2251	OMG	C5-C4-N3	-5.88	118.93	128.46
1	1	1618	6MZ	C5-C4-N3	-5.79	119.20	126.75
1	1	2069	G7M	N9-C4-N3	5.77	137.53	125.94
2	2	1518	MA6	C5-C4-N3	-5.76	119.23	126.75
1	1	2030	6MZ	N1-C2-N3	-5.70	119.69	128.60
1	1	1939	5MU	C4-N3-C2	-5.66	120.02	127.35
1	1	1917	PSU	N1-C2-N3	5.65	121.53	115.13
2	2	527	7MG	N9-C8-N7	-5.61	95.35	103.38
1	1	745	1MG	C5-C4-N3	-5.61	119.35	128.46
1	1	2069	G7M	C5-C4-N3	-5.51	117.58	128.15
1	1	1915	3TD	N1-C2-N3	5.41	120.41	116.14
2	2	527	7MG	C5-C4-N3	-5.34	117.96	128.13
1	1	747	5MU	N3-C2-N1	5.28	121.89	114.89
1	1	2580	PSU	O2-C2-N1	-5.25	117.01	122.79
2	2	967	5MC	C5-C6-N1	-5.22	117.97	123.34
2	2	1519	MA6	C5-C4-N3	-5.18	120.00	126.75
1	1	747	5MU	C4-N3-C2	-5.17	120.66	127.35
2	2	1407	5MC	C5-C6-N1	-5.06	118.13	123.34
2	2	1207	2MG	N9-C4-N3	5.06	136.09	125.94
1	1	1939	5MU	C5-C4-N3	5.03	119.61	115.31
1	1	2552	OMU	N3-C2-N1	5.01	121.54	114.89
1	1	1835	2MG	N9-C4-N3	4.99	135.95	125.94
1	1	1939	5MU	N3-C2-N1	4.97	121.48	114.89
1	1	2445	2MG	N9-C4-N3	4.88	135.73	125.94
1	1	2552	OMU	C4-N3-C2	-4.81	120.24	126.58
2	2	1519	MA6	N1-C2-N3	-4.77	121.14	128.60
1	1	1835	2MG	C2-N1-C6	-4.70	119.07	124.48
2	2	1518	MA6	C2-N1-C6	4.65	122.75	111.75
1	1	2030	6MZ	C6-C5-N7	4.65	137.42	132.39
1	1	2457	PSU	O2-C2-N1	-4.64	117.68	122.79
2	2	966	2MG	N9-C4-N3	4.61	135.20	125.94
1	1	1618	6MZ	C5-N7-C8	4.59	110.03	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2457	PSU	C4-N3-C2	-4.59	119.73	126.34
1	1	2251	OMG	C2-N3-C4	4.59	120.47	112.30
1	1	1939	5MU	C5-C6-N1	-4.56	118.65	123.34
2	2	1516	2MG	N9-C4-N3	4.54	135.06	125.94
1	1	745	1MG	C2-N3-C4	4.54	122.18	111.98
1	1	2445	2MG	C2-N1-C6	-4.53	119.27	124.48
1	1	2605	PSU	C4-N3-C2	-4.49	119.87	126.34
1	1	2069	G7M	C2-N3-C4	4.48	120.27	112.30
2	2	1518	MA6	N1-C2-N3	-4.47	121.61	128.60
1	1	1618	6MZ	N1-C2-N3	-4.44	121.66	128.60
1	1	955	PSU	C4-N3-C2	-4.38	120.03	126.34
1	1	2498	OMC	C1'-N1-C2	4.36	128.14	118.42
1	1	1939	5MU	O4-C4-C5	-4.34	119.87	124.90
1	1	2030	6MZ	C5-C4-N3	-4.31	121.13	126.75
1	1	2504	PSU	C4-N3-C2	-4.29	120.16	126.34
1	1	745	1MG	N9-C4-N3	4.24	134.45	125.94
1	1	2030	6MZ	N9-C8-N7	-4.20	108.17	113.91
1	1	1911	PSU	O2-C2-N1	-4.17	118.20	122.79
2	2	1516	2MG	C2-N1-C6	-4.14	119.71	124.48
2	2	1519	MA6	C2-N1-C6	4.14	121.53	111.75
2	2	516	PSU	C4-N3-C2	-4.13	120.39	126.34
1	1	747	5MU	C5-C4-N3	4.12	118.83	115.31
1	1	746	PSU	C4-N3-C2	-4.11	120.41	126.34
47	q	89	0TD	OD2-CG-CB	4.10	122.01	113.15
2	2	527	7MG	C2-N3-C4	4.09	119.59	112.30
1	1	1911	PSU	C4-N3-C2	-4.06	120.49	126.34
1	1	2251	OMG	N9-C4-N3	4.00	133.97	125.94
1	1	2498	OMC	O2-C2-N1	3.99	127.12	118.89
1	1	1618	6MZ	C4-C5-N7	-3.98	105.78	110.62
1	1	2030	6MZ	C2-N3-C4	3.95	121.08	111.75
2	2	1518	MA6	N3-C4-N9	3.94	133.58	127.08
1	1	1618	6MZ	N3-C4-N9	3.92	133.54	127.08
1	1	2445	2MG	CM2-N2-C2	-3.86	115.33	123.86
1	1	1618	6MZ	N9-C8-N7	-3.84	108.66	113.91
1	1	2580	PSU	C4-N3-C2	-3.79	120.89	126.34
2	2	1498	UR3	C4-N3-C2	-3.78	121.01	124.56
1	1	2504	PSU	O2-C2-N1	-3.76	118.65	122.79
2	2	1519	MA6	C2-N3-C4	3.76	120.62	111.75
1	1	747	5MU	C5-C6-N1	-3.73	119.50	123.34
1	1	1917	PSU	O2-C2-N1	-3.73	118.69	122.79
1	1	747	5MU	O4-C4-C5	-3.71	120.60	124.90
2	2	1518	MA6	C2-N3-C4	3.69	120.48	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1618	6MZ	C2-N3-C4	3.68	120.44	111.75
1	1	2580	PSU	C6-C5-C4	-3.68	115.63	118.20
1	1	2030	6MZ	C5-N7-C8	3.64	108.68	103.51
1	1	2552	OMU	C5-C4-N3	3.61	120.25	114.84
2	2	1519	MA6	N3-C4-N9	3.61	133.03	127.08
2	2	966	2MG	C2-N1-C6	-3.59	120.35	124.48
1	1	1917	PSU	C4-N3-C2	-3.57	121.20	126.34
2	2	516	PSU	O2-C2-N1	-3.55	118.88	122.79
1	1	2503	2MA	N9-C8-N7	-3.51	109.11	113.91
1	1	955	PSU	O2-C2-N1	-3.49	118.95	122.79
2	2	1519	MA6	N9-C8-N7	-3.47	109.17	113.91
1	1	746	PSU	O2'-C2'-C1'	-3.46	102.98	111.23
2	2	1402	4OC	C2'-C1'-N1	-3.46	107.51	114.22
1	1	1939	5MU	O2-C2-N1	-3.41	118.25	122.79
1	1	746	PSU	O2-C2-N1	-3.40	119.04	122.79
2	2	1518	MA6	C4-C5-N7	-3.38	106.50	110.62
1	1	2030	6MZ	C4-C5-N7	-3.38	106.51	110.62
2	2	1519	MA6	C5-N7-C8	3.34	108.25	103.51
1	1	2030	6MZ	C4-N9-C8	3.30	109.31	105.73
47	q	89	0TD	CSB-SB-CB	3.30	108.41	102.44
1	1	747	5MU	O2-C2-N1	-3.29	118.41	122.79
1	1	2503	2MA	C5-N7-C8	3.27	108.15	103.51
1	1	2605	PSU	O2-C2-N1	-3.24	119.22	122.79
2	2	1519	MA6	C4-C5-N7	-3.23	106.68	110.62
1	1	2552	OMU	CM2-O2'-C2'	-3.18	106.19	114.52
1	1	2498	OMC	C6-N1-C2	-3.15	115.02	120.49
2	2	1207	2MG	C2-N1-C6	-3.15	120.85	124.48
2	2	1518	MA6	C5-N7-C8	3.12	107.94	103.51
1	1	1835	2MG	CM2-N2-C2	-3.10	117.02	123.86
1	1	2251	OMG	C2-N1-C6	-3.08	119.49	125.10
47	q	89	0TD	OD1-CG-CB	-3.06	116.03	122.44
1	1	745	1MG	C4-C5-N7	-3.01	105.96	110.72
1	1	1618	6MZ	C6-C5-N7	3.01	135.64	132.39
1	1	1835	2MG	C5-C6-N1	2.97	120.73	113.19
2	2	1519	MA6	C4-N9-C8	2.94	108.92	105.73
1	1	2069	G7M	O6-C6-C5	-2.88	121.56	128.06
1	1	2552	OMU	O4-C4-C5	-2.88	120.09	125.16
1	1	2580	PSU	C6-N1-C2	-2.86	119.76	122.68
2	2	1407	5MC	O2-C2-N3	-2.86	117.69	122.33
2	2	1516	2MG	O6-C6-C5	-2.84	119.07	126.60
2	2	516	PSU	O3'-C3'-C2'	2.81	120.93	111.82
1	1	2503	2MA	N3-C2-N1	-2.80	120.57	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2503	2MA	C4-N9-C8	2.79	108.75	105.73
1	1	745	1MG	C6-C5-N7	2.78	135.65	129.35
1	1	2251	OMG	O6-C6-C5	-2.78	119.22	126.60
1	1	2030	6MZ	N3-C4-N9	2.70	131.53	127.08
2	2	1518	MA6	C4-C5-C6	2.69	118.89	115.88
2	2	1402	4OC	O4'-C1'-N1	2.67	114.46	108.36
1	1	2552	OMU	O3'-C3'-C4'	2.66	118.74	111.05
2	2	527	7MG	O3'-C3'-C4'	2.65	118.72	111.05
2	2	966	2MG	C5-C6-N1	2.64	119.88	113.19
1	1	2251	OMG	C5-C6-N1	2.63	119.87	113.19
2	2	967	5MC	O2-C2-N3	-2.63	118.06	122.33
1	1	747	5MU	C2'-C1'-N1	-2.63	105.78	113.22
1	1	1939	5MU	O3'-C3'-C4'	-2.62	103.47	111.05
1	1	2251	OMG	CM2-O2'-C2'	-2.62	107.66	114.52
2	2	527	7MG	C5-C6-N1	2.61	115.59	110.99
1	1	1962	5MC	O2-C2-N3	-2.55	118.18	122.33
1	1	1911	PSU	C6-N1-C2	-2.54	120.08	122.68
1	1	955	PSU	C2'-C3'-C4'	2.53	107.56	102.64
1	1	2445	2MG	C5-C6-N1	2.52	119.59	113.19
2	2	966	2MG	O6-C6-C5	-2.51	119.94	126.60
2	2	1207	2MG	CM2-N2-C2	-2.48	118.38	123.86
1	1	1835	2MG	O6-C6-C5	-2.48	120.03	126.60
2	2	1518	MA6	C9-N6-C6	2.46	126.78	120.40
1	1	1835	2MG	N9-C8-N7	-2.45	108.78	113.39
1	1	746	PSU	O3'-C3'-C2'	2.43	119.69	111.82
1	1	746	PSU	C5-C6-N1	-2.41	118.50	122.11
1	1	2503	2MA	C4-C5-N7	-2.41	107.69	110.62
2	2	1207	2MG	O6-C6-C5	-2.37	120.30	126.60
2	2	1516	2MG	C5-C6-N1	2.37	119.20	113.19
1	1	2069	G7M	C5-C6-N1	2.34	116.67	111.79
1	1	1618	6MZ	C4-N9-C8	2.31	108.24	105.73
2	2	1498	UR3	C3U-N3-C2	2.31	121.36	117.31
2	2	1516	2MG	CM2-N2-C2	-2.30	118.79	123.86
2	2	1518	MA6	C1'-N9-C8	-2.29	121.96	127.14
1	1	2498	OMC	CM2-O2'-C2'	-2.29	108.53	114.52
2	2	1402	4OC	C6-C5-C4	2.28	119.75	116.96
2	2	1207	2MG	C5-C6-N1	2.28	118.99	113.19
1	1	1618	6MZ	C4-C5-C6	2.26	118.56	116.81
2	2	966	2MG	N9-C8-N7	-2.26	109.13	113.39
2	2	967	5MC	C5-C4-N3	-2.24	119.25	121.67
2	2	527	7MG	O6-C6-C5	-2.23	122.06	127.54
2	2	967	5MC	N1-C2-N3	2.22	122.86	118.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2504	PSU	C6-N1-C2	-2.22	120.41	122.68
1	1	745	1MG	C8-N7-C5	2.22	108.25	104.24
1	1	1835	2MG	C8-N7-C5	2.21	108.24	104.24
1	1	2503	2MA	C2-N3-C4	2.21	122.42	116.99
1	1	2457	PSU	O3'-C3'-C4'	2.20	117.40	111.05
1	1	1917	PSU	C6-N1-C2	-2.17	120.47	122.68
1	1	2457	PSU	C6-N1-C2	-2.15	120.48	122.68
2	2	516	PSU	O2'-C2'-C1'	-2.14	106.12	111.23
1	1	2552	OMU	O2-C2-N3	-2.14	117.51	121.50
2	2	966	2MG	C6-C5-N7	2.14	134.23	130.25
2	2	966	2MG	C8-N7-C5	2.14	108.11	104.24
2	2	527	7MG	C5-C4-N9	-2.14	103.57	106.35
1	1	1917	PSU	C6-C5-C4	-2.12	116.72	118.20
2	2	966	2MG	C4-C5-N7	-2.08	107.43	110.72
1	1	2445	2MG	C4-C5-N7	-2.07	107.44	110.72
1	1	2580	PSU	C3'-C2'-C1'	-2.07	99.22	101.64
1	1	1835	2MG	C4-C5-N7	-2.07	107.44	110.72
1	1	955	PSU	C5-C6-N1	-2.07	119.00	122.11
2	2	1407	5MC	N1-C2-N3	2.06	122.56	118.81
1	1	2030	6MZ	C4-N9-C1'	-2.06	121.69	126.59
1	1	2504	PSU	O4-C4-C5	-2.02	118.77	124.05
1	1	1835	2MG	C6-C5-N7	2.02	134.00	130.25
1	1	2498	OMC	C4-N3-C2	2.01	123.51	120.25
1	1	2030	6MZ	C5-C6-N1	2.01	120.34	118.20
2	2	1402	4OC	CM4-N4-C4	-2.01	118.53	122.45
1	1	2069	G7M	C3'-C2'-C1'	2.00	105.23	101.43

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	1618	6MZ	C2'
1	1	1618	6MZ	C3'
1	1	1911	PSU	C3'
1	1	1911	PSU	C4'
1	1	1915	3TD	C3'
1	1	1917	PSU	C3'
1	1	1917	PSU	C4'
1	1	2030	6MZ	C2'
1	1	2030	6MZ	C3'
1	1	2069	G7M	C2'
1	1	2069	G7M	C3'
1	1	2069	G7M	C4'

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Mol	Chain	Res	Type	Atom
1	1	2251	OMG	C2'
1	1	2457	PSU	C3'
1	1	2457	PSU	C4'
1	1	2498	OMC	C4'
1	1	2503	2MA	C2'
1	1	2503	2MA	C3'
1	1	2504	PSU	C3'
1	1	2504	PSU	C4'
1	1	2552	OMU	C2'
1	1	2552	OMU	C3'
1	1	2580	PSU	C3'
1	1	2580	PSU	C4'
1	1	2605	PSU	C3'
1	1	2605	PSU	C4'

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	955	PSU	C2'-C1'-C5-C4
1	1	955	PSU	C4'-C5'-O5'-P
1	1	1618	6MZ	C5-C6-N6-C9
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	1835	2MG	N1-C2-N2-CM2
1	1	1835	2MG	N3-C2-N2-CM2
1	1	1911	PSU	C4'-C5'-O5'-P
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	1962	5MC	O4'-C4'-C5'-O5'
1	1	1962	5MC	C3'-C4'-C5'-O5'
1	1	2030	6MZ	N1-C6-N6-C9
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2069	G7M	C3'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2445	2MG	N1-C2-N2-CM2
1	1	2445	2MG	N3-C2-N2-CM2
1	1	2498	OMC	C3'-C4'-C5'-O5'
1	1	2498	OMC	C4'-C5'-O5'-P
1	1	2504	PSU	C2'-C1'-C5-C6
1	1	2552	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	2580	PSU	C2'-C1'-C5-C4
1	1	2580	PSU	C2'-C1'-C5-C6
1	1	2605	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	516	PSU	C4'-C5'-O5'-P
2	2	527	7MG	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1207	2MG	N1-C2-N2-CM2
2	2	1207	2MG	N3-C2-N2-CM2
2	2	1402	4OC	C1'-C2'-O2'-CM2
2	2	1407	5MC	O4'-C4'-C5'-O5'
2	2	1516	2MG	N3-C2-N2-CM2
2	2	1518	MA6	O4'-C4'-C5'-O5'
2	2	1518	MA6	C3'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
1	1	2504	PSU	C4'-C5'-O5'-P
1	1	1915	3TD	O4'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
1	1	2552	OMU	C3'-C4'-C5'-O5'
2	2	1407	5MC	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C1'-N9-C8
1	1	2503	2MA	O4'-C1'-N9-C4
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
1	1	2605	PSU	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
1	1	1911	PSU	C3'-C4'-C5'-O5'
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	2251	OMG	O4'-C4'-C5'-O5'
1	1	1917	PSU	C4'-C5'-O5'-P
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	2605	PSU	C4'-C5'-O5'-P
2	2	1402	4OC	C4'-C5'-O5'-P
1	1	2030	6MZ	C5-C6-N6-C9
1	1	1911	PSU	O4'-C4'-C5'-O5'
1	1	2498	OMC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	C4'-C5'-O5'-P
1	1	2552	OMU	C4'-C5'-O5'-P
47	q	89	0TD	SB-CB-CG-OD1
2	2	1402	4OC	C3'-C2'-O2'-CM2
2	2	1498	UR3	C2'-C1'-N1-C6
1	1	2498	OMC	C2'-C1'-N1-C2
2	2	1519	MA6	C5-C6-N6-C9
2	2	967	5MC	C4'-C5'-O5'-P
1	1	2503	2MA	C4'-C5'-O5'-P
1	1	746	PSU	O4'-C1'-C5-C4
1	1	955	PSU	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C1'-N1-C6
47	q	89	0TD	CA-CB-SB-CSB
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2251	OMG	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
2	2	1518	MA6	C4'-C5'-O5'-P
1	1	746	PSU	O4'-C1'-C5-C6
2	2	1498	UR3	C2'-C1'-N1-C2
2	2	1498	UR3	O4'-C1'-N1-C2
2	2	1498	UR3	C3'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	q	89	0TD	1	0
2	2	527	7MG	5	0
1	1	1962	5MC	1	0
2	2	1516	2MG	3	0
1	1	745	1MG	1	0
2	2	516	PSU	3	0
1	1	2251	OMG	3	0
1	1	2069	G7M	3	0
1	1	1618	6MZ	1	0
2	2	1207	2MG	1	0
2	2	1402	4OC	4	0
1	1	746	PSU	4	0
2	2	1407	5MC	1	0
1	1	1915	3TD	1	0
1	1	955	PSU	3	0
1	1	2580	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 431 ligands modelled in this entry, 431 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
57	4	1
1	1	1
17	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	342:U	O3'	343:C	P	3.61
1	2	1276:G	O3'	1277:C	P	3.26
1	1	2314:A	O3'	2315:G	P	3.25
1	2	147:G	O3'	148:G	P	3.25
1	2	1383:C	O3'	1384:C	P	3.17
1	M	2:LEU	C	3:GLN	N	1.13

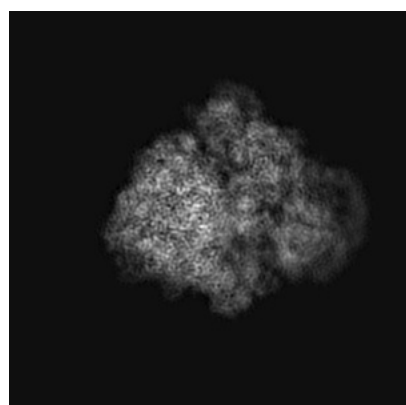
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4477. These allow visual inspection of the internal detail of the map and identification of artifacts.

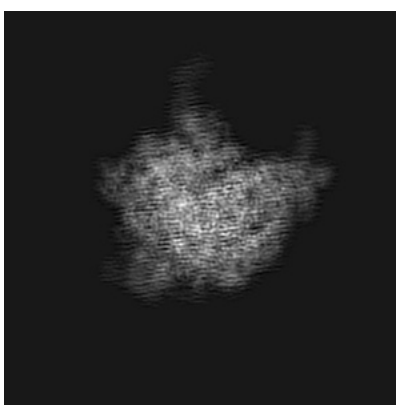
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

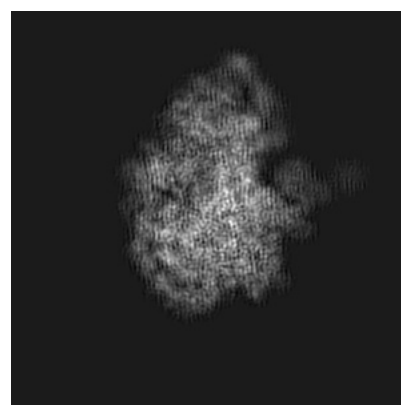
6.1.1 Primary map



X



Y

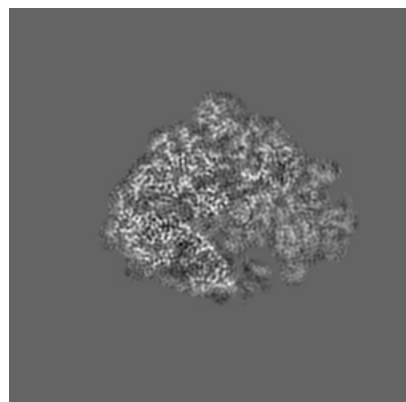


Z

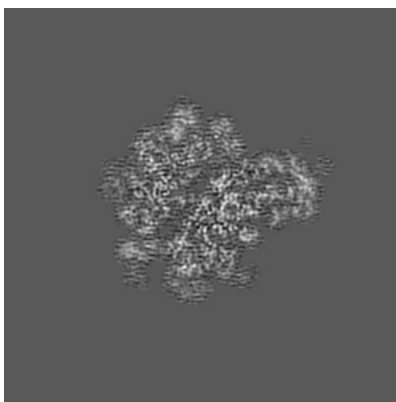
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

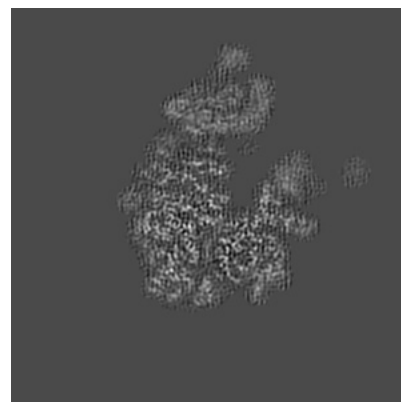
6.2.1 Primary map



X Index: 190



Y Index: 190

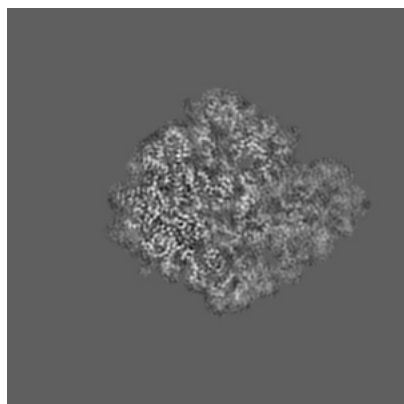


Z Index: 190

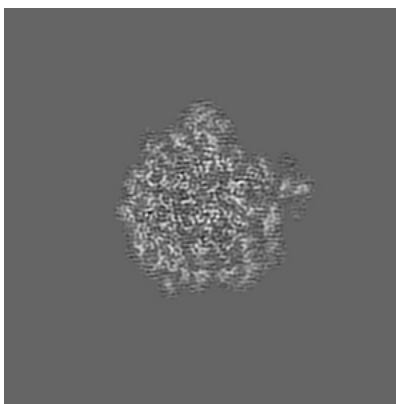
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

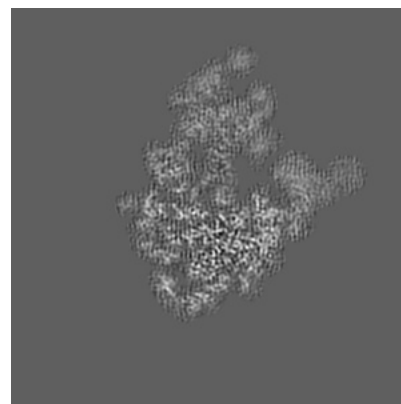
6.3.1 Primary map



X Index: 199



Y Index: 176

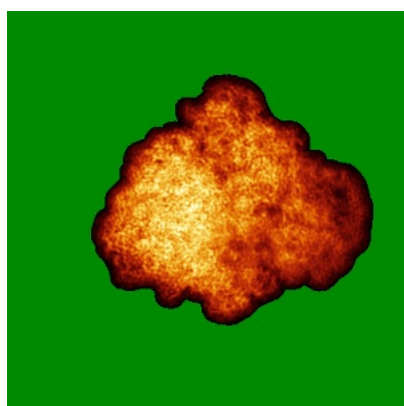


Z Index: 174

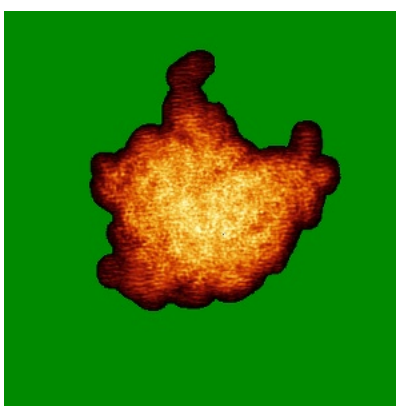
The images above show the largest variance slices of the map in three orthogonal directions.

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

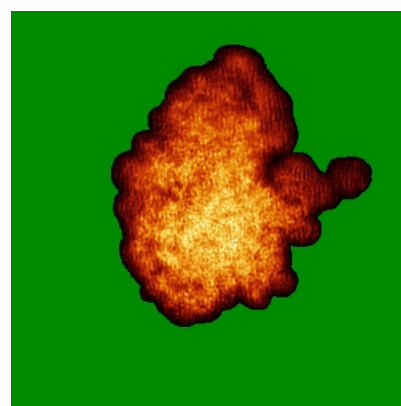
6.4.1 Primary map



X



Y

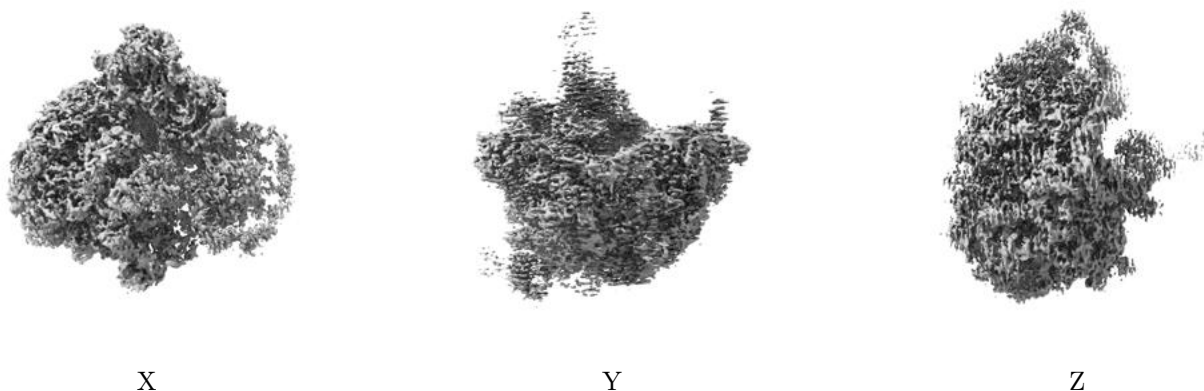


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0934. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

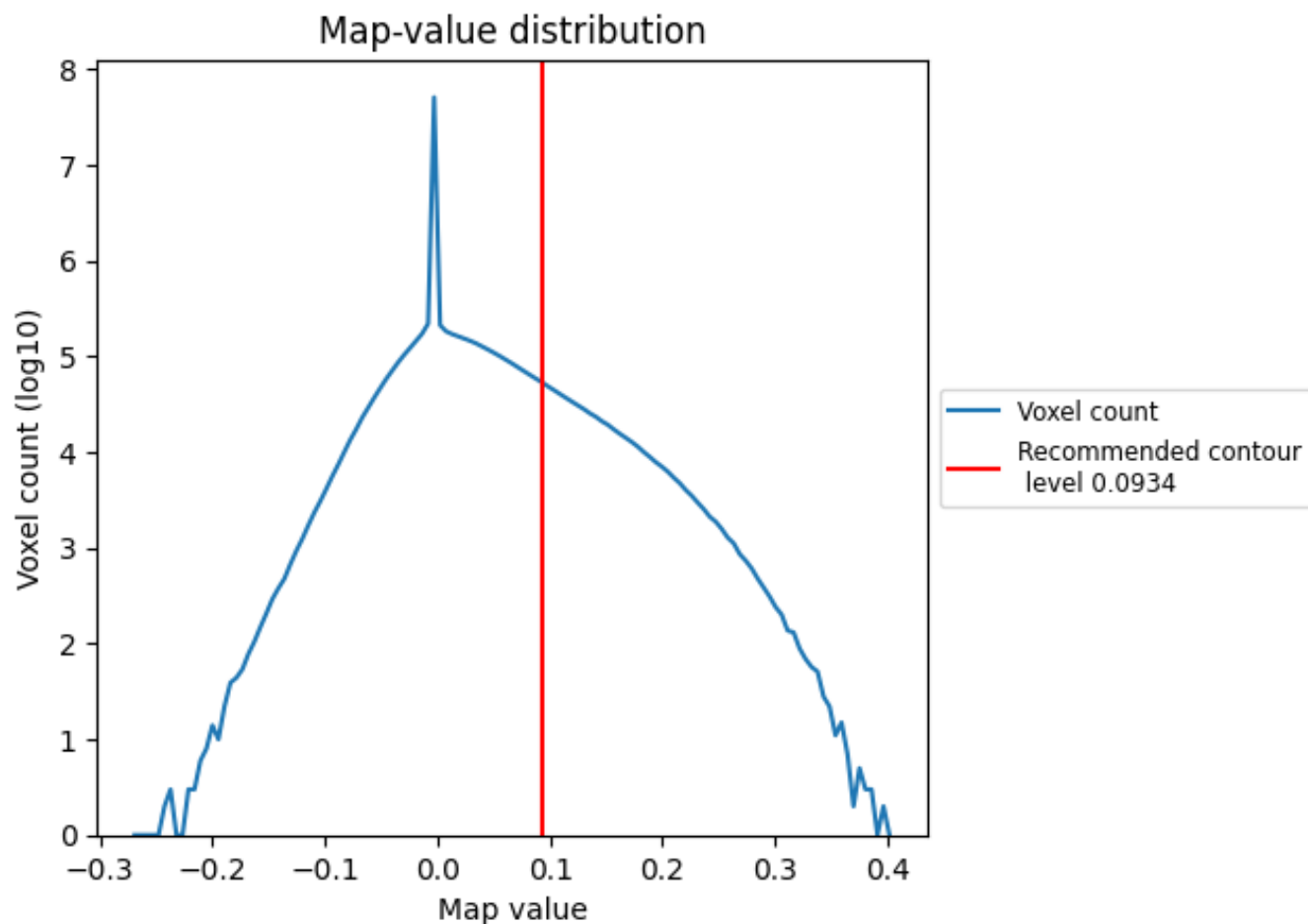
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

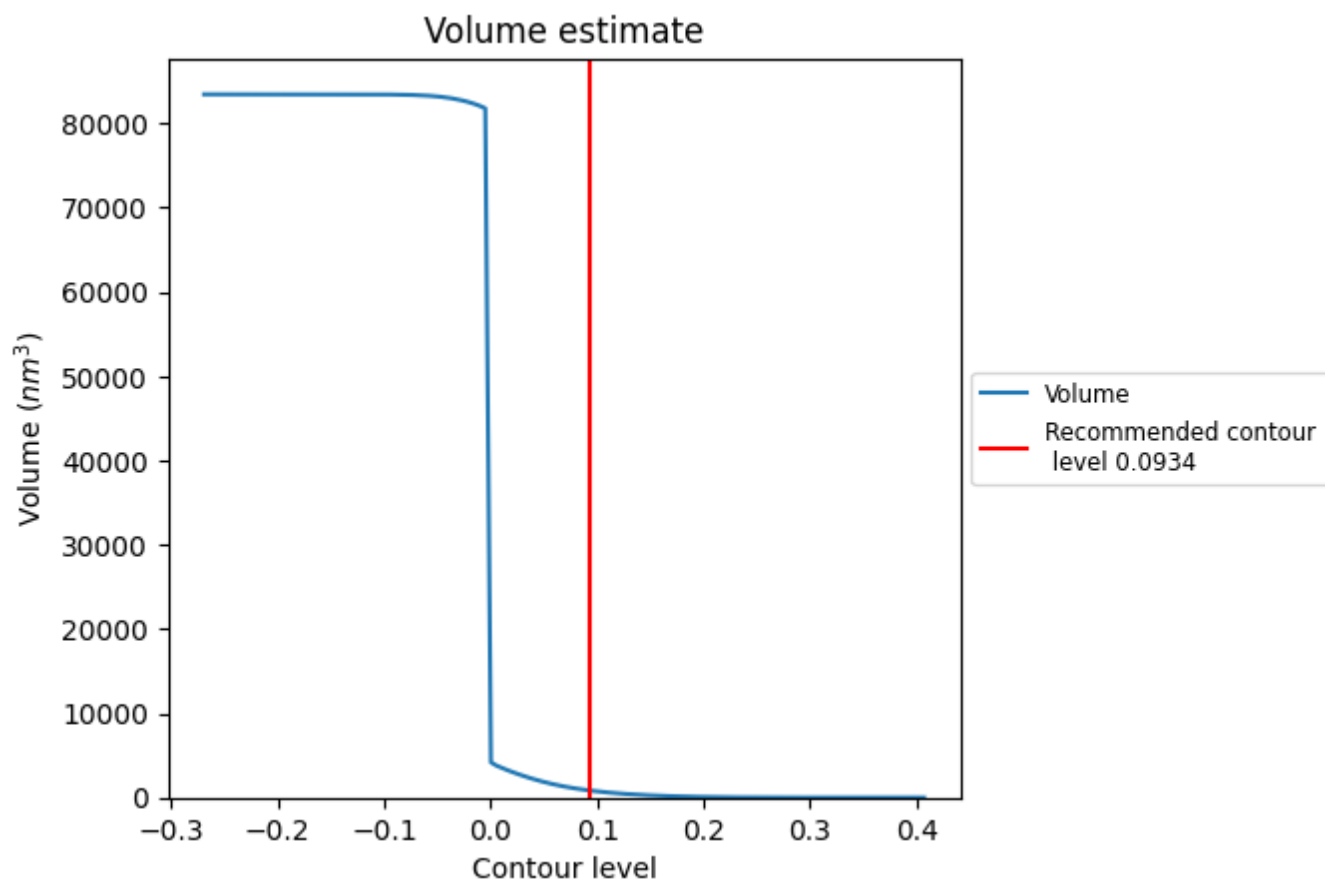
This section contains the results of statistical analysis of the map.

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.

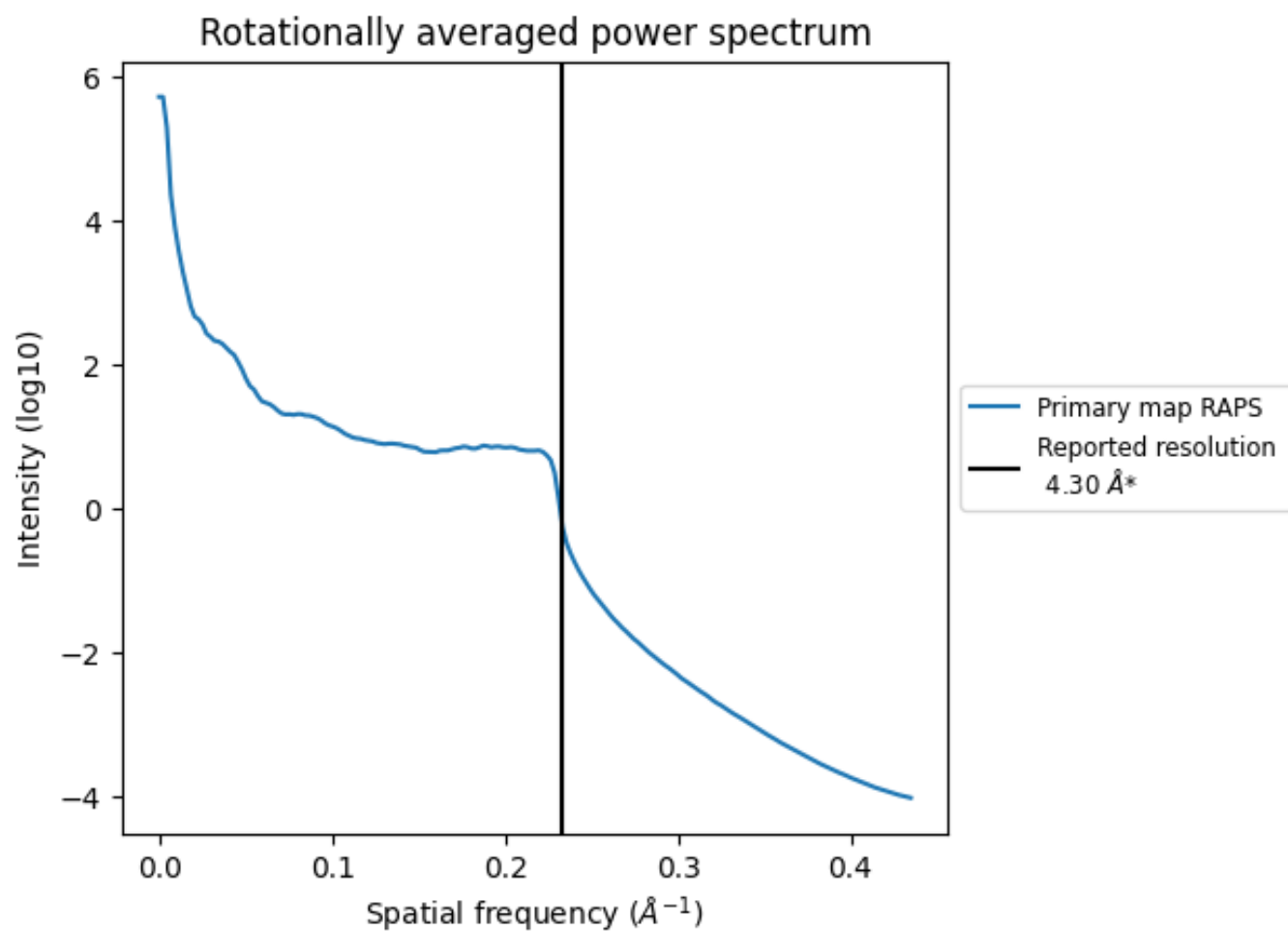
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm³; this corresponds to an approximate mass of 755 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 0.233 $\text{\AA}^{-1}$

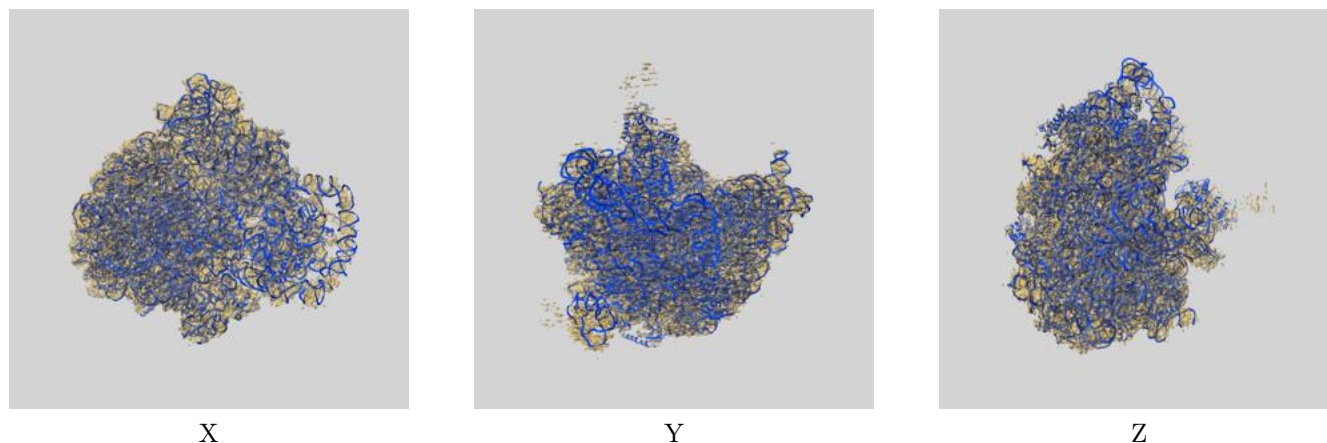
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

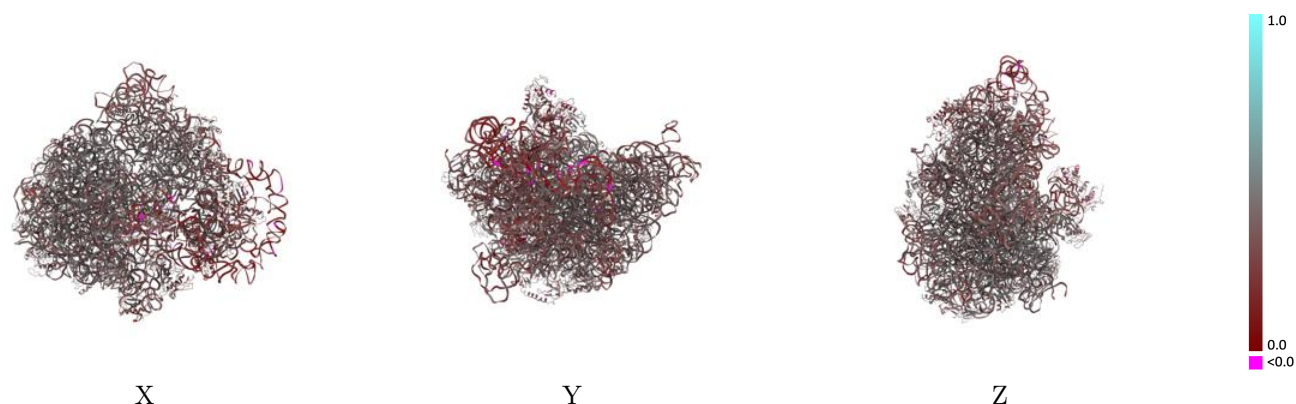
This section contains information regarding the fit between EMDB map EMD-4477 and PDB model 6Q98. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



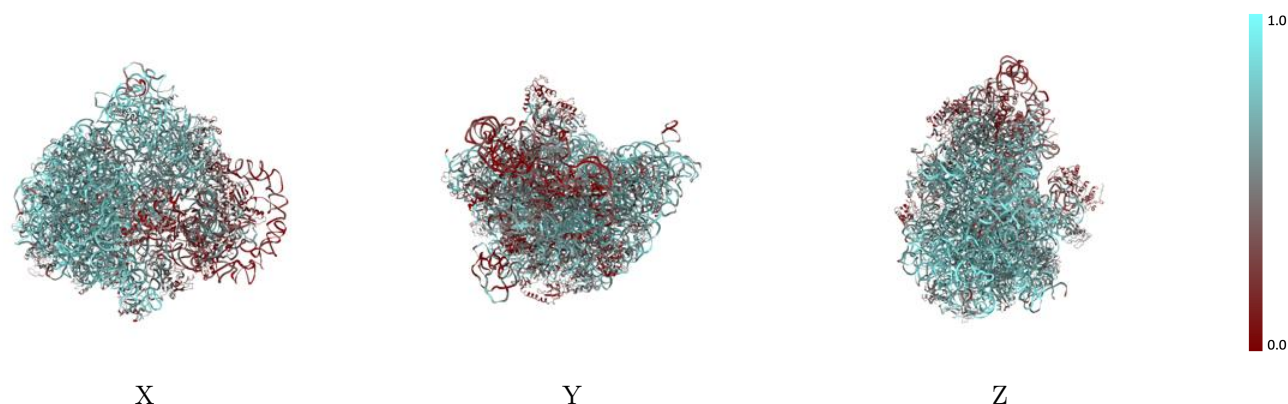
The images above show the 3D surface view of the map at the recommended contour level 0.0934 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



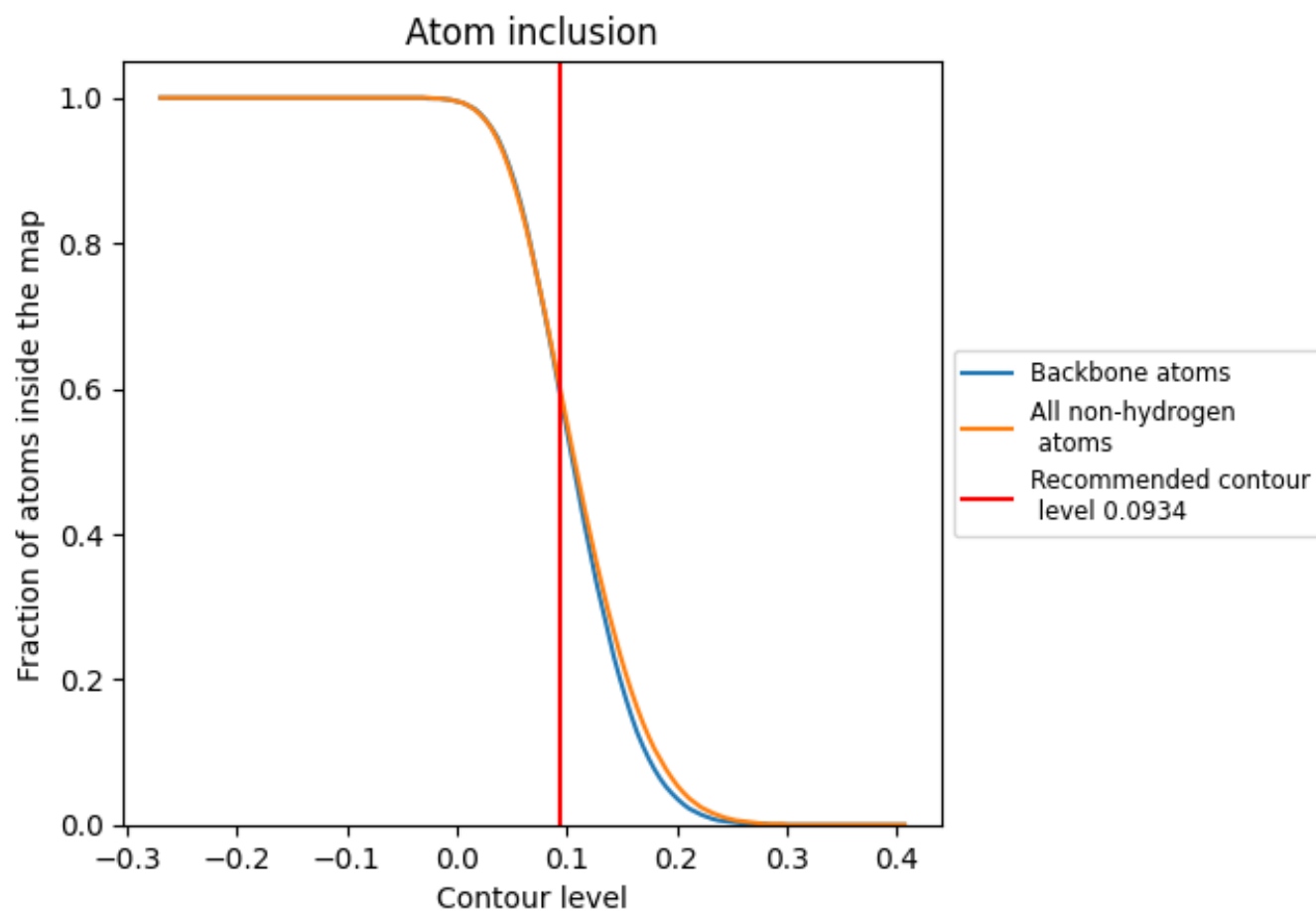
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0934).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 60% 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 (0.0934) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6050	 0.3700
1	 0.7470	 0.3840
2	 0.6730	 0.3560
3	 0.7410	 0.3560
4	 0.2510	 0.2110
5	 0.3400	 0.3730
6	 0.1910	 0.4410
B	 0.5360	 0.4340
C	 0.5700	 0.4370
D	 0.5280	 0.4110
E	 0.3970	 0.3660
F	 0.4770	 0.3860
G	 0.2300	 0.3420
H	 0.1950	 0.2960
I	 0.1690	 0.2730
J	 0.5620	 0.4220
K	 0.5360	 0.4430
L	 0.5580	 0.4400
M	 0.5440	 0.4230
N	 0.5940	 0.4280
O	 0.4770	 0.3820
P	 0.4830	 0.4250
Q	 0.6410	 0.4180
R	 0.5480	 0.4200
S	 0.5730	 0.4420
T	 0.5000	 0.4190
U	 0.5020	 0.4070
V	 0.5470	 0.3970
W	 0.5620	 0.4470
X	 0.5440	 0.4330
Y	 0.4930	 0.3830
Z	 0.5620	 0.4200
a	 0.2390	 0.3390
b	 0.5940	 0.4320
c	 0.4330	 0.3920



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Chain	Atom inclusion	Q-score
d	 0.5630	 0.4400
e	 0.5930	 0.4470
f	 0.5750	 0.4300
g	 0.2340	 0.3290
h	 0.2910	 0.3610
i	 0.3530	 0.3770
j	 0.4890	 0.4080
k	 0.4870	 0.3860
l	 0.2300	 0.3090
m	 0.4980	 0.4040
n	 0.2160	 0.3150
o	 0.1920	 0.3170
p	 0.4850	 0.3970
q	 0.4700	 0.4110
r	 0.1890	 0.3050
s	 0.2520	 0.3260
t	 0.4940	 0.3850
u	 0.4880	 0.4060
v	 0.4710	 0.4050
w	 0.4910	 0.3970
x	 0.2100	 0.3250
y	 0.4680	 0.3570
z	 0.3790	 0.3840